



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:02 AM UTC

PDB ID : 1YE9 / pdb\_00001ye9  
Title : Crystal structure of proteolytically truncated catalase HP11 from E. coli  
Authors : Loewen, P.C.; Chelikani, P.; Carpena, X.; Fita, I.; Perez-Luque, R.; Donald, L.J.; Switala, J.; Duckworth, H.W.  
Deposited on : 2004-12-28  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

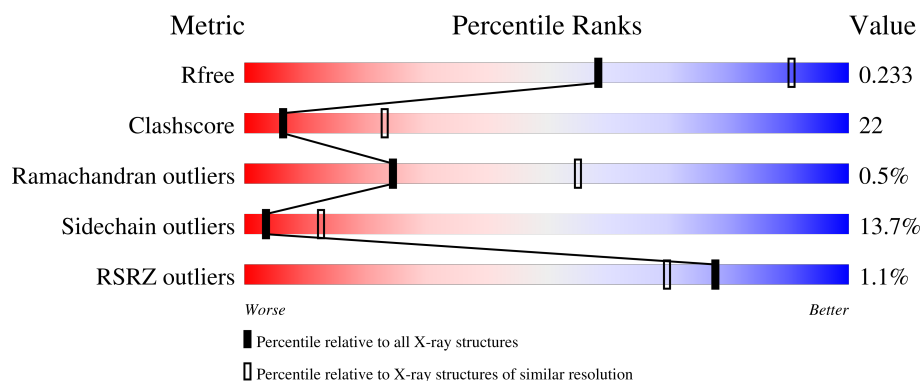
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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     | 226    | <br>61% 34% 5% . . |
| 1   | B     | 226    | <br>55% 38% 5% . . |
| 1   | C     | 226    | <br>66% 29% . .    |
| 1   | D     | 226    | <br>61% 33% . .    |
| 1   | I     | 226    | <br>56% 35% 8% .   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | J     | 226    |                  |
| 1   | K     | 226    |                  |
| 1   | L     | 226    |                  |
| 2   | E     | 259    |                  |
| 2   | F     | 259    |                  |
| 2   | G     | 259    |                  |
| 2   | H     | 259    |                  |
| 2   | M     | 259    |                  |
| 2   | N     | 259    |                  |
| 2   | O     | 259    |                  |
| 2   | P     | 259    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | HDD  | F     | 760 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31715 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 catalase HPIL.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1796  | 1148 | 319 | 326 | 3 |         |         |       |
| 1   | B     | 223      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1803  | 1152 | 322 | 326 | 3 |         |         |       |
| 1   | C     | 223      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1800  | 1151 | 320 | 326 | 3 |         |         |       |
| 1   | D     | 223      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1802  | 1151 | 322 | 326 | 3 |         |         |       |
| 1   | I     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1796  | 1148 | 319 | 326 | 3 |         |         |       |
| 1   | J     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1796  | 1148 | 319 | 326 | 3 |         |         |       |
| 1   | K     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1796  | 1148 | 319 | 326 | 3 |         |         |       |
| 1   | L     | 223      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1801  | 1150 | 322 | 326 | 3 |         |         |       |

- Molecule 2 is a protein called catalase HPIL.

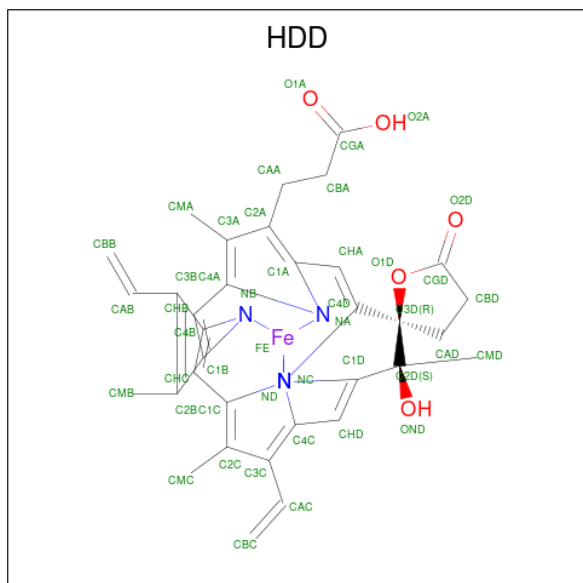
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | E     | 256      | Total | C    | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 2107  | 1340 | 370 | 393 | 4 |         |         |       |
| 2   | F     | 256      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2094  | 1333 | 367 | 390 | 4 |         |         |       |
| 2   | G     | 256      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2106  | 1340 | 372 | 390 | 4 |         |         |       |
| 2   | H     | 256      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2100  | 1337 | 369 | 390 | 4 |         |         |       |
| 2   | M     | 256      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2098  | 1336 | 368 | 390 | 4 |         |         |       |
| 2   | N     | 256      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2100  | 1337 | 369 | 390 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | O     | 256      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2094  | 1333 | 367 | 390 | 4 |         |         |       |
| 2   | P     | 256      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2094  | 1333 | 367 | 390 | 4 |         |         |       |

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula:  $C_{34}H_{32}FeN_4O_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 3   | E     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | F     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | G     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | H     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | M     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | O     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |
| 3   | P     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 44    | 34 | 1  | 4 | 5 |         |         |

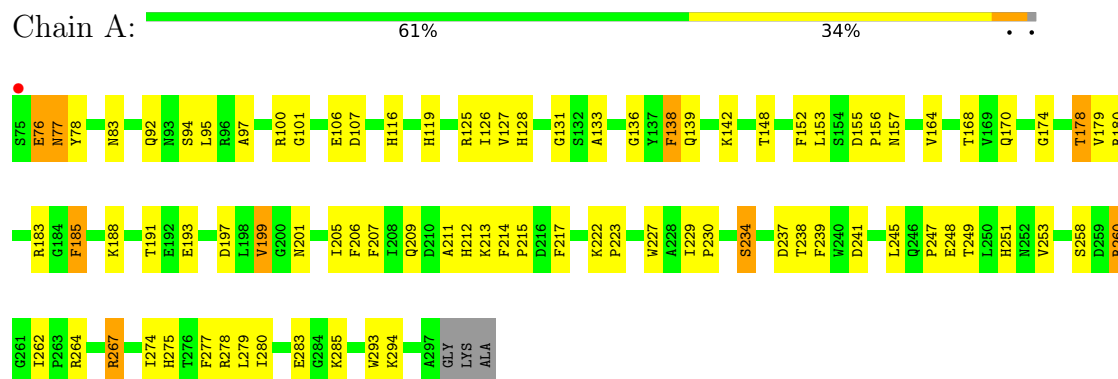
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 21       | Total O<br>21 21 | 0       | 0       |
| 4   | E     | 20       | Total O<br>20 20 | 0       | 0       |
| 4   | B     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | F     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | C     | 20       | Total O<br>20 20 | 0       | 0       |
| 4   | G     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | D     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | H     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | I     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | M     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | J     | 12       | Total O<br>12 12 | 0       | 0       |
| 4   | N     | 12       | Total O<br>12 12 | 0       | 0       |
| 4   | K     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | O     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | L     | 16       | Total O<br>16 16 | 0       | 0       |
| 4   | P     | 13       | Total O<br>13 13 | 0       | 0       |

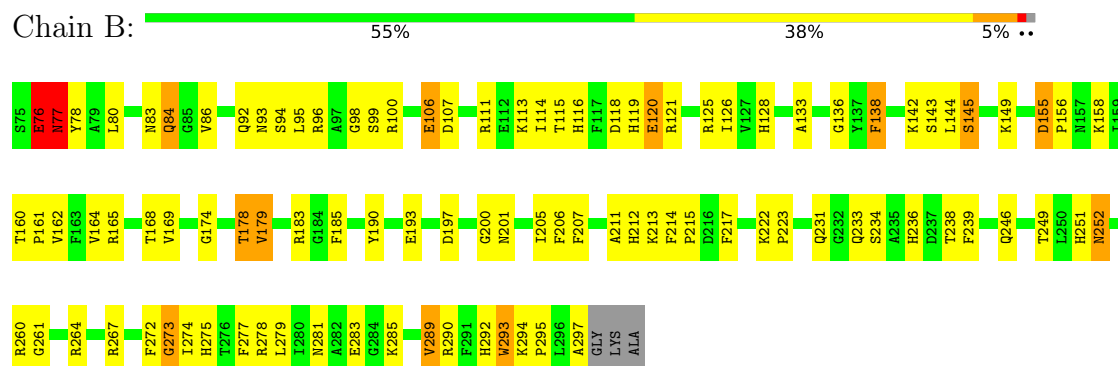
### 3 Residue-property plots

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.

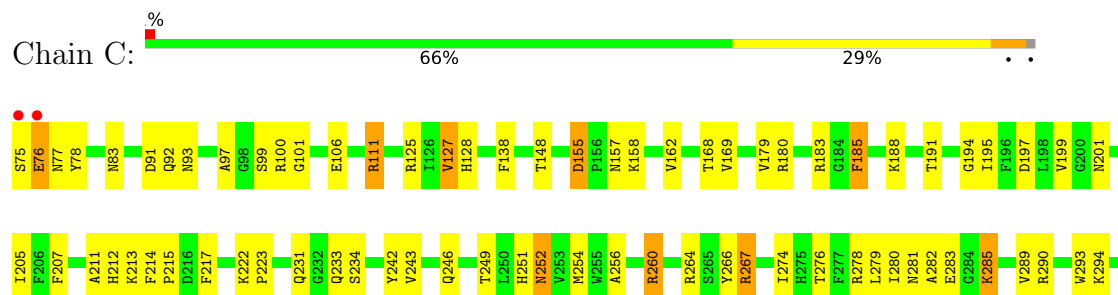
#### • Molecule 1: catalase HP11



#### • Molecule 1: catalase HP11



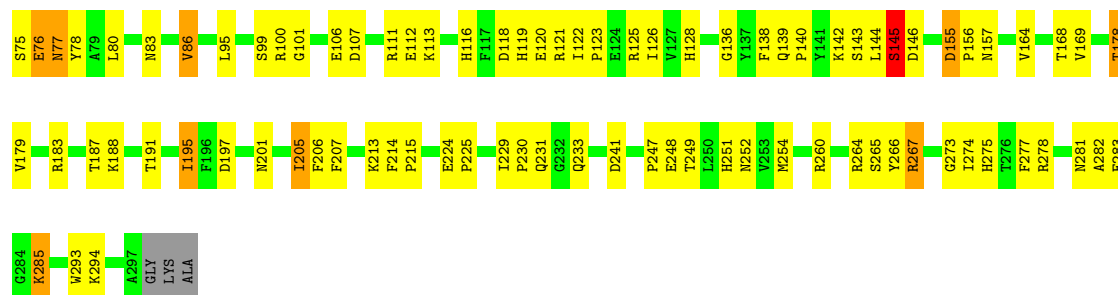
#### • Molecule 1: catalase HP11





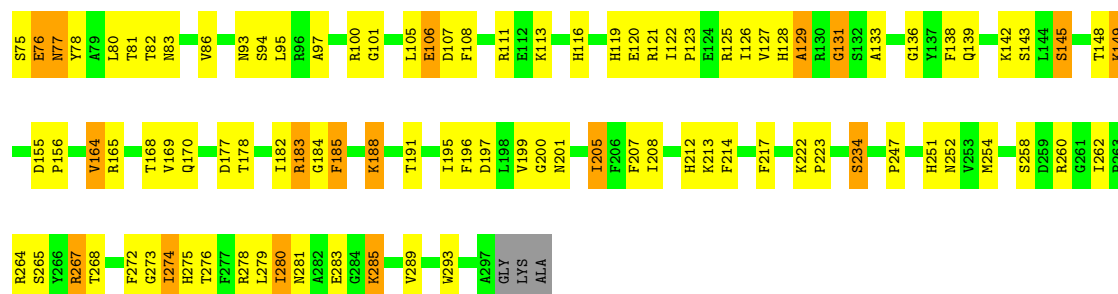
• Molecule 1: catalase HP1I

Chain D:  61% 33%



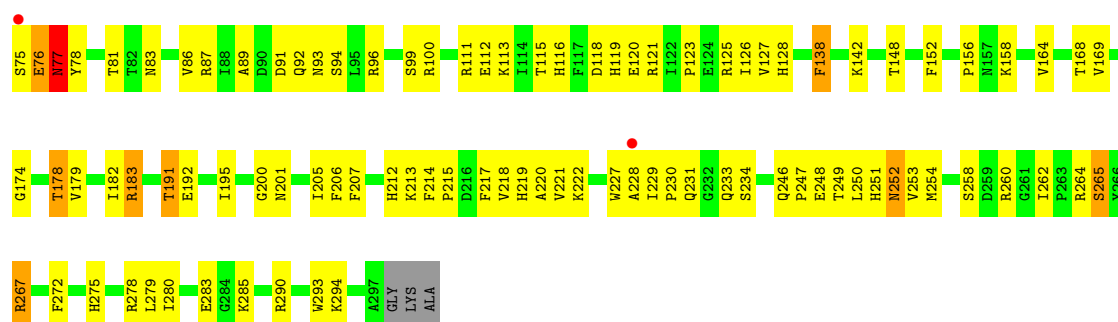
• Molecule 1: catalase HP1I

Chain I:  56% 35% 8%



• Molecule 1: catalase HP1I

Chain J:  57% 38%

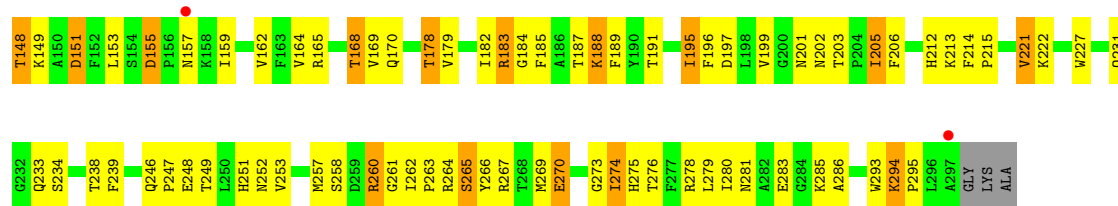


• Molecule 1: catalase HP1I

Chain K:  47% 43% 8%



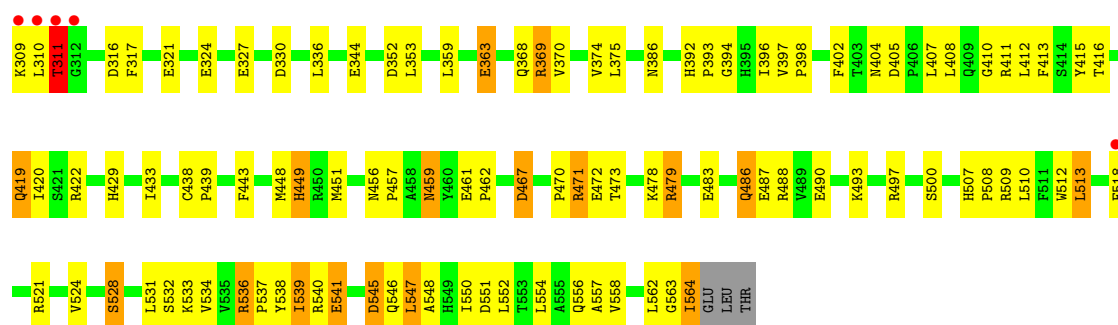




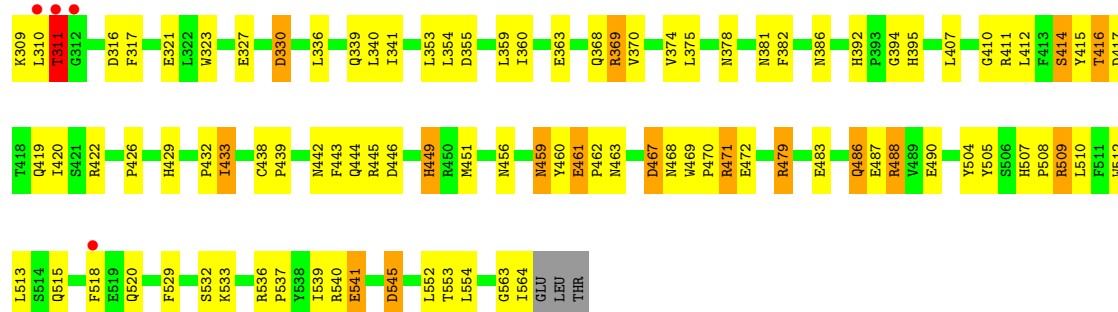
● Molecule 1: catalase HPII



● Molecule 2: catalase HPII

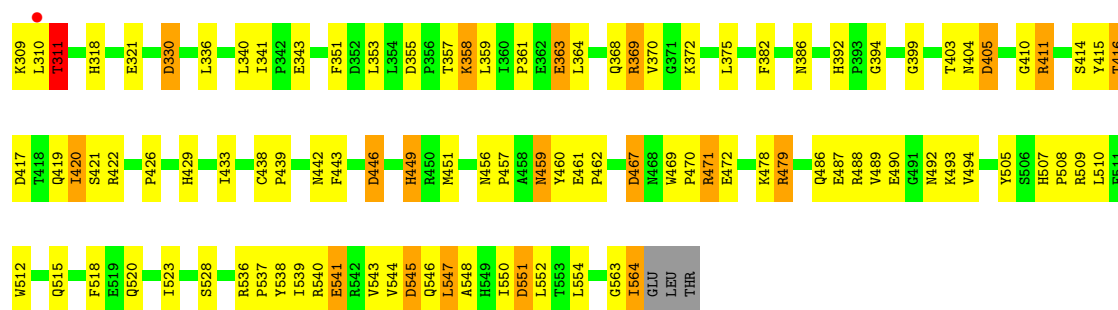


● Molecule 2: catalase HPII



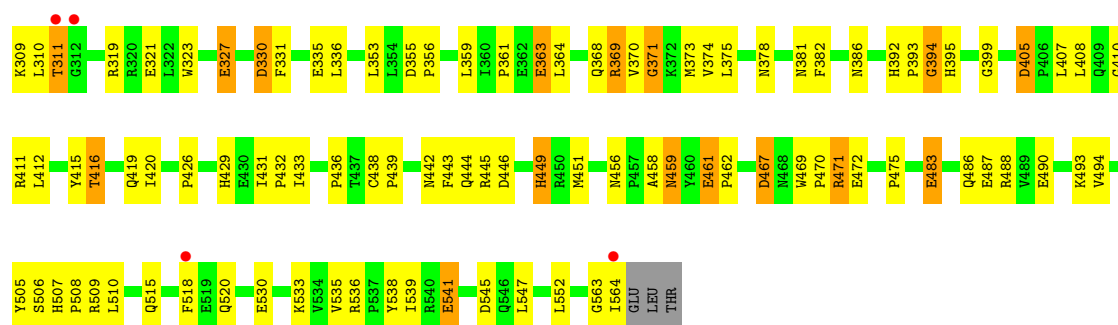
● Molecule 2: catalase HPII

Chain G:  59% 32% 7% .



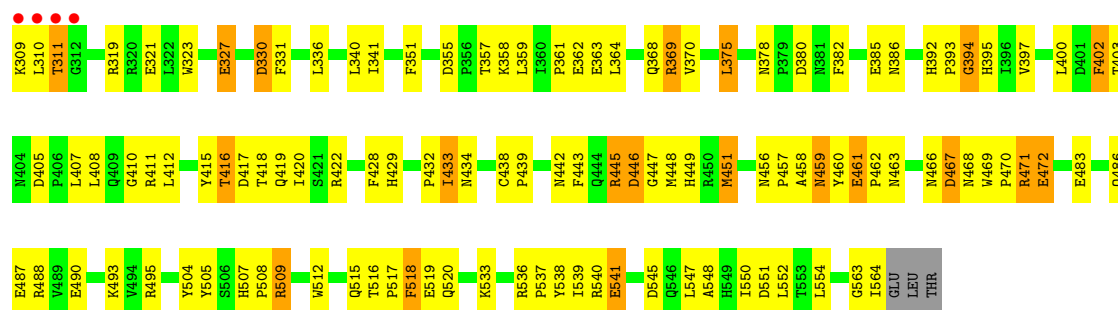
• Molecule 2: catalase HPII

Chain H:  61% 32% 6% .



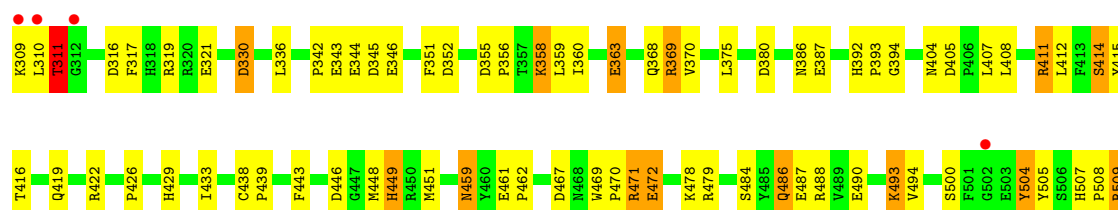
• Molecule 2: catalase HPII

Chain M:  54% 37% 8% .



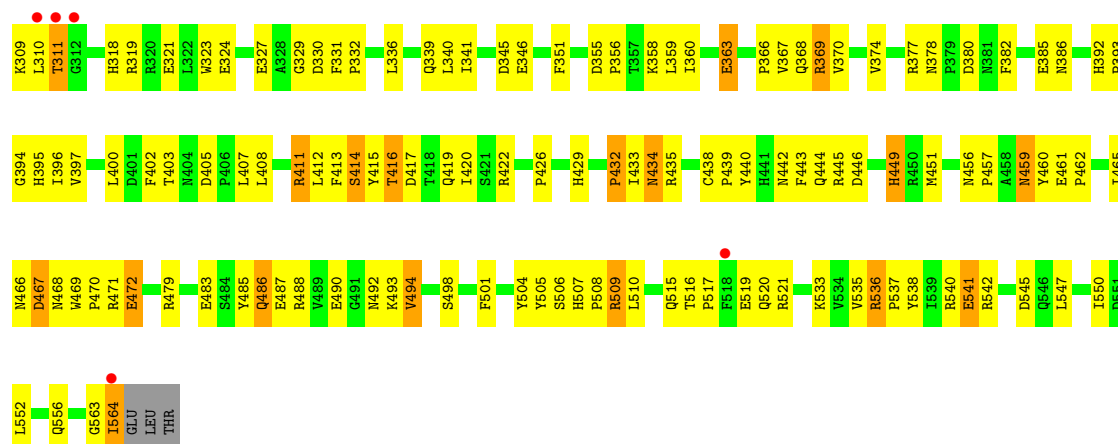
• Molecule 2: catalase HPII

Chain N:  60% 31% 8% .

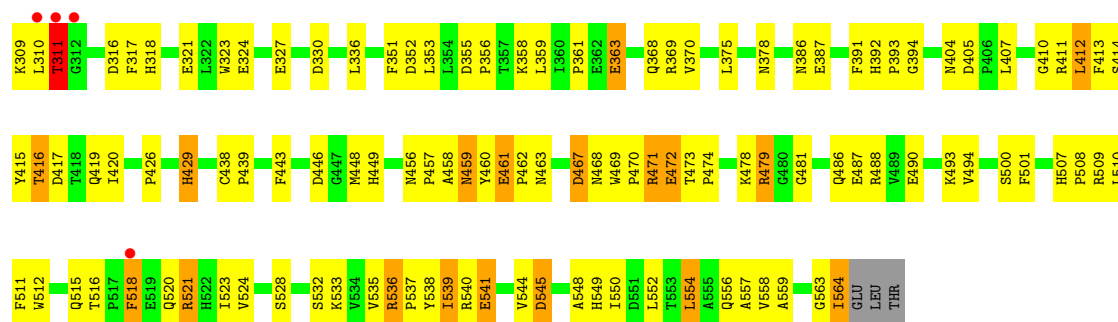




● Molecule 2: catalase HPII



● Molecule 2: catalase HPII



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 111.01Å 152.89Å 135.29Å<br>90.00° 97.54° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.80<br>30.00 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (30.00-2.80)<br>95.3 (30.00-2.80)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | 0.11                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.86 (at 2.80Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.1.24                                               | Depositor        |
| R, $R_{free}$                                                           | 0.217 , 0.269<br>(Not available) , 0.233                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5289 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.139                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 45.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 31715                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 43.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.94         | 0/1851          | 1.09        | 4/2513 (0.2%)   |
| 1   | B     | 0.91         | 1/1862 (0.1%)   | 1.15        | 8/2527 (0.3%)   |
| 1   | C     | 0.92         | 0/1860          | 1.11        | 3/2525 (0.1%)   |
| 1   | D     | 0.91         | 1/1862 (0.1%)   | 1.15        | 2/2527 (0.1%)   |
| 1   | I     | 0.95         | 1/1851 (0.1%)   | 1.17        | 9/2513 (0.4%)   |
| 1   | J     | 0.89         | 2/1851 (0.1%)   | 1.15        | 3/2513 (0.1%)   |
| 1   | K     | 0.98         | 0/1851          | 1.16        | 6/2513 (0.2%)   |
| 1   | L     | 0.88         | 0/1862          | 1.09        | 3/2527 (0.1%)   |
| 2   | E     | 0.90         | 1/2188 (0.0%)   | 1.07        | 0/2975          |
| 2   | F     | 0.88         | 1/2159 (0.0%)   | 1.10        | 4/2936 (0.1%)   |
| 2   | G     | 0.92         | 2/2181 (0.1%)   | 1.08        | 5/2965 (0.2%)   |
| 2   | H     | 0.89         | 0/2170          | 1.11        | 4/2951 (0.1%)   |
| 2   | M     | 0.88         | 0/2168          | 1.12        | 5/2947 (0.2%)   |
| 2   | N     | 0.89         | 2/2170 (0.1%)   | 1.08        | 4/2951 (0.1%)   |
| 2   | O     | 0.91         | 1/2159 (0.0%)   | 1.13        | 5/2936 (0.2%)   |
| 2   | P     | 0.88         | 1/2159 (0.0%)   | 1.09        | 4/2936 (0.1%)   |
| All | All   | 0.91         | 13/32204 (0.0%) | 1.11        | 69/43755 (0.2%) |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | E     | 311 | THR  | CA-CB | 6.70  | 1.65        | 1.53     |
| 1   | B     | 178 | THR  | CA-C  | -6.60 | 1.46        | 1.53     |
| 2   | O     | 451 | MET  | SD-CE | 6.08  | 1.94        | 1.79     |
| 1   | J     | 164 | VAL  | CA-CB | -5.94 | 1.47        | 1.54     |
| 2   | G     | 442 | ASN  | C-O   | -5.69 | 1.18        | 1.24     |
| 1   | I     | 268 | THR  | CA-CB | 5.68  | 1.60        | 1.53     |
| 2   | N     | 451 | MET  | SD-CE | 5.57  | 1.93        | 1.79     |
| 2   | N     | 311 | THR  | CA-CB | 5.54  | 1.63        | 1.53     |
| 2   | F     | 311 | THR  | CA-CB | 5.25  | 1.62        | 1.53     |
| 2   | P     | 311 | THR  | CA-CB | 5.22  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | G     | 311 | THR  | CA-CB | 5.17  | 1.62        | 1.53     |
| 1   | J     | 220 | ALA  | CA-CB | -5.15 | 1.45        | 1.53     |
| 1   | D     | 254 | MET  | SD-CE | -5.08 | 1.66        | 1.79     |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 76  | GLU  | N-CA-C    | 7.40  | 122.37      | 112.30   |
| 2   | F     | 414 | SER  | N-CA-C    | 6.79  | 118.48      | 111.14   |
| 2   | H     | 371 | GLY  | N-CA-C    | 6.67  | 121.62      | 110.56   |
| 2   | M     | 428 | PHE  | N-CA-C    | -6.64 | 105.14      | 113.18   |
| 2   | M     | 394 | GLY  | N-CA-C    | -6.62 | 107.38      | 114.67   |
| 2   | P     | 474 | PRO  | O-C-N     | 6.52  | 124.22      | 121.15   |
| 1   | C     | 77  | ASN  | N-CA-C    | 6.45  | 120.11      | 107.98   |
| 1   | I     | 111 | ARG  | NE-CZ-NH2 | 6.45  | 125.00      | 119.20   |
| 1   | I     | 82  | THR  | N-CA-C    | -6.41 | 102.52      | 110.41   |
| 1   | K     | 94  | SER  | N-CA-C    | -6.36 | 102.33      | 110.53   |
| 2   | G     | 414 | SER  | N-CA-C    | 6.34  | 118.27      | 111.36   |
| 1   | B     | 98  | GLY  | N-CA-C    | -6.34 | 104.81      | 112.48   |
| 1   | K     | 131 | GLY  | N-CA-C    | 6.26  | 120.82      | 111.18   |
| 1   | B     | 84  | GLN  | N-CA-C    | -6.24 | 105.53      | 113.02   |
| 2   | G     | 411 | ARG  | N-CA-C    | -6.24 | 104.48      | 111.28   |
| 1   | L     | 131 | GLY  | N-CA-C    | 6.16  | 120.67      | 111.18   |
| 1   | D     | 77  | ASN  | N-CA-C    | 5.99  | 117.96      | 108.67   |
| 1   | J     | 93  | ASN  | N-CA-C    | 5.98  | 118.50      | 109.23   |
| 1   | I     | 131 | GLY  | N-CA-C    | 5.89  | 119.74      | 110.96   |
| 1   | B     | 273 | GLY  | N-CA-C    | -5.87 | 105.58      | 115.62   |
| 2   | H     | 416 | THR  | N-CA-C    | -5.86 | 106.17      | 113.55   |
| 1   | B     | 93  | ASN  | N-CA-C    | 5.85  | 118.07      | 109.24   |
| 1   | A     | 77  | ASN  | N-CA-C    | 5.84  | 117.55      | 109.15   |
| 1   | C     | 93  | ASN  | N-CA-C    | 5.84  | 118.72      | 109.50   |
| 1   | L     | 199 | VAL  | CB-CA-C   | -5.81 | 103.85      | 111.81   |
| 2   | G     | 528 | SER  | N-CA-C    | -5.75 | 104.94      | 111.14   |
| 1   | I     | 129 | ALA  | N-CA-C    | -5.73 | 104.94      | 111.07   |
| 1   | B     | 76  | GLU  | N-CA-C    | 5.67  | 119.30      | 111.71   |
| 1   | C     | 162 | VAL  | N-CA-C    | 5.65  | 117.96      | 108.81   |
| 1   | B     | 77  | ASN  | N-CA-C    | 5.64  | 122.81      | 110.80   |
| 1   | B     | 293 | TRP  | N-CA-C    | -5.61 | 99.14       | 108.34   |
| 2   | O     | 535 | VAL  | N-CA-C    | 5.60  | 115.80      | 110.42   |
| 1   | I     | 77  | ASN  | N-CA-C    | 5.58  | 117.79      | 109.25   |
| 2   | N     | 330 | ASP  | N-CA-CB   | 5.58  | 118.39      | 110.46   |
| 1   | D     | 241 | ASP  | N-CA-C    | -5.58 | 105.10      | 111.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 394 | GLY  | N-CA-C  | -5.57 | 108.54      | 114.67   |
| 2   | N     | 504 | TYR  | N-CA-C  | 5.54  | 120.04      | 113.16   |
| 1   | B     | 162 | VAL  | N-CA-C  | 5.54  | 117.79      | 108.81   |
| 2   | O     | 494 | VAL  | N-CA-C  | 5.52  | 115.12      | 108.06   |
| 2   | O     | 414 | SER  | N-CA-C  | 5.47  | 116.93      | 111.07   |
| 1   | L     | 77  | ASN  | N-CA-C  | 5.42  | 122.34      | 110.80   |
| 2   | P     | 518 | PHE  | CB-CA-C | 5.40  | 121.04      | 110.67   |
| 1   | J     | 77  | ASN  | N-CA-C  | 5.38  | 122.25      | 110.80   |
| 2   | O     | 367 | VAL  | CB-CA-C | -5.35 | 106.13      | 111.80   |
| 2   | F     | 420 | ILE  | N-CA-C  | 5.32  | 116.68      | 110.62   |
| 2   | F     | 504 | TYR  | N-CA-C  | 5.29  | 119.88      | 113.38   |
| 1   | K     | 121 | ARG  | N-CA-C  | 5.25  | 118.49      | 110.20   |
| 1   | I     | 234 | SER  | N-CA-C  | -5.25 | 106.56      | 113.17   |
| 2   | M     | 446 | ASP  | CB-CA-C | -5.23 | 108.98      | 115.89   |
| 2   | H     | 399 | GLY  | N-CA-C  | -5.22 | 107.99      | 113.58   |
| 2   | G     | 399 | GLY  | N-CA-C  | -5.22 | 108.27      | 114.48   |
| 2   | O     | 556 | GLN  | N-CA-C  | 5.20  | 116.63      | 111.07   |
| 2   | P     | 429 | HIS  | N-CA-C  | -5.19 | 106.90      | 113.18   |
| 2   | G     | 330 | ASP  | N-CA-CB | 5.16  | 117.79      | 110.46   |
| 2   | F     | 394 | GLY  | N-CA-C  | -5.16 | 107.53      | 115.73   |
| 2   | M     | 447 | GLY  | N-CA-C  | -5.15 | 105.28      | 112.18   |
| 1   | A     | 170 | GLN  | N-CA-C  | 5.14  | 116.57      | 111.07   |
| 1   | I     | 170 | GLN  | N-CA-C  | 5.14  | 116.69      | 111.14   |
| 1   | I     | 164 | VAL  | N-CA-C  | 5.13  | 115.37      | 107.77   |
| 1   | A     | 199 | VAL  | CB-CA-C | -5.10 | 102.93      | 111.29   |
| 2   | N     | 380 | ASP  | N-CA-C  | -5.09 | 105.91      | 112.68   |
| 2   | N     | 422 | ARG  | N-CA-C  | 5.08  | 116.81      | 111.28   |
| 2   | P     | 414 | SER  | N-CA-C  | 5.07  | 116.61      | 111.14   |
| 1   | K     | 162 | VAL  | N-CA-C  | 5.06  | 115.66      | 108.42   |
| 1   | I     | 93  | ASN  | N-CA-C  | 5.05  | 117.48      | 109.50   |
| 2   | M     | 445 | ARG  | N-CA-C  | 5.03  | 117.05      | 109.41   |
| 1   | K     | 77  | ASN  | N-CA-C  | 5.03  | 116.46      | 108.67   |
| 1   | K     | 81  | THR  | N-CA-C  | 5.03  | 117.05      | 109.41   |
| 1   | A     | 131 | GLY  | N-CA-C  | 5.02  | 118.43      | 111.10   |

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     | 1796  | 0        | 1720     | 77      | 0            |
| 1   | B     | 1803  | 0        | 1729     | 106     | 0            |
| 1   | C     | 1800  | 0        | 1729     | 68      | 0            |
| 1   | D     | 1802  | 0        | 1729     | 99      | 1            |
| 1   | I     | 1796  | 0        | 1720     | 102     | 0            |
| 1   | J     | 1796  | 0        | 1720     | 80      | 0            |
| 1   | K     | 1796  | 0        | 1720     | 117     | 0            |
| 1   | L     | 1801  | 0        | 1725     | 85      | 0            |
| 2   | E     | 2107  | 0        | 1980     | 84      | 0            |
| 2   | F     | 2094  | 0        | 1975     | 109     | 0            |
| 2   | G     | 2106  | 0        | 1987     | 97      | 0            |
| 2   | H     | 2100  | 0        | 1978     | 92      | 0            |
| 2   | M     | 2098  | 0        | 1984     | 128     | 0            |
| 2   | N     | 2100  | 0        | 1978     | 99      | 0            |
| 2   | O     | 2094  | 0        | 1975     | 138     | 3            |
| 2   | P     | 2094  | 0        | 1975     | 123     | 2            |
| 3   | E     | 44    | 0        | 28       | 12      | 0            |
| 3   | F     | 44    | 0        | 28       | 25      | 0            |
| 3   | G     | 44    | 0        | 28       | 8       | 0            |
| 3   | H     | 44    | 0        | 28       | 14      | 0            |
| 3   | M     | 44    | 0        | 28       | 15      | 0            |
| 3   | N     | 44    | 0        | 28       | 8       | 0            |
| 3   | O     | 44    | 0        | 28       | 20      | 0            |
| 3   | P     | 44    | 0        | 28       | 9       | 0            |
| 4   | A     | 21    | 0        | 0        | 2       | 0            |
| 4   | B     | 8     | 0        | 0        | 3       | 0            |
| 4   | C     | 20    | 0        | 0        | 5       | 0            |
| 4   | D     | 11    | 0        | 0        | 5       | 0            |
| 4   | E     | 20    | 0        | 0        | 6       | 0            |
| 4   | F     | 11    | 0        | 0        | 9       | 0            |
| 4   | G     | 11    | 0        | 0        | 1       | 0            |
| 4   | H     | 11    | 0        | 0        | 2       | 0            |
| 4   | I     | 5     | 0        | 0        | 4       | 0            |
| 4   | J     | 12    | 0        | 0        | 4       | 0            |
| 4   | K     | 3     | 0        | 0        | 1       | 0            |
| 4   | L     | 16    | 0        | 0        | 4       | 0            |
| 4   | M     | 2     | 0        | 0        | 2       | 0            |
| 4   | N     | 12    | 0        | 0        | 3       | 0            |
| 4   | O     | 4     | 0        | 0        | 2       | 0            |
| 4   | P     | 13    | 0        | 0        | 4       | 0            |
| All | All   | 31715 | 0        | 29848    | 1352    | 3            |



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 22.

All (1352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:L:267:ARG:HH11    | 1:L:267:ARG:CB      | 1.11                     | 1.61              |
| 2:O:392:HIS:ND1     | 2:O:415:TYR:CB      | 1.71                     | 1.53              |
| 2:P:392:HIS:ND1     | 2:P:415:TYR:CB      | 1.72                     | 1.50              |
| 2:G:392:HIS:ND1     | 2:G:415:TYR:CB      | 1.74                     | 1.48              |
| 2:N:392:HIS:ND1     | 2:N:415:TYR:CB      | 1.74                     | 1.48              |
| 1:L:267:ARG:NH1     | 1:L:267:ARG:HB3     | 1.31                     | 1.38              |
| 2:F:392:HIS:ND1     | 2:F:415:TYR:CB      | 1.88                     | 1.35              |
| 1:L:267:ARG:CB      | 1:L:267:ARG:NH1     | 1.90                     | 1.25              |
| 2:P:392:HIS:CE1     | 2:P:415:TYR:HB2     | 1.70                     | 1.25              |
| 2:F:392:HIS:ND1     | 2:F:415:TYR:HB2     | 0.91                     | 1.22              |
| 1:I:83:ASN:HB3      | 2:O:429:HIS:CD2     | 1.76                     | 1.20              |
| 1:B:165:ARG:HD3     | 3:F:760:HDD:O1A     | 1.38                     | 1.18              |
| 2:G:369:ARG:HG3     | 4:G:767:HOH:O       | 1.42                     | 1.18              |
| 2:P:392:HIS:ND1     | 2:P:415:TYR:HB2     | 0.86                     | 1.17              |
| 3:P:760:HDD:HBB1    | 3:P:760:HDD:HMB3    | 1.17                     | 1.16              |
| 2:N:392:HIS:ND1     | 2:N:415:TYR:HB2     | 0.84                     | 1.15              |
| 2:N:392:HIS:CE1     | 2:N:415:TYR:HB2     | 1.82                     | 1.15              |
| 2:O:392:HIS:ND1     | 2:O:415:TYR:HB2     | 0.80                     | 1.13              |
| 2:N:412:LEU:O       | 1:L:111:ARG:NH2     | 1.82                     | 1.11              |
| 2:G:392:HIS:ND1     | 2:G:415:TYR:HB2     | 0.79                     | 1.11              |
| 2:G:392:HIS:CE1     | 2:G:415:TYR:HB2     | 1.84                     | 1.10              |
| 2:O:392:HIS:CG      | 2:O:415:TYR:HB2     | 1.87                     | 1.07              |
| 1:B:267[B]:ARG:HH22 | 2:F:330:ASP:HB2     | 1.13                     | 1.07              |
| 1:B:267[B]:ARG:NH2  | 2:F:330:ASP:HB2     | 1.69                     | 1.06              |
| 2:M:309:LYS:CB      | 2:M:311:THR:HG23    | 1.84                     | 1.06              |
| 2:F:451:MET:HE2     | 2:H:451:MET:HE2     | 1.39                     | 1.05              |
| 2:G:449[B]:HIS:HE1  | 2:G:451:MET:SD      | 1.79                     | 1.05              |
| 2:O:392:HIS:CE1     | 2:O:415:TYR:HB2     | 1.90                     | 1.05              |
| 2:G:309:LYS:CB      | 2:G:311:THR:HG23    | 1.86                     | 1.05              |
| 2:F:509:ARG:HG3     | 2:F:509:ARG:HH11    | 1.22                     | 1.03              |
| 3:P:760:HDD:HBB1    | 3:P:760:HDD:CMB     | 1.87                     | 1.03              |
| 1:D:267[B]:ARG:HG3  | 1:D:267[B]:ARG:NH1  | 1.64                     | 1.02              |
| 2:O:355:ASP:OD1     | 2:O:358:LYS:HE2     | 1.58                     | 1.02              |
| 1:B:76:GLU:OE1      | 1:B:76:GLU:O        | 1.77                     | 1.01              |
| 1:D:267[B]:ARG:HG3  | 1:D:267[B]:ARG:HH11 | 0.83                     | 1.00              |
| 1:B:77:ASN:H        | 1:B:77:ASN:HD22     | 1.03                     | 1.00              |
| 2:G:392:HIS:CG      | 2:G:415:TYR:HB2     | 1.97                     | 0.99              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:D:267[B]:ARG:HH11 | 1:D:267[B]:ARG:CG | 1.76                     | 0.99              |
| 2:F:392:HIS:CG      | 2:F:415:TYR:HB2   | 1.99                     | 0.98              |
| 2:E:419:GLN:NE2     | 2:E:419:GLN:HA    | 1.76                     | 0.98              |
| 2:M:438:CYS:HB2     | 2:M:439:PRO:HD2   | 1.46                     | 0.98              |
| 2:G:449[B]:HIS:CE1  | 2:G:451:MET:SD    | 2.58                     | 0.96              |
| 2:O:366:PRO:HA      | 4:O:763:HOH:O     | 1.63                     | 0.96              |
| 2:N:419:GLN:NE2     | 2:N:419:GLN:HA    | 1.80                     | 0.96              |
| 2:M:416:THR:HG22    | 2:M:417:ASP:N     | 1.81                     | 0.95              |
| 2:N:309:LYS:CB      | 2:N:311:THR:HG23  | 1.96                     | 0.95              |
| 2:F:309:LYS:CB      | 2:F:311:THR:HG23  | 1.96                     | 0.95              |
| 1:L:77:ASN:HD22     | 1:L:77:ASN:N      | 1.63                     | 0.94              |
| 1:I:267:ARG:HH21    | 2:M:330:ASP:HB2   | 1.30                     | 0.94              |
| 2:P:392:HIS:CD2     | 2:P:394:GLY:H     | 1.84                     | 0.94              |
| 2:G:369:ARG:HG2     | 2:G:369:ARG:HH11  | 1.31                     | 0.93              |
| 1:K:293:TRP:CZ3     | 2:O:336:LEU:HB2   | 2.02                     | 0.93              |
| 2:O:411:ARG:HG2     | 2:O:415:TYR:HE2   | 1.31                     | 0.93              |
| 2:F:488:ARG:CD      | 4:F:761:HOH:O     | 2.15                     | 0.93              |
| 2:P:459:ASN:HD22    | 2:P:459:ASN:H     | 1.01                     | 0.93              |
| 1:C:267:ARG:CB      | 1:C:267:ARG:HH11  | 1.82                     | 0.92              |
| 2:N:392:HIS:CG      | 2:N:415:TYR:HB2   | 2.03                     | 0.92              |
| 2:F:392:HIS:CE1     | 2:F:415:TYR:HB2   | 2.03                     | 0.92              |
| 2:M:416:THR:HG22    | 2:M:417:ASP:H     | 1.32                     | 0.92              |
| 2:G:419:GLN:HA      | 2:G:419:GLN:NE2   | 1.82                     | 0.92              |
| 1:L:267:ARG:NH1     | 1:L:267:ARG:HB2   | 1.81                     | 0.91              |
| 1:K:294:LYS:HD3     | 1:K:295:PRO:HD2   | 1.53                     | 0.90              |
| 2:E:309:LYS:CB      | 2:E:311:THR:HG23  | 2.01                     | 0.90              |
| 1:K:276:THR:O       | 2:O:403:THR:CG2   | 2.20                     | 0.90              |
| 2:F:414:SER:CB      | 3:F:760:HDD:HBC1  | 2.01                     | 0.89              |
| 1:J:77:ASN:N        | 1:J:77:ASN:HD22   | 1.68                     | 0.89              |
| 1:K:201:ASN:CG      | 3:O:760:HDD:HMB1  | 1.97                     | 0.89              |
| 2:F:459:ASN:HD22    | 2:F:459:ASN:H     | 1.15                     | 0.89              |
| 1:I:125:ARG:HB3     | 3:M:760:HDD:HBD1  | 1.54                     | 0.89              |
| 2:P:459:ASN:HD22    | 2:P:459:ASN:N     | 1.70                     | 0.88              |
| 1:I:127:VAL:HA      | 4:I:304:HOH:O     | 1.70                     | 0.88              |
| 2:O:419:GLN:HA      | 2:O:419:GLN:NE2   | 1.87                     | 0.88              |
| 2:M:429:HIS:CD2     | 1:K:83:ASN:HB3    | 2.09                     | 0.88              |
| 1:A:267:ARG:HH11    | 1:A:267:ARG:HG2   | 1.38                     | 0.88              |
| 2:G:493:LYS:HE3     | 2:H:487:GLU:OE2   | 1.71                     | 0.87              |
| 1:K:201:ASN:OD1     | 3:O:760:HDD:HMB1  | 1.74                     | 0.87              |
| 2:P:458:ALA:HA      | 4:P:761:HOH:O     | 1.73                     | 0.87              |
| 2:M:487:GLU:OE2     | 2:N:493:LYS:HE3   | 1.75                     | 0.86              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:K:249:THR:O      | 1:K:253:VAL:HG23   | 1.76                     | 0.86              |
| 1:B:125:ARG:HB3    | 3:F:760:HDD:HBD1   | 1.54                     | 0.86              |
| 1:B:267[B]:ARG:HD3 | 1:B:297:ALA:HB2    | 1.58                     | 0.86              |
| 1:A:274:ILE:HD12   | 3:E:760:HDD:HBB1   | 1.59                     | 0.85              |
| 1:I:77:ASN:HB3     | 2:O:469:TRP:CZ3    | 2.11                     | 0.85              |
| 2:M:456:ASN:ND2    | 2:M:458:ALA:H      | 1.73                     | 0.85              |
| 2:M:351:PHE:HB2    | 2:M:358[B]:LYS:CD  | 2.07                     | 0.85              |
| 2:H:309:LYS:CB     | 2:H:311:THR:HG23   | 2.06                     | 0.85              |
| 1:J:278:ARG:NH2    | 2:N:487:GLU:OE1    | 2.09                     | 0.84              |
| 2:E:419:GLN:HA     | 2:E:419:GLN:HE21   | 1.43                     | 0.84              |
| 2:P:392:HIS:CG     | 2:P:415:TYR:HB2    | 2.06                     | 0.84              |
| 2:H:467:ASP:O      | 2:H:471:ARG:NH1    | 2.11                     | 0.82              |
| 2:P:419:GLN:HA     | 2:P:419:GLN:NE2    | 1.93                     | 0.82              |
| 1:K:276:THR:O      | 2:O:403:THR:HG21   | 1.77                     | 0.82              |
| 1:B:267[B]:ARG:HD3 | 1:B:297:ALA:CB     | 2.09                     | 0.82              |
| 2:N:467:ASP:O      | 2:N:471:ARG:NH1    | 2.13                     | 0.82              |
| 2:N:509:ARG:HH11   | 2:N:509:ARG:HB2    | 1.43                     | 0.82              |
| 1:K:183:ARG:O      | 1:K:201:ASN:HB3    | 1.80                     | 0.81              |
| 1:J:77:ASN:HD22    | 1:J:77:ASN:H       | 1.24                     | 0.81              |
| 2:M:407:LEU:HD23   | 3:M:760:HDD:HBB2   | 1.62                     | 0.81              |
| 2:M:416:THR:CG2    | 2:M:417:ASP:N      | 2.44                     | 0.81              |
| 2:E:419:GLN:HE22   | 2:E:422:ARG:HH11   | 1.28                     | 0.81              |
| 1:B:76:GLU:O       | 1:B:76:GLU:CD      | 2.24                     | 0.81              |
| 1:C:214:PHE:HB3    | 1:C:215:PRO:HD3    | 1.63                     | 0.81              |
| 3:M:760:HDD:HMC1   | 3:M:760:HDD:HBC1   | 1.62                     | 0.80              |
| 2:O:309:LYS:CB     | 2:O:311:THR:HG23   | 2.12                     | 0.80              |
| 2:P:392:HIS:ND1    | 2:P:415:TYR:HB3    | 1.96                     | 0.80              |
| 1:A:212:HIS:O      | 1:D:113:LYS:HE2    | 1.82                     | 0.80              |
| 1:L:183[B]:ARG:NH1 | 2:P:318:HIS:ND1    | 2.30                     | 0.80              |
| 2:M:351:PHE:HB2    | 2:M:358[B]:LYS:HD3 | 1.64                     | 0.80              |
| 2:M:419:GLN:HE22   | 2:M:422:ARG:NH1    | 1.80                     | 0.80              |
| 1:K:165:ARG:HH11   | 3:O:760:HDD:CGA    | 1.93                     | 0.79              |
| 1:B:77:ASN:H       | 1:B:77:ASN:ND2     | 1.78                     | 0.79              |
| 2:H:456:ASN:OD1    | 2:H:458:ALA:N      | 2.13                     | 0.79              |
| 1:C:125:ARG:HB3    | 3:G:760:HDD:HBD1   | 1.64                     | 0.79              |
| 2:E:467:ASP:O      | 2:E:471:ARG:NH1    | 2.16                     | 0.79              |
| 2:N:448:MET:HG3    | 2:N:449[B]:HIS:CD2 | 2.18                     | 0.79              |
| 2:P:309:LYS:CB     | 2:P:311:THR:HG23   | 2.12                     | 0.79              |
| 2:F:354:LEU:HA     | 4:F:767:HOH:O      | 1.83                     | 0.78              |
| 1:I:125:ARG:HB3    | 3:M:760:HDD:CBD    | 2.13                     | 0.78              |
| 2:E:369:ARG:HG2    | 2:E:369:ARG:HH11   | 1.47                     | 0.78              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:N:355:ASP:OD1  | 2:N:358:LYS:HE2     | 1.84                     | 0.78              |
| 2:M:467:ASP:O    | 2:M:471:ARG:NH1     | 2.16                     | 0.78              |
| 2:M:412:LEU:O    | 1:K:111:ARG:NH2     | 2.17                     | 0.78              |
| 1:B:76:GLU:O     | 1:B:76:GLU:CG       | 2.30                     | 0.78              |
| 2:F:449:HIS:CD2  | 2:H:449[A]:HIS:HD2  | 2.00                     | 0.78              |
| 2:P:416:THR:HG22 | 2:P:417:ASP:N       | 1.97                     | 0.78              |
| 1:C:76:GLU:HG3   | 1:C:78:TYR:CE2      | 2.19                     | 0.77              |
| 1:I:83:ASN:HB3   | 2:O:429:HIS:HD2     | 1.44                     | 0.77              |
| 2:M:456:ASN:HD22 | 2:M:457:PRO:N       | 1.81                     | 0.77              |
| 4:B:305:HOH:O    | 2:F:422:ARG:HD2     | 1.84                     | 0.77              |
| 1:B:77:ASN:HD22  | 1:B:77:ASN:N        | 1.75                     | 0.77              |
| 2:E:412:LEU:O    | 1:C:111:ARG:NH2     | 2.18                     | 0.77              |
| 2:F:488:ARG:HD3  | 4:F:761:HOH:O       | 1.81                     | 0.77              |
| 2:M:456:ASN:HD22 | 2:M:456:ASN:C       | 1.89                     | 0.77              |
| 2:M:438:CYS:HB2  | 2:M:439:PRO:CD      | 2.14                     | 0.77              |
| 1:I:267:ARG:NH2  | 2:M:330:ASP:HB2     | 2.00                     | 0.77              |
| 1:K:101:GLY:O    | 4:K:302:HOH:O       | 2.04                     | 0.76              |
| 3:P:760:HDD:HMB3 | 3:P:760:HDD:CBB     | 2.09                     | 0.76              |
| 2:M:392:HIS:O    | 2:M:395:HIS:HB2     | 1.84                     | 0.76              |
| 2:P:327:GLU:OE1  | 4:P:767:HOH:O       | 2.03                     | 0.76              |
| 2:H:419:GLN:HA   | 2:H:419:GLN:NE2     | 1.99                     | 0.75              |
| 2:O:382:PHE:CZ   | 2:O:386:ASN:ND2     | 2.53                     | 0.75              |
| 1:D:206:PHE:CG   | 3:H:760:HDD:CBB     | 2.68                     | 0.75              |
| 1:C:207:PHE:CD1  | 1:C:217:PHE:CZ      | 2.75                     | 0.74              |
| 2:M:419:GLN:HE22 | 2:M:422:ARG:HH11    | 1.34                     | 0.74              |
| 1:B:206:PHE:HB2  | 3:F:760:HDD:HBB2    | 1.69                     | 0.74              |
| 1:D:282:ALA:N    | 4:D:310:HOH:O       | 2.07                     | 0.74              |
| 1:B:201:ASN:OD1  | 3:F:760:HDD:HMB1    | 1.86                     | 0.74              |
| 1:C:267:ARG:HH11 | 1:C:267:ARG:HB3     | 1.53                     | 0.74              |
| 1:J:231:GLN:O    | 1:J:233:GLN:HG3     | 1.88                     | 0.74              |
| 2:O:411:ARG:HG2  | 2:O:415:TYR:CE2     | 2.21                     | 0.74              |
| 2:M:309:LYS:CB   | 2:M:311:THR:CG2     | 2.65                     | 0.73              |
| 2:M:461:GLU:HA   | 2:M:462:PRO:C       | 2.12                     | 0.72              |
| 2:N:419:GLN:HA   | 2:N:419:GLN:HE21    | 1.52                     | 0.72              |
| 1:K:294:LYS:HD3  | 1:K:295:PRO:CD      | 2.17                     | 0.72              |
| 2:O:392:HIS:ND1  | 2:O:415:TYR:CA      | 2.52                     | 0.72              |
| 2:P:563:GLY:C    | 2:P:564:ILE:HG13    | 2.14                     | 0.72              |
| 2:F:381:ASN:CG   | 4:F:763:HOH:O       | 2.32                     | 0.72              |
| 1:D:266:TYR:HB2  | 1:D:267[B]:ARG:HH12 | 1.54                     | 0.72              |
| 2:P:563:GLY:O    | 2:P:564:ILE:HG13    | 1.89                     | 0.72              |
| 2:F:414:SER:CB   | 3:F:760:HDD:CBC     | 2.67                     | 0.72              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:D:214:PHE:HB3     | 1:D:215:PRO:HD3    | 1.71                     | 0.72              |
| 2:H:407:LEU:HD21    | 3:H:760:HDD:HBB2   | 1.70                     | 0.72              |
| 1:J:125:ARG:HB3     | 3:N:760:HDD:HBD1   | 1.72                     | 0.71              |
| 1:K:125:ARG:HB3     | 3:O:760:HDD:HBD1   | 1.72                     | 0.71              |
| 2:G:493:LYS:CE      | 2:H:487:GLU:OE2    | 2.37                     | 0.71              |
| 1:L:77:ASN:HD22     | 1:L:77:ASN:H       | 1.39                     | 0.71              |
| 1:B:293:TRP:CZ3     | 2:F:336:LEU:HB2    | 2.24                     | 0.71              |
| 1:K:131:GLY:O       | 2:O:319:ARG:NH2    | 2.23                     | 0.71              |
| 2:O:414:SER:HB3     | 3:O:760:HDD:HBC1   | 1.73                     | 0.71              |
| 1:A:251:HIS:CE1     | 2:E:359:LEU:HD23   | 2.26                     | 0.71              |
| 1:B:111:ARG:NH2     | 2:H:412:LEU:O      | 2.23                     | 0.71              |
| 2:G:416:THR:HG22    | 2:G:417:ASP:N      | 2.06                     | 0.71              |
| 1:K:278:ARG:HH22    | 2:O:487:GLU:CD     | 1.99                     | 0.71              |
| 1:J:206:PHE:HB2     | 3:N:760:HDD:HBB2   | 1.73                     | 0.71              |
| 2:O:457:PRO:O       | 2:O:465:ILE:HD11   | 1.91                     | 0.71              |
| 1:L:183[B]:ARG:NH1  | 2:P:318:HIS:CE1    | 2.59                     | 0.71              |
| 1:I:119:HIS:HB2     | 2:O:426:PRO:HG3    | 1.72                     | 0.70              |
| 1:L:183[B]:ARG:HH11 | 2:P:318:HIS:CE1    | 2.09                     | 0.70              |
| 1:L:279:LEU:C       | 1:L:280:ILE:HD13   | 2.14                     | 0.70              |
| 2:F:449:HIS:CD2     | 2:H:449[A]:HIS:CD2 | 2.79                     | 0.70              |
| 2:F:512:TRP:CZ3     | 2:F:554:LEU:HD13   | 2.26                     | 0.70              |
| 2:P:392:HIS:CD2     | 2:P:394:GLY:N      | 2.59                     | 0.70              |
| 4:B:306:HOH:O       | 2:F:422:ARG:HD3    | 1.91                     | 0.70              |
| 2:F:381:ASN:ND2     | 4:F:763:HOH:O      | 2.24                     | 0.70              |
| 2:G:363:GLU:CD      | 2:G:363:GLU:H      | 1.99                     | 0.70              |
| 1:I:201:ASN:CG      | 3:M:760:HDD:HMB2   | 2.16                     | 0.70              |
| 2:O:323:TRP:CZ3     | 2:O:378:ASN:HB3    | 2.27                     | 0.70              |
| 1:L:77:ASN:N        | 1:L:77:ASN:ND2     | 2.38                     | 0.70              |
| 1:D:142:LYS:HA      | 1:D:156:PRO:HG3    | 1.74                     | 0.70              |
| 2:F:412:LEU:O       | 1:D:111:ARG:NH2    | 2.25                     | 0.70              |
| 1:C:267:ARG:HH11    | 1:C:267:ARG:HB2    | 1.57                     | 0.70              |
| 2:G:537:PRO:O       | 2:G:540:ARG:HB2    | 1.92                     | 0.70              |
| 1:K:273:GLY:O       | 1:K:275:HIS:N      | 2.25                     | 0.70              |
| 2:G:419:GLN:HA      | 2:G:419:GLN:HE21   | 1.55                     | 0.69              |
| 2:P:392:HIS:CG      | 2:P:415:TYR:CB     | 2.72                     | 0.69              |
| 2:N:449[B]:HIS:HD1  | 2:P:449:HIS:CG     | 2.11                     | 0.69              |
| 2:G:467:ASP:O       | 2:G:471:ARG:NH1    | 2.24                     | 0.69              |
| 1:I:77:ASN:HB3      | 2:O:469:TRP:CE3    | 2.27                     | 0.69              |
| 2:E:419:GLN:NE2     | 2:E:419:GLN:CA     | 2.55                     | 0.69              |
| 2:E:396:ILE:HD13    | 2:E:402:PHE:CE2    | 2.28                     | 0.69              |
| 1:B:76:GLU:OE1      | 1:B:76:GLU:C       | 2.36                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:M:461:GLU:OE2    | 2:M:461:GLU:C      | 2.36                     | 0.69              |
| 2:O:355:ASP:OD1    | 2:O:358:LYS:CE     | 2.40                     | 0.69              |
| 1:K:276:THR:O      | 2:O:403:THR:HG23   | 1.90                     | 0.69              |
| 1:B:206:PHE:CG     | 3:F:760:HDD:CBB    | 2.76                     | 0.68              |
| 2:O:416:THR:HG22   | 2:O:417:ASP:N      | 2.08                     | 0.68              |
| 2:G:419:GLN:HE22   | 2:G:422:ARG:NH1    | 1.91                     | 0.68              |
| 2:O:392:HIS:HB2    | 2:O:415:TYR:HB3    | 1.75                     | 0.68              |
| 2:P:467:ASP:O      | 2:P:471:ARG:NH1    | 2.26                     | 0.68              |
| 2:G:438:CYS:HB2    | 2:G:439:PRO:HD2    | 1.76                     | 0.68              |
| 2:F:509:ARG:HH11   | 2:F:509:ARG:CG     | 2.04                     | 0.68              |
| 2:G:419:GLN:NE2    | 2:G:419:GLN:CA     | 2.53                     | 0.68              |
| 1:I:279:LEU:C      | 1:I:280:ILE:HD13   | 2.18                     | 0.68              |
| 2:N:449[B]:HIS:ND1 | 2:P:449:HIS:HB2    | 2.09                     | 0.68              |
| 2:G:392:HIS:ND1    | 2:G:415:TYR:CG     | 2.61                     | 0.68              |
| 2:M:402:PHE:HB3    | 2:M:408:LEU:HD21   | 1.76                     | 0.68              |
| 3:E:760:HDD:HBD2   | 4:E:137:HOH:O      | 1.94                     | 0.67              |
| 2:G:443:PHE:CZ     | 2:G:470:PRO:HD2    | 2.29                     | 0.67              |
| 1:K:125:ARG:HB3    | 3:O:760:HDD:CBD    | 2.24                     | 0.67              |
| 2:P:404:ASN:O      | 2:P:405:ASP:C      | 2.38                     | 0.67              |
| 1:K:165:ARG:NH1    | 3:O:760:HDD:O2A    | 2.24                     | 0.67              |
| 2:P:456:ASN:OD1    | 2:P:457:PRO:HD2    | 1.95                     | 0.67              |
| 1:J:120:GLU:HG2    | 2:P:446:ASP:HB2    | 1.75                     | 0.67              |
| 2:F:414:SER:HB3    | 3:F:760:HDD:HBC1   | 1.76                     | 0.67              |
| 2:E:392:HIS:CD2    | 2:E:394:GLY:H      | 2.11                     | 0.67              |
| 3:E:760:HDD:HBB1   | 3:E:760:HDD:HMB3   | 1.74                     | 0.67              |
| 1:K:201:ASN:CG     | 3:O:760:HDD:CMB    | 2.68                     | 0.67              |
| 1:L:267:ARG:HH11   | 1:L:267:ARG:HB3    | 0.50                     | 0.67              |
| 1:C:279:LEU:O      | 1:C:280:ILE:HD13   | 1.95                     | 0.66              |
| 2:M:505:TYR:C      | 2:M:508:PRO:HD2    | 2.20                     | 0.66              |
| 2:G:369:ARG:HH11   | 2:G:369:ARG:CG     | 2.07                     | 0.66              |
| 2:P:351:PHE:HB2    | 4:P:773:HOH:O      | 1.94                     | 0.66              |
| 1:B:125:ARG:CB     | 3:F:760:HDD:HBD1   | 2.25                     | 0.66              |
| 2:F:323:TRP:CZ3    | 2:F:378:ASN:HB3    | 2.29                     | 0.66              |
| 2:N:449[B]:HIS:CE1 | 2:P:449:HIS:HB2    | 2.31                     | 0.66              |
| 1:K:286:ALA:HB2    | 2:O:485:TYR:CE1    | 2.30                     | 0.66              |
| 2:N:392:HIS:CD2    | 2:N:394:GLY:H      | 2.13                     | 0.66              |
| 2:O:461:GLU:HA     | 2:O:462:PRO:C      | 2.19                     | 0.66              |
| 2:E:449[B]:HIS:HB2 | 2:G:449[B]:HIS:CD2 | 2.30                     | 0.66              |
| 2:F:509:ARG:HG3    | 2:F:509:ARG:NH1    | 2.00                     | 0.66              |
| 1:I:265:SER:OG     | 1:I:267:ARG:HB2    | 1.95                     | 0.66              |
| 1:B:76:GLU:HG3     | 1:B:78:TYR:CE2     | 2.31                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:P:438:CYS:HB2   | 2:P:439:PRO:CD     | 2.26                     | 0.66              |
| 1:A:127:VAL:HG22  | 3:E:760:HDD:HMD2   | 1.77                     | 0.66              |
| 4:A:315:HOH:O     | 2:E:478:LYS:HD2    | 1.94                     | 0.66              |
| 2:H:563:GLY:C     | 2:H:564:ILE:HG13   | 2.21                     | 0.66              |
| 2:O:414:SER:CB    | 3:O:760:HDD:CBC    | 2.74                     | 0.66              |
| 2:O:438:CYS:HB2   | 2:O:439:PRO:HD2    | 1.78                     | 0.66              |
| 2:P:356:PRO:HG3   | 2:P:407:LEU:HB2    | 1.76                     | 0.66              |
| 1:A:76:GLU:HG3    | 1:A:78:TYR:CE2     | 2.30                     | 0.65              |
| 2:M:419:GLN:HE21  | 2:M:419:GLN:HA     | 1.61                     | 0.65              |
| 2:N:461:GLU:HA    | 2:N:462:PRO:C      | 2.20                     | 0.65              |
| 2:O:382:PHE:CE1   | 2:O:386:ASN:ND2    | 2.62                     | 0.65              |
| 1:A:251:HIS:HE1   | 2:E:359:LEU:HD23   | 1.60                     | 0.65              |
| 1:K:196:PHE:CE1   | 2:O:400:LEU:HD13   | 2.31                     | 0.65              |
| 2:H:392:HIS:O     | 2:H:395:HIS:HB2    | 1.96                     | 0.65              |
| 2:N:438:CYS:HB2   | 2:N:439:PRO:CD     | 2.26                     | 0.65              |
| 1:D:278:ARG:HH22  | 2:H:487:GLU:CD     | 2.04                     | 0.65              |
| 1:I:121:ARG:HH21  | 1:L:222:LYS:HZ1    | 1.43                     | 0.65              |
| 1:I:165:ARG:HD3   | 3:M:760:HDD:O2A    | 1.97                     | 0.65              |
| 1:I:273:GLY:C     | 4:I:303:HOH:O      | 2.39                     | 0.65              |
| 2:M:419:GLN:HA    | 2:M:419:GLN:NE2    | 2.11                     | 0.65              |
| 1:L:158:LYS:CE    | 4:L:310:HOH:O      | 2.43                     | 0.65              |
| 2:E:461:GLU:O     | 1:B:213:LYS:NZ     | 2.27                     | 0.65              |
| 1:J:76:GLU:HG3    | 1:J:78:TYR:CE2     | 2.31                     | 0.65              |
| 1:A:95:LEU:HB3    | 1:A:107:ASP:HB2    | 1.79                     | 0.65              |
| 2:F:414:SER:HB2   | 3:F:760:HDD:CBC    | 2.27                     | 0.65              |
| 1:D:265:SER:HB2   | 1:D:267[B]:ARG:NH2 | 2.11                     | 0.65              |
| 2:F:382:PHE:N     | 4:F:763:HOH:O      | 2.30                     | 0.64              |
| 2:F:416:THR:HG22  | 2:F:417:ASP:N      | 2.12                     | 0.64              |
| 1:B:267[B]:ARG:CD | 1:B:297:ALA:CB     | 2.75                     | 0.64              |
| 1:K:279:LEU:O     | 1:K:280:ILE:HD13   | 1.97                     | 0.64              |
| 1:A:92:GLN:HA     | 1:D:213:LYS:HD3    | 1.80                     | 0.64              |
| 1:B:76:GLU:O      | 1:B:76:GLU:HG3     | 1.97                     | 0.64              |
| 2:G:361:PRO:HG2   | 2:G:364:LEU:HD12   | 1.77                     | 0.64              |
| 1:I:196:PHE:CE1   | 2:M:400:LEU:HD13   | 2.32                     | 0.64              |
| 2:E:443:PHE:CZ    | 2:E:470:PRO:HD2    | 2.32                     | 0.64              |
| 1:D:128:HIS:CE1   | 1:D:169:VAL:HG22   | 2.33                     | 0.64              |
| 1:D:206:PHE:CG    | 3:H:760:HDD:HBB2   | 2.32                     | 0.64              |
| 1:L:158:LYS:HE3   | 4:L:310:HOH:O      | 1.97                     | 0.64              |
| 2:F:467:ASP:O     | 2:F:471:ARG:NH1    | 2.31                     | 0.64              |
| 1:A:138:PHE:C     | 1:A:138:PHE:CD2    | 2.76                     | 0.64              |
| 2:N:404:ASN:O     | 2:N:405:ASP:C      | 2.40                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:77:ASN:HB3     | 2:G:469:TRP:CZ3    | 2.33                     | 0.64              |
| 1:J:213:LYS:HD3    | 1:K:92:GLN:HA      | 1.79                     | 0.64              |
| 2:E:369:ARG:HH11   | 2:E:369:ARG:CG     | 2.11                     | 0.64              |
| 2:F:449:HIS:HB2    | 2:H:449[B]:HIS:CD2 | 2.33                     | 0.63              |
| 1:J:222:LYS:NZ     | 1:K:121:ARG:HH21   | 1.96                     | 0.63              |
| 2:P:416:THR:CG2    | 2:P:417:ASP:N      | 2.60                     | 0.63              |
| 1:B:142:LYS:HA     | 1:B:156:PRO:HG3    | 1.80                     | 0.63              |
| 1:B:83:ASN:HB3     | 2:H:429:HIS:CD2    | 2.34                     | 0.63              |
| 2:H:323:TRP:CD2    | 2:H:378:ASN:ND2    | 2.66                     | 0.63              |
| 2:M:451:MET:HE3    | 2:O:432:PRO:HD3    | 1.80                     | 0.63              |
| 2:M:459:ASN:HD22   | 2:M:459:ASN:H      | 1.44                     | 0.63              |
| 2:M:469:TRP:CE3    | 1:K:77:ASN:HB3     | 2.32                     | 0.63              |
| 1:K:164:VAL:CG2    | 1:K:187:THR:HG23   | 2.29                     | 0.63              |
| 2:E:483[B]:GLU:OE1 | 2:E:486[B]:GLN:OE1 | 2.17                     | 0.63              |
| 2:O:509:ARG:HG2    | 2:O:550:ILE:O      | 1.99                     | 0.63              |
| 2:M:456:ASN:HD22   | 2:M:458:ALA:H      | 1.46                     | 0.63              |
| 3:P:760:HDD:CMB    | 3:P:760:HDD:CBB    | 2.71                     | 0.63              |
| 2:F:429:HIS:CD2    | 1:D:83:ASN:HB3     | 2.34                     | 0.63              |
| 2:G:509[A]:ARG:HG3 | 2:G:550:ILE:O      | 1.98                     | 0.63              |
| 1:I:293:TRP:CZ3    | 2:M:336:LEU:HB2    | 2.34                     | 0.63              |
| 1:I:201:ASN:ND2    | 3:M:760:HDD:HMB2   | 2.13                     | 0.62              |
| 2:P:461:GLU:HA     | 2:P:462:PRO:C      | 2.22                     | 0.62              |
| 1:A:179:VAL:O      | 1:A:183:ARG:NH2    | 2.32                     | 0.62              |
| 1:I:105:LEU:HD11   | 2:O:413:PHE:HB2    | 1.80                     | 0.62              |
| 1:J:111:ARG:NH2    | 2:P:412:LEU:O      | 2.32                     | 0.62              |
| 2:P:355:ASP:HB3    | 2:P:358:LYS:HG3    | 1.81                     | 0.62              |
| 2:F:461:GLU:HA     | 2:F:462:PRO:C      | 2.24                     | 0.62              |
| 2:H:461:GLU:HA     | 2:H:462:PRO:C      | 2.23                     | 0.62              |
| 1:K:148:THR:HG23   | 1:K:148:THR:O      | 1.97                     | 0.62              |
| 2:E:545:ASP:O      | 2:E:548:ALA:HB3    | 2.00                     | 0.62              |
| 2:F:438:CYS:HB2    | 2:F:439:PRO:HD2    | 1.80                     | 0.62              |
| 2:H:438:CYS:HB2    | 2:H:439:PRO:CD     | 2.28                     | 0.62              |
| 2:H:471:ARG:HA     | 4:H:771:HOH:O      | 1.98                     | 0.62              |
| 2:N:392:HIS:CG     | 2:N:415:TYR:CB     | 2.73                     | 0.62              |
| 1:A:249:THR:O      | 1:A:253:VAL:HG23   | 1.99                     | 0.62              |
| 1:D:201:ASN:CG     | 3:H:760:HDD:HMB1   | 2.24                     | 0.62              |
| 2:O:459:ASN:H      | 2:O:459:ASN:HD22   | 1.46                     | 0.62              |
| 1:B:201:ASN:CG     | 3:F:760:HDD:HMB1   | 2.24                     | 0.62              |
| 1:D:265:SER:HB2    | 1:D:267[B]:ARG:CZ  | 2.30                     | 0.62              |
| 2:M:512:TRP:CZ3    | 2:M:554:LEU:HD13   | 2.34                     | 0.62              |
| 1:J:214:PHE:HB3    | 1:J:215:PRO:HD3    | 1.80                     | 0.62              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:O:419:GLN:HA      | 2:O:419:GLN:HE21   | 1.64                     | 0.62              |
| 1:L:197:ASP:HB2     | 2:P:392:HIS:O      | 1.99                     | 0.62              |
| 2:P:416:THR:HG22    | 2:P:417:ASP:H      | 1.64                     | 0.62              |
| 2:G:392:HIS:CD2     | 2:G:394:GLY:H      | 2.18                     | 0.62              |
| 2:H:419:GLN:HA      | 2:H:419:GLN:HE21   | 1.65                     | 0.62              |
| 1:I:83:ASN:CB       | 2:O:429:HIS:CD2    | 2.69                     | 0.62              |
| 2:M:382:PHE:CE1     | 2:M:386:ASN:ND2    | 2.67                     | 0.62              |
| 1:B:120:GLU:HG2     | 2:H:446:ASP:HB2    | 1.82                     | 0.62              |
| 1:B:267[B]:ARG:HH11 | 1:B:267[B]:ARG:CG  | 2.12                     | 0.62              |
| 2:N:411:ARG:HG2     | 2:N:415:TYR:HE2    | 1.65                     | 0.62              |
| 1:K:136:GLY:HA3     | 2:O:374:VAL:O      | 1.98                     | 0.62              |
| 1:L:214:PHE:HB3     | 1:L:215:PRO:HD3    | 1.82                     | 0.62              |
| 2:E:419:GLN:HE22    | 2:E:422:ARG:NH1    | 1.97                     | 0.61              |
| 2:M:493:LYS:HE3     | 2:N:487:GLU:OE2    | 2.00                     | 0.61              |
| 2:N:459:ASN:HD22    | 2:N:459:ASN:H      | 1.48                     | 0.61              |
| 2:O:392:HIS:CG      | 2:O:415:TYR:CB     | 2.62                     | 0.61              |
| 2:F:563:GLY:C       | 2:F:564:ILE:HG13   | 2.24                     | 0.61              |
| 1:B:278:ARG:NH2     | 2:F:487:GLU:OE1    | 2.34                     | 0.61              |
| 2:F:419:GLN:NE2     | 2:F:419:GLN:HA     | 2.15                     | 0.61              |
| 2:G:369:ARG:HG2     | 2:G:369:ARG:NH1    | 2.10                     | 0.61              |
| 1:B:114:ILE:O       | 1:B:115:THR:C      | 2.44                     | 0.61              |
| 1:J:123:PRO:HG3     | 1:K:123:PRO:HD3    | 1.83                     | 0.61              |
| 1:K:231:GLN:O       | 1:K:233:GLN:HG3    | 2.00                     | 0.61              |
| 1:A:209:GLN:N       | 4:A:311:HOH:O      | 2.34                     | 0.61              |
| 1:I:188:LYS:HG3     | 1:I:197:ASP:OD2    | 2.00                     | 0.61              |
| 1:K:122:ILE:HB      | 1:K:123:PRO:HD2    | 1.82                     | 0.61              |
| 1:C:278:ARG:NH1     | 4:C:317:HOH:O      | 2.14                     | 0.60              |
| 2:M:355:ASP:OD1     | 2:M:358[B]:LYS:NZ  | 2.33                     | 0.60              |
| 2:M:469:TRP:CZ3     | 1:K:77:ASN:HB3     | 2.36                     | 0.60              |
| 1:I:212:HIS:O       | 1:L:113:LYS:HE2    | 2.00                     | 0.60              |
| 1:B:206:PHE:CG      | 3:F:760:HDD:HBB2   | 2.36                     | 0.60              |
| 2:N:505:TYR:C       | 2:N:508:PRO:HD2    | 2.25                     | 0.60              |
| 1:I:273:GLY:O       | 1:I:275:HIS:N      | 2.33                     | 0.60              |
| 2:M:448:MET:HE2     | 1:K:122:ILE:HG22   | 1.83                     | 0.60              |
| 2:F:449:HIS:HB3     | 2:H:449[A]:HIS:CD2 | 2.36                     | 0.60              |
| 1:L:95:LEU:HB3      | 1:L:107:ASP:HB2    | 1.84                     | 0.60              |
| 1:L:229:ILE:HG23    | 1:L:230:PRO:HA     | 1.83                     | 0.60              |
| 2:F:369:ARG:HG2     | 2:F:369:ARG:HH11   | 1.67                     | 0.60              |
| 1:C:293:TRP:CZ3     | 2:G:336:LEU:HB2    | 2.36                     | 0.60              |
| 2:E:363:GLU:CD      | 2:E:363:GLU:H      | 2.10                     | 0.60              |
| 2:H:530:GLU:OE2     | 4:H:765:HOH:O      | 2.17                     | 0.60              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:I:121:ARG:HH21    | 1:L:222:LYS:NZ     | 1.99                     | 0.60              |
| 2:M:411:ARG:HG2     | 2:M:415:TYR:HE2    | 1.66                     | 0.60              |
| 1:J:87:ARG:N        | 4:J:305:HOH:O      | 1.99                     | 0.60              |
| 2:O:363:GLU:H       | 2:O:363:GLU:CD     | 2.10                     | 0.60              |
| 1:I:116:HIS:CD2     | 2:O:426:PRO:HB2    | 2.37                     | 0.60              |
| 1:A:279:LEU:O       | 1:A:280:ILE:HD13   | 2.01                     | 0.60              |
| 2:O:323:TRP:CH2     | 2:O:378:ASN:HB3    | 2.36                     | 0.60              |
| 1:B:77:ASN:ND2      | 1:B:77:ASN:N       | 2.40                     | 0.59              |
| 1:C:260:ARG:HH11    | 1:C:260:ARG:CG     | 2.15                     | 0.59              |
| 1:L:168:THR:CG2     | 1:L:183[B]:ARG:NH2 | 2.65                     | 0.59              |
| 2:E:413:PHE:CE1     | 1:D:111:ARG:HG2    | 2.37                     | 0.59              |
| 1:L:279:LEU:O       | 1:L:280:ILE:HD13   | 2.01                     | 0.59              |
| 2:E:512:TRP:CZ3     | 2:E:554:LEU:HD13   | 2.37                     | 0.59              |
| 1:D:267[A]:ARG:HH22 | 2:H:330:ASP:HB2    | 1.68                     | 0.59              |
| 1:I:279:LEU:O       | 1:I:280:ILE:HD13   | 2.01                     | 0.59              |
| 1:J:128:HIS:HA      | 1:J:168:THR:O      | 2.01                     | 0.59              |
| 1:D:206:PHE:CD1     | 3:H:760:HDD:CBB    | 2.85                     | 0.59              |
| 2:N:438:CYS:HB2     | 2:N:439:PRO:HD2    | 1.85                     | 0.59              |
| 2:O:467:ASP:O       | 2:O:469:TRP:CD1    | 2.55                     | 0.59              |
| 2:P:363:GLU:CD      | 2:P:363:GLU:H      | 2.11                     | 0.59              |
| 1:D:267[B]:ARG:NH1  | 1:D:267[B]:ARG:CG  | 2.47                     | 0.59              |
| 1:I:133:ALA:HA      | 1:I:164:VAL:O      | 2.02                     | 0.59              |
| 1:I:276:THR:O       | 2:M:403:THR:CG2    | 2.51                     | 0.59              |
| 2:G:405:ASP:C       | 2:G:405:ASP:OD1    | 2.46                     | 0.59              |
| 1:D:179:VAL:O       | 1:D:183:ARG:NH2    | 2.35                     | 0.59              |
| 1:I:251:HIS:CE1     | 2:M:359:LEU:HD23   | 2.38                     | 0.59              |
| 1:J:207:PHE:CD1     | 1:J:217:PHE:CZ     | 2.91                     | 0.59              |
| 2:N:433:ILE:HG13    | 2:N:433:ILE:O      | 2.02                     | 0.59              |
| 2:O:414:SER:CB      | 3:O:760:HDD:HBC1   | 2.32                     | 0.59              |
| 2:H:323:TRP:CG      | 2:H:378:ASN:ND2    | 2.71                     | 0.59              |
| 1:K:164:VAL:HG22    | 1:K:187:THR:HG23   | 1.85                     | 0.59              |
| 1:K:201:ASN:ND2     | 3:O:760:HDD:HMB3   | 2.18                     | 0.59              |
| 2:F:449:HIS:CB      | 2:H:449[B]:HIS:CD2 | 2.86                     | 0.58              |
| 1:D:281:ASN:ND2     | 1:D:285:LYS:HB3    | 2.18                     | 0.58              |
| 1:D:281:ASN:HD21    | 1:D:285:LYS:HB3    | 1.67                     | 0.58              |
| 2:P:545:ASP:O       | 2:P:548:ALA:HB3    | 2.03                     | 0.58              |
| 1:B:206:PHE:CB      | 3:F:760:HDD:HBB2   | 2.34                     | 0.58              |
| 2:N:538:TYR:HA      | 2:N:541:GLU:CG     | 2.34                     | 0.58              |
| 1:K:269:MET:HG2     | 1:K:270:GLU:O      | 2.04                     | 0.58              |
| 2:O:493:LYS:HE3     | 2:P:487:GLU:OE2    | 2.04                     | 0.58              |
| 1:L:169:VAL:HG23    | 1:L:182:ILE:O      | 2.03                     | 0.58              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:D:178:THR:O    | 2:H:311:THR:HG22   | 2.03                     | 0.58              |
| 1:C:179:VAL:O    | 1:C:183:ARG:NH2    | 2.36                     | 0.58              |
| 2:M:448:MET:CE   | 1:K:122:ILE:HG22   | 2.34                     | 0.58              |
| 2:N:494:VAL:O    | 2:N:494:VAL:HG23   | 2.03                     | 0.58              |
| 2:E:473:THR:CB   | 4:E:93:HOH:O       | 2.51                     | 0.58              |
| 2:G:461:GLU:HA   | 2:G:462:PRO:C      | 2.27                     | 0.58              |
| 2:G:493:LYS:NZ   | 2:H:487:GLU:OE2    | 2.36                     | 0.58              |
| 1:D:293:TRP:CZ3  | 2:H:336:LEU:HB2    | 2.38                     | 0.58              |
| 1:J:121:ARG:HH21 | 1:K:222:LYS:HE3    | 1.68                     | 0.58              |
| 1:D:266:TYR:H    | 1:D:267[B]:ARG:NH2 | 2.02                     | 0.58              |
| 2:M:351:PHE:CB   | 2:M:358[B]:LYS:HD3 | 2.32                     | 0.58              |
| 2:O:507:HIS:N    | 2:O:508:PRO:HD2    | 2.18                     | 0.58              |
| 1:A:214:PHE:HB3  | 1:A:215:PRO:HD3    | 1.85                     | 0.58              |
| 1:I:120:GLU:HG2  | 2:O:446:ASP:HB2    | 1.86                     | 0.58              |
| 1:I:177:ASP:O    | 1:I:183:ARG:NH2    | 2.37                     | 0.58              |
| 2:O:507:HIS:N    | 2:O:508:PRO:CD     | 2.66                     | 0.58              |
| 1:A:201:ASN:CG   | 3:E:760:HDD:HMB1   | 2.29                     | 0.58              |
| 1:C:260:ARG:NH1  | 1:C:260:ARG:HG3    | 2.18                     | 0.58              |
| 1:C:290:ARG:HD2  | 4:C:314:HOH:O      | 2.02                     | 0.58              |
| 2:G:461:GLU:O    | 1:D:213:LYS:NZ     | 2.37                     | 0.58              |
| 1:D:164:VAL:HG22 | 1:D:187:THR:OG1    | 2.04                     | 0.58              |
| 1:I:76:GLU:OE1   | 1:I:77:ASN:N       | 2.36                     | 0.58              |
| 1:I:272:PHE:C    | 1:I:274:ILE:H      | 2.12                     | 0.58              |
| 2:P:438:CYS:HB2  | 2:P:439:PRO:HD2    | 1.86                     | 0.57              |
| 1:A:83:ASN:HB3   | 2:G:429:HIS:CD2    | 2.39                     | 0.57              |
| 2:G:419:GLN:HE22 | 2:G:422:ARG:HH11   | 1.52                     | 0.57              |
| 3:N:760:HDD:HBC1 | 3:N:760:HDD:CMC    | 2.33                     | 0.57              |
| 1:B:292:HIS:O    | 2:F:336:LEU:HD12   | 2.04                     | 0.57              |
| 2:N:563:GLY:C    | 2:N:564:ILE:HG13   | 2.29                     | 0.57              |
| 1:C:76:GLU:HG3   | 1:C:78:TYR:CZ      | 2.38                     | 0.57              |
| 2:P:463:ASN:ND2  | 2:P:468:ASN:HA     | 2.19                     | 0.57              |
| 1:A:267:ARG:HG2  | 1:A:267:ARG:NH1    | 2.15                     | 0.57              |
| 2:M:351:PHE:HB2  | 2:M:358[B]:LYS:HD2 | 1.86                     | 0.57              |
| 1:J:142:LYS:HA   | 1:J:156:PRO:HG3    | 1.85                     | 0.57              |
| 2:O:490:GLU:HG2  | 2:P:490:GLU:HG2    | 1.85                     | 0.57              |
| 1:A:274:ILE:HD12 | 3:E:760:HDD:CBB    | 2.32                     | 0.57              |
| 2:M:537:PRO:O    | 2:M:540:ARG:HB2    | 2.05                     | 0.57              |
| 1:J:118:ASP:O    | 1:K:126:ILE:HD11   | 2.03                     | 0.57              |
| 1:K:155:ASP:OD2  | 1:K:157:ASN:N      | 2.35                     | 0.57              |
| 1:A:293:TRP:CZ3  | 2:E:336:LEU:HB2    | 2.39                     | 0.57              |
| 1:C:207:PHE:CD2  | 1:C:252:ASN:HB3    | 2.40                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I:199:VAL:HB     | 2:M:411:ARG:HH22   | 1.69                     | 0.57              |
| 2:N:515:GLN:HB2    | 2:N:520:GLN:HG2    | 1.86                     | 0.57              |
| 1:K:281:ASN:OD1    | 1:K:281:ASN:C      | 2.47                     | 0.57              |
| 1:A:178:THR:O      | 2:E:311:THR:HG22   | 2.05                     | 0.57              |
| 2:F:469:TRP:CZ3    | 1:D:77:ASN:HB3     | 2.40                     | 0.57              |
| 1:B:77:ASN:HB3     | 2:H:469:TRP:CZ3    | 2.40                     | 0.57              |
| 1:D:120:GLU:HB3    | 1:D:121:ARG:NH1    | 2.20                     | 0.57              |
| 1:I:113:LYS:HE2    | 1:L:212:HIS:O      | 2.05                     | 0.57              |
| 1:C:76:GLU:OE2     | 1:C:76:GLU:HA      | 2.05                     | 0.56              |
| 1:C:274:ILE:HD12   | 3:G:760:HDD:HMB3   | 1.86                     | 0.56              |
| 1:I:95:LEU:HB3     | 1:I:107:ASP:HB2    | 1.87                     | 0.56              |
| 2:M:461:GLU:OE2    | 2:M:462:PRO:N      | 2.38                     | 0.56              |
| 1:B:267[B]:ARG:NH1 | 1:B:267[B]:ARG:HG3 | 2.20                     | 0.56              |
| 2:E:473:THR:HB     | 4:E:93:HOH:O       | 2.04                     | 0.56              |
| 1:J:278:ARG:HH22   | 2:N:487:GLU:CD     | 2.09                     | 0.56              |
| 1:L:267:ARG:CB     | 1:L:267:ARG:CZ     | 2.75                     | 0.56              |
| 2:P:419:GLN:HA     | 2:P:419:GLN:HE21   | 1.67                     | 0.56              |
| 1:D:128:HIS:HA     | 1:D:168:THR:O      | 2.05                     | 0.56              |
| 1:D:195:ILE:HD11   | 2:H:436:PRO:HA     | 1.87                     | 0.56              |
| 2:M:362:GLU:HG3    | 4:M:214:HOH:O      | 2.05                     | 0.56              |
| 2:P:512:TRP:CZ3    | 2:P:554:LEU:HD13   | 2.40                     | 0.56              |
| 2:E:459:ASN:H      | 2:E:459:ASN:HD22   | 1.52                     | 0.56              |
| 2:G:478:LYS:O      | 2:G:479:ARG:HB2    | 2.05                     | 0.56              |
| 2:M:487:GLU:OE2    | 2:N:493:LYS:CE     | 2.51                     | 0.56              |
| 1:A:116:HIS:CD2    | 2:G:426:PRO:HB2    | 2.40                     | 0.56              |
| 1:D:95:LEU:HB3     | 1:D:107:ASP:HB2    | 1.88                     | 0.56              |
| 2:M:340:LEU:C      | 2:M:341:ILE:HG13   | 2.31                     | 0.56              |
| 2:F:463:ASN:ND2    | 2:F:468:ASN:HA     | 2.20                     | 0.56              |
| 2:H:461:GLU:OE2    | 2:H:461:GLU:C      | 2.49                     | 0.56              |
| 1:I:207:PHE:CD1    | 1:I:217:PHE:CZ     | 2.94                     | 0.56              |
| 1:J:113:LYS:HE2    | 1:K:212:HIS:O      | 2.06                     | 0.56              |
| 1:J:119:HIS:CE1    | 2:P:420:ILE:HG21   | 2.41                     | 0.56              |
| 2:O:537:PRO:O      | 2:O:540:ARG:HB2    | 2.05                     | 0.56              |
| 1:L:293:TRP:CZ3    | 2:P:336:LEU:HB2    | 2.41                     | 0.56              |
| 2:H:438:CYS:HB2    | 2:H:439:PRO:HD2    | 1.87                     | 0.56              |
| 2:G:563:GLY:C      | 2:G:564:ILE:HG13   | 2.29                     | 0.56              |
| 1:J:179:VAL:O      | 1:J:183:ARG:NH2    | 2.39                     | 0.56              |
| 2:N:369:ARG:NH2    | 4:N:104:HOH:O      | 1.83                     | 0.56              |
| 2:M:407:LEU:CD2    | 3:M:760:HDD:HBB2   | 2.34                     | 0.56              |
| 1:J:201:ASN:CG     | 3:N:760:HDD:HMB1   | 2.31                     | 0.56              |
| 2:E:537:PRO:O      | 2:E:540:ARG:HB2    | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:F:541:GLU:O      | 2:F:545:ASP:HB2    | 2.05                     | 0.55              |
| 1:C:242:TYR:O      | 1:C:243:VAL:C      | 2.46                     | 0.55              |
| 2:P:355:ASP:OD1    | 2:P:358:LYS:HE2    | 2.05                     | 0.55              |
| 1:A:97:ALA:O       | 1:A:101:GLY:HA3    | 2.06                     | 0.55              |
| 2:E:419:GLN:NE2    | 2:E:422:ARG:HH11   | 2.02                     | 0.55              |
| 2:N:449[B]:HIS:ND1 | 2:P:449:HIS:CB     | 2.70                     | 0.55              |
| 1:J:212:HIS:HE1    | 1:K:109:ILE:HG22   | 1.72                     | 0.55              |
| 2:O:392:HIS:CE1    | 2:O:412:LEU:O      | 2.59                     | 0.55              |
| 1:D:125:ARG:HB3    | 3:H:760:HDD:HBD1   | 1.88                     | 0.55              |
| 1:I:138:PHE:C      | 1:I:138:PHE:CD2    | 2.85                     | 0.55              |
| 2:M:469:TRP:HA     | 2:M:470:PRO:C      | 2.31                     | 0.55              |
| 1:K:199:VAL:HG21   | 2:O:393:PRO:HD3    | 1.89                     | 0.55              |
| 2:P:448:MET:O      | 4:P:763:HOH:O      | 2.18                     | 0.55              |
| 1:J:213:LYS:O      | 1:J:214:PHE:C      | 2.50                     | 0.55              |
| 1:K:165:ARG:NH1    | 3:O:760:HDD:CGA    | 2.68                     | 0.55              |
| 1:C:231:GLN:O      | 1:C:233:GLN:HG3    | 2.07                     | 0.55              |
| 1:D:247:PRO:O      | 1:D:248:GLU:C      | 2.50                     | 0.55              |
| 2:M:461:GLU:C      | 2:M:461:GLU:CD     | 2.74                     | 0.55              |
| 1:L:168:THR:HG22   | 1:L:183[B]:ARG:NH2 | 2.22                     | 0.55              |
| 1:C:281:ASN:ND2    | 1:C:285:LYS:HB3    | 2.22                     | 0.55              |
| 2:N:363:GLU:CD     | 2:N:363:GLU:H      | 2.15                     | 0.55              |
| 1:J:138:PHE:C      | 1:J:138:PHE:CD2    | 2.84                     | 0.55              |
| 1:K:95:LEU:HB3     | 1:K:107:ASP:HB2    | 1.89                     | 0.55              |
| 1:K:201:ASN:ND2    | 3:O:760:HDD:CMB    | 2.70                     | 0.55              |
| 2:E:493:LYS:HE3    | 2:F:487:GLU:OE2    | 2.07                     | 0.55              |
| 1:L:260:ARG:HG3    | 1:L:260:ARG:NH1    | 2.21                     | 0.55              |
| 2:G:392:HIS:HB2    | 2:G:415:TYR:HB3    | 1.89                     | 0.54              |
| 1:I:213:LYS:NZ     | 2:N:461:GLU:O      | 2.36                     | 0.54              |
| 1:L:251:HIS:N      | 4:L:302:HOH:O      | 2.41                     | 0.54              |
| 1:B:128:HIS:HA     | 1:B:168:THR:O      | 2.07                     | 0.54              |
| 2:F:446:ASP:HB2    | 1:D:120:GLU:HG2    | 1.87                     | 0.54              |
| 1:I:199:VAL:HB     | 2:M:411:ARG:NH2    | 2.22                     | 0.54              |
| 2:N:392:HIS:ND1    | 2:N:415:TYR:HB3    | 2.04                     | 0.54              |
| 2:N:563:GLY:O      | 2:N:564:ILE:HG13   | 2.08                     | 0.54              |
| 1:K:147:ILE:C      | 1:K:281:ASN:HB3    | 2.32                     | 0.54              |
| 1:B:95:LEU:HB3     | 1:B:107:ASP:HB2    | 1.89                     | 0.54              |
| 1:C:281:ASN:HD21   | 1:C:285:LYS:HB3    | 1.71                     | 0.54              |
| 2:G:392:HIS:CG     | 2:G:415:TYR:CB     | 2.70                     | 0.54              |
| 2:O:392:HIS:CD2    | 2:O:394:GLY:H      | 2.25                     | 0.54              |
| 1:A:278:ARG:NH2    | 2:E:487:GLU:OE1    | 2.38                     | 0.54              |
| 2:E:536:ARG:HB3    | 2:E:539:ILE:HG13   | 1.89                     | 0.54              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:F:459:ASN:HD22    | 2:F:459:ASN:N      | 1.88                     | 0.54              |
| 1:J:246:GLN:O       | 1:J:249:THR:HG23   | 2.06                     | 0.54              |
| 2:O:457:PRO:O       | 2:O:465:ILE:CD1    | 2.55                     | 0.54              |
| 1:B:113:LYS:HE2     | 1:C:212:HIS:O      | 2.08                     | 0.54              |
| 1:B:125:ARG:HB3     | 3:F:760:HDD:CBD    | 2.33                     | 0.54              |
| 2:F:426:PRO:HB2     | 1:D:116:HIS:CD2    | 2.42                     | 0.54              |
| 1:C:260:ARG:HH11    | 1:C:260:ARG:HG3    | 1.72                     | 0.54              |
| 1:L:181:ASP:HB3     | 1:L:183[A]:ARG:NH2 | 2.22                     | 0.54              |
| 1:L:185:PHE:HD1     | 1:L:185:PHE:C      | 2.14                     | 0.54              |
| 2:P:405:ASP:C       | 2:P:405:ASP:OD1    | 2.50                     | 0.54              |
| 1:B:144:LEU:HD21    | 4:F:770:HOH:O      | 2.07                     | 0.54              |
| 2:M:442:ASN:HA      | 1:K:80:LEU:CD1     | 2.38                     | 0.54              |
| 2:E:528:SER:O       | 2:E:532:SER:HB3    | 2.07                     | 0.54              |
| 1:D:125:ARG:HG3     | 1:D:125:ARG:HH11   | 1.73                     | 0.54              |
| 1:I:278:ARG:HH22    | 2:M:487:GLU:CD     | 2.15                     | 0.54              |
| 2:E:369:ARG:CG      | 2:E:369:ARG:NH1    | 2.70                     | 0.54              |
| 2:F:442:ASN:HA      | 1:D:80:LEU:HD12    | 1.90                     | 0.54              |
| 1:D:251:HIS:CE1     | 2:H:359:LEU:HD23   | 2.43                     | 0.54              |
| 2:M:449:HIS:CD2     | 2:O:449:HIS:CD2    | 2.95                     | 0.54              |
| 4:J:303:HOH:O       | 2:N:393:PRO:HB3    | 2.08                     | 0.54              |
| 2:P:461:GLU:CD      | 2:P:461:GLU:C      | 2.76                     | 0.54              |
| 1:B:183:ARG:NH2     | 1:B:261:GLY:O      | 2.41                     | 0.54              |
| 1:C:246:GLN:O       | 1:C:249:THR:HG23   | 2.07                     | 0.54              |
| 2:M:509:ARG:HG3     | 2:M:550:ILE:O      | 2.08                     | 0.54              |
| 2:O:351:PHE:CD1     | 2:O:351:PHE:C      | 2.86                     | 0.54              |
| 1:L:138:PHE:C       | 1:L:138:PHE:CD2    | 2.86                     | 0.53              |
| 2:F:443:PHE:CE1     | 2:F:461:GLU:HB3    | 2.43                     | 0.53              |
| 2:G:411:ARG:HA      | 3:G:760:HDD:HBC1   | 1.89                     | 0.53              |
| 2:P:393:PRO:HD2     | 2:P:415:TYR:CG     | 2.43                     | 0.53              |
| 2:P:411:ARG:HG2     | 2:P:415:TYR:HE2    | 1.73                     | 0.53              |
| 2:M:405:ASP:OD1     | 2:M:405:ASP:C      | 2.52                     | 0.53              |
| 1:J:126:ILE:HD11    | 1:K:118:ASP:O      | 2.07                     | 0.53              |
| 2:H:382:PHE:CE1     | 2:H:386:ASN:ND2    | 2.77                     | 0.53              |
| 1:I:128:HIS:CE1     | 1:I:169:VAL:HG22   | 2.43                     | 0.53              |
| 1:K:165:ARG:HD3     | 3:O:760:HDD:O1A    | 2.08                     | 0.53              |
| 1:A:222:LYS:O       | 1:A:223:PRO:C      | 2.52                     | 0.53              |
| 1:C:155:ASP:OD2     | 1:C:157:ASN:N      | 2.33                     | 0.53              |
| 1:K:179:VAL:O       | 1:K:183:ARG:NH2    | 2.42                     | 0.53              |
| 1:B:267[B]:ARG:HH22 | 2:F:330:ASP:CB     | 2.03                     | 0.53              |
| 1:I:106:GLU:O       | 1:I:108:PHE:N      | 2.42                     | 0.53              |
| 2:M:407:LEU:CD2     | 3:M:760:HDD:CBB    | 2.86                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:414:SER:HB2  | 3:O:760:HDD:CBC  | 2.38                     | 0.53              |
| 2:P:493:LYS:C    | 2:P:494:VAL:HG13 | 2.33                     | 0.53              |
| 1:A:77:ASN:HB3   | 2:G:469:TRP:CE3  | 2.44                     | 0.53              |
| 2:F:470:PRO:HB3  | 1:D:78:TYR:O     | 2.09                     | 0.53              |
| 1:I:128:HIS:HA   | 1:I:168:THR:O    | 2.07                     | 0.53              |
| 2:M:446:ASP:HB2  | 1:K:120:GLU:HG2  | 1.90                     | 0.53              |
| 1:L:125:ARG:HB3  | 1:L:127:VAL:O    | 2.09                     | 0.53              |
| 1:C:222:LYS:HB3  | 1:C:223:PRO:HD2  | 1.90                     | 0.53              |
| 2:O:392:HIS:O    | 2:O:395:HIS:HB2  | 2.08                     | 0.53              |
| 2:O:396:ILE:HD13 | 2:O:402:PHE:CE2  | 2.44                     | 0.53              |
| 2:P:538:TYR:HA   | 2:P:541:GLU:CG   | 2.38                     | 0.53              |
| 1:A:119:HIS:HB2  | 2:G:426:PRO:HG3  | 1.90                     | 0.53              |
| 1:A:185:PHE:C    | 1:A:185:PHE:CD1  | 2.87                     | 0.53              |
| 1:B:116:HIS:CD2  | 2:H:426:PRO:HB2  | 2.43                     | 0.53              |
| 2:F:505:TYR:C    | 2:F:508:PRO:HD2  | 2.33                     | 0.53              |
| 1:I:142:LYS:HA   | 1:I:156:PRO:HG3  | 1.89                     | 0.53              |
| 1:I:213:LYS:HD3  | 1:L:92:GLN:HA    | 1.91                     | 0.53              |
| 2:M:516:THR:O    | 2:M:517:PRO:C    | 2.51                     | 0.53              |
| 2:O:457:PRO:HA   | 4:O:764:HOH:O    | 2.09                     | 0.53              |
| 1:B:165:ARG:HD3  | 3:F:760:HDD:CGA  | 2.31                     | 0.52              |
| 1:B:179:VAL:O    | 1:B:183:ARG:NH2  | 2.37                     | 0.52              |
| 1:B:206:PHE:CD2  | 3:F:760:HDD:CBB  | 2.92                     | 0.52              |
| 2:N:356:PRO:HG3  | 2:N:407:LEU:HB2  | 1.90                     | 0.52              |
| 2:P:351:PHE:HB2  | 2:P:358:LYS:HD2  | 1.90                     | 0.52              |
| 2:G:512:TRP:CZ3  | 2:G:554:LEU:HD13 | 2.44                     | 0.52              |
| 1:I:125:ARG:CB   | 3:M:760:HDD:HBD1 | 2.33                     | 0.52              |
| 1:K:76:GLU:HG3   | 1:K:78:TYR:CE2   | 2.44                     | 0.52              |
| 2:O:445:ARG:HB3  | 2:O:446:ASP:OD1  | 2.09                     | 0.52              |
| 2:P:556:GLN:O    | 2:P:557:ALA:C    | 2.52                     | 0.52              |
| 1:A:206:PHE:HD1  | 2:E:407:LEU:HD21 | 1.75                     | 0.52              |
| 2:E:405:ASP:C    | 2:E:405:ASP:OD1  | 2.53                     | 0.52              |
| 2:F:392:HIS:ND1  | 2:F:415:TYR:CG   | 2.74                     | 0.52              |
| 1:D:76:GLU:HG3   | 1:D:78:TYR:CE2   | 2.44                     | 0.52              |
| 1:I:222:LYS:HB3  | 1:I:223:PRO:HD2  | 1.91                     | 0.52              |
| 2:N:538:TYR:HA   | 2:N:541:GLU:HG3  | 1.92                     | 0.52              |
| 1:K:278:ARG:NH2  | 2:O:487:GLU:CD   | 2.67                     | 0.52              |
| 2:E:509:ARG:HD2  | 2:E:550:ILE:O    | 2.09                     | 0.52              |
| 1:D:136:GLY:HA3  | 2:H:374:VAL:O    | 2.09                     | 0.52              |
| 1:L:260:ARG:HG3  | 1:L:260:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:185:PHE:C    | 1:A:185:PHE:HD1  | 2.18                     | 0.52              |
| 1:B:119:HIS:CE1  | 2:H:420:ILE:HG21 | 2.45                     | 0.52              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:D:266:TYR:H     | 1:D:267[B]:ARG:HH22 | 1.57                     | 0.52              |
| 1:I:251:HIS:HE1   | 2:M:359:LEU:HD23    | 1.73                     | 0.52              |
| 1:J:249:THR:O     | 1:J:250:LEU:C       | 2.50                     | 0.52              |
| 1:L:185:PHE:C     | 1:L:185:PHE:CD1     | 2.85                     | 0.52              |
| 1:C:128:HIS:HA    | 1:C:168:THR:O       | 2.09                     | 0.52              |
| 1:I:76:GLU:HG3    | 1:I:78:TYR:CE2      | 2.44                     | 0.52              |
| 2:O:438:CYS:HB2   | 2:O:439:PRO:CD      | 2.40                     | 0.52              |
| 2:E:563:GLY:C     | 2:E:564:ILE:HG13    | 2.33                     | 0.52              |
| 1:D:76:GLU:OE1    | 1:D:77:ASN:N        | 2.43                     | 0.52              |
| 1:J:229:ILE:HD11  | 2:O:319:ARG:HG2     | 1.92                     | 0.52              |
| 2:O:392:HIS:HE1   | 2:O:412:LEU:O       | 1.93                     | 0.52              |
| 1:A:214:PHE:CD1   | 3:E:760:HDD:CAC     | 2.93                     | 0.52              |
| 2:F:433:ILE:HG13  | 2:F:433:ILE:O       | 2.08                     | 0.52              |
| 4:C:317:HOH:O     | 2:G:343:GLU:OE2     | 2.19                     | 0.52              |
| 1:K:206:PHE:CD1   | 2:O:407:LEU:HD21    | 2.45                     | 0.52              |
| 2:H:443:PHE:HB3   | 2:H:459:ASN:O       | 2.08                     | 0.52              |
| 1:L:177:ASP:O     | 1:L:183[B]:ARG:NH1  | 2.42                     | 0.52              |
| 2:H:361:PRO:HG2   | 2:H:364:LEU:HD12    | 1.91                     | 0.51              |
| 2:M:357:THR:C     | 2:M:358[A]:LYS:HD3  | 2.35                     | 0.51              |
| 1:J:77:ASN:N      | 1:J:77:ASN:ND2      | 2.42                     | 0.51              |
| 1:L:128:HIS:HA    | 1:L:168:THR:O       | 2.09                     | 0.51              |
| 1:B:125:ARG:HG2   | 3:F:760:HDD:HBD1    | 1.92                     | 0.51              |
| 1:B:273:GLY:O     | 1:B:275:HIS:N       | 2.42                     | 0.51              |
| 2:F:459:ASN:H     | 2:F:459:ASN:ND2     | 1.97                     | 0.51              |
| 1:C:251:HIS:CE1   | 2:G:359:LEU:HD23    | 2.45                     | 0.51              |
| 2:N:448:MET:CG    | 2:N:449[B]:HIS:CD2  | 2.91                     | 0.51              |
| 2:N:459:ASN:HD22  | 2:N:459:ASN:N       | 2.07                     | 0.51              |
| 1:B:267[B]:ARG:CG | 1:B:267[B]:ARG:NH1  | 2.72                     | 0.51              |
| 1:C:127:VAL:HG23  | 3:G:760:HDD:HAD1    | 1.92                     | 0.51              |
| 2:O:443:PHE:CZ    | 2:O:470:PRO:HD2     | 2.46                     | 0.51              |
| 2:O:515:GLN:HB2   | 2:O:520:GLN:HG2     | 1.92                     | 0.51              |
| 1:L:278:ARG:HH22  | 2:P:487:GLU:CD      | 2.18                     | 0.51              |
| 2:E:438:CYS:HB2   | 2:E:439:PRO:CD      | 2.40                     | 0.51              |
| 1:B:206:PHE:CD2   | 3:F:760:HDD:HBB1    | 2.44                     | 0.51              |
| 2:G:382:PHE:CE1   | 2:G:386:ASN:ND2     | 2.78                     | 0.51              |
| 2:M:382:PHE:O     | 2:M:386:ASN:HB3     | 2.11                     | 0.51              |
| 2:N:443:PHE:CZ    | 2:N:470:PRO:HD2     | 2.46                     | 0.51              |
| 1:C:214:PHE:HB3   | 1:C:215:PRO:CD      | 2.38                     | 0.51              |
| 1:I:122:ILE:HB    | 1:I:123:PRO:CD      | 2.41                     | 0.51              |
| 1:B:119:HIS:HB2   | 2:H:426:PRO:HG3     | 1.93                     | 0.51              |
| 1:B:214:PHE:HB3   | 1:B:215:PRO:HD3     | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:392:HIS:CD2  | 2:H:394:GLY:H    | 2.28                     | 0.51              |
| 2:O:505:TYR:C    | 2:O:508:PRO:HD2  | 2.35                     | 0.51              |
| 2:M:361:PRO:HG2  | 2:M:364:LEU:HD12 | 1.92                     | 0.51              |
| 2:O:392:HIS:CB   | 2:O:415:TYR:HB3  | 2.39                     | 0.51              |
| 2:P:461:GLU:C    | 2:P:461:GLU:OE2  | 2.54                     | 0.51              |
| 1:C:185:PHE:HD1  | 1:C:185:PHE:C    | 2.19                     | 0.51              |
| 1:C:207:PHE:CD1  | 1:C:217:PHE:HZ   | 2.28                     | 0.51              |
| 1:C:290:ARG:CD   | 4:C:314:HOH:O    | 2.58                     | 0.51              |
| 1:D:275:HIS:CG   | 2:H:408:LEU:HB2  | 2.46                     | 0.51              |
| 1:J:212:HIS:O    | 1:K:113:LYS:HE2  | 2.10                     | 0.51              |
| 1:A:76:GLU:OE1   | 1:A:77:ASN:N     | 2.44                     | 0.51              |
| 1:A:188:LYS:HG3  | 1:A:197:ASP:OD2  | 2.11                     | 0.51              |
| 1:C:185:PHE:C    | 1:C:185:PHE:CD1  | 2.89                     | 0.51              |
| 2:H:369:ARG:HG2  | 2:H:369:ARG:HH11 | 1.75                     | 0.51              |
| 2:N:405:ASP:C    | 2:N:405:ASP:OD1  | 2.54                     | 0.51              |
| 1:K:214:PHE:CD1  | 3:O:760:HDD:HAC  | 2.46                     | 0.51              |
| 2:O:414:SER:HB2  | 3:O:760:HDD:HBC2 | 1.93                     | 0.51              |
| 3:E:760:HDD:HBB1 | 3:E:760:HDD:CMB  | 2.41                     | 0.50              |
| 2:F:369:ARG:HH11 | 2:F:369:ARG:CG   | 2.25                     | 0.50              |
| 2:G:459:ASN:HD22 | 2:G:459:ASN:H    | 1.58                     | 0.50              |
| 1:I:273:GLY:CA   | 4:I:303:HOH:O    | 2.59                     | 0.50              |
| 1:K:128:HIS:CD2  | 3:O:760:HDD:C1A  | 2.94                     | 0.50              |
| 2:P:544:VAL:HG11 | 2:P:559:ALA:HB2  | 1.93                     | 0.50              |
| 1:A:126:ILE:HD11 | 1:D:118:ASP:O    | 2.11                     | 0.50              |
| 2:F:426:PRO:HG3  | 1:D:119:HIS:HB2  | 1.93                     | 0.50              |
| 1:C:155:ASP:OD2  | 1:C:155:ASP:C    | 2.54                     | 0.50              |
| 2:N:536:ARG:HB3  | 2:N:539:ILE:HG13 | 1.92                     | 0.50              |
| 2:O:339:GLN:HE22 | 2:O:360:ILE:HG22 | 1.76                     | 0.50              |
| 2:E:461:GLU:HA   | 2:E:462:PRO:C    | 2.36                     | 0.50              |
| 1:D:275:HIS:HB2  | 1:D:277:PHE:CE2  | 2.46                     | 0.50              |
| 1:I:276:THR:O    | 2:M:403:THR:HG21 | 2.11                     | 0.50              |
| 1:J:249:THR:O    | 1:J:253:VAL:HG23 | 2.12                     | 0.50              |
| 2:N:316:ASP:O    | 2:N:317:PHE:C    | 2.53                     | 0.50              |
| 2:N:429:HIS:CD2  | 1:L:83:ASN:HB3   | 2.47                     | 0.50              |
| 2:P:493:LYS:O    | 2:P:494:VAL:CG1  | 2.59                     | 0.50              |
| 1:D:122:ILE:HB   | 1:D:123:PRO:HD2  | 1.94                     | 0.50              |
| 1:D:251:HIS:HE1  | 2:H:359:LEU:HD23 | 1.76                     | 0.50              |
| 1:I:182:ILE:C    | 1:I:183:ARG:HD2  | 2.36                     | 0.50              |
| 1:K:251:HIS:CE1  | 2:O:359:LEU:HD23 | 2.46                     | 0.50              |
| 2:E:524:VAL:O    | 2:E:528:SER:OG   | 2.29                     | 0.50              |
| 2:F:316:ASP:O    | 2:F:317:PHE:C    | 2.54                     | 0.50              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:F:340:LEU:C       | 2:F:341:ILE:HG13   | 2.36                     | 0.50              |
| 2:M:469:TRP:NE1     | 2:M:471:ARG:NH1    | 2.60                     | 0.50              |
| 1:C:211:ALA:CB      | 2:G:410:GLY:HA3    | 2.41                     | 0.50              |
| 1:J:86:VAL:HA       | 4:J:305:HOH:O      | 2.11                     | 0.50              |
| 2:N:449[B]:HIS:ND1  | 2:P:449:HIS:CG     | 2.79                     | 0.50              |
| 2:P:352:ASP:HB2     | 2:P:500:SER:HB2    | 1.94                     | 0.50              |
| 2:P:469:TRP:CE3     | 2:P:471:ARG:HG3    | 2.47                     | 0.50              |
| 2:E:507:HIS:N       | 2:E:508:PRO:HD2    | 2.27                     | 0.50              |
| 1:B:212:HIS:NE2     | 1:C:91:ASP:OD2     | 2.45                     | 0.50              |
| 2:M:357:THR:O       | 2:M:358[A]:LYS:HD3 | 2.11                     | 0.50              |
| 1:L:222:LYS:HD3     | 1:L:223:PRO:HD2    | 1.93                     | 0.50              |
| 1:A:229:ILE:HG23    | 1:A:230:PRO:HA     | 1.93                     | 0.50              |
| 2:E:538:TYR:HA      | 2:E:541:GLU:HG2    | 1.93                     | 0.50              |
| 2:F:469:TRP:CE3     | 1:D:77:ASN:HB3     | 2.46                     | 0.50              |
| 1:C:97:ALA:O        | 1:C:101:GLY:HA3    | 2.12                     | 0.50              |
| 1:K:206:PHE:HD1     | 2:O:407:LEU:HD21   | 1.76                     | 0.50              |
| 1:A:207:PHE:CD1     | 1:A:217:PHE:CZ     | 3.00                     | 0.49              |
| 2:E:392:HIS:CD2     | 2:E:394:GLY:N      | 2.80                     | 0.49              |
| 2:H:410:GLY:O       | 2:H:411:ARG:C      | 2.55                     | 0.49              |
| 2:P:469:TRP:HA      | 2:P:470:PRO:C      | 2.37                     | 0.49              |
| 1:B:133:ALA:HA      | 1:B:164:VAL:O      | 2.12                     | 0.49              |
| 1:B:267[B]:ARG:HH11 | 1:B:267[B]:ARG:HG3 | 1.77                     | 0.49              |
| 2:F:488:ARG:HD2     | 4:F:761:HOH:O      | 1.97                     | 0.49              |
| 2:G:446:ASP:OD1     | 2:G:446:ASP:N      | 2.42                     | 0.49              |
| 2:M:411:ARG:HD2     | 3:M:760:HDD:CHC    | 2.42                     | 0.49              |
| 2:E:524:VAL:HG13    | 2:E:558:VAL:HG22   | 1.95                     | 0.49              |
| 2:F:449:HIS:HD2     | 2:H:449[A]:HIS:HD2 | 1.55                     | 0.49              |
| 1:D:144:LEU:O       | 1:D:146:ASP:N      | 2.45                     | 0.49              |
| 2:N:352:ASP:HB2     | 2:N:500:SER:HB2    | 1.94                     | 0.49              |
| 1:L:168:THR:HG23    | 1:L:183[B]:ARG:NH2 | 2.27                     | 0.49              |
| 1:A:213:LYS:NZ      | 2:F:461:GLU:O      | 2.27                     | 0.49              |
| 1:B:201:ASN:CG      | 3:F:760:HDD:CMB    | 2.85                     | 0.49              |
| 1:J:251:HIS:CE1     | 2:N:359:LEU:HD23   | 2.47                     | 0.49              |
| 1:K:178:THR:O       | 2:O:311:THR:HG22   | 2.11                     | 0.49              |
| 1:A:206:PHE:CD1     | 2:E:407:LEU:HD21   | 2.47                     | 0.49              |
| 2:E:404:ASN:O       | 2:E:405:ASP:C      | 2.53                     | 0.49              |
| 1:I:205:ILE:HD13    | 1:I:205:ILE:H      | 1.77                     | 0.49              |
| 1:I:276:THR:O       | 2:M:403:THR:HG23   | 2.12                     | 0.49              |
| 2:E:473:THR:N       | 4:E:93:HOH:O       | 2.45                     | 0.49              |
| 4:E:148:HOH:O       | 1:C:106:GLU:HG2    | 2.12                     | 0.49              |
| 2:H:461:GLU:C       | 2:H:461:GLU:CD     | 2.81                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:492:ASN:O    | 2:G:494:VAL:HG22 | 2.13                     | 0.49              |
| 1:J:265:SER:OG   | 1:J:267:ARG:HG3  | 2.13                     | 0.49              |
| 1:K:221:VAL:HG23 | 1:K:239:PHE:CD1  | 2.48                     | 0.49              |
| 1:A:138:PHE:CD2  | 1:A:139:GLN:N    | 2.81                     | 0.49              |
| 1:D:206:PHE:CD1  | 3:H:760:HDD:HBB2 | 2.48                     | 0.49              |
| 1:I:143:SER:OG   | 1:I:145:SER:HB3  | 2.13                     | 0.49              |
| 2:P:516:THR:O    | 2:P:520:GLN:HG3  | 2.12                     | 0.49              |
| 1:I:247:PRO:HB2  | 2:M:504:TYR:CD2  | 2.47                     | 0.49              |
| 2:M:363:GLU:H    | 2:M:363:GLU:CD   | 2.21                     | 0.49              |
| 2:M:563:GLY:C    | 2:M:564:ILE:HG13 | 2.38                     | 0.49              |
| 2:N:411:ARG:NE   | 3:N:760:HDD:C4B  | 2.75                     | 0.49              |
| 2:N:512:TRP:CZ3  | 2:N:554:LEU:HD13 | 2.47                     | 0.49              |
| 2:O:433:ILE:O    | 2:O:433:ILE:HG13 | 2.12                     | 0.49              |
| 2:N:386:ASN:O    | 2:N:387:GLU:C    | 2.52                     | 0.49              |
| 2:E:536:ARG:HG2  | 2:E:538:TYR:CE2  | 2.48                     | 0.48              |
| 1:B:190:TYR:HE1  | 4:F:771:HOH:O    | 1.95                     | 0.48              |
| 1:D:143:SER:OG   | 1:D:145:SER:HB3  | 2.13                     | 0.48              |
| 1:K:183:ARG:NH2  | 1:K:261:GLY:O    | 2.46                     | 0.48              |
| 1:L:125:ARG:HB2  | 1:L:129:ALA:HA   | 1.94                     | 0.48              |
| 1:B:278:ARG:HH22 | 2:F:487:GLU:CD   | 2.21                     | 0.48              |
| 2:G:507:HIS:N    | 2:G:508:PRO:CD   | 2.76                     | 0.48              |
| 1:K:155:ASP:OD2  | 1:K:155:ASP:C    | 2.56                     | 0.48              |
| 2:G:438:CYS:HB2  | 2:G:439:PRO:CD   | 2.40                     | 0.48              |
| 1:I:275:HIS:CG   | 2:M:408:LEU:HB2  | 2.48                     | 0.48              |
| 2:M:538:TYR:HA   | 2:M:541:GLU:HG2  | 1.95                     | 0.48              |
| 2:P:386:ASN:O    | 2:P:387:GLU:C    | 2.55                     | 0.48              |
| 2:P:419:GLN:NE2  | 2:P:419:GLN:CA   | 2.66                     | 0.48              |
| 1:A:142:LYS:HA   | 1:A:156:PRO:HG3  | 1.94                     | 0.48              |
| 1:A:214:PHE:CD1  | 3:E:760:HDD:HAC  | 2.48                     | 0.48              |
| 1:B:138:PHE:C    | 1:B:138:PHE:CD2  | 2.91                     | 0.48              |
| 2:G:355:ASP:OD2  | 2:G:357:THR:OG1  | 2.31                     | 0.48              |
| 2:H:433:ILE:O    | 2:H:433:ILE:HG13 | 2.13                     | 0.48              |
| 2:M:564:ILE:HG22 | 2:M:564:ILE:O    | 2.13                     | 0.48              |
| 2:O:493:LYS:O    | 2:O:494:VAL:HG13 | 2.12                     | 0.48              |
| 2:P:461:GLU:OE2  | 2:P:462:PRO:N    | 2.47                     | 0.48              |
| 2:E:451:MET:HE2  | 2:G:451:MET:HE2  | 1.94                     | 0.48              |
| 1:B:197:ASP:HB2  | 2:F:395:HIS:HB2  | 1.95                     | 0.48              |
| 1:B:207:PHE:CD1  | 1:B:217:PHE:CZ   | 3.02                     | 0.48              |
| 1:B:246:GLN:O    | 1:B:249:THR:HG23 | 2.13                     | 0.48              |
| 2:H:363:GLU:H    | 2:H:363:GLU:CD   | 2.21                     | 0.48              |
| 2:M:323:TRP:CZ3  | 2:M:378:ASN:HB3  | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:N:411:ARG:O      | 2:N:415:TYR:HD2    | 1.97                     | 0.48              |
| 2:N:537:PRO:O      | 2:N:541:GLU:HG2    | 2.12                     | 0.48              |
| 2:O:460:TYR:N      | 2:O:460:TYR:CD2    | 2.80                     | 0.48              |
| 2:E:429:HIS:CD2    | 1:C:83:ASN:HB3     | 2.49                     | 0.48              |
| 2:F:449:HIS:CG     | 2:H:449[A]:HIS:CD2 | 3.01                     | 0.48              |
| 2:G:469:TRP:HA     | 2:G:470:PRO:C      | 2.39                     | 0.48              |
| 1:D:214:PHE:CB     | 1:D:215:PRO:HD3    | 2.43                     | 0.48              |
| 2:M:548:ALA:C      | 2:M:550:ILE:H      | 2.22                     | 0.48              |
| 2:O:493:LYS:CE     | 2:P:487:GLU:OE2    | 2.61                     | 0.48              |
| 2:O:563:GLY:C      | 2:O:564:ILE:HG13   | 2.38                     | 0.48              |
| 1:L:229:ILE:CG2    | 1:L:230:PRO:HA     | 2.43                     | 0.48              |
| 2:P:443:PHE:CZ     | 2:P:470:PRO:HD2    | 2.49                     | 0.48              |
| 2:E:490:GLU:HG2    | 2:F:490:GLU:HG2    | 1.95                     | 0.48              |
| 1:B:267[B]:ARG:NH2 | 2:F:330:ASP:CB     | 2.60                     | 0.48              |
| 2:F:416:THR:CG2    | 2:F:417:ASP:N      | 2.77                     | 0.48              |
| 1:C:125:ARG:CB     | 3:G:760:HDD:HBD1   | 2.41                     | 0.48              |
| 1:D:265:SER:HB2    | 1:D:267[B]:ARG:NE  | 2.29                     | 0.48              |
| 2:H:405:ASP:OD1    | 2:H:405:ASP:C      | 2.56                     | 0.48              |
| 1:I:222:LYS:NZ     | 1:L:121:ARG:HH21   | 2.12                     | 0.48              |
| 1:K:294:LYS:HD3    | 1:K:295:PRO:N      | 2.27                     | 0.48              |
| 2:O:339:GLN:NE2    | 2:O:360:ILE:HG22   | 2.29                     | 0.48              |
| 2:E:449[A]:HIS:CD2 | 2:E:451:MET:SD     | 3.06                     | 0.48              |
| 1:B:213:LYS:HD3    | 1:C:92:GLN:HA      | 1.96                     | 0.48              |
| 2:N:531:LEU:HA     | 2:N:534:VAL:HG23   | 1.96                     | 0.48              |
| 1:K:260:ARG:HH22   | 1:K:270:GLU:HG3    | 1.78                     | 0.48              |
| 2:P:359:LEU:O      | 2:P:361:PRO:HD3    | 2.14                     | 0.48              |
| 3:G:760:HDD:HMD2   | 3:G:760:HDD:HAD2   | 1.54                     | 0.48              |
| 2:H:335:GLU:HA     | 2:H:371:GLY:O      | 2.13                     | 0.48              |
| 2:O:345:ASP:O      | 2:O:346:GLU:C      | 2.57                     | 0.48              |
| 2:O:538:TYR:HA     | 2:O:541:GLU:HG2    | 1.95                     | 0.48              |
| 2:P:473:THR:O      | 2:P:481:GLY:HA3    | 2.13                     | 0.48              |
| 2:F:411:ARG:NE     | 2:F:415:TYR:OH     | 2.38                     | 0.48              |
| 1:C:76:GLU:OE2     | 1:C:76:GLU:CA      | 2.62                     | 0.48              |
| 1:D:76:GLU:OE1     | 1:D:76:GLU:C       | 2.57                     | 0.48              |
| 1:K:189:PHE:CD1    | 1:K:196:PHE:HD2    | 2.32                     | 0.48              |
| 1:B:125:ARG:HA     | 4:B:306:HOH:O      | 2.13                     | 0.47              |
| 2:F:382:PHE:O      | 2:F:386:ASN:HB3    | 2.14                     | 0.47              |
| 1:K:265:SER:OG     | 1:K:267:ARG:HB2    | 2.14                     | 0.47              |
| 2:O:493:LYS:NZ     | 2:P:487:GLU:OE2    | 2.46                     | 0.47              |
| 2:E:546:GLN:O      | 2:E:547:LEU:C      | 2.56                     | 0.47              |
| 1:C:289:VAL:HG22   | 1:C:290:ARG:N      | 2.28                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I:120:GLU:HB3    | 1:I:121:ARG:NH1    | 2.29                     | 0.47              |
| 2:N:459:ASN:H      | 2:N:459:ASN:ND2    | 2.12                     | 0.47              |
| 1:K:246:GLN:O      | 1:K:249:THR:HG23   | 2.14                     | 0.47              |
| 1:L:260:ARG:HH11   | 1:L:260:ARG:CG     | 2.28                     | 0.47              |
| 1:I:222:LYS:HB3    | 1:I:223:PRO:CD     | 2.44                     | 0.47              |
| 2:O:462:PRO:HA     | 2:O:468:ASN:OD1    | 2.15                     | 0.47              |
| 2:M:495:ARG:HD2    | 4:M:129:HOH:O      | 2.15                     | 0.47              |
| 1:J:290:ARG:CD     | 2:N:360:ILE:HD12   | 2.44                     | 0.47              |
| 1:K:189:PHE:CD1    | 1:K:196:PHE:CD2    | 3.03                     | 0.47              |
| 2:H:431:ILE:CG2    | 2:H:432:PRO:HD2    | 2.45                     | 0.47              |
| 2:M:460:TYR:N      | 2:M:460:TYR:CD2    | 2.83                     | 0.47              |
| 1:J:279:LEU:O      | 1:J:280:ILE:HD13   | 2.14                     | 0.47              |
| 1:L:254:MET:HE3    | 2:P:523:ILE:HG21   | 1.96                     | 0.47              |
| 2:F:449:HIS:HB2    | 2:H:449[B]:HIS:NE2 | 2.30                     | 0.47              |
| 1:I:155:ASP:OD2    | 1:I:155:ASP:C      | 2.57                     | 0.47              |
| 2:M:449:HIS:CD2    | 2:O:449:HIS:HD2    | 2.32                     | 0.47              |
| 2:M:490:GLU:HG2    | 2:N:490:GLU:HG2    | 1.96                     | 0.47              |
| 2:O:460:TYR:CE2    | 1:L:238:THR:HG22   | 2.49                     | 0.47              |
| 2:P:528:SER:O      | 2:P:532:SER:HB3    | 2.15                     | 0.47              |
| 2:G:507:HIS:N      | 2:G:508:PRO:HD2    | 2.29                     | 0.47              |
| 1:D:138:PHE:CD2    | 1:D:138:PHE:C      | 2.93                     | 0.47              |
| 2:H:505:TYR:C      | 2:H:508:PRO:HD2    | 2.40                     | 0.47              |
| 1:J:121:ARG:NH2    | 1:K:222:LYS:HE3    | 2.30                     | 0.47              |
| 1:K:197:ASP:HB2    | 2:O:395:HIS:HB2    | 1.95                     | 0.47              |
| 1:K:260:ARG:NH2    | 1:K:270:GLU:HG3    | 2.29                     | 0.47              |
| 2:O:433:ILE:HG23   | 2:O:434:ASN:OD1    | 2.14                     | 0.47              |
| 2:E:316:ASP:O      | 2:E:317:PHE:C      | 2.57                     | 0.47              |
| 2:F:515:GLN:HB2    | 2:F:520:GLN:HG2    | 1.97                     | 0.47              |
| 3:F:760:HDD:HAD2   | 3:F:760:HDD:HMD2   | 1.23                     | 0.47              |
| 2:H:410:GLY:C      | 2:H:412:LEU:N      | 2.71                     | 0.47              |
| 1:L:249:THR:O      | 1:L:253:VAL:HG23   | 2.15                     | 0.47              |
| 2:E:404:ASN:ND2    | 1:D:101:GLY:HA2    | 2.29                     | 0.47              |
| 1:B:267[B]:ARG:NH2 | 2:F:330:ASP:O      | 2.43                     | 0.47              |
| 2:F:410:GLY:O      | 2:F:411:ARG:C      | 2.56                     | 0.47              |
| 1:I:281:ASN:OD1    | 1:I:281:ASN:C      | 2.57                     | 0.47              |
| 1:J:254:MET:HE3    | 2:N:523:ILE:HG21   | 1.97                     | 0.47              |
| 2:N:352:ASP:C      | 2:N:352:ASP:OD2    | 2.57                     | 0.47              |
| 1:K:275:HIS:CG     | 2:O:408:LEU:HB2    | 2.49                     | 0.47              |
| 1:L:97:ALA:O       | 1:L:101:GLY:HA3    | 2.15                     | 0.47              |
| 1:A:76:GLU:OE1     | 1:A:76:GLU:C       | 2.58                     | 0.47              |
| 1:A:275:HIS:CG     | 2:E:408:LEU:HB2    | 2.50                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:188:LYS:HB2  | 1:C:188:LYS:HE2   | 1.74                     | 0.47              |
| 2:G:544:VAL:O    | 2:G:547:LEU:HB2   | 2.14                     | 0.47              |
| 2:M:459:ASN:HD22 | 2:M:459:ASN:N     | 2.05                     | 0.47              |
| 1:L:251:HIS:CE1  | 2:P:359:LEU:HD23  | 2.49                     | 0.47              |
| 1:J:119:HIS:HB2  | 2:P:426:PRO:HG3   | 1.96                     | 0.46              |
| 1:K:183:ARG:O    | 1:K:201:ASN:CB    | 2.59                     | 0.46              |
| 1:K:247:PRO:O    | 1:K:249:THR:N     | 2.48                     | 0.46              |
| 1:L:127:VAL:HA   | 4:L:301:HOH:O     | 2.14                     | 0.46              |
| 1:I:97:ALA:O     | 1:I:101:GLY:HA3   | 2.15                     | 0.46              |
| 2:P:355:ASP:HA   | 2:P:501:PHE:CE2   | 2.50                     | 0.46              |
| 2:P:493:LYS:O    | 2:P:494:VAL:HG13  | 2.15                     | 0.46              |
| 2:E:531:LEU:HA   | 2:E:534:VAL:HG23  | 1.98                     | 0.46              |
| 1:D:155:ASP:OD2  | 1:D:155:ASP:C     | 2.58                     | 0.46              |
| 1:I:80:LEU:CD1   | 2:O:442:ASN:HA    | 2.45                     | 0.46              |
| 1:I:81:THR:OG1   | 2:O:440:TYR:HA    | 2.16                     | 0.46              |
| 2:M:507:HIS:N    | 2:M:508:PRO:CD    | 2.79                     | 0.46              |
| 1:J:293:TRP:CZ3  | 2:N:336:LEU:HB2   | 2.51                     | 0.46              |
| 2:P:538:TYR:HA   | 2:P:541:GLU:HG3   | 1.97                     | 0.46              |
| 2:H:459:ASN:H    | 2:H:459:ASN:HD22  | 1.63                     | 0.46              |
| 2:F:456:ASN:OD1  | 2:F:456:ASN:C     | 2.59                     | 0.46              |
| 1:I:275:HIS:CD2  | 2:M:408:LEU:HB2   | 2.51                     | 0.46              |
| 2:N:472:GLU:HG2  | 4:N:136:HOH:O     | 2.15                     | 0.46              |
| 1:K:205:ILE:HB   | 2:O:356:PRO:O     | 2.14                     | 0.46              |
| 2:E:419:GLN:NE2  | 2:E:422:ARG:NH1   | 2.62                     | 0.46              |
| 2:F:444:GLN:C    | 2:F:445:ARG:HG2   | 2.40                     | 0.46              |
| 1:K:138:PHE:CD2  | 1:K:138:PHE:C     | 2.94                     | 0.46              |
| 2:P:537:PRO:O    | 2:P:540:ARG:HB2   | 2.16                     | 0.46              |
| 1:A:212:HIS:O    | 1:D:113:LYS:CE    | 2.58                     | 0.46              |
| 2:F:509:ARG:CG   | 2:F:509:ARG:NH1   | 2.68                     | 0.46              |
| 2:G:369:ARG:CG   | 2:G:369:ARG:NH1   | 2.69                     | 0.46              |
| 2:G:456:ASN:OD1  | 2:G:457:PRO:HD2   | 2.16                     | 0.46              |
| 2:M:355:ASP:OD1  | 2:M:358[B]:LYS:CE | 2.63                     | 0.46              |
| 2:M:411:ARG:O    | 2:M:415:TYR:HD2   | 1.98                     | 0.46              |
| 1:J:279:LEU:C    | 1:J:280:ILE:HD13  | 2.41                     | 0.46              |
| 2:N:351:PHE:CD1  | 2:N:351:PHE:C     | 2.94                     | 0.46              |
| 1:A:107:ASP:OD2  | 1:A:107:ASP:C     | 2.57                     | 0.46              |
| 1:A:275:HIS:CD2  | 2:E:408:LEU:HB2   | 2.51                     | 0.46              |
| 2:E:433:ILE:HG13 | 2:E:433:ILE:O     | 2.16                     | 0.46              |
| 1:C:214:PHE:CD1  | 3:G:760:HDD:HAC   | 2.51                     | 0.46              |
| 2:M:516:THR:O    | 2:M:519:GLU:N     | 2.48                     | 0.46              |
| 1:J:92:GLN:NE2   | 2:P:472:GLU:OE2   | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:116:HIS:CD2  | 2:P:426:PRO:HB2  | 2.50                     | 0.46              |
| 1:K:155:ASP:OD2  | 1:K:157:ASN:HB2  | 2.15                     | 0.46              |
| 2:P:392:HIS:HD2  | 2:P:394:GLY:N    | 2.09                     | 0.46              |
| 1:D:206:PHE:CG   | 1:D:207:PHE:N    | 2.84                     | 0.46              |
| 2:H:407:LEU:CD2  | 3:H:760:HDD:HBB2 | 2.45                     | 0.46              |
| 1:I:131:GLY:HA3  | 1:I:165:ARG:CZ   | 2.46                     | 0.46              |
| 2:M:380:ASP:N    | 2:M:385:GLU:OE2  | 2.37                     | 0.46              |
| 1:J:229:ILE:HG23 | 1:J:230:PRO:HA   | 1.98                     | 0.46              |
| 2:O:331:PHE:N    | 2:O:331:PHE:CD2  | 2.81                     | 0.46              |
| 1:A:119:HIS:CE1  | 2:G:420:ILE:HG21 | 2.51                     | 0.46              |
| 1:A:234:SER:HB2  | 1:A:239:PHE:CD2  | 2.51                     | 0.46              |
| 1:A:241:ASP:O    | 1:A:245:LEU:HD12 | 2.16                     | 0.46              |
| 1:D:140:PRO:O    | 1:D:156:PRO:HB3  | 2.16                     | 0.46              |
| 1:D:197:ASP:HB2  | 2:H:392:HIS:O    | 2.16                     | 0.46              |
| 1:I:185:PHE:CD1  | 1:I:185:PHE:C    | 2.94                     | 0.46              |
| 1:J:227:TRP:H    | 1:J:227:TRP:CD1  | 2.34                     | 0.46              |
| 2:G:309:LYS:CB   | 2:G:311:THR:CG2  | 2.76                     | 0.45              |
| 2:G:411:ARG:HG2  | 2:G:415:TYR:HE2  | 1.80                     | 0.45              |
| 2:M:456:ASN:ND2  | 2:M:456:ASN:C    | 2.64                     | 0.45              |
| 2:N:355:ASP:OD1  | 2:N:358:LYS:CE   | 2.61                     | 0.45              |
| 1:L:207:PHE:CD1  | 1:L:217:PHE:CZ   | 3.04                     | 0.45              |
| 1:L:280:ILE:HD13 | 1:L:280:ILE:N    | 2.30                     | 0.45              |
| 1:A:211:ALA:CB   | 2:E:410:GLY:HA3  | 2.46                     | 0.45              |
| 1:C:278:ARG:NH2  | 2:G:487:GLU:OE1  | 2.39                     | 0.45              |
| 1:I:101:GLY:HA2  | 2:P:404:ASN:ND2  | 2.31                     | 0.45              |
| 2:P:392:HIS:ND1  | 2:P:415:TYR:CA   | 2.68                     | 0.45              |
| 2:P:410:GLY:O    | 2:P:411:ARG:C    | 2.59                     | 0.45              |
| 1:B:211:ALA:CB   | 2:F:410:GLY:HA3  | 2.47                     | 0.45              |
| 2:G:351:PHE:HB2  | 2:G:358:LYS:HD2  | 1.96                     | 0.45              |
| 2:G:392:HIS:CD2  | 2:G:394:GLY:N    | 2.84                     | 0.45              |
| 2:H:356:PRO:HG3  | 2:H:407:LEU:HB2  | 1.98                     | 0.45              |
| 2:M:407:LEU:HD23 | 3:M:760:HDD:CBB  | 2.37                     | 0.45              |
| 1:J:229:ILE:CG2  | 1:J:230:PRO:HA   | 2.46                     | 0.45              |
| 1:J:230:PRO:HG2  | 1:J:233:GLN:HB2  | 1.98                     | 0.45              |
| 2:O:369:ARG:HG2  | 2:O:369:ARG:HH11 | 1.81                     | 0.45              |
| 2:O:402:PHE:HB3  | 2:O:408:LEU:HD21 | 1.97                     | 0.45              |
| 2:G:536:ARG:HA   | 2:G:537:PRO:HD3  | 1.78                     | 0.45              |
| 1:D:278:ARG:NH2  | 2:H:487:GLU:CD   | 2.73                     | 0.45              |
| 1:J:89:ALA:HA    | 2:P:473:THR:O    | 2.17                     | 0.45              |
| 2:N:446:ASP:HB2  | 1:L:120:GLU:HG2  | 1.99                     | 0.45              |
| 1:K:81:THR:HB    | 1:K:86:VAL:O     | 2.17                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:P:393:PRO:HD2  | 2:P:415:TYR:CD2    | 2.52                     | 0.45              |
| 1:B:120:GLU:HB3  | 1:B:121:ARG:NH1    | 2.31                     | 0.45              |
| 1:D:265:SER:OG   | 1:D:267[A]:ARG:HG3 | 2.17                     | 0.45              |
| 1:A:128:HIS:HA   | 1:A:168:THR:O      | 2.17                     | 0.45              |
| 1:B:77:ASN:HB3   | 2:H:469:TRP:CH2    | 2.51                     | 0.45              |
| 2:F:323:TRP:CH2  | 2:F:378:ASN:HB3    | 2.51                     | 0.45              |
| 2:M:386:ASN:C    | 2:M:386:ASN:OD1    | 2.60                     | 0.45              |
| 2:M:443:PHE:CE2  | 2:M:460:TYR:O      | 2.69                     | 0.45              |
| 1:K:136:GLY:CA   | 2:O:374:VAL:O      | 2.65                     | 0.45              |
| 2:P:391:PHE:CD2  | 2:P:391:PHE:N      | 2.85                     | 0.45              |
| 2:E:556:GLN:O    | 2:E:557:ALA:C      | 2.60                     | 0.45              |
| 2:F:392:HIS:HB2  | 2:F:415:TYR:HB3    | 1.97                     | 0.45              |
| 1:D:229:ILE:HG23 | 1:D:230:PRO:HA     | 1.98                     | 0.45              |
| 2:M:463:ASN:ND2  | 2:M:468:ASN:HA     | 2.31                     | 0.45              |
| 3:M:760:HDD:HMD3 | 3:M:760:HDD:HAD2   | 1.79                     | 0.45              |
| 1:J:125:ARG:HA   | 4:J:309:HOH:O      | 2.16                     | 0.45              |
| 2:P:524:VAL:HG13 | 2:P:558:VAL:CG2    | 2.47                     | 0.45              |
| 1:B:115:THR:O    | 1:B:118:ASP:HB2    | 2.17                     | 0.45              |
| 2:F:414:SER:OG   | 3:F:760:HDD:HBC1   | 2.16                     | 0.45              |
| 2:F:564:ILE:HG22 | 2:F:564:ILE:O      | 2.17                     | 0.45              |
| 1:C:213:LYS:O    | 1:C:214:PHE:C      | 2.57                     | 0.45              |
| 1:I:131:GLY:HA3  | 1:I:165:ARG:NH2    | 2.32                     | 0.45              |
| 1:I:196:PHE:HA   | 2:M:395:HIS:O      | 2.17                     | 0.45              |
| 1:K:202:ASN:OD1  | 1:K:202:ASN:C      | 2.60                     | 0.45              |
| 1:L:274:ILE:HD12 | 3:P:760:HDD:HMB3   | 1.98                     | 0.45              |
| 2:P:459:ASN:N    | 2:P:459:ASN:ND2    | 2.44                     | 0.45              |
| 1:D:281:ASN:OD1  | 1:D:281:ASN:C      | 2.60                     | 0.45              |
| 2:H:323:TRP:CZ3  | 2:H:378:ASN:HB3    | 2.51                     | 0.45              |
| 2:M:448:MET:HE2  | 2:M:448:MET:HB2    | 1.91                     | 0.45              |
| 2:M:459:ASN:CG   | 1:J:219:HIS:HB3    | 2.42                     | 0.45              |
| 1:J:178:THR:O    | 2:N:311:THR:HG22   | 2.17                     | 0.45              |
| 1:J:290:ARG:HD2  | 2:N:360:ILE:HD12   | 1.98                     | 0.45              |
| 2:N:355:ASP:OD1  | 2:N:358:LYS:CG     | 2.65                     | 0.45              |
| 1:K:133:ALA:HA   | 1:K:164:VAL:O      | 2.17                     | 0.45              |
| 2:F:363:GLU:CD   | 2:F:363:GLU:H      | 2.25                     | 0.45              |
| 3:H:760:HDD:HBC1 | 3:H:760:HDD:HMC1   | 1.99                     | 0.45              |
| 2:M:443:PHE:HA   | 2:M:445:ARG:HH12   | 1.82                     | 0.45              |
| 2:M:462:PRO:HA   | 2:M:468:ASN:OD1    | 2.17                     | 0.45              |
| 1:J:158:LYS:HE2  | 1:J:192:GLU:OE1    | 2.17                     | 0.45              |
| 1:J:247:PRO:HB2  | 2:N:504:TYR:CD2    | 2.52                     | 0.45              |
| 2:N:556:GLN:O    | 2:N:557:ALA:C      | 2.60                     | 0.45              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:442:ASN:OD1     | 2:O:444:GLN:HB2  | 2.17                     | 0.45              |
| 1:D:205:ILE:HD12    | 1:D:251:HIS:CE1  | 2.53                     | 0.44              |
| 1:I:78:TYR:O        | 2:O:470:PRO:HB3  | 2.17                     | 0.44              |
| 1:K:184:GLY:HA3     | 3:O:760:HDD:HMA3 | 1.99                     | 0.44              |
| 2:P:353:LEU:HD23    | 2:P:353:LEU:HA   | 1.79                     | 0.44              |
| 1:A:227:TRP:O       | 2:H:319:ARG:HD3  | 2.17                     | 0.44              |
| 1:B:106:GLU:OE2     | 2:G:493:LYS:NZ   | 2.49                     | 0.44              |
| 1:B:251:HIS:CE1     | 2:F:359:LEU:HD23 | 2.52                     | 0.44              |
| 2:G:386:ASN:OD1     | 2:G:386:ASN:C    | 2.60                     | 0.44              |
| 2:M:472:GLU:H       | 2:M:472:GLU:HG2  | 1.32                     | 0.44              |
| 1:J:91:ASP:OD2      | 1:K:212:HIS:NE2  | 2.50                     | 0.44              |
| 2:O:340:LEU:C       | 2:O:341:ILE:HG13 | 2.42                     | 0.44              |
| 2:O:392:HIS:CB      | 2:O:415:TYR:CB   | 2.96                     | 0.44              |
| 2:O:459:ASN:HD22    | 2:O:459:ASN:N    | 2.09                     | 0.44              |
| 1:B:165:ARG:CD      | 3:F:760:HDD:O1A  | 2.34                     | 0.44              |
| 2:G:419:GLN:HE21    | 2:G:419:GLN:CA   | 2.20                     | 0.44              |
| 2:M:449:HIS:HD2     | 2:O:449:HIS:HD2  | 1.66                     | 0.44              |
| 1:J:252:ASN:HD22    | 1:J:252:ASN:HA   | 1.64                     | 0.44              |
| 1:J:275:HIS:CG      | 2:N:408:LEU:HB2  | 2.52                     | 0.44              |
| 1:K:188:LYS:NZ      | 1:K:197:ASP:OD2  | 2.42                     | 0.44              |
| 1:L:207:PHE:CD2     | 1:L:252:ASN:HB3  | 2.52                     | 0.44              |
| 1:I:182:ILE:O       | 1:I:183:ARG:HD2  | 2.18                     | 0.44              |
| 1:J:228:ALA:HB2     | 2:O:382:PHE:CG   | 2.52                     | 0.44              |
| 1:K:115:THR:O       | 1:K:116:HIS:C    | 2.57                     | 0.44              |
| 2:O:456:ASN:OD1     | 2:O:456:ASN:C    | 2.61                     | 0.44              |
| 2:O:490:GLU:CG      | 2:P:490:GLU:HG2  | 2.47                     | 0.44              |
| 2:F:513:LEU:HD23    | 2:F:513:LEU:HA   | 1.84                     | 0.44              |
| 1:C:191:THR:OG1     | 1:C:194:GLY:O    | 2.30                     | 0.44              |
| 1:C:254:MET:HE3     | 2:G:523:ILE:HG21 | 1.98                     | 0.44              |
| 1:I:106:GLU:HB3     | 2:O:412:LEU:HD12 | 1.99                     | 0.44              |
| 2:M:419:GLN:NE2     | 2:M:419:GLN:CA   | 2.75                     | 0.44              |
| 1:L:183[B]:ARG:HH11 | 2:P:318:HIS:HE1  | 1.63                     | 0.44              |
| 1:A:152:PHE:CE1     | 1:A:153:LEU:HD21 | 2.53                     | 0.44              |
| 1:A:279:LEU:C       | 1:A:280:ILE:HD13 | 2.42                     | 0.44              |
| 1:B:193:GLU:OE1     | 2:F:479:ARG:HD3  | 2.17                     | 0.44              |
| 2:H:331:PHE:CD2     | 2:H:331:PHE:N    | 2.85                     | 0.44              |
| 1:I:128:HIS:O       | 1:I:129:ALA:C    | 2.58                     | 0.44              |
| 2:M:538:TYR:HA      | 2:M:541:GLU:CG   | 2.47                     | 0.44              |
| 1:J:246:GLN:O       | 1:J:248:GLU:N    | 2.50                     | 0.44              |
| 1:L:114:ILE:HD13    | 1:L:114:ILE:HA   | 1.81                     | 0.44              |
| 1:L:199:VAL:HB      | 2:P:411:ARG:NH2  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:251:HIS:HE1  | 2:G:359:LEU:HD23 | 1.82                     | 0.44              |
| 2:G:355:ASP:HB3  | 2:G:358:LYS:HG3  | 1.99                     | 0.44              |
| 2:M:327:GLU:OE1  | 2:M:327:GLU:HA   | 2.17                     | 0.44              |
| 1:J:218:VAL:O    | 1:J:221:VAL:HG12 | 2.18                     | 0.44              |
| 2:N:392:HIS:HB2  | 2:N:415:TYR:HB3  | 2.00                     | 0.44              |
| 2:E:507:HIS:N    | 2:E:508:PRO:CD   | 2.81                     | 0.44              |
| 1:C:278:ARG:HH22 | 2:G:487:GLU:CD   | 2.24                     | 0.44              |
| 2:H:382:PHE:CZ   | 2:H:386:ASN:ND2  | 2.86                     | 0.44              |
| 1:I:76:GLU:OE1   | 1:I:76:GLU:C     | 2.61                     | 0.44              |
| 2:M:394:GLY:HA2  | 2:M:412:LEU:HD22 | 1.98                     | 0.44              |
| 2:N:486:GLN:O    | 2:N:487:GLU:C    | 2.61                     | 0.44              |
| 1:K:238:THR:HG22 | 2:P:460:TYR:CE2  | 2.53                     | 0.44              |
| 1:A:247:PRO:O    | 1:A:248:GLU:C    | 2.61                     | 0.44              |
| 2:F:339:GLN:HE22 | 2:F:360:ILE:HG22 | 1.83                     | 0.44              |
| 1:C:201:ASN:CG   | 3:G:760:HDD:HMB1 | 2.42                     | 0.44              |
| 1:D:273:GLY:O    | 1:D:275:HIS:N    | 2.46                     | 0.44              |
| 2:H:506:SER:HA   | 2:H:509:ARG:HG2  | 2.00                     | 0.44              |
| 2:M:393:PRO:HD2  | 2:M:415:TYR:CG   | 2.53                     | 0.44              |
| 1:K:202:ASN:OD1  | 1:K:203:THR:HG23 | 2.18                     | 0.44              |
| 1:L:82:THR:OG1   | 1:L:86:VAL:HB    | 2.18                     | 0.44              |
| 2:E:396:ILE:HD13 | 2:E:402:PHE:CZ   | 2.52                     | 0.43              |
| 2:E:397:VAL:HB   | 2:E:398:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:128:HIS:CE1  | 1:C:169:VAL:HG22 | 2.53                     | 0.43              |
| 2:H:327:GLU:OE1  | 2:H:327:GLU:HA   | 2.19                     | 0.43              |
| 2:M:515:GLN:HB2  | 2:M:520:GLN:HG2  | 2.00                     | 0.43              |
| 1:K:188:LYS:HZ2  | 1:K:195:ILE:HG21 | 1.82                     | 0.43              |
| 1:L:252:ASN:HD22 | 1:L:252:ASN:HA   | 1.65                     | 0.43              |
| 2:P:478:LYS:O    | 2:P:479:ARG:HB2  | 2.18                     | 0.43              |
| 1:B:289:VAL:CG2  | 1:B:290:ARG:N    | 2.81                     | 0.43              |
| 1:B:289:VAL:HG22 | 1:B:290:ARG:N    | 2.31                     | 0.43              |
| 1:J:174:GLY:O    | 1:K:231:GLN:HG2  | 2.18                     | 0.43              |
| 2:N:392:HIS:CD2  | 2:N:394:GLY:N    | 2.86                     | 0.43              |
| 2:N:426:PRO:HB2  | 1:L:116:HIS:CD2  | 2.52                     | 0.43              |
| 1:K:213:LYS:NZ   | 2:P:461:GLU:O    | 2.42                     | 0.43              |
| 1:L:289:VAL:HG22 | 1:L:290:ARG:N    | 2.33                     | 0.43              |
| 2:P:540:ARG:O    | 2:P:544:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:213:LYS:O    | 1:A:214:PHE:C    | 2.61                     | 0.43              |
| 2:G:543:VAL:O    | 2:G:546:GLN:N    | 2.52                     | 0.43              |
| 2:N:369:ARG:HH11 | 2:N:369:ARG:HG2  | 1.84                     | 0.43              |
| 1:K:280:ILE:CD1  | 1:K:286:ALA:HA   | 2.48                     | 0.43              |
| 1:A:260:ARG:HH11 | 1:A:260:ARG:HB3  | 1.83                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:D:267[A]:ARG:NH2 | 2:H:330:ASP:HB2  | 2.33                     | 0.43              |
| 2:H:475:PRO:HG3    | 2:H:483:GLU:OE2  | 2.19                     | 0.43              |
| 1:I:136:GLY:HA3    | 2:M:375:LEU:HA   | 1.99                     | 0.43              |
| 1:I:199:VAL:HG21   | 2:M:393:PRO:HD3  | 1.99                     | 0.43              |
| 1:K:246:GLN:O      | 1:K:247:PRO:C    | 2.61                     | 0.43              |
| 2:O:443:PHE:CD2    | 2:O:460:TYR:O    | 2.72                     | 0.43              |
| 2:O:516:THR:HG23   | 2:O:519:GLU:OE2  | 2.18                     | 0.43              |
| 1:B:92:GLN:HA      | 1:C:213:LYS:HD3  | 2.00                     | 0.43              |
| 2:H:507:HIS:N      | 2:H:508:PRO:CD   | 2.81                     | 0.43              |
| 1:I:214:PHE:CD1    | 3:M:760:HDD:CAC  | 3.01                     | 0.43              |
| 1:J:81:THR:HG22    | 1:J:87:ARG:HA    | 2.00                     | 0.43              |
| 2:P:548:ALA:C      | 2:P:550:ILE:H    | 2.26                     | 0.43              |
| 1:A:199:VAL:HG21   | 2:E:393:PRO:HD3  | 2.00                     | 0.43              |
| 1:I:185:PHE:C      | 1:I:185:PHE:HD1  | 2.25                     | 0.43              |
| 1:J:247:PRO:HG2    | 2:N:504:TYR:CE2  | 2.53                     | 0.43              |
| 1:K:94:SER:HB2     | 1:K:103:THR:HG23 | 2.00                     | 0.43              |
| 2:O:492:ASN:O      | 2:O:494:VAL:HG22 | 2.17                     | 0.43              |
| 1:A:174:GLY:O      | 1:D:231:GLN:HG2  | 2.18                     | 0.43              |
| 1:D:187:THR:HB     | 4:D:305:HOH:O    | 2.18                     | 0.43              |
| 2:H:469:TRP:HA     | 2:H:470:PRO:C    | 2.44                     | 0.43              |
| 2:H:547:LEU:HD23   | 2:H:547:LEU:HA   | 1.58                     | 0.43              |
| 1:I:131:GLY:O      | 2:M:319:ARG:NH2  | 2.51                     | 0.43              |
| 2:M:459:ASN:ND2    | 1:J:219:HIS:HB3  | 2.34                     | 0.43              |
| 1:J:125:ARG:CB     | 3:N:760:HDD:HBD1 | 2.45                     | 0.43              |
| 2:N:449[A]:HIS:CE1 | 4:N:48:HOH:O     | 2.72                     | 0.43              |
| 2:O:329:GLY:HA2    | 2:O:331:PHE:CE2  | 2.54                     | 0.43              |
| 2:O:411:ARG:O      | 2:O:412:LEU:C    | 2.61                     | 0.43              |
| 1:L:125:ARG:HG2    | 3:P:760:HDD:HBD1 | 2.01                     | 0.43              |
| 1:A:180:ARG:NH1    | 1:A:180:ARG:HG3  | 2.34                     | 0.43              |
| 2:E:353:LEU:HD23   | 2:E:353:LEU:HA   | 1.67                     | 0.43              |
| 2:E:393:PRO:HD2    | 2:E:415:TYR:CG   | 2.54                     | 0.43              |
| 1:B:125:ARG:CG     | 3:F:760:HDD:HBD1 | 2.47                     | 0.43              |
| 2:G:433:ILE:O      | 2:G:433:ILE:HG13 | 2.18                     | 0.43              |
| 2:H:393:PRO:HD2    | 2:H:415:TYR:CG   | 2.53                     | 0.43              |
| 2:M:410:GLY:O      | 2:M:411:ARG:C    | 2.62                     | 0.43              |
| 2:M:516:THR:O      | 2:M:518:PHE:N    | 2.52                     | 0.43              |
| 2:N:545:ASP:O      | 2:N:548:ALA:HB3  | 2.19                     | 0.43              |
| 1:K:128:HIS:NE2    | 3:O:760:HDD:C4A  | 2.82                     | 0.43              |
| 1:K:253:VAL:O      | 1:K:257:MET:HG2  | 2.18                     | 0.43              |
| 3:P:760:HDD:HMD3   | 3:P:760:HDD:HAD2 | 1.31                     | 0.43              |
| 1:A:238:THR:HG22   | 2:F:460:TYR:CE2  | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:115:THR:O    | 1:B:116:HIS:C    | 2.61                     | 0.43              |
| 1:B:119:HIS:ND1  | 2:G:421:SER:HB3  | 2.34                     | 0.43              |
| 1:B:214:PHE:CD1  | 3:F:760:HDD:CAC  | 3.02                     | 0.43              |
| 2:F:414:SER:HB2  | 3:F:760:HDD:HBC2 | 2.01                     | 0.43              |
| 1:C:282:ALA:N    | 4:C:315:HOH:O    | 2.36                     | 0.43              |
| 2:G:548:ALA:C    | 2:G:550:ILE:H    | 2.27                     | 0.43              |
| 2:G:551:ASP:OD1  | 2:G:551:ASP:C    | 2.62                     | 0.43              |
| 1:D:139:GLN:HA   | 1:D:140:PRO:HD3  | 1.88                     | 0.43              |
| 1:I:200:GLY:HA2  | 3:M:760:HDD:HMB3 | 2.00                     | 0.43              |
| 1:J:127:VAL:O    | 1:J:128:HIS:C    | 2.62                     | 0.43              |
| 2:N:393:PRO:HD2  | 2:N:415:TYR:CG   | 2.54                     | 0.43              |
| 2:G:340:LEU:C    | 2:G:341:ILE:HG13 | 2.44                     | 0.43              |
| 2:M:397:VAL:CG2  | 2:M:400:LEU:HD12 | 2.49                     | 0.43              |
| 2:N:536:ARG:HA   | 2:N:537:PRO:HD3  | 1.88                     | 0.43              |
| 1:K:205:ILE:HA   | 1:K:274:ILE:HG23 | 1.99                     | 0.43              |
| 1:L:275:HIS:HE1  | 2:P:407:LEU:HB3  | 1.82                     | 0.43              |
| 2:P:316:ASP:O    | 2:P:317:PHE:C    | 2.62                     | 0.43              |
| 1:D:111:ARG:O    | 1:D:112:GLU:C    | 2.62                     | 0.42              |
| 2:M:443:PHE:CZ   | 2:M:461:GLU:HB3  | 2.54                     | 0.42              |
| 1:J:200:GLY:HA3  | 1:J:272:PHE:O    | 2.19                     | 0.42              |
| 2:N:392:HIS:ND1  | 2:N:415:TYR:CA   | 2.70                     | 0.42              |
| 1:K:151:ASP:O    | 1:K:153:LEU:N    | 2.52                     | 0.42              |
| 2:O:459:ASN:H    | 2:O:459:ASN:ND2  | 2.15                     | 0.42              |
| 1:L:206:PHE:CG   | 1:L:207:PHE:N    | 2.86                     | 0.42              |
| 1:B:207:PHE:O    | 1:B:249:THR:HA   | 2.19                     | 0.42              |
| 1:B:275:HIS:HB2  | 1:B:277:PHE:CE2  | 2.54                     | 0.42              |
| 1:D:86:VAL:O     | 1:D:86:VAL:HG12  | 2.19                     | 0.42              |
| 1:D:224:GLU:HB3  | 1:D:225:PRO:HD2  | 2.01                     | 0.42              |
| 1:D:293:TRP:CZ3  | 2:H:373:MET:HE2  | 2.54                     | 0.42              |
| 1:K:279:LEU:C    | 1:K:280:ILE:HD13 | 2.43                     | 0.42              |
| 2:O:536:ARG:HA   | 2:O:537:PRO:HD3  | 1.89                     | 0.42              |
| 2:P:351:PHE:CD1  | 2:P:351:PHE:C    | 2.96                     | 0.42              |
| 2:P:472:GLU:H    | 2:P:472:GLU:HG2  | 1.46                     | 0.42              |
| 1:A:155:ASP:HA   | 1:A:156:PRO:HD3  | 1.88                     | 0.42              |
| 2:F:419:GLN:HA   | 2:F:419:GLN:HE21 | 1.83                     | 0.42              |
| 1:C:199:VAL:HB   | 2:G:411:ARG:HH22 | 1.84                     | 0.42              |
| 1:I:208:ILE:HG22 | 4:I:302:HOH:O    | 2.19                     | 0.42              |
| 2:O:547:LEU:HD23 | 2:O:547:LEU:HA   | 1.68                     | 0.42              |
| 2:G:490:GLU:HG2  | 2:H:490:GLU:HG2  | 2.00                     | 0.42              |
| 1:D:206:PHE:CD1  | 3:H:760:HDD:HBB1 | 2.54                     | 0.42              |
| 2:H:323:TRP:CG   | 2:H:378:ASN:HD21 | 2.38                     | 0.42              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:247:PRO:C      | 1:K:249:THR:N    | 2.77                     | 0.42              |
| 1:L:82:THR:C       | 1:L:84:GLN:H     | 2.27                     | 0.42              |
| 1:L:201:ASN:CG     | 3:P:760:HDD:HMB1 | 2.44                     | 0.42              |
| 1:B:126:ILE:H      | 1:B:126:ILE:HG12 | 1.67                     | 0.42              |
| 1:B:174:GLY:O      | 1:C:231:GLN:HG2  | 2.20                     | 0.42              |
| 2:G:541:GLU:H      | 2:G:541:GLU:HG2  | 1.72                     | 0.42              |
| 1:J:222:LYS:HZ1    | 1:K:121:ARG:HH21 | 1.66                     | 0.42              |
| 1:A:193:GLU:OE1    | 2:E:479:ARG:HD3  | 2.20                     | 0.42              |
| 1:D:214:PHE:CD1    | 3:H:760:HDD:CAC  | 3.03                     | 0.42              |
| 1:I:272:PHE:C      | 1:I:274:ILE:N    | 2.78                     | 0.42              |
| 1:K:97:ALA:O       | 1:K:101:GLY:HA3  | 2.20                     | 0.42              |
| 1:K:213:LYS:O      | 1:K:214:PHE:C    | 2.62                     | 0.42              |
| 2:P:536:ARG:HA     | 2:P:537:PRO:HD3  | 1.82                     | 0.42              |
| 1:B:252:ASN:HD22   | 1:B:252:ASN:HA   | 1.63                     | 0.42              |
| 2:F:507:HIS:N      | 2:F:508:PRO:CD   | 2.82                     | 0.42              |
| 2:F:537:PRO:O      | 2:F:540:ARG:HB2  | 2.20                     | 0.42              |
| 2:H:493:LYS:O      | 2:H:494:VAL:HG13 | 2.19                     | 0.42              |
| 2:N:319:ARG:HD3    | 1:K:227:TRP:O    | 2.20                     | 0.42              |
| 2:N:505:TYR:O      | 2:N:508:PRO:HD2  | 2.20                     | 0.42              |
| 1:K:247:PRO:HB2    | 2:O:504:TYR:CD2  | 2.55                     | 0.42              |
| 1:L:169:VAL:HG21   | 1:L:182:ILE:HB   | 2.02                     | 0.42              |
| 1:L:199:VAL:HB     | 2:P:411:ARG:HH22 | 1.84                     | 0.42              |
| 1:L:222:LYS:O      | 1:L:223:PRO:C    | 2.63                     | 0.42              |
| 2:P:539:ILE:O      | 2:P:540:ARG:C    | 2.63                     | 0.42              |
| 1:B:160:THR:HG22   | 1:B:161:PRO:O    | 2.20                     | 0.42              |
| 2:G:404:ASN:O      | 2:G:405:ASP:C    | 2.62                     | 0.42              |
| 1:I:106:GLU:OE2    | 2:P:493:LYS:NZ   | 2.52                     | 0.42              |
| 1:I:149:LYS:O      | 1:I:149:LYS:HG3  | 2.20                     | 0.42              |
| 1:L:247:PRO:O      | 1:L:250:LEU:HG   | 2.18                     | 0.42              |
| 2:P:443:PHE:HB3    | 2:P:459:ASN:C    | 2.45                     | 0.42              |
| 2:F:353:LEU:HD23   | 2:F:353:LEU:HA   | 1.79                     | 0.42              |
| 2:F:469:TRP:HA     | 2:F:470:PRO:C    | 2.45                     | 0.42              |
| 1:C:197:ASP:HB2    | 2:G:392:HIS:O    | 2.20                     | 0.42              |
| 2:G:515:GLN:HB2    | 2:G:520:GLN:HG2  | 2.02                     | 0.42              |
| 2:G:547:LEU:HA     | 2:G:547:LEU:HD23 | 1.56                     | 0.42              |
| 1:D:125:ARG:HG3    | 1:D:125:ARG:NH1  | 2.34                     | 0.42              |
| 1:D:144:LEU:O      | 1:D:145:SER:C    | 2.62                     | 0.42              |
| 1:I:142:LYS:O      | 1:I:143:SER:C    | 2.63                     | 0.42              |
| 2:N:449[B]:HIS:HD1 | 2:P:449:HIS:CB   | 2.32                     | 0.42              |
| 2:O:516:THR:O      | 2:O:517:PRO:C    | 2.63                     | 0.42              |
| 1:L:82:THR:C       | 1:L:84:GLN:N     | 2.76                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:190:TYR:CD2  | 1:B:190:TYR:N    | 2.87                     | 0.42              |
| 2:F:355:ASP:OD2  | 2:F:355:ASP:C    | 2.63                     | 0.42              |
| 2:F:412:LEU:HD23 | 2:F:412:LEU:HA   | 1.64                     | 0.42              |
| 1:C:266:TYR:CE2  | 2:G:318:HIS:HB3  | 2.55                     | 0.42              |
| 1:C:276:THR:O    | 2:G:403:THR:CG2  | 2.68                     | 0.42              |
| 1:C:281:ASN:OD1  | 1:C:281:ASN:C    | 2.63                     | 0.42              |
| 2:H:493:LYS:C    | 2:H:494:VAL:HG13 | 2.44                     | 0.42              |
| 1:B:155:ASP:OD2  | 1:B:155:ASP:C    | 2.63                     | 0.41              |
| 1:B:206:PHE:CD1  | 2:F:407:LEU:HD21 | 2.55                     | 0.41              |
| 1:B:231:GLN:O    | 1:B:233:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:281:ASN:OD1  | 1:B:281:ASN:C    | 2.63                     | 0.41              |
| 2:F:486:GLN:H    | 2:F:486:GLN:HG2  | 1.55                     | 0.41              |
| 1:D:155:ASP:HA   | 1:D:156:PRO:HD3  | 1.90                     | 0.41              |
| 2:M:548:ALA:C    | 2:M:550:ILE:N    | 2.78                     | 0.41              |
| 2:O:380:ASP:N    | 2:O:385:GLU:OE2  | 2.41                     | 0.41              |
| 1:L:242:TYR:O    | 1:L:243:VAL:C    | 2.63                     | 0.41              |
| 2:P:411:ARG:O    | 2:P:413:PHE:N    | 2.53                     | 0.41              |
| 2:P:524:VAL:O    | 2:P:528:SER:OG   | 2.32                     | 0.41              |
| 1:A:125:ARG:HG2  | 3:E:760:HDD:HBD1 | 2.02                     | 0.41              |
| 1:A:148:THR:HB   | 1:A:279:LEU:HB3  | 2.01                     | 0.41              |
| 2:E:456:ASN:HA   | 2:E:457:PRO:HD2  | 1.96                     | 0.41              |
| 1:B:136:GLY:HA3  | 2:F:374:VAL:O    | 2.20                     | 0.41              |
| 1:C:180:ARG:NH1  | 1:C:256:ALA:O    | 2.54                     | 0.41              |
| 1:C:289:VAL:CG2  | 1:C:290:ARG:N    | 2.82                     | 0.41              |
| 1:D:282:ALA:CB   | 4:D:310:HOH:O    | 2.68                     | 0.41              |
| 2:H:459:ASN:HD22 | 2:H:459:ASN:N    | 2.18                     | 0.41              |
| 3:H:760:HDD:HAD2 | 3:H:760:HDD:HMD2 | 1.71                     | 0.41              |
| 1:I:184:GLY:HA2  | 1:I:201:ASN:HA   | 2.02                     | 0.41              |
| 1:I:185:PHE:N    | 1:I:200:GLY:O    | 2.52                     | 0.41              |
| 2:M:432:PRO:O    | 2:M:433:ILE:C    | 2.61                     | 0.41              |
| 1:J:206:PHE:CD1  | 2:N:407:LEU:HD21 | 2.55                     | 0.41              |
| 2:N:411:ARG:NE   | 3:N:760:HDD:CHC  | 2.83                     | 0.41              |
| 2:O:331:PHE:HA   | 2:O:332:PRO:HD3  | 1.92                     | 0.41              |
| 1:B:84:GLN:HG3   | 2:H:395:HIS:CD2  | 2.55                     | 0.41              |
| 1:B:128:HIS:CE1  | 1:B:169:VAL:HG22 | 2.55                     | 0.41              |
| 1:D:122:ILE:HB   | 1:D:123:PRO:CD   | 2.49                     | 0.41              |
| 1:D:230:PRO:HG2  | 1:D:233:GLN:HB2  | 2.02                     | 0.41              |
| 2:H:323:TRP:CE2  | 2:H:378:ASN:ND2  | 2.88                     | 0.41              |
| 2:H:444:GLN:O    | 2:H:445:ARG:HD3  | 2.20                     | 0.41              |
| 2:H:515:GLN:HB2  | 2:H:520:GLN:HG2  | 2.01                     | 0.41              |
| 1:I:125:ARG:O    | 1:I:126:ILE:C    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:281:ASN:HD21 | 1:I:285:LYS:HB3  | 1.86                     | 0.41              |
| 2:M:397:VAL:HG22 | 2:M:400:LEU:HD12 | 2.02                     | 0.41              |
| 1:J:251:HIS:CE1  | 2:N:507:HIS:HB3  | 2.56                     | 0.41              |
| 2:O:443:PHE:CE2  | 2:O:460:TYR:O    | 2.73                     | 0.41              |
| 1:A:180:ARG:HG3  | 1:A:180:ARG:HH11 | 1.84                     | 0.41              |
| 1:A:213:LYS:HD2  | 1:A:213:LYS:HA   | 1.74                     | 0.41              |
| 1:A:237:ASP:O    | 1:A:238:THR:C    | 2.63                     | 0.41              |
| 2:E:459:ASN:HD22 | 2:E:459:ASN:N    | 2.13                     | 0.41              |
| 1:B:222:LYS:O    | 1:B:223:PRO:C    | 2.64                     | 0.41              |
| 1:D:125:ARG:CB   | 3:H:760:HDD:HBD1 | 2.49                     | 0.41              |
| 1:I:213:LYS:HB3  | 1:I:213:LYS:HE3  | 1.72                     | 0.41              |
| 2:M:466:ASN:O    | 2:M:466:ASN:ND2  | 2.54                     | 0.41              |
| 2:O:509:ARG:CG   | 2:O:550:ILE:O    | 2.68                     | 0.41              |
| 1:B:236:HIS:CD2  | 1:B:236:HIS:N    | 2.89                     | 0.41              |
| 2:F:459:ASN:N    | 2:F:459:ASN:ND2  | 2.60                     | 0.41              |
| 2:H:355:ASP:OD2  | 2:H:355:ASP:C    | 2.63                     | 0.41              |
| 2:H:461:GLU:OE2  | 2:H:462:PRO:N    | 2.54                     | 0.41              |
| 1:I:122:ILE:HB   | 1:I:123:PRO:HD2  | 2.02                     | 0.41              |
| 1:K:135:HIS:HB2  | 2:O:377:ARG:HB3  | 2.01                     | 0.41              |
| 2:P:407:LEU:HD12 | 2:P:407:LEU:HA   | 1.77                     | 0.41              |
| 2:P:508:PRO:O    | 2:P:511:PHE:HB3  | 2.20                     | 0.41              |
| 1:B:238:THR:O    | 1:B:239:PHE:C    | 2.63                     | 0.41              |
| 2:F:461:GLU:C    | 2:F:461:GLU:CD   | 2.88                     | 0.41              |
| 2:F:529:PHE:O    | 2:F:532:SER:OG   | 2.31                     | 0.41              |
| 1:C:138:PHE:CD2  | 1:C:138:PHE:C    | 2.98                     | 0.41              |
| 2:M:331:PHE:CD2  | 2:M:331:PHE:N    | 2.85                     | 0.41              |
| 2:M:547:LEU:HD23 | 2:M:547:LEU:HA   | 1.75                     | 0.41              |
| 1:J:158:LYS:HE2  | 1:J:192:GLU:CD   | 2.46                     | 0.41              |
| 2:O:397:VAL:HG22 | 2:O:400:LEU:HD12 | 2.01                     | 0.41              |
| 2:O:516:THR:O    | 2:O:519:GLU:N    | 2.53                     | 0.41              |
| 1:L:178:THR:O    | 2:P:311:THR:HG22 | 2.20                     | 0.41              |
| 2:E:359:LEU:HD21 | 4:E:92:HOH:O     | 2.20                     | 0.41              |
| 2:E:438:CYS:HB2  | 2:E:439:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:126:ILE:H    | 1:D:126:ILE:HG12 | 1.62                     | 0.41              |
| 1:J:169:VAL:HG21 | 1:J:182:ILE:HB   | 2.02                     | 0.41              |
| 2:P:392:HIS:HB2  | 2:P:415:TYR:HB3  | 2.02                     | 0.41              |
| 3:E:760:HDD:HMC1 | 3:E:760:HDD:HBC1 | 2.03                     | 0.41              |
| 1:B:279:LEU:HD12 | 2:F:340:LEU:HD21 | 2.03                     | 0.41              |
| 2:F:444:GLN:O    | 2:F:445:ARG:HG2  | 2.21                     | 0.41              |
| 2:G:538:TYR:HA   | 2:G:541:GLU:CG   | 2.51                     | 0.41              |
| 2:M:394:GLY:CA   | 2:M:412:LEU:HD22 | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:541:GLU:HG2  | 2:N:541:GLU:H    | 1.52                     | 0.41              |
| 1:K:260:ARG:O    | 1:K:263:PRO:HD3  | 2.21                     | 0.41              |
| 1:L:246:GLN:O    | 1:L:249:THR:HG23 | 2.20                     | 0.41              |
| 1:L:281:ASN:OD1  | 1:L:281:ASN:C    | 2.64                     | 0.41              |
| 1:A:274:ILE:CD1  | 3:E:760:HDD:CBB  | 2.98                     | 0.41              |
| 2:E:352:ASP:HB2  | 2:E:500:SER:HB2  | 2.03                     | 0.41              |
| 2:E:410:GLY:O    | 2:E:411:ARG:C    | 2.64                     | 0.41              |
| 1:B:76:GLU:O     | 1:B:77:ASN:C     | 2.63                     | 0.41              |
| 1:B:80:LEU:CD1   | 2:H:442:ASN:HA   | 2.51                     | 0.41              |
| 1:B:294:LYS:HG3  | 1:B:295:PRO:N    | 2.35                     | 0.41              |
| 2:G:459:ASN:HD22 | 2:G:460:TYR:HD2  | 1.67                     | 0.41              |
| 2:G:505:TYR:C    | 2:G:508:PRO:HD2  | 2.46                     | 0.41              |
| 2:G:545:ASP:O    | 2:G:548:ALA:HB3  | 2.21                     | 0.41              |
| 2:H:353:LEU:HD23 | 2:H:353:LEU:HA   | 1.89                     | 0.41              |
| 2:H:381:ASN:O    | 2:H:382:PHE:C    | 2.63                     | 0.41              |
| 2:H:538:TYR:HA   | 2:H:541:GLU:CG   | 2.51                     | 0.41              |
| 1:I:279:LEU:HG   | 1:I:289:VAL:CG1  | 2.51                     | 0.41              |
| 2:M:392:HIS:CD2  | 2:M:394:GLY:H    | 2.38                     | 0.41              |
| 1:J:111:ARG:O    | 1:J:112:GLU:C    | 2.63                     | 0.41              |
| 2:N:342:PRO:O    | 2:N:343:GLU:C    | 2.64                     | 0.41              |
| 2:N:469:TRP:HA   | 2:N:470:PRO:C    | 2.46                     | 0.41              |
| 3:N:760:HDD:HMD2 | 3:N:760:HDD:HAD2 | 1.82                     | 0.41              |
| 1:K:214:PHE:HB3  | 1:K:215:PRO:HD3  | 2.03                     | 0.41              |
| 2:O:419:GLN:HE22 | 2:O:422:ARG:HH11 | 1.69                     | 0.41              |
| 2:O:419:GLN:HE22 | 2:O:422:ARG:NH1  | 2.19                     | 0.41              |
| 1:L:180:ARG:NH1  | 1:L:256:ALA:O    | 2.53                     | 0.41              |
| 2:P:456:ASN:OD1  | 2:P:457:PRO:CD   | 2.67                     | 0.41              |
| 1:A:136:GLY:HA3  | 2:E:374:VAL:O    | 2.21                     | 0.41              |
| 1:D:188:LYS:HG3  | 1:D:197:ASP:OD2  | 2.21                     | 0.41              |
| 1:I:116:HIS:HE1  | 2:O:446:ASP:O    | 2.04                     | 0.41              |
| 2:M:369:ARG:HG2  | 2:M:369:ARG:HH11 | 1.86                     | 0.41              |
| 1:J:152:PHE:HB3  | 1:J:191:THR:HB   | 2.03                     | 0.41              |
| 2:O:498:SER:O    | 2:O:501:PHE:HB2  | 2.20                     | 0.41              |
| 2:P:524:VAL:HG13 | 2:P:558:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:155:ASP:OD2  | 1:A:157:ASN:HB2  | 2.21                     | 0.40              |
| 1:D:144:LEU:C    | 1:D:146:ASP:N    | 2.77                     | 0.40              |
| 1:D:282:ALA:HB2  | 4:D:310:HOH:O    | 2.21                     | 0.40              |
| 1:I:77:ASN:HB3   | 2:O:469:TRP:CH2  | 2.53                     | 0.40              |
| 2:O:507:HIS:H    | 2:O:508:PRO:HD2  | 1.83                     | 0.40              |
| 1:L:229:ILE:CG2  | 1:L:230:PRO:CA   | 2.98                     | 0.40              |
| 1:A:77:ASN:N     | 1:A:77:ASN:ND2   | 2.67                     | 0.40              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:A:138:PHE:CG   | 1:A:139:GLN:N       | 2.89                     | 0.40              |
| 1:A:222:LYS:HG3  | 4:D:308:HOH:O       | 2.20                     | 0.40              |
| 1:D:207:PHE:O    | 1:D:249:THR:HA      | 2.21                     | 0.40              |
| 1:K:168:THR:HB   | 1:K:169:VAL:H       | 1.75                     | 0.40              |
| 2:O:466:ASN:O    | 2:O:467:ASP:C       | 2.63                     | 0.40              |
| 1:L:125:ARG:HB3  | 3:P:760:HDD:HBD1    | 2.02                     | 0.40              |
| 1:L:181:ASP:HB3  | 1:L:183[A]:ARG:HH21 | 1.83                     | 0.40              |
| 1:A:133:ALA:HA   | 1:A:164:VAL:O       | 2.21                     | 0.40              |
| 1:B:200:GLY:HA3  | 1:B:272:PHE:O       | 2.22                     | 0.40              |
| 1:I:183:ARG:HD2  | 1:I:183:ARG:N       | 2.36                     | 0.40              |
| 2:M:505:TYR:O    | 2:M:508:PRO:HD2     | 2.20                     | 0.40              |
| 1:J:83:ASN:HB3   | 2:P:429:HIS:CD2     | 2.55                     | 0.40              |
| 2:N:412:LEU:HD23 | 2:N:412:LEU:HA      | 1.79                     | 0.40              |
| 1:K:169:VAL:HG21 | 1:K:182:ILE:HB      | 2.03                     | 0.40              |
| 2:O:506:SER:HA   | 2:O:509:ARG:HB2     | 2.02                     | 0.40              |
| 2:P:323:TRP:CZ3  | 2:P:378:ASN:HB3     | 2.56                     | 0.40              |
| 2:P:515:GLN:HB2  | 2:P:520:GLN:HG2     | 2.02                     | 0.40              |
| 1:A:275:HIS:HB2  | 1:A:277:PHE:CE2     | 2.57                     | 0.40              |
| 2:F:507:HIS:N    | 2:F:508:PRO:HD2     | 2.36                     | 0.40              |
| 2:G:353:LEU:HD23 | 2:G:353:LEU:HA      | 1.80                     | 0.40              |
| 1:D:206:PHE:CG   | 3:H:760:HDD:HBB1    | 2.54                     | 0.40              |
| 1:I:155:ASP:HA   | 1:I:156:PRO:HD3     | 1.80                     | 0.40              |
| 1:I:279:LEU:HD23 | 1:I:279:LEU:HA      | 1.87                     | 0.40              |
| 1:J:115:THR:O    | 1:J:116:HIS:C       | 2.64                     | 0.40              |
| 1:J:115:THR:O    | 1:J:119:HIS:HD2     | 2.05                     | 0.40              |
| 2:N:345:ASP:O    | 2:N:346:GLU:C       | 2.64                     | 0.40              |
| 1:K:247:PRO:C    | 1:K:249:THR:H       | 2.30                     | 0.40              |
| 1:K:251:HIS:CE1  | 2:O:507:HIS:HB3     | 2.55                     | 0.40              |
| 2:E:386:ASN:OD1  | 2:E:386:ASN:C       | 2.64                     | 0.40              |
| 2:E:513:LEU:HD23 | 2:E:513:LEU:HA      | 1.89                     | 0.40              |
| 1:B:143:SER:OG   | 1:B:145:SER:HB3     | 2.22                     | 0.40              |
| 1:C:199:VAL:HB   | 2:G:411:ARG:NH2     | 2.37                     | 0.40              |
| 2:N:414:SER:O    | 2:N:415:TYR:C       | 2.64                     | 0.40              |
| 1:K:266:TYR:CE2  | 2:O:318:HIS:HB3     | 2.56                     | 0.40              |
| 1:L:246:GLN:O    | 1:L:247:PRO:C       | 2.65                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 2:O:509:ARG:NH1 | 2:P:521:ARG:NE[2_756] | 1.70                     | 0.50              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:D:157:ASN:OD1 | 2:O:369:ARG:NH2[2_645] | 2.16                     | 0.04              |
| 2:O:509:ARG:NH1 | 2:P:521:ARG:CD[2_756]  | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 221/226 (98%)   | 208 (94%)  | 12 (5%)  | 1 (0%)   | 24          | 55  |
| 1   | B     | 222/226 (98%)   | 207 (93%)  | 13 (6%)  | 2 (1%)   | 14          | 41  |
| 1   | C     | 222/226 (98%)   | 214 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | D     | 222/226 (98%)   | 209 (94%)  | 11 (5%)  | 2 (1%)   | 14          | 41  |
| 1   | I     | 221/226 (98%)   | 206 (93%)  | 13 (6%)  | 2 (1%)   | 14          | 41  |
| 1   | J     | 221/226 (98%)   | 207 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 1   | K     | 221/226 (98%)   | 202 (91%)  | 17 (8%)  | 2 (1%)   | 14          | 41  |
| 1   | L     | 222/226 (98%)   | 206 (93%)  | 15 (7%)  | 1 (0%)   | 24          | 55  |
| 2   | E     | 257/259 (99%)   | 240 (93%)  | 15 (6%)  | 2 (1%)   | 16          | 44  |
| 2   | F     | 254/259 (98%)   | 238 (94%)  | 15 (6%)  | 1 (0%)   | 30          | 60  |
| 2   | G     | 256/259 (99%)   | 237 (93%)  | 19 (7%)  | 0        | 100         | 100 |
| 2   | H     | 255/259 (98%)   | 237 (93%)  | 18 (7%)  | 0        | 100         | 100 |
| 2   | M     | 255/259 (98%)   | 230 (90%)  | 23 (9%)  | 2 (1%)   | 16          | 44  |
| 2   | N     | 255/259 (98%)   | 237 (93%)  | 17 (7%)  | 1 (0%)   | 30          | 60  |
| 2   | O     | 254/259 (98%)   | 228 (90%)  | 23 (9%)  | 3 (1%)   | 10          | 34  |
| 2   | P     | 254/259 (98%)   | 233 (92%)  | 19 (8%)  | 2 (1%)   | 16          | 44  |
| All | All   | 3812/3880 (98%) | 3539 (93%) | 252 (7%) | 21 (1%)  | 24          | 51  |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 258    | SER  |
| 1   | I     | 274    | ILE  |
| 1   | B     | 77     | ASN  |
| 1   | B     | 274    | ILE  |
| 1   | D     | 145    | SER  |
| 1   | K     | 274    | ILE  |
| 2   | P     | 549    | HIS  |
| 1   | I     | 258    | SER  |
| 2   | N     | 493    | LYS  |
| 2   | O     | 432    | PRO  |
| 2   | P     | 412    | LEU  |
| 1   | K     | 248    | GLU  |
| 2   | O     | 472    | GLU  |
| 2   | O     | 486    | GLN  |
| 2   | M     | 551    | ASP  |
| 1   | L     | 248    | GLU  |
| 2   | E     | 449[A] | HIS  |
| 2   | E     | 449[B] | HIS  |
| 2   | F     | 432    | PRO  |
| 2   | M     | 486    | GLN  |
| 1   | D     | 274    | ILE  |

### 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     | 189/190 (100%) | 172 (91%) | 17 (9%)  | 9           | 28 |
| 1   | B     | 190/190 (100%) | 165 (87%) | 25 (13%) | 4           | 14 |
| 1   | C     | 190/190 (100%) | 169 (89%) | 21 (11%) | 6           | 20 |
| 1   | D     | 190/190 (100%) | 170 (90%) | 20 (10%) | 6           | 22 |
| 1   | I     | 189/190 (100%) | 162 (86%) | 27 (14%) | 3           | 11 |
| 1   | J     | 189/190 (100%) | 165 (87%) | 24 (13%) | 4           | 15 |
| 1   | K     | 189/190 (100%) | 155 (82%) | 34 (18%) | 2           | 6  |
| 1   | L     | 190/190 (100%) | 169 (89%) | 21 (11%) | 6           | 20 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | E     | 229/231 (99%)   | 190 (83%)  | 39 (17%)  | 2           | 7  |
| 2   | F     | 226/231 (98%)   | 195 (86%)  | 31 (14%)  | 3           | 13 |
| 2   | G     | 228/231 (99%)   | 194 (85%)  | 34 (15%)  | 3           | 10 |
| 2   | H     | 227/231 (98%)   | 196 (86%)  | 31 (14%)  | 3           | 13 |
| 2   | M     | 227/231 (98%)   | 196 (86%)  | 31 (14%)  | 3           | 13 |
| 2   | N     | 227/231 (98%)   | 190 (84%)  | 37 (16%)  | 2           | 8  |
| 2   | O     | 226/231 (98%)   | 191 (84%)  | 35 (16%)  | 2           | 9  |
| 2   | P     | 226/231 (98%)   | 193 (85%)  | 33 (15%)  | 3           | 11 |
| All | All   | 3332/3368 (99%) | 2872 (86%) | 460 (14%) | 3           | 12 |

All (460) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 76  | GLU  |
| 1   | A     | 94  | SER  |
| 1   | A     | 100 | ARG  |
| 1   | A     | 106 | GLU  |
| 1   | A     | 138 | PHE  |
| 1   | A     | 178 | THR  |
| 1   | A     | 185 | PHE  |
| 1   | A     | 191 | THR  |
| 1   | A     | 205 | ILE  |
| 1   | A     | 234 | SER  |
| 1   | A     | 260 | ARG  |
| 1   | A     | 262 | ILE  |
| 1   | A     | 264 | ARG  |
| 1   | A     | 267 | ARG  |
| 1   | A     | 283 | GLU  |
| 1   | A     | 285 | LYS  |
| 1   | A     | 294 | LYS  |
| 2   | E     | 310 | LEU  |
| 2   | E     | 311 | THR  |
| 2   | E     | 321 | GLU  |
| 2   | E     | 324 | GLU  |
| 2   | E     | 327 | GLU  |
| 2   | E     | 330 | ASP  |
| 2   | E     | 344 | GLU  |
| 2   | E     | 363 | GLU  |
| 2   | E     | 368 | GLN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | E     | 369    | ARG  |
| 2   | E     | 370    | VAL  |
| 2   | E     | 375    | LEU  |
| 2   | E     | 416    | THR  |
| 2   | E     | 419    | GLN  |
| 2   | E     | 420    | ILE  |
| 2   | E     | 459    | ASN  |
| 2   | E     | 467    | ASP  |
| 2   | E     | 471    | ARG  |
| 2   | E     | 472    | GLU  |
| 2   | E     | 479    | ARG  |
| 2   | E     | 486[A] | GLN  |
| 2   | E     | 486[B] | GLN  |
| 2   | E     | 488    | ARG  |
| 2   | E     | 497    | ARG  |
| 2   | E     | 510    | LEU  |
| 2   | E     | 513    | LEU  |
| 2   | E     | 518    | PHE  |
| 2   | E     | 521    | ARG  |
| 2   | E     | 528    | SER  |
| 2   | E     | 533    | LYS  |
| 2   | E     | 536    | ARG  |
| 2   | E     | 539    | ILE  |
| 2   | E     | 541    | GLU  |
| 2   | E     | 545    | ASP  |
| 2   | E     | 547    | LEU  |
| 2   | E     | 551    | ASP  |
| 2   | E     | 552    | LEU  |
| 2   | E     | 562    | LEU  |
| 2   | E     | 564    | ILE  |
| 1   | B     | 76     | GLU  |
| 1   | B     | 77     | ASN  |
| 1   | B     | 86     | VAL  |
| 1   | B     | 94     | SER  |
| 1   | B     | 96     | ARG  |
| 1   | B     | 99     | SER  |
| 1   | B     | 100    | ARG  |
| 1   | B     | 106    | GLU  |
| 1   | B     | 120    | GLU  |
| 1   | B     | 138    | PHE  |
| 1   | B     | 145    | SER  |
| 1   | B     | 149    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 155 | ASP  |
| 1   | B     | 158 | LYS  |
| 1   | B     | 178 | THR  |
| 1   | B     | 179 | VAL  |
| 1   | B     | 185 | PHE  |
| 1   | B     | 205 | ILE  |
| 1   | B     | 234 | SER  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 260 | ARG  |
| 1   | B     | 264 | ARG  |
| 1   | B     | 283 | GLU  |
| 1   | B     | 285 | LYS  |
| 1   | B     | 289 | VAL  |
| 2   | F     | 310 | LEU  |
| 2   | F     | 311 | THR  |
| 2   | F     | 321 | GLU  |
| 2   | F     | 327 | GLU  |
| 2   | F     | 330 | ASP  |
| 2   | F     | 368 | GLN  |
| 2   | F     | 369 | ARG  |
| 2   | F     | 370 | VAL  |
| 2   | F     | 375 | LEU  |
| 2   | F     | 416 | THR  |
| 2   | F     | 433 | ILE  |
| 2   | F     | 449 | HIS  |
| 2   | F     | 459 | ASN  |
| 2   | F     | 461 | GLU  |
| 2   | F     | 467 | ASP  |
| 2   | F     | 471 | ARG  |
| 2   | F     | 472 | GLU  |
| 2   | F     | 479 | ARG  |
| 2   | F     | 483 | GLU  |
| 2   | F     | 486 | GLN  |
| 2   | F     | 488 | ARG  |
| 2   | F     | 509 | ARG  |
| 2   | F     | 510 | LEU  |
| 2   | F     | 518 | PHE  |
| 2   | F     | 533 | LYS  |
| 2   | F     | 536 | ARG  |
| 2   | F     | 539 | ILE  |
| 2   | F     | 541 | GLU  |
| 2   | F     | 545 | ASP  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | F     | 552    | LEU  |
| 2   | F     | 553    | THR  |
| 1   | C     | 75     | SER  |
| 1   | C     | 76     | GLU  |
| 1   | C     | 99     | SER  |
| 1   | C     | 100    | ARG  |
| 1   | C     | 111    | ARG  |
| 1   | C     | 127    | VAL  |
| 1   | C     | 148    | THR  |
| 1   | C     | 155    | ASP  |
| 1   | C     | 158    | LYS  |
| 1   | C     | 185    | PHE  |
| 1   | C     | 195    | ILE  |
| 1   | C     | 205    | ILE  |
| 1   | C     | 234    | SER  |
| 1   | C     | 252    | ASN  |
| 1   | C     | 260    | ARG  |
| 1   | C     | 264    | ARG  |
| 1   | C     | 267    | ARG  |
| 1   | C     | 283    | GLU  |
| 1   | C     | 285    | LYS  |
| 1   | C     | 294[A] | LYS  |
| 1   | C     | 294[B] | LYS  |
| 2   | G     | 310    | LEU  |
| 2   | G     | 311    | THR  |
| 2   | G     | 321    | GLU  |
| 2   | G     | 330    | ASP  |
| 2   | G     | 358    | LYS  |
| 2   | G     | 363    | GLU  |
| 2   | G     | 368    | GLN  |
| 2   | G     | 369    | ARG  |
| 2   | G     | 370    | VAL  |
| 2   | G     | 372    | LYS  |
| 2   | G     | 375    | LEU  |
| 2   | G     | 405    | ASP  |
| 2   | G     | 416    | THR  |
| 2   | G     | 420    | ILE  |
| 2   | G     | 446    | ASP  |
| 2   | G     | 449[A] | HIS  |
| 2   | G     | 449[B] | HIS  |
| 2   | G     | 459    | ASN  |
| 2   | G     | 467    | ASP  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | G     | 471    | ARG  |
| 2   | G     | 472    | GLU  |
| 2   | G     | 479    | ARG  |
| 2   | G     | 486    | GLN  |
| 2   | G     | 488    | ARG  |
| 2   | G     | 489    | VAL  |
| 2   | G     | 510    | LEU  |
| 2   | G     | 518    | PHE  |
| 2   | G     | 539    | ILE  |
| 2   | G     | 541    | GLU  |
| 2   | G     | 545    | ASP  |
| 2   | G     | 547    | LEU  |
| 2   | G     | 551    | ASP  |
| 2   | G     | 552    | LEU  |
| 2   | G     | 564    | ILE  |
| 1   | D     | 75     | SER  |
| 1   | D     | 76     | GLU  |
| 1   | D     | 86     | VAL  |
| 1   | D     | 99     | SER  |
| 1   | D     | 100    | ARG  |
| 1   | D     | 106    | GLU  |
| 1   | D     | 145    | SER  |
| 1   | D     | 155    | ASP  |
| 1   | D     | 178    | THR  |
| 1   | D     | 191    | THR  |
| 1   | D     | 195    | ILE  |
| 1   | D     | 205    | ILE  |
| 1   | D     | 252    | ASN  |
| 1   | D     | 260    | ARG  |
| 1   | D     | 264    | ARG  |
| 1   | D     | 267[A] | ARG  |
| 1   | D     | 267[B] | ARG  |
| 1   | D     | 283    | GLU  |
| 1   | D     | 285    | LYS  |
| 1   | D     | 294    | LYS  |
| 2   | H     | 310    | LEU  |
| 2   | H     | 311    | THR  |
| 2   | H     | 321    | GLU  |
| 2   | H     | 327    | GLU  |
| 2   | H     | 330    | ASP  |
| 2   | H     | 363    | GLU  |
| 2   | H     | 368    | GLN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | H     | 369    | ARG  |
| 2   | H     | 370    | VAL  |
| 2   | H     | 375    | LEU  |
| 2   | H     | 405    | ASP  |
| 2   | H     | 416    | THR  |
| 2   | H     | 449[A] | HIS  |
| 2   | H     | 449[B] | HIS  |
| 2   | H     | 459    | ASN  |
| 2   | H     | 461    | GLU  |
| 2   | H     | 467    | ASP  |
| 2   | H     | 471    | ARG  |
| 2   | H     | 472    | GLU  |
| 2   | H     | 483    | GLU  |
| 2   | H     | 486    | GLN  |
| 2   | H     | 488    | ARG  |
| 2   | H     | 510    | LEU  |
| 2   | H     | 518    | PHE  |
| 2   | H     | 533    | LYS  |
| 2   | H     | 535    | VAL  |
| 2   | H     | 536    | ARG  |
| 2   | H     | 539    | ILE  |
| 2   | H     | 541    | GLU  |
| 2   | H     | 545    | ASP  |
| 2   | H     | 552    | LEU  |
| 1   | I     | 75     | SER  |
| 1   | I     | 76     | GLU  |
| 1   | I     | 86     | VAL  |
| 1   | I     | 94     | SER  |
| 1   | I     | 100    | ARG  |
| 1   | I     | 106    | GLU  |
| 1   | I     | 139    | GLN  |
| 1   | I     | 145    | SER  |
| 1   | I     | 148    | THR  |
| 1   | I     | 149    | LYS  |
| 1   | I     | 178    | THR  |
| 1   | I     | 183    | ARG  |
| 1   | I     | 185    | PHE  |
| 1   | I     | 188    | LYS  |
| 1   | I     | 191    | THR  |
| 1   | I     | 195    | ILE  |
| 1   | I     | 205    | ILE  |
| 1   | I     | 234    | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 252 | ASN  |
| 1   | I     | 254 | MET  |
| 1   | I     | 260 | ARG  |
| 1   | I     | 262 | ILE  |
| 1   | I     | 264 | ARG  |
| 1   | I     | 267 | ARG  |
| 1   | I     | 280 | ILE  |
| 1   | I     | 283 | GLU  |
| 1   | I     | 285 | LYS  |
| 2   | M     | 310 | LEU  |
| 2   | M     | 311 | THR  |
| 2   | M     | 321 | GLU  |
| 2   | M     | 327 | GLU  |
| 2   | M     | 330 | ASP  |
| 2   | M     | 368 | GLN  |
| 2   | M     | 369 | ARG  |
| 2   | M     | 370 | VAL  |
| 2   | M     | 375 | LEU  |
| 2   | M     | 402 | PHE  |
| 2   | M     | 416 | THR  |
| 2   | M     | 418 | THR  |
| 2   | M     | 420 | ILE  |
| 2   | M     | 433 | ILE  |
| 2   | M     | 434 | ASN  |
| 2   | M     | 451 | MET  |
| 2   | M     | 459 | ASN  |
| 2   | M     | 461 | GLU  |
| 2   | M     | 467 | ASP  |
| 2   | M     | 471 | ARG  |
| 2   | M     | 472 | GLU  |
| 2   | M     | 483 | GLU  |
| 2   | M     | 488 | ARG  |
| 2   | M     | 509 | ARG  |
| 2   | M     | 518 | PHE  |
| 2   | M     | 533 | LYS  |
| 2   | M     | 536 | ARG  |
| 2   | M     | 539 | ILE  |
| 2   | M     | 541 | GLU  |
| 2   | M     | 545 | ASP  |
| 2   | M     | 552 | LEU  |
| 1   | J     | 75  | SER  |
| 1   | J     | 77  | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | J     | 94     | SER  |
| 1   | J     | 96     | ARG  |
| 1   | J     | 99     | SER  |
| 1   | J     | 100    | ARG  |
| 1   | J     | 138    | PHE  |
| 1   | J     | 148    | THR  |
| 1   | J     | 178    | THR  |
| 1   | J     | 183    | ARG  |
| 1   | J     | 191    | THR  |
| 1   | J     | 195    | ILE  |
| 1   | J     | 205    | ILE  |
| 1   | J     | 234    | SER  |
| 1   | J     | 252    | ASN  |
| 1   | J     | 258    | SER  |
| 1   | J     | 260    | ARG  |
| 1   | J     | 262    | ILE  |
| 1   | J     | 264    | ARG  |
| 1   | J     | 265    | SER  |
| 1   | J     | 267    | ARG  |
| 1   | J     | 283    | GLU  |
| 1   | J     | 285    | LYS  |
| 1   | J     | 294    | LYS  |
| 2   | N     | 310    | LEU  |
| 2   | N     | 311    | THR  |
| 2   | N     | 321    | GLU  |
| 2   | N     | 330    | ASP  |
| 2   | N     | 344    | GLU  |
| 2   | N     | 358    | LYS  |
| 2   | N     | 363    | GLU  |
| 2   | N     | 368    | GLN  |
| 2   | N     | 369    | ARG  |
| 2   | N     | 370    | VAL  |
| 2   | N     | 375    | LEU  |
| 2   | N     | 411    | ARG  |
| 2   | N     | 414    | SER  |
| 2   | N     | 416    | THR  |
| 2   | N     | 449[A] | HIS  |
| 2   | N     | 449[B] | HIS  |
| 2   | N     | 459    | ASN  |
| 2   | N     | 471    | ARG  |
| 2   | N     | 472    | GLU  |
| 2   | N     | 478    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 479 | ARG  |
| 2   | N     | 484 | SER  |
| 2   | N     | 486 | GLN  |
| 2   | N     | 488 | ARG  |
| 2   | N     | 509 | ARG  |
| 2   | N     | 510 | LEU  |
| 2   | N     | 532 | SER  |
| 2   | N     | 533 | LYS  |
| 2   | N     | 535 | VAL  |
| 2   | N     | 536 | ARG  |
| 2   | N     | 539 | ILE  |
| 2   | N     | 541 | GLU  |
| 2   | N     | 545 | ASP  |
| 2   | N     | 551 | ASP  |
| 2   | N     | 552 | LEU  |
| 2   | N     | 554 | LEU  |
| 2   | N     | 564 | ILE  |
| 1   | K     | 75  | SER  |
| 1   | K     | 94  | SER  |
| 1   | K     | 96  | ARG  |
| 1   | K     | 99  | SER  |
| 1   | K     | 100 | ARG  |
| 1   | K     | 106 | GLU  |
| 1   | K     | 127 | VAL  |
| 1   | K     | 139 | GLN  |
| 1   | K     | 148 | THR  |
| 1   | K     | 149 | LYS  |
| 1   | K     | 151 | ASP  |
| 1   | K     | 155 | ASP  |
| 1   | K     | 159 | ILE  |
| 1   | K     | 168 | THR  |
| 1   | K     | 170 | GLN  |
| 1   | K     | 178 | THR  |
| 1   | K     | 183 | ARG  |
| 1   | K     | 185 | PHE  |
| 1   | K     | 188 | LYS  |
| 1   | K     | 191 | THR  |
| 1   | K     | 195 | ILE  |
| 1   | K     | 205 | ILE  |
| 1   | K     | 221 | VAL  |
| 1   | K     | 234 | SER  |
| 1   | K     | 252 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 258 | SER  |
| 1   | K     | 260 | ARG  |
| 1   | K     | 262 | ILE  |
| 1   | K     | 264 | ARG  |
| 1   | K     | 265 | SER  |
| 1   | K     | 270 | GLU  |
| 1   | K     | 283 | GLU  |
| 1   | K     | 285 | LYS  |
| 1   | K     | 294 | LYS  |
| 2   | O     | 310 | LEU  |
| 2   | O     | 311 | THR  |
| 2   | O     | 321 | GLU  |
| 2   | O     | 324 | GLU  |
| 2   | O     | 327 | GLU  |
| 2   | O     | 330 | ASP  |
| 2   | O     | 363 | GLU  |
| 2   | O     | 368 | GLN  |
| 2   | O     | 369 | ARG  |
| 2   | O     | 370 | VAL  |
| 2   | O     | 405 | ASP  |
| 2   | O     | 411 | ARG  |
| 2   | O     | 416 | THR  |
| 2   | O     | 420 | ILE  |
| 2   | O     | 434 | ASN  |
| 2   | O     | 435 | ARG  |
| 2   | O     | 449 | HIS  |
| 2   | O     | 459 | ASN  |
| 2   | O     | 467 | ASP  |
| 2   | O     | 471 | ARG  |
| 2   | O     | 472 | GLU  |
| 2   | O     | 479 | ARG  |
| 2   | O     | 483 | GLU  |
| 2   | O     | 486 | GLN  |
| 2   | O     | 488 | ARG  |
| 2   | O     | 509 | ARG  |
| 2   | O     | 510 | LEU  |
| 2   | O     | 521 | ARG  |
| 2   | O     | 533 | LYS  |
| 2   | O     | 536 | ARG  |
| 2   | O     | 541 | GLU  |
| 2   | O     | 542 | ARG  |
| 2   | O     | 545 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 552 | LEU  |
| 2   | O     | 564 | ILE  |
| 1   | L     | 75  | SER  |
| 1   | L     | 76  | GLU  |
| 1   | L     | 77  | ASN  |
| 1   | L     | 94  | SER  |
| 1   | L     | 99  | SER  |
| 1   | L     | 100 | ARG  |
| 1   | L     | 106 | GLU  |
| 1   | L     | 127 | VAL  |
| 1   | L     | 145 | SER  |
| 1   | L     | 178 | THR  |
| 1   | L     | 179 | VAL  |
| 1   | L     | 185 | PHE  |
| 1   | L     | 205 | ILE  |
| 1   | L     | 252 | ASN  |
| 1   | L     | 260 | ARG  |
| 1   | L     | 262 | ILE  |
| 1   | L     | 264 | ARG  |
| 1   | L     | 267 | ARG  |
| 1   | L     | 280 | ILE  |
| 1   | L     | 283 | GLU  |
| 1   | L     | 285 | LYS  |
| 2   | P     | 310 | LEU  |
| 2   | P     | 311 | THR  |
| 2   | P     | 321 | GLU  |
| 2   | P     | 324 | GLU  |
| 2   | P     | 330 | ASP  |
| 2   | P     | 363 | GLU  |
| 2   | P     | 368 | GLN  |
| 2   | P     | 369 | ARG  |
| 2   | P     | 370 | VAL  |
| 2   | P     | 375 | LEU  |
| 2   | P     | 416 | THR  |
| 2   | P     | 459 | ASN  |
| 2   | P     | 461 | GLU  |
| 2   | P     | 467 | ASP  |
| 2   | P     | 471 | ARG  |
| 2   | P     | 472 | GLU  |
| 2   | P     | 479 | ARG  |
| 2   | P     | 486 | GLN  |
| 2   | P     | 488 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 507 | HIS  |
| 2   | P     | 509 | ARG  |
| 2   | P     | 510 | LEU  |
| 2   | P     | 518 | PHE  |
| 2   | P     | 521 | ARG  |
| 2   | P     | 533 | LYS  |
| 2   | P     | 535 | VAL  |
| 2   | P     | 536 | ARG  |
| 2   | P     | 539 | ILE  |
| 2   | P     | 541 | GLU  |
| 2   | P     | 545 | ASP  |
| 2   | P     | 552 | LEU  |
| 2   | P     | 554 | LEU  |
| 2   | P     | 564 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 77  | ASN  |
| 1   | A     | 252 | ASN  |
| 2   | E     | 419 | GLN  |
| 2   | E     | 459 | ASN  |
| 2   | E     | 549 | HIS  |
| 1   | B     | 77  | ASN  |
| 1   | B     | 231 | GLN  |
| 1   | B     | 252 | ASN  |
| 2   | F     | 318 | HIS  |
| 2   | F     | 449 | HIS  |
| 2   | F     | 459 | ASN  |
| 2   | F     | 522 | HIS  |
| 2   | F     | 549 | HIS  |
| 1   | C     | 77  | ASN  |
| 1   | C     | 128 | HIS  |
| 1   | C     | 233 | GLN  |
| 1   | C     | 252 | ASN  |
| 2   | G     | 318 | HIS  |
| 2   | G     | 419 | GLN  |
| 2   | G     | 459 | ASN  |
| 2   | G     | 522 | HIS  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 128 | HIS  |
| 1   | D     | 233 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 252 | ASN  |
| 2   | H     | 419 | GLN  |
| 2   | H     | 429 | HIS  |
| 2   | H     | 459 | ASN  |
| 2   | H     | 466 | ASN  |
| 2   | H     | 507 | HIS  |
| 2   | H     | 556 | GLN  |
| 1   | I     | 77  | ASN  |
| 1   | I     | 128 | HIS  |
| 1   | I     | 252 | ASN  |
| 2   | M     | 419 | GLN  |
| 2   | M     | 449 | HIS  |
| 2   | M     | 456 | ASN  |
| 2   | M     | 459 | ASN  |
| 2   | M     | 466 | ASN  |
| 2   | M     | 549 | HIS  |
| 2   | M     | 556 | GLN  |
| 1   | J     | 77  | ASN  |
| 1   | J     | 252 | ASN  |
| 2   | N     | 318 | HIS  |
| 2   | N     | 419 | GLN  |
| 2   | N     | 459 | ASN  |
| 2   | N     | 486 | GLN  |
| 2   | N     | 507 | HIS  |
| 1   | K     | 77  | ASN  |
| 1   | K     | 251 | HIS  |
| 1   | K     | 252 | ASN  |
| 2   | O     | 318 | HIS  |
| 2   | O     | 419 | GLN  |
| 2   | O     | 429 | HIS  |
| 2   | O     | 449 | HIS  |
| 2   | O     | 459 | ASN  |
| 1   | L     | 77  | ASN  |
| 1   | L     | 246 | GLN  |
| 1   | L     | 252 | ASN  |
| 2   | P     | 419 | GLN  |
| 2   | P     | 459 | ASN  |

### 5.3.3 RNA ⓘ

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](#)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | HDD  | P     | 760 | 2    | 46,52,52     | 2.93 | 24 (52%)    | 62,89,89    | 4.79 | 39 (62%)    |
| 3   | HDD  | O     | 760 | 2    | 46,52,52     | 2.89 | 24 (52%)    | 62,89,89    | 4.62 | 33 (53%)    |
| 3   | HDD  | H     | 760 | 2    | 46,52,52     | 2.90 | 23 (50%)    | 62,89,89    | 4.33 | 32 (51%)    |
| 3   | HDD  | E     | 760 | 2    | 46,52,52     | 3.11 | 24 (52%)    | 62,89,89    | 4.95 | 36 (58%)    |
| 3   | HDD  | M     | 760 | 2    | 46,52,52     | 2.76 | 23 (50%)    | 62,89,89    | 4.54 | 32 (51%)    |
| 3   | HDD  | F     | 760 | 2    | 46,52,52     | 2.64 | 21 (45%)    | 62,89,89    | 4.57 | 34 (54%)    |
| 3   | HDD  | N     | 760 | 2    | 46,52,52     | 3.03 | 22 (47%)    | 62,89,89    | 4.49 | 34 (54%)    |
| 3   | HDD  | G     | 760 | 2    | 46,52,52     | 2.80 | 25 (54%)    | 62,89,89    | 4.16 | 29 (46%)    |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | HDD  | P     | 760 | 2    | -       | 4/9/89/89 | 0/1/9/9 |
| 3   | HDD  | O     | 760 | 2    | -       | 8/9/89/89 | 0/1/9/9 |
| 3   | HDD  | H     | 760 | 2    | -       | 4/9/89/89 | 0/1/9/9 |
| 3   | HDD  | E     | 760 | 2    | -       | 2/9/89/89 | 0/1/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | HDD  | M     | 760 | 2    | -       | 2/9/89/89 | 0/1/9/9 |
| 3   | HDD  | F     | 760 | 2    | -       | 5/9/89/89 | 0/1/9/9 |
| 3   | HDD  | N     | 760 | 2    | -       | 2/9/89/89 | 0/1/9/9 |
| 3   | HDD  | G     | 760 | 2    | -       | 5/9/89/89 | 0/1/9/9 |

All (186) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | P     | 760 | HDD  | O1D-CGD | 7.50  | 1.47        | 1.35     |
| 3   | E     | 760 | HDD  | C4C-NC  | -7.03 | 1.26        | 1.39     |
| 3   | O     | 760 | HDD  | O1D-CGD | 6.67  | 1.46        | 1.35     |
| 3   | H     | 760 | HDD  | O1D-CGD | 6.63  | 1.46        | 1.35     |
| 3   | F     | 760 | HDD  | O1D-CGD | 6.62  | 1.46        | 1.35     |
| 3   | M     | 760 | HDD  | O1D-CGD | 6.59  | 1.45        | 1.35     |
| 3   | N     | 760 | HDD  | C4C-NC  | -6.59 | 1.27        | 1.39     |
| 3   | E     | 760 | HDD  | C3B-C2B | 6.24  | 1.49        | 1.37     |
| 3   | E     | 760 | HDD  | O1D-CGD | 6.16  | 1.45        | 1.35     |
| 3   | H     | 760 | HDD  | C3B-C2B | 5.99  | 1.49        | 1.37     |
| 3   | G     | 760 | HDD  | C3B-C2B | 5.96  | 1.49        | 1.37     |
| 3   | N     | 760 | HDD  | C3B-C2B | 5.95  | 1.49        | 1.37     |
| 3   | N     | 760 | HDD  | O1D-CGD | 5.86  | 1.44        | 1.35     |
| 3   | G     | 760 | HDD  | O1D-CGD | 5.66  | 1.44        | 1.35     |
| 3   | P     | 760 | HDD  | CHD-C1D | -5.60 | 1.20        | 1.37     |
| 3   | M     | 760 | HDD  | C3B-C2B | 5.56  | 1.48        | 1.37     |
| 3   | P     | 760 | HDD  | C2A-C3A | 5.46  | 1.53        | 1.38     |
| 3   | F     | 760 | HDD  | C3B-C2B | 5.42  | 1.48        | 1.37     |
| 3   | N     | 760 | HDD  | C3B-C4B | -5.33 | 1.36        | 1.46     |
| 3   | E     | 760 | HDD  | CHD-C1D | -5.32 | 1.21        | 1.37     |
| 3   | P     | 760 | HDD  | C3B-C2B | 5.20  | 1.47        | 1.37     |
| 3   | O     | 760 | HDD  | CHD-C1D | -5.17 | 1.21        | 1.37     |
| 3   | O     | 760 | HDD  | C3B-C2B | 5.17  | 1.47        | 1.37     |
| 3   | M     | 760 | HDD  | CHD-C1D | -5.16 | 1.21        | 1.37     |
| 3   | E     | 760 | HDD  | C1D-ND  | -5.14 | 1.29        | 1.37     |
| 3   | G     | 760 | HDD  | CHD-C1D | -5.06 | 1.22        | 1.37     |
| 3   | O     | 760 | HDD  | C4C-NC  | -5.01 | 1.30        | 1.39     |
| 3   | P     | 760 | HDD  | CHA-C4D | -4.99 | 1.22        | 1.37     |
| 3   | N     | 760 | HDD  | CHC-C1C | -4.98 | 1.28        | 1.39     |
| 3   | N     | 760 | HDD  | CHC-C4B | -4.91 | 1.28        | 1.38     |
| 3   | E     | 760 | HDD  | C1A-NA  | -4.87 | 1.30        | 1.39     |
| 3   | E     | 760 | HDD  | CHD-C4C | -4.82 | 1.28        | 1.39     |
| 3   | P     | 760 | HDD  | C4C-NC  | -4.82 | 1.30        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 760 | HDD  | CHA-C4D | -4.81 | 1.23        | 1.37     |
| 3   | N     | 760 | HDD  | CHD-C1D | -4.78 | 1.23        | 1.37     |
| 3   | M     | 760 | HDD  | CHA-C4D | -4.76 | 1.23        | 1.37     |
| 3   | E     | 760 | HDD  | CHA-C4D | -4.76 | 1.23        | 1.37     |
| 3   | O     | 760 | HDD  | C3B-C4B | -4.70 | 1.37        | 1.46     |
| 3   | G     | 760 | HDD  | CHD-C4C | -4.67 | 1.28        | 1.39     |
| 3   | N     | 760 | HDD  | CHA-C4D | -4.66 | 1.23        | 1.37     |
| 3   | G     | 760 | HDD  | CHA-C4D | -4.65 | 1.23        | 1.37     |
| 3   | H     | 760 | HDD  | C1C-NC  | -4.65 | 1.30        | 1.39     |
| 3   | O     | 760 | HDD  | CHB-C1B | 4.63  | 1.47        | 1.38     |
| 3   | H     | 760 | HDD  | C4C-NC  | -4.62 | 1.30        | 1.39     |
| 3   | M     | 760 | HDD  | C4C-NC  | -4.62 | 1.30        | 1.39     |
| 3   | F     | 760 | HDD  | CHA-C4D | -4.60 | 1.23        | 1.37     |
| 3   | O     | 760 | HDD  | CHD-C4C | -4.60 | 1.29        | 1.39     |
| 3   | F     | 760 | HDD  | CHD-C1D | -4.57 | 1.23        | 1.37     |
| 3   | H     | 760 | HDD  | C3B-C4B | -4.57 | 1.38        | 1.46     |
| 3   | O     | 760 | HDD  | CHA-C4D | -4.53 | 1.23        | 1.37     |
| 3   | H     | 760 | HDD  | CHD-C1D | -4.52 | 1.23        | 1.37     |
| 3   | H     | 760 | HDD  | CHB-C1B | 4.46  | 1.47        | 1.38     |
| 3   | G     | 760 | HDD  | C4C-NC  | -4.45 | 1.31        | 1.39     |
| 3   | E     | 760 | HDD  | C3B-C4B | -4.42 | 1.38        | 1.46     |
| 3   | P     | 760 | HDD  | C1C-NC  | -4.37 | 1.31        | 1.39     |
| 3   | G     | 760 | HDD  | C2A-C3A | 4.35  | 1.50        | 1.38     |
| 3   | N     | 760 | HDD  | C1C-NC  | -4.35 | 1.31        | 1.39     |
| 3   | M     | 760 | HDD  | CHD-C4C | -4.34 | 1.29        | 1.39     |
| 3   | P     | 760 | HDD  | CHD-C4C | -4.28 | 1.29        | 1.39     |
| 3   | P     | 760 | HDD  | C4A-NA  | -4.27 | 1.31        | 1.39     |
| 3   | O     | 760 | HDD  | C1C-NC  | -4.27 | 1.31        | 1.39     |
| 3   | P     | 760 | HDD  | C1A-NA  | -4.26 | 1.31        | 1.39     |
| 3   | N     | 760 | HDD  | CHD-C4C | -4.21 | 1.30        | 1.39     |
| 3   | M     | 760 | HDD  | C1A-NA  | -4.14 | 1.31        | 1.39     |
| 3   | E     | 760 | HDD  | C4A-NA  | -4.13 | 1.31        | 1.39     |
| 3   | M     | 760 | HDD  | CHB-C1B | 4.09  | 1.46        | 1.38     |
| 3   | F     | 760 | HDD  | C1C-NC  | -4.09 | 1.31        | 1.39     |
| 3   | E     | 760 | HDD  | CHA-C1A | -4.08 | 1.30        | 1.39     |
| 3   | M     | 760 | HDD  | C4A-NA  | -4.06 | 1.32        | 1.39     |
| 3   | G     | 760 | HDD  | C3B-C4B | -4.03 | 1.39        | 1.46     |
| 3   | E     | 760 | HDD  | CHC-C1C | -3.98 | 1.30        | 1.39     |
| 3   | E     | 760 | HDD  | C1C-NC  | -3.97 | 1.32        | 1.39     |
| 3   | P     | 760 | HDD  | CHB-C1B | 3.97  | 1.46        | 1.38     |
| 3   | P     | 760 | HDD  | C1A-C2A | -3.95 | 1.36        | 1.44     |
| 3   | H     | 760 | HDD  | CHC-C1C | -3.95 | 1.30        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 760 | HDD  | C1A-NA  | -3.94 | 1.32        | 1.39     |
| 3   | F     | 760 | HDD  | CHC-C1C | -3.91 | 1.30        | 1.39     |
| 3   | F     | 760 | HDD  | CHC-C4B | -3.80 | 1.30        | 1.38     |
| 3   | O     | 760 | HDD  | C2A-C3A | 3.79  | 1.48        | 1.38     |
| 3   | H     | 760 | HDD  | CHC-C4B | -3.79 | 1.30        | 1.38     |
| 3   | E     | 760 | HDD  | CHB-C1B | 3.78  | 1.45        | 1.38     |
| 3   | G     | 760 | HDD  | CHB-C1B | 3.78  | 1.45        | 1.38     |
| 3   | G     | 760 | HDD  | C1A-NA  | -3.77 | 1.32        | 1.39     |
| 3   | N     | 760 | HDD  | C4B-NB  | -3.76 | 1.32        | 1.39     |
| 3   | O     | 760 | HDD  | C4B-NB  | -3.74 | 1.32        | 1.39     |
| 3   | M     | 760 | HDD  | C1C-NC  | -3.73 | 1.32        | 1.39     |
| 3   | O     | 760 | HDD  | CHC-C4B | -3.73 | 1.31        | 1.38     |
| 3   | G     | 760 | HDD  | C1C-NC  | -3.72 | 1.32        | 1.39     |
| 3   | N     | 760 | HDD  | CHA-C1A | -3.72 | 1.31        | 1.39     |
| 3   | F     | 760 | HDD  | C4B-NB  | -3.71 | 1.32        | 1.39     |
| 3   | O     | 760 | HDD  | CHC-C1C | -3.70 | 1.31        | 1.39     |
| 3   | N     | 760 | HDD  | C1B-NB  | -3.70 | 1.32        | 1.39     |
| 3   | F     | 760 | HDD  | C1B-C2B | -3.67 | 1.38        | 1.45     |
| 3   | F     | 760 | HDD  | C4A-NA  | -3.66 | 1.32        | 1.39     |
| 3   | E     | 760 | HDD  | C1B-NB  | -3.66 | 1.32        | 1.39     |
| 3   | M     | 760 | HDD  | CHC-C1C | -3.65 | 1.31        | 1.39     |
| 3   | P     | 760 | HDD  | CHA-C1A | -3.65 | 1.31        | 1.39     |
| 3   | H     | 760 | HDD  | CHA-C1A | -3.64 | 1.31        | 1.39     |
| 3   | H     | 760 | HDD  | C2A-C3A | 3.64  | 1.48        | 1.38     |
| 3   | G     | 760 | HDD  | CHC-C1C | -3.63 | 1.31        | 1.39     |
| 3   | N     | 760 | HDD  | C4A-NA  | -3.63 | 1.32        | 1.39     |
| 3   | N     | 760 | HDD  | C1A-NA  | -3.63 | 1.32        | 1.39     |
| 3   | E     | 760 | HDD  | CHC-C4B | -3.62 | 1.31        | 1.38     |
| 3   | H     | 760 | HDD  | C4B-NB  | -3.60 | 1.32        | 1.39     |
| 3   | M     | 760 | HDD  | CHA-C1A | -3.59 | 1.31        | 1.39     |
| 3   | F     | 760 | HDD  | C4C-NC  | -3.58 | 1.32        | 1.39     |
| 3   | H     | 760 | HDD  | CHD-C4C | -3.56 | 1.31        | 1.39     |
| 3   | F     | 760 | HDD  | CHB-C1B | 3.55  | 1.45        | 1.38     |
| 3   | G     | 760 | HDD  | C4A-NA  | -3.54 | 1.33        | 1.39     |
| 3   | O     | 760 | HDD  | C1A-NA  | -3.52 | 1.33        | 1.39     |
| 3   | F     | 760 | HDD  | C2A-C3A | 3.52  | 1.48        | 1.38     |
| 3   | N     | 760 | HDD  | C2A-C3A | 3.50  | 1.48        | 1.38     |
| 3   | N     | 760 | HDD  | CHB-C1B | 3.49  | 1.45        | 1.38     |
| 3   | P     | 760 | HDD  | CHC-C1C | -3.43 | 1.31        | 1.39     |
| 3   | M     | 760 | HDD  | C2A-C3A | 3.42  | 1.47        | 1.38     |
| 3   | M     | 760 | HDD  | CHC-C4B | -3.42 | 1.31        | 1.38     |
| 3   | F     | 760 | HDD  | CHA-C1A | -3.41 | 1.31        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | N     | 760 | HDD  | C1D-ND  | -3.40 | 1.31        | 1.37     |
| 3   | G     | 760 | HDD  | CHA-C1A | -3.40 | 1.31        | 1.39     |
| 3   | O     | 760 | HDD  | CHB-C4A | 3.40  | 1.47        | 1.39     |
| 3   | G     | 760 | HDD  | C1B-C2B | -3.31 | 1.38        | 1.45     |
| 3   | G     | 760 | HDD  | C1B-NB  | -3.30 | 1.33        | 1.39     |
| 3   | F     | 760 | HDD  | C3B-C4B | -3.22 | 1.40        | 1.46     |
| 3   | P     | 760 | HDD  | C1D-ND  | -3.21 | 1.32        | 1.37     |
| 3   | O     | 760 | HDD  | C4A-NA  | -3.20 | 1.33        | 1.39     |
| 3   | F     | 760 | HDD  | CHD-C4C | -3.19 | 1.32        | 1.39     |
| 3   | E     | 760 | HDD  | CHB-C4A | 3.17  | 1.46        | 1.39     |
| 3   | G     | 760 | HDD  | CHC-C4B | -3.15 | 1.32        | 1.38     |
| 3   | H     | 760 | HDD  | C4A-NA  | -3.14 | 1.33        | 1.39     |
| 3   | O     | 760 | HDD  | C4A-C3A | 3.12  | 1.50        | 1.43     |
| 3   | H     | 760 | HDD  | C3C-C2C | 3.01  | 1.51        | 1.41     |
| 3   | F     | 760 | HDD  | C1B-NB  | -3.01 | 1.34        | 1.39     |
| 3   | O     | 760 | HDD  | CHA-C1A | -2.98 | 1.32        | 1.39     |
| 3   | P     | 760 | HDD  | C1B-NB  | -2.98 | 1.34        | 1.39     |
| 3   | O     | 760 | HDD  | C4D-ND  | -2.93 | 1.32        | 1.37     |
| 3   | M     | 760 | HDD  | C3C-C2C | 2.90  | 1.51        | 1.41     |
| 3   | M     | 760 | HDD  | C4D-ND  | -2.89 | 1.32        | 1.37     |
| 3   | E     | 760 | HDD  | C4A-C3A | 2.88  | 1.49        | 1.43     |
| 3   | E     | 760 | HDD  | C4B-NB  | -2.88 | 1.34        | 1.39     |
| 3   | H     | 760 | HDD  | C1A-C2A | -2.87 | 1.38        | 1.44     |
| 3   | G     | 760 | HDD  | C4B-NB  | -2.86 | 1.34        | 1.39     |
| 3   | H     | 760 | HDD  | C4A-C3A | 2.86  | 1.49        | 1.43     |
| 3   | O     | 760 | HDD  | C1B-C2B | -2.85 | 1.39        | 1.45     |
| 3   | M     | 760 | HDD  | CHB-C4A | 2.83  | 1.45        | 1.39     |
| 3   | N     | 760 | HDD  | C3C-C2C | 2.83  | 1.50        | 1.41     |
| 3   | O     | 760 | HDD  | C1D-ND  | -2.74 | 1.33        | 1.37     |
| 3   | M     | 760 | HDD  | C3B-C4B | -2.73 | 1.41        | 1.46     |
| 3   | H     | 760 | HDD  | C1C-C2C | -2.71 | 1.36        | 1.43     |
| 3   | F     | 760 | HDD  | C1A-NA  | -2.71 | 1.34        | 1.39     |
| 3   | N     | 760 | HDD  | C1B-C2B | -2.69 | 1.40        | 1.45     |
| 3   | G     | 760 | HDD  | C3C-C2C | 2.66  | 1.50        | 1.41     |
| 3   | H     | 760 | HDD  | C1B-C2B | -2.64 | 1.40        | 1.45     |
| 3   | H     | 760 | HDD  | CHB-C4A | 2.61  | 1.45        | 1.39     |
| 3   | E     | 760 | HDD  | C2A-C3A | 2.58  | 1.45        | 1.38     |
| 3   | G     | 760 | HDD  | C3C-C4C | -2.58 | 1.35        | 1.42     |
| 3   | M     | 760 | HDD  | C1B-NB  | -2.57 | 1.34        | 1.39     |
| 3   | P     | 760 | HDD  | O1A-CGA | 2.55  | 1.30        | 1.22     |
| 3   | G     | 760 | HDD  | O1D-C3D | -2.53 | 1.42        | 1.46     |
| 3   | E     | 760 | HDD  | C3C-C2C | 2.53  | 1.49        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | N     | 760 | HDD  | CHB-C4A | 2.52  | 1.45        | 1.39     |
| 3   | O     | 760 | HDD  | C1B-NB  | -2.46 | 1.35        | 1.39     |
| 3   | P     | 760 | HDD  | C3C-C2C | 2.44  | 1.49        | 1.41     |
| 3   | G     | 760 | HDD  | CHB-C4A | 2.43  | 1.44        | 1.39     |
| 3   | F     | 760 | HDD  | C4A-C3A | 2.36  | 1.48        | 1.43     |
| 3   | P     | 760 | HDD  | C3B-C4B | -2.33 | 1.42        | 1.46     |
| 3   | M     | 760 | HDD  | C1A-C2A | -2.32 | 1.39        | 1.44     |
| 3   | M     | 760 | HDD  | C4B-NB  | -2.30 | 1.35        | 1.39     |
| 3   | P     | 760 | HDD  | C4B-NB  | -2.23 | 1.35        | 1.39     |
| 3   | E     | 760 | HDD  | C4D-ND  | -2.23 | 1.33        | 1.37     |
| 3   | P     | 760 | HDD  | CHC-C4B | -2.22 | 1.34        | 1.38     |
| 3   | P     | 760 | HDD  | CHB-C4A | 2.21  | 1.44        | 1.39     |
| 3   | G     | 760 | HDD  | C1A-C2A | -2.21 | 1.40        | 1.44     |
| 3   | P     | 760 | HDD  | C1B-C2B | -2.20 | 1.41        | 1.45     |
| 3   | E     | 760 | HDD  | C1B-C2B | -2.15 | 1.41        | 1.45     |
| 3   | O     | 760 | HDD  | C3C-C2C | 2.14  | 1.48        | 1.41     |
| 3   | F     | 760 | HDD  | C3C-C2C | 2.12  | 1.48        | 1.41     |
| 3   | M     | 760 | HDD  | C1B-C2B | -2.11 | 1.41        | 1.45     |
| 3   | P     | 760 | HDD  | C3C-C4C | -2.09 | 1.36        | 1.42     |
| 3   | N     | 760 | HDD  | C1C-C2C | -2.08 | 1.38        | 1.43     |
| 3   | G     | 760 | HDD  | C4A-C3A | 2.07  | 1.48        | 1.43     |
| 3   | O     | 760 | HDD  | CBA-CGA | 2.06  | 1.55        | 1.50     |
| 3   | F     | 760 | HDD  | C4D-ND  | -2.05 | 1.34        | 1.37     |
| 3   | H     | 760 | HDD  | C1D-ND  | -2.04 | 1.34        | 1.37     |
| 3   | E     | 760 | HDD  | C1A-C2A | -2.02 | 1.40        | 1.44     |
| 3   | G     | 760 | HDD  | C4D-ND  | -2.00 | 1.34        | 1.37     |
| 3   | M     | 760 | HDD  | C1D-ND  | -2.00 | 1.34        | 1.37     |

All (269) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | O     | 760 | HDD  | C1A-CHA-C4D | 16.46 | 157.77      | 125.81   |
| 3   | E     | 760 | HDD  | C4C-CHD-C1D | 16.37 | 157.61      | 125.81   |
| 3   | E     | 760 | HDD  | C1A-CHA-C4D | 15.91 | 156.71      | 125.81   |
| 3   | M     | 760 | HDD  | C1A-CHA-C4D | 15.83 | 156.55      | 125.81   |
| 3   | N     | 760 | HDD  | C4C-CHD-C1D | 15.71 | 156.33      | 125.81   |
| 3   | H     | 760 | HDD  | C1A-CHA-C4D | 15.70 | 156.30      | 125.81   |
| 3   | G     | 760 | HDD  | C1A-CHA-C4D | 15.40 | 155.73      | 125.81   |
| 3   | F     | 760 | HDD  | C1A-CHA-C4D | 15.26 | 155.46      | 125.81   |
| 3   | P     | 760 | HDD  | C4C-CHD-C1D | 15.04 | 155.03      | 125.81   |
| 3   | P     | 760 | HDD  | C1A-CHA-C4D | 14.64 | 154.25      | 125.81   |
| 3   | O     | 760 | HDD  | C4C-CHD-C1D | 14.31 | 153.61      | 125.81   |

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| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | N     | 760 | HDD  | C1A-CHA-C4D | 14.05  | 153.10      | 125.81   |
| 3   | M     | 760 | HDD  | C4C-CHD-C1D | 13.78  | 152.57      | 125.81   |
| 3   | F     | 760 | HDD  | C4C-CHD-C1D | 13.32  | 151.69      | 125.81   |
| 3   | H     | 760 | HDD  | C4C-CHD-C1D | 12.49  | 150.06      | 125.81   |
| 3   | G     | 760 | HDD  | C4C-CHD-C1D | 11.96  | 149.04      | 125.81   |
| 3   | M     | 760 | HDD  | CHC-C4B-NB  | -10.79 | 112.70      | 124.45   |
| 3   | P     | 760 | HDD  | CHA-C4D-ND  | -10.22 | 110.19      | 124.28   |
| 3   | O     | 760 | HDD  | C1C-CHC-C4B | 9.94   | 155.35      | 124.66   |
| 3   | F     | 760 | HDD  | C1C-CHC-C4B | 9.91   | 155.24      | 124.66   |
| 3   | H     | 760 | HDD  | C1C-CHC-C4B | 9.72   | 154.67      | 124.66   |
| 3   | F     | 760 | HDD  | CHC-C4B-NB  | -9.66  | 113.94      | 124.45   |
| 3   | M     | 760 | HDD  | C1C-CHC-C4B | 9.64   | 154.40      | 124.66   |
| 3   | H     | 760 | HDD  | CHC-C4B-NB  | -9.62  | 113.98      | 124.45   |
| 3   | E     | 760 | HDD  | CHA-C4D-ND  | -9.42  | 111.30      | 124.28   |
| 3   | E     | 760 | HDD  | C1C-CHC-C4B | 9.41   | 153.70      | 124.66   |
| 3   | G     | 760 | HDD  | C1C-CHC-C4B | 9.29   | 153.34      | 124.66   |
| 3   | N     | 760 | HDD  | C1C-CHC-C4B | 9.28   | 153.29      | 124.66   |
| 3   | P     | 760 | HDD  | CHD-C1D-ND  | -9.17  | 111.64      | 124.28   |
| 3   | P     | 760 | HDD  | C1C-CHC-C4B | 9.08   | 152.67      | 124.66   |
| 3   | O     | 760 | HDD  | CHC-C4B-NB  | -8.98  | 114.68      | 124.45   |
| 3   | E     | 760 | HDD  | CHD-C4C-NC  | -8.89  | 107.73      | 123.86   |
| 3   | O     | 760 | HDD  | CHA-C4D-ND  | -8.68  | 112.32      | 124.28   |
| 3   | N     | 760 | HDD  | CHD-C4C-NC  | -8.60  | 108.26      | 123.86   |
| 3   | M     | 760 | HDD  | CHA-C4D-ND  | -8.56  | 112.47      | 124.28   |
| 3   | G     | 760 | HDD  | CHC-C4B-NB  | -8.41  | 115.29      | 124.45   |
| 3   | P     | 760 | HDD  | CHC-C4B-NB  | -8.32  | 115.39      | 124.45   |
| 3   | E     | 760 | HDD  | CHC-C1C-NC  | -8.20  | 108.99      | 123.86   |
| 3   | P     | 760 | HDD  | CHC-C1C-NC  | -8.17  | 109.05      | 123.86   |
| 3   | O     | 760 | HDD  | CHA-C1A-NA  | -8.14  | 109.10      | 123.86   |
| 3   | F     | 760 | HDD  | CHC-C1C-NC  | -7.89  | 109.55      | 123.86   |
| 3   | H     | 760 | HDD  | CHA-C4D-ND  | -7.88  | 113.42      | 124.28   |
| 3   | F     | 760 | HDD  | CHA-C4D-ND  | -7.86  | 113.45      | 124.28   |
| 3   | E     | 760 | HDD  | CHA-C1A-NA  | -7.84  | 109.63      | 123.86   |
| 3   | O     | 760 | HDD  | CHC-C1C-NC  | -7.79  | 109.73      | 123.86   |
| 3   | N     | 760 | HDD  | CHC-C4B-NB  | -7.76  | 116.01      | 124.45   |
| 3   | G     | 760 | HDD  | CHA-C4D-ND  | -7.73  | 113.62      | 124.28   |
| 3   | O     | 760 | HDD  | CHD-C4C-NC  | -7.72  | 109.87      | 123.86   |
| 3   | F     | 760 | HDD  | CHA-C1A-NA  | -7.68  | 109.93      | 123.86   |
| 3   | E     | 760 | HDD  | CHC-C4B-NB  | -7.64  | 116.14      | 124.45   |
| 3   | F     | 760 | HDD  | CHD-C4C-NC  | -7.59  | 110.10      | 123.86   |
| 3   | N     | 760 | HDD  | C3C-C2C-C1C | -7.49  | 98.35       | 107.17   |
| 3   | N     | 760 | HDD  | CHA-C1A-NA  | -7.48  | 110.30      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 760 | HDD  | CHA-C1A-NA  | -7.43 | 110.38      | 123.86   |
| 3   | E     | 760 | HDD  | C2A-C1A-NA  | 7.40  | 118.36      | 110.15   |
| 3   | G     | 760 | HDD  | CHA-C1A-NA  | -7.34 | 110.55      | 123.86   |
| 3   | P     | 760 | HDD  | O1D-CGD-O2D | 7.22  | 126.89      | 120.81   |
| 3   | N     | 760 | HDD  | CHC-C1C-NC  | -7.10 | 110.99      | 123.86   |
| 3   | N     | 760 | HDD  | CHA-C4D-ND  | -7.09 | 114.50      | 124.28   |
| 3   | M     | 760 | HDD  | CHD-C1D-ND  | -7.07 | 114.53      | 124.28   |
| 3   | E     | 760 | HDD  | C3C-C2C-C1C | -7.05 | 98.86       | 107.17   |
| 3   | N     | 760 | HDD  | CHD-C1D-ND  | -7.04 | 114.58      | 124.28   |
| 3   | G     | 760 | HDD  | CHC-C1C-NC  | -6.99 | 111.18      | 123.86   |
| 3   | H     | 760 | HDD  | CHD-C4C-NC  | -6.97 | 111.21      | 123.86   |
| 3   | M     | 760 | HDD  | CHD-C4C-NC  | -6.93 | 111.28      | 123.86   |
| 3   | E     | 760 | HDD  | CHD-C1D-ND  | -6.92 | 114.74      | 124.28   |
| 3   | P     | 760 | HDD  | CMC-C2C-C1C | 6.84  | 135.83      | 125.42   |
| 3   | O     | 760 | HDD  | CHD-C1D-ND  | -6.77 | 114.95      | 124.28   |
| 3   | M     | 760 | HDD  | CHC-C1C-NC  | -6.73 | 111.66      | 123.86   |
| 3   | H     | 760 | HDD  | CHA-C1A-NA  | -6.58 | 111.93      | 123.86   |
| 3   | F     | 760 | HDD  | CHD-C1D-ND  | -6.56 | 115.23      | 124.28   |
| 3   | M     | 760 | HDD  | O1D-CGD-O2D | 6.52  | 126.30      | 120.81   |
| 3   | H     | 760 | HDD  | CHD-C1D-ND  | -6.51 | 115.30      | 124.28   |
| 3   | E     | 760 | HDD  | O1D-CGD-O2D | 6.19  | 126.02      | 120.81   |
| 3   | G     | 760 | HDD  | C3C-C2C-C1C | -6.13 | 99.94       | 107.17   |
| 3   | O     | 760 | HDD  | O1D-CGD-O2D | 6.06  | 125.92      | 120.81   |
| 3   | O     | 760 | HDD  | C2A-C1A-NA  | 5.96  | 116.76      | 110.15   |
| 3   | N     | 760 | HDD  | CAA-CBA-CGA | -5.88 | 98.06       | 113.67   |
| 3   | H     | 760 | HDD  | CHC-C1C-NC  | -5.86 | 113.22      | 123.86   |
| 3   | G     | 760 | HDD  | CHD-C1D-ND  | -5.76 | 116.34      | 124.28   |
| 3   | O     | 760 | HDD  | CMC-C2C-C1C | 5.76  | 134.19      | 125.42   |
| 3   | G     | 760 | HDD  | CHD-C4C-NC  | -5.69 | 113.54      | 123.86   |
| 3   | M     | 760 | HDD  | C3C-C2C-C1C | -5.66 | 100.50      | 107.17   |
| 3   | H     | 760 | HDD  | O1D-CGD-O2D | 5.65  | 125.57      | 120.81   |
| 3   | H     | 760 | HDD  | C2A-C1A-NA  | 5.63  | 116.40      | 110.15   |
| 3   | E     | 760 | HDD  | CBD-CAD-C3D | 5.60  | 111.96      | 103.98   |
| 3   | F     | 760 | HDD  | C2A-C1A-NA  | 5.58  | 116.34      | 110.15   |
| 3   | F     | 760 | HDD  | CAA-CBA-CGA | -5.43 | 99.26       | 113.67   |
| 3   | P     | 760 | HDD  | C3C-C2C-C1C | -5.43 | 100.77      | 107.17   |
| 3   | H     | 760 | HDD  | C3C-C2C-C1C | -5.43 | 100.77      | 107.17   |
| 3   | P     | 760 | HDD  | CHD-C4C-NC  | -5.41 | 114.04      | 123.86   |
| 3   | P     | 760 | HDD  | CMA-C3A-C2A | 5.40  | 137.08      | 125.62   |
| 3   | H     | 760 | HDD  | C2D-C1D-CHD | 5.37  | 132.62      | 124.27   |
| 3   | P     | 760 | HDD  | CHC-C4B-C3B | 5.35  | 134.23      | 125.21   |
| 3   | O     | 760 | HDD  | C3C-C2C-C1C | -5.33 | 100.88      | 107.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 760 | HDD  | CHC-C4B-C3B | 5.32  | 134.19      | 125.21   |
| 3   | P     | 760 | HDD  | OND-C2D-CMD | -5.27 | 99.26       | 109.45   |
| 3   | P     | 760 | HDD  | CHA-C1A-NA  | -5.17 | 114.49      | 123.86   |
| 3   | P     | 760 | HDD  | C3B-C2B-C1B | -5.16 | 102.17      | 107.05   |
| 3   | G     | 760 | HDD  | C2A-C1A-NA  | 5.15  | 115.86      | 110.15   |
| 3   | F     | 760 | HDD  | CHC-C4B-C3B | 5.13  | 133.86      | 125.21   |
| 3   | P     | 760 | HDD  | CBD-CAD-C3D | 5.12  | 111.29      | 103.98   |
| 3   | N     | 760 | HDD  | C3B-C2B-C1B | -5.05 | 102.27      | 107.05   |
| 3   | F     | 760 | HDD  | C3C-C2C-C1C | -5.04 | 101.23      | 107.17   |
| 3   | P     | 760 | HDD  | C2D-C1D-CHD | 4.99  | 132.03      | 124.27   |
| 3   | E     | 760 | HDD  | OND-C2D-C3D | 4.96  | 122.08      | 110.46   |
| 3   | E     | 760 | HDD  | C3C-C4C-NC  | 4.95  | 113.97      | 109.80   |
| 3   | N     | 760 | HDD  | C2D-C1D-CHD | 4.93  | 131.94      | 124.27   |
| 3   | F     | 760 | HDD  | CAA-C2A-C1A | 4.88  | 134.46      | 124.94   |
| 3   | H     | 760 | HDD  | CHC-C4B-C3B | 4.87  | 133.42      | 125.21   |
| 3   | E     | 760 | HDD  | C2D-C1D-CHD | 4.84  | 131.79      | 124.27   |
| 3   | F     | 760 | HDD  | CMC-C2C-C1C | 4.77  | 132.68      | 125.42   |
| 3   | M     | 760 | HDD  | C2A-C1A-NA  | 4.75  | 115.42      | 110.15   |
| 3   | O     | 760 | HDD  | CHC-C4B-C3B | 4.73  | 133.18      | 125.21   |
| 3   | G     | 760 | HDD  | CHC-C4B-C3B | 4.71  | 133.15      | 125.21   |
| 3   | M     | 760 | HDD  | CAB-C3B-C4B | 4.69  | 136.01      | 124.82   |
| 3   | O     | 760 | HDD  | CBD-CAD-C3D | 4.67  | 110.63      | 103.98   |
| 3   | E     | 760 | HDD  | CMC-C2C-C1C | 4.64  | 132.48      | 125.42   |
| 3   | F     | 760 | HDD  | O1D-CGD-O2D | 4.57  | 124.66      | 120.81   |
| 3   | E     | 760 | HDD  | CMD-C2D-C3D | -4.48 | 103.33      | 115.11   |
| 3   | E     | 760 | HDD  | CAA-C2A-C1A | 4.48  | 133.69      | 124.94   |
| 3   | N     | 760 | HDD  | CHA-C1A-C2A | 4.48  | 135.10      | 125.30   |
| 3   | F     | 760 | HDD  | C2D-C1D-CHD | 4.45  | 131.19      | 124.27   |
| 3   | F     | 760 | HDD  | CBD-CAD-C3D | 4.37  | 110.21      | 103.98   |
| 3   | H     | 760 | HDD  | C3B-C2B-C1B | -4.34 | 102.94      | 107.05   |
| 3   | E     | 760 | HDD  | C3D-O1D-CGD | 4.31  | 115.16      | 111.14   |
| 3   | M     | 760 | HDD  | C2D-C1D-CHD | 4.25  | 130.88      | 124.27   |
| 3   | P     | 760 | HDD  | C2A-C1A-NA  | 4.22  | 114.83      | 110.15   |
| 3   | F     | 760 | HDD  | CBA-CAA-C2A | 4.19  | 124.12      | 112.53   |
| 3   | H     | 760 | HDD  | CAA-CBA-CGA | -4.18 | 102.57      | 113.67   |
| 3   | N     | 760 | HDD  | O1D-CGD-O2D | 4.15  | 124.31      | 120.81   |
| 3   | E     | 760 | HDD  | C4B-C3B-C2B | -4.12 | 103.24      | 106.81   |
| 3   | F     | 760 | HDD  | C4B-C3B-C2B | -4.12 | 103.24      | 106.81   |
| 3   | O     | 760 | HDD  | C3C-C4C-NC  | 4.06  | 113.22      | 109.80   |
| 3   | M     | 760 | HDD  | CHA-C1A-C2A | 4.06  | 134.19      | 125.30   |
| 3   | O     | 760 | HDD  | C3B-C2B-C1B | -4.04 | 103.22      | 107.05   |
| 3   | G     | 760 | HDD  | C2D-C1D-CHD | 4.04  | 130.55      | 124.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | O     | 760 | HDD  | CHA-C1A-C2A | 4.04  | 134.13      | 125.30   |
| 3   | N     | 760 | HDD  | CAA-C2A-C1A | 4.02  | 132.79      | 124.94   |
| 3   | N     | 760 | HDD  | C2A-C1A-NA  | 3.99  | 114.58      | 110.15   |
| 3   | O     | 760 | HDD  | CAA-C2A-C1A | 3.98  | 132.72      | 124.94   |
| 3   | P     | 760 | HDD  | CAB-C3B-C4B | 3.97  | 134.31      | 124.82   |
| 3   | P     | 760 | HDD  | CHC-C1C-C2C | 3.96  | 138.92      | 127.43   |
| 3   | M     | 760 | HDD  | CMC-C2C-C1C | 3.95  | 131.44      | 125.42   |
| 3   | H     | 760 | HDD  | C4A-C3A-C2A | -3.94 | 102.31      | 106.82   |
| 3   | G     | 760 | HDD  | CBD-CAD-C3D | 3.94  | 109.59      | 103.98   |
| 3   | E     | 760 | HDD  | CAA-CBA-CGA | -3.93 | 103.24      | 113.67   |
| 3   | G     | 760 | HDD  | CMC-C2C-C1C | 3.93  | 131.40      | 125.42   |
| 3   | H     | 760 | HDD  | CMA-C3A-C4A | 3.87  | 131.32      | 125.42   |
| 3   | F     | 760 | HDD  | CHA-C1A-C2A | 3.85  | 133.72      | 125.30   |
| 3   | N     | 760 | HDD  | CBD-CAD-C3D | 3.83  | 109.44      | 103.98   |
| 3   | O     | 760 | HDD  | C2D-C1D-CHD | 3.81  | 130.19      | 124.27   |
| 3   | G     | 760 | HDD  | CHA-C1A-C2A | 3.79  | 133.59      | 125.30   |
| 3   | F     | 760 | HDD  | CHB-C1B-NB  | 3.79  | 128.58      | 124.45   |
| 3   | P     | 760 | HDD  | C4A-C3A-C2A | -3.78 | 102.49      | 106.82   |
| 3   | E     | 760 | HDD  | C1A-C2A-C3A | -3.73 | 101.10      | 106.87   |
| 3   | N     | 760 | HDD  | C2C-C1C-NC  | 3.68  | 116.03      | 110.14   |
| 3   | M     | 760 | HDD  | C4B-C3B-C2B | -3.63 | 103.67      | 106.81   |
| 3   | H     | 760 | HDD  | CBD-CAD-C3D | 3.60  | 109.12      | 103.98   |
| 3   | G     | 760 | HDD  | CBC-CAC-C3C | -3.60 | 109.56      | 127.53   |
| 3   | P     | 760 | HDD  | C3C-C4C-NC  | 3.58  | 112.82      | 109.80   |
| 3   | P     | 760 | HDD  | CAA-CBA-CGA | -3.51 | 104.35      | 113.67   |
| 3   | E     | 760 | HDD  | CMA-C3A-C4A | 3.48  | 130.72      | 125.42   |
| 3   | O     | 760 | HDD  | C1A-C2A-C3A | -3.48 | 101.49      | 106.87   |
| 3   | M     | 760 | HDD  | CBD-CAD-C3D | 3.47  | 108.93      | 103.98   |
| 3   | F     | 760 | HDD  | C1A-C2A-C3A | -3.46 | 101.51      | 106.87   |
| 3   | E     | 760 | HDD  | C3B-C2B-C1B | -3.46 | 103.77      | 107.05   |
| 3   | G     | 760 | HDD  | C4A-C3A-C2A | -3.38 | 102.95      | 106.82   |
| 3   | F     | 760 | HDD  | CAB-C3B-C4B | 3.34  | 132.79      | 124.82   |
| 3   | M     | 760 | HDD  | CAA-C2A-C1A | 3.30  | 131.39      | 124.94   |
| 3   | G     | 760 | HDD  | CMD-C2D-C1D | 3.30  | 118.27      | 112.68   |
| 3   | E     | 760 | HDD  | C3D-C4D-CHA | 3.29  | 133.70      | 124.14   |
| 3   | M     | 760 | HDD  | C3B-C2B-C1B | -3.29 | 103.93      | 107.05   |
| 3   | P     | 760 | HDD  | CMA-C3A-C4A | -3.28 | 120.42      | 125.42   |
| 3   | G     | 760 | HDD  | C4B-C3B-C2B | -3.27 | 103.98      | 106.81   |
| 3   | N     | 760 | HDD  | C4B-C3B-C2B | -3.26 | 103.99      | 106.81   |
| 3   | O     | 760 | HDD  | C3D-C4D-CHA | 3.25  | 133.58      | 124.14   |
| 3   | M     | 760 | HDD  | C3D-C4D-CHA | 3.22  | 133.47      | 124.14   |
| 3   | E     | 760 | HDD  | C2C-C1C-NC  | 3.16  | 115.21      | 110.14   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | E     | 760 | HDD  | CMD-C2D-C1D | -3.12 | 107.41      | 112.68   |
| 3   | O     | 760 | HDD  | CHC-C1C-C2C | 3.09  | 136.41      | 127.43   |
| 3   | E     | 760 | HDD  | CHC-C4B-C3B | 3.09  | 130.42      | 125.21   |
| 3   | E     | 760 | HDD  | CHA-C1A-C2A | 3.07  | 132.01      | 125.30   |
| 3   | P     | 760 | HDD  | CMB-C2B-C1B | 3.03  | 130.06      | 124.73   |
| 3   | N     | 760 | HDD  | C3D-C4D-CHA | 3.02  | 132.89      | 124.14   |
| 3   | G     | 760 | HDD  | O1D-CGD-O2D | 3.01  | 123.35      | 120.81   |
| 3   | G     | 760 | HDD  | C3D-C4D-CHA | 3.00  | 132.84      | 124.14   |
| 3   | N     | 760 | HDD  | CHD-C4C-C3C | 2.98  | 140.29      | 127.37   |
| 3   | N     | 760 | HDD  | C4A-C3A-C2A | -2.97 | 103.41      | 106.82   |
| 3   | P     | 760 | HDD  | C3D-C4D-CHA | 2.96  | 132.73      | 124.14   |
| 3   | H     | 760 | HDD  | CBA-CAA-C2A | -2.95 | 104.39      | 112.53   |
| 3   | F     | 760 | HDD  | CHB-C1B-C2B | -2.95 | 119.36      | 125.49   |
| 3   | F     | 760 | HDD  | CHC-C1C-C2C | 2.94  | 135.96      | 127.43   |
| 3   | M     | 760 | HDD  | CMB-C2B-C1B | 2.94  | 129.90      | 124.73   |
| 3   | G     | 760 | HDD  | C3B-C2B-C1B | -2.91 | 104.29      | 107.05   |
| 3   | H     | 760 | HDD  | CHA-C1A-C2A | 2.91  | 131.66      | 125.30   |
| 3   | P     | 760 | HDD  | CMD-C2D-C1D | 2.89  | 117.57      | 112.68   |
| 3   | E     | 760 | HDD  | CHC-C1C-C2C | 2.88  | 135.78      | 127.43   |
| 3   | P     | 760 | HDD  | CBA-CAA-C2A | -2.87 | 104.58      | 112.53   |
| 3   | G     | 760 | HDD  | CMA-C3A-C2A | 2.86  | 131.68      | 125.62   |
| 3   | N     | 760 | HDD  | CMC-C2C-C1C | 2.85  | 129.77      | 125.42   |
| 3   | H     | 760 | HDD  | CMC-C2C-C3C | 2.85  | 133.25      | 126.55   |
| 3   | M     | 760 | HDD  | C1A-C2A-C3A | -2.84 | 102.48      | 106.87   |
| 3   | F     | 760 | HDD  | C3D-C4D-CHA | 2.83  | 132.35      | 124.14   |
| 3   | G     | 760 | HDD  | C1A-C2A-C3A | -2.83 | 102.49      | 106.87   |
| 3   | N     | 760 | HDD  | CHC-C4B-C3B | 2.83  | 129.98      | 125.21   |
| 3   | G     | 760 | HDD  | CHC-C1C-C2C | 2.78  | 135.50      | 127.43   |
| 3   | H     | 760 | HDD  | CAA-C2A-C1A | 2.76  | 130.33      | 124.94   |
| 3   | P     | 760 | HDD  | CAB-C3B-C2B | -2.74 | 119.53      | 128.43   |
| 3   | F     | 760 | HDD  | C2C-C1C-NC  | 2.71  | 114.49      | 110.14   |
| 3   | M     | 760 | HDD  | C4A-C3A-C2A | -2.71 | 103.72      | 106.82   |
| 3   | M     | 760 | HDD  | C3C-C4C-NC  | 2.68  | 112.06      | 109.80   |
| 3   | H     | 760 | HDD  | CHD-C4C-C3C | 2.66  | 138.93      | 127.37   |
| 3   | P     | 760 | HDD  | C1A-C2A-C3A | -2.66 | 102.76      | 106.87   |
| 3   | N     | 760 | HDD  | CBB-CAB-C3B | -2.65 | 114.26      | 127.53   |
| 3   | H     | 760 | HDD  | OND-C2D-C3D | -2.61 | 104.33      | 110.46   |
| 3   | F     | 760 | HDD  | CHD-C4C-C3C | 2.60  | 138.67      | 127.37   |
| 3   | H     | 760 | HDD  | CBB-CAB-C3B | -2.56 | 114.75      | 127.53   |
| 3   | N     | 760 | HDD  | CBC-CAC-C3C | -2.52 | 114.93      | 127.53   |
| 3   | E     | 760 | HDD  | CHD-C4C-C3C | 2.52  | 138.29      | 127.37   |
| 3   | N     | 760 | HDD  | CMD-C2D-C1D | -2.50 | 108.44      | 112.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | M     | 760 | HDD  | CAB-C3B-C2B | -2.50 | 120.29      | 128.43   |
| 3   | E     | 760 | HDD  | C4A-C3A-C2A | -2.50 | 103.95      | 106.82   |
| 3   | G     | 760 | HDD  | CAA-CBA-CGA | -2.48 | 107.09      | 113.67   |
| 3   | F     | 760 | HDD  | C3B-C2B-C1B | -2.48 | 104.70      | 107.05   |
| 3   | H     | 760 | HDD  | C4C-NC-C1C  | 2.47  | 109.85      | 105.82   |
| 3   | P     | 760 | HDD  | CHA-C1A-C2A | 2.45  | 130.65      | 125.30   |
| 3   | M     | 760 | HDD  | C2C-C1C-NC  | 2.44  | 114.06      | 110.14   |
| 3   | N     | 760 | HDD  | C1A-C2A-C3A | -2.44 | 103.09      | 106.87   |
| 3   | M     | 760 | HDD  | O1A-CGA-CBA | -2.43 | 115.39      | 123.09   |
| 3   | P     | 760 | HDD  | O1A-CGA-CBA | -2.42 | 115.42      | 123.09   |
| 3   | F     | 760 | HDD  | C4A-C3A-C2A | -2.40 | 104.06      | 106.82   |
| 3   | H     | 760 | HDD  | C3D-C4D-CHA | 2.39  | 131.07      | 124.14   |
| 3   | P     | 760 | HDD  | C4A-NA-C1A  | 2.39  | 109.72      | 105.82   |
| 3   | P     | 760 | HDD  | C2B-C1B-NB  | 2.36  | 114.01      | 109.64   |
| 3   | M     | 760 | HDD  | CHC-C1C-C2C | 2.36  | 134.28      | 127.43   |
| 3   | O     | 760 | HDD  | C2C-C1C-NC  | 2.32  | 113.87      | 110.14   |
| 3   | P     | 760 | HDD  | O2A-CGA-O1A | 2.32  | 129.30      | 123.33   |
| 3   | O     | 760 | HDD  | CMB-C2B-C1B | 2.31  | 128.79      | 124.73   |
| 3   | H     | 760 | HDD  | C2C-C1C-NC  | 2.30  | 113.82      | 110.14   |
| 3   | P     | 760 | HDD  | CAA-C2A-C3A | 2.29  | 132.22      | 127.07   |
| 3   | O     | 760 | HDD  | C4A-C3A-C2A | -2.29 | 104.19      | 106.82   |
| 3   | E     | 760 | HDD  | CMB-C2B-C1B | 2.29  | 128.76      | 124.73   |
| 3   | P     | 760 | HDD  | CHB-C4A-NA  | 2.29  | 128.01      | 123.86   |
| 3   | E     | 760 | HDD  | CBC-CAC-C3C | -2.27 | 116.17      | 127.53   |
| 3   | N     | 760 | HDD  | CMC-C2C-C3C | 2.27  | 131.88      | 126.55   |
| 3   | E     | 760 | HDD  | OND-C2D-CMD | 2.26  | 113.83      | 109.45   |
| 3   | F     | 760 | HDD  | CMD-C2D-C3D | -2.25 | 109.21      | 115.11   |
| 3   | O     | 760 | HDD  | CBB-CAB-C3B | -2.24 | 116.33      | 127.53   |
| 3   | M     | 760 | HDD  | CAA-CBA-CGA | -2.22 | 107.77      | 113.67   |
| 3   | G     | 760 | HDD  | CAB-C3B-C4B | 2.21  | 130.11      | 124.82   |
| 3   | O     | 760 | HDD  | O2A-CGA-CBA | 2.21  | 120.99      | 114.00   |
| 3   | O     | 760 | HDD  | CHD-C4C-C3C | 2.20  | 136.91      | 127.37   |
| 3   | H     | 760 | HDD  | O1A-CGA-CBA | -2.19 | 116.16      | 123.09   |
| 3   | O     | 760 | HDD  | CAB-C3B-C4B | 2.17  | 130.01      | 124.82   |
| 3   | G     | 760 | HDD  | CAA-C2A-C1A | 2.16  | 129.16      | 124.94   |
| 3   | M     | 760 | HDD  | CHD-C4C-C3C | 2.14  | 136.66      | 127.37   |
| 3   | F     | 760 | HDD  | O1A-CGA-CBA | -2.14 | 116.31      | 123.09   |
| 3   | H     | 760 | HDD  | C1A-C2A-C3A | -2.13 | 103.58      | 106.87   |
| 3   | O     | 760 | HDD  | CMA-C3A-C4A | 2.12  | 128.65      | 125.42   |
| 3   | P     | 760 | HDD  | OND-C2D-C3D | 2.11  | 115.41      | 110.46   |
| 3   | N     | 760 | HDD  | C2B-C1B-NB  | 2.06  | 113.45      | 109.64   |
| 3   | N     | 760 | HDD  | CMA-C3A-C2A | 2.06  | 129.99      | 125.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | N     | 760 | HDD  | O1A-CGA-CBA | -2.06 | 116.57      | 123.09   |
| 3   | N     | 760 | HDD  | O1D-CGD-CBD | 2.05  | 112.05      | 110.17   |
| 3   | O     | 760 | HDD  | C4C-C3C-C2C | -2.05 | 104.75      | 107.30   |
| 3   | F     | 760 | HDD  | CBB-CAB-C3B | -2.04 | 117.33      | 127.53   |
| 3   | O     | 760 | HDD  | C3D-O1D-CGD | 2.04  | 113.04      | 111.14   |
| 3   | H     | 760 | HDD  | C4B-C3B-C2B | -2.02 | 105.06      | 106.81   |

There are no chirality outliers.

All (32) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 760 | HDD  | C2C-C3C-CAC-CBC |
| 3   | G     | 760 | HDD  | C4C-C3C-CAC-CBC |
| 3   | H     | 760 | HDD  | C2B-C3B-CAB-CBB |
| 3   | O     | 760 | HDD  | C2B-C3B-CAB-CBB |
| 3   | O     | 760 | HDD  | C4B-C3B-CAB-CBB |
| 3   | P     | 760 | HDD  | C3A-C2A-CAA-CBA |
| 3   | O     | 760 | HDD  | C4C-C3C-CAC-CBC |
| 3   | O     | 760 | HDD  | C2C-C3C-CAC-CBC |
| 3   | H     | 760 | HDD  | C4B-C3B-CAB-CBB |
| 3   | F     | 760 | HDD  | C2A-CAA-CBA-CGA |
| 3   | P     | 760 | HDD  | C1A-C2A-CAA-CBA |
| 3   | F     | 760 | HDD  | C2B-C3B-CAB-CBB |
| 3   | O     | 760 | HDD  | C3A-C2A-CAA-CBA |
| 3   | F     | 760 | HDD  | C4B-C3B-CAB-CBB |
| 3   | P     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | H     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | H     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | O     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | P     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | O     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | F     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | N     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | G     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | E     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | G     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | E     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | M     | 760 | HDD  | CAA-CBA-CGA-O2A |
| 3   | M     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | N     | 760 | HDD  | CAA-CBA-CGA-O1A |
| 3   | O     | 760 | HDD  | C1A-C2A-CAA-CBA |
| 3   | F     | 760 | HDD  | CAA-CBA-CGA-O2A |

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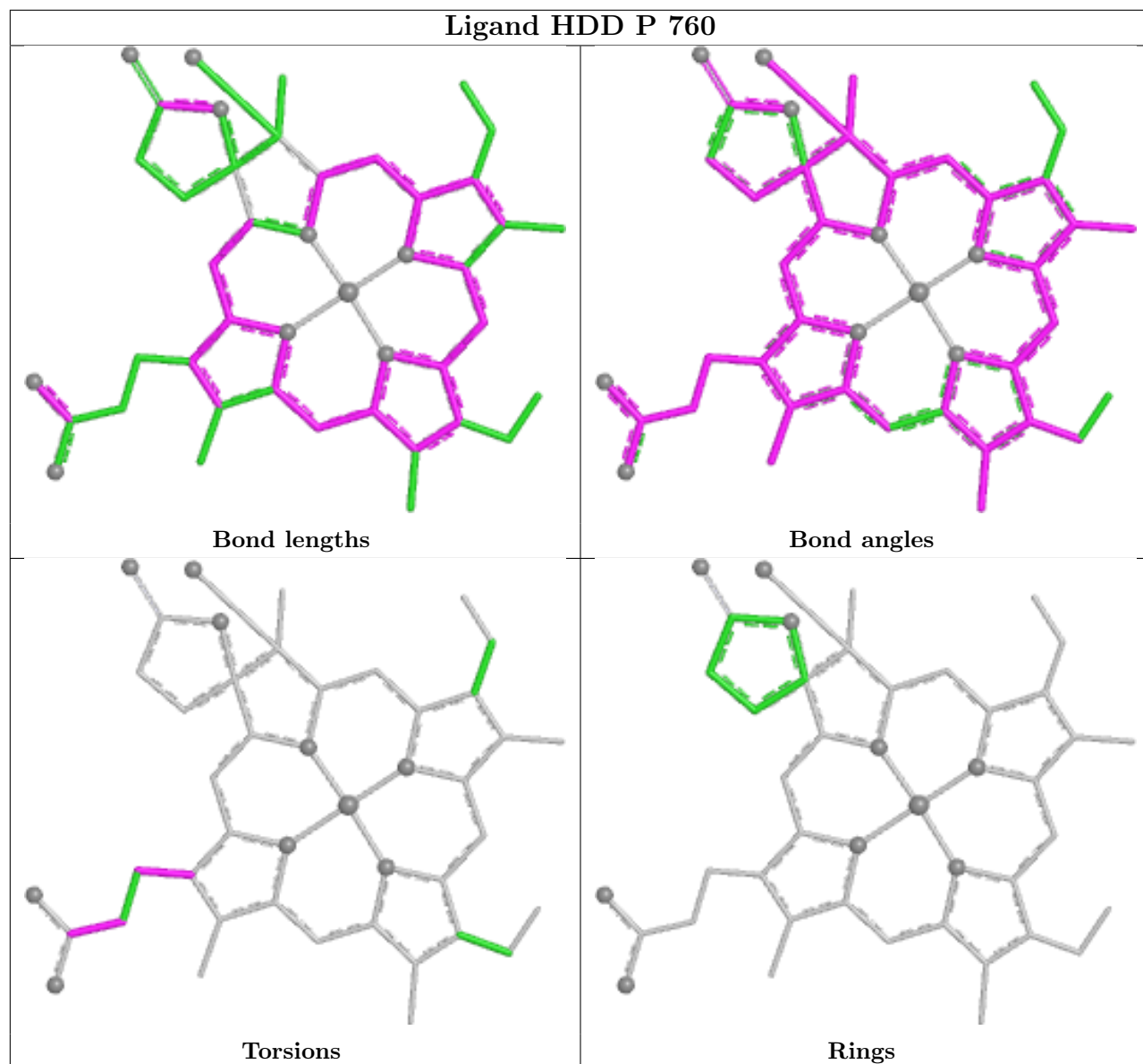
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 760 | HDD  | C2B-C3B-CAB-CBB |

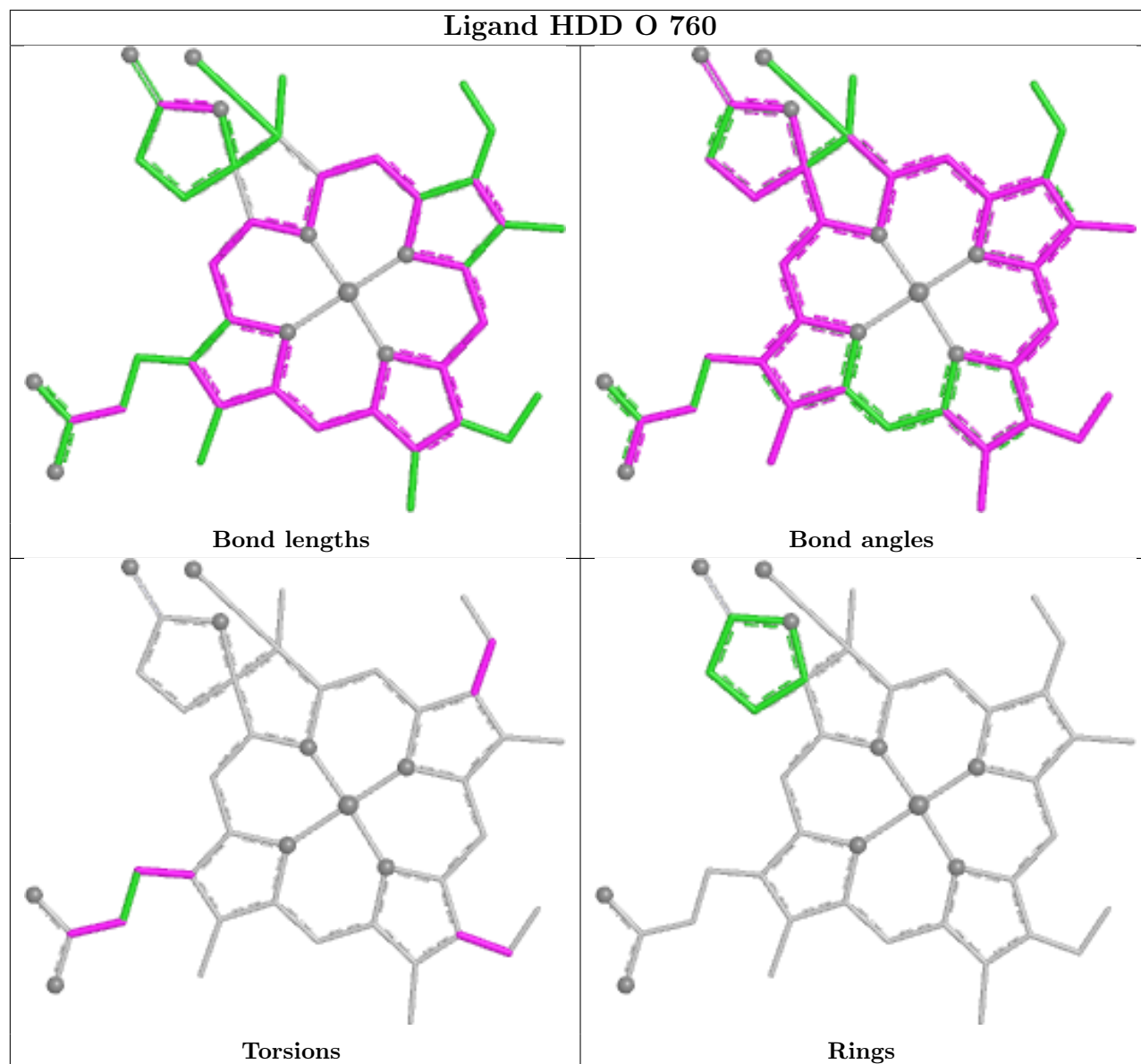
There are no ring outliers.

8 monomers are involved in 111 short contacts:

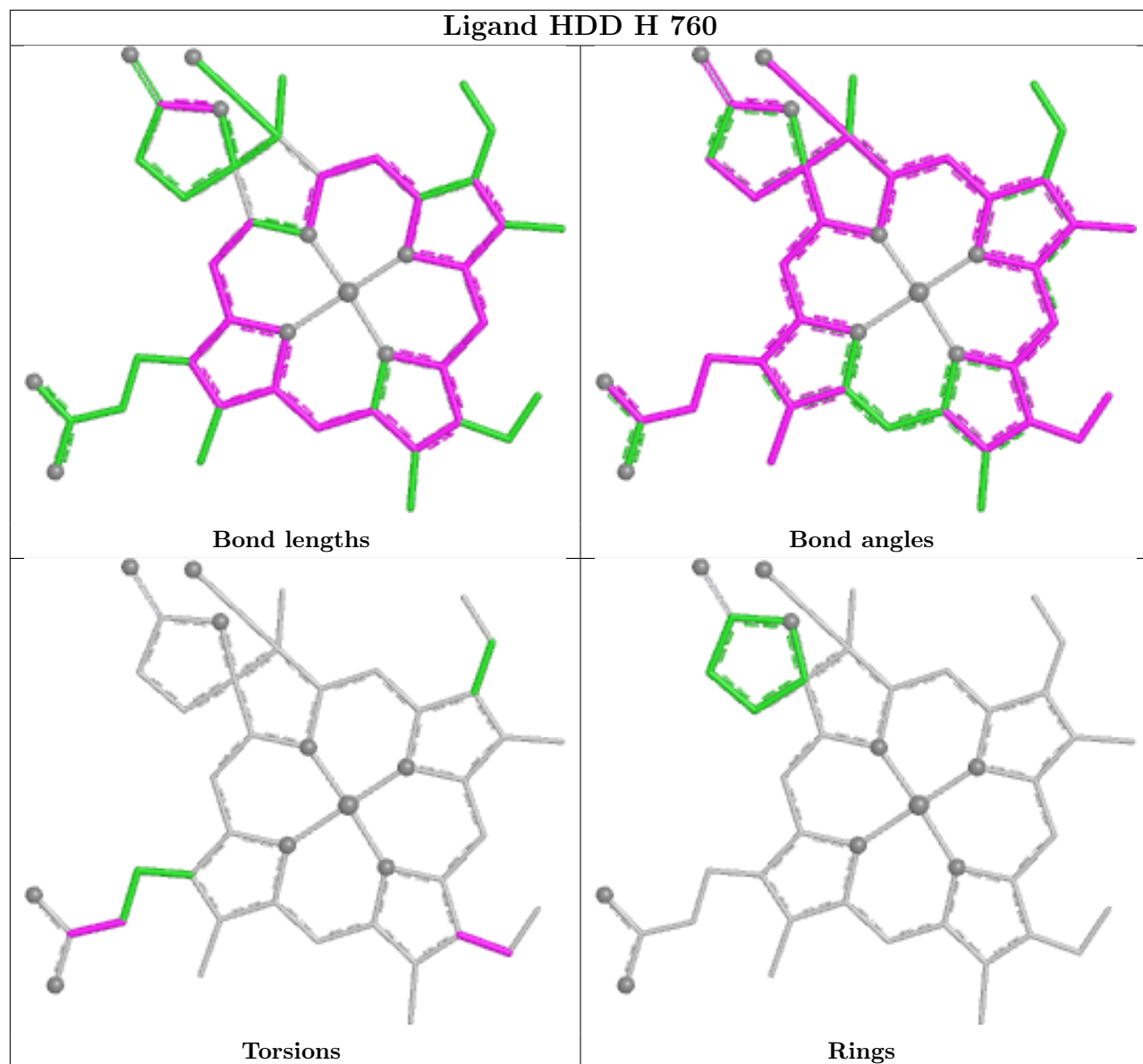
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | P     | 760 | HDD  | 9       | 0            |
| 3   | O     | 760 | HDD  | 20      | 0            |
| 3   | H     | 760 | HDD  | 14      | 0            |
| 3   | E     | 760 | HDD  | 12      | 0            |
| 3   | M     | 760 | HDD  | 15      | 0            |
| 3   | F     | 760 | HDD  | 25      | 0            |
| 3   | N     | 760 | HDD  | 8       | 0            |
| 3   | G     | 760 | HDD  | 8       | 0            |

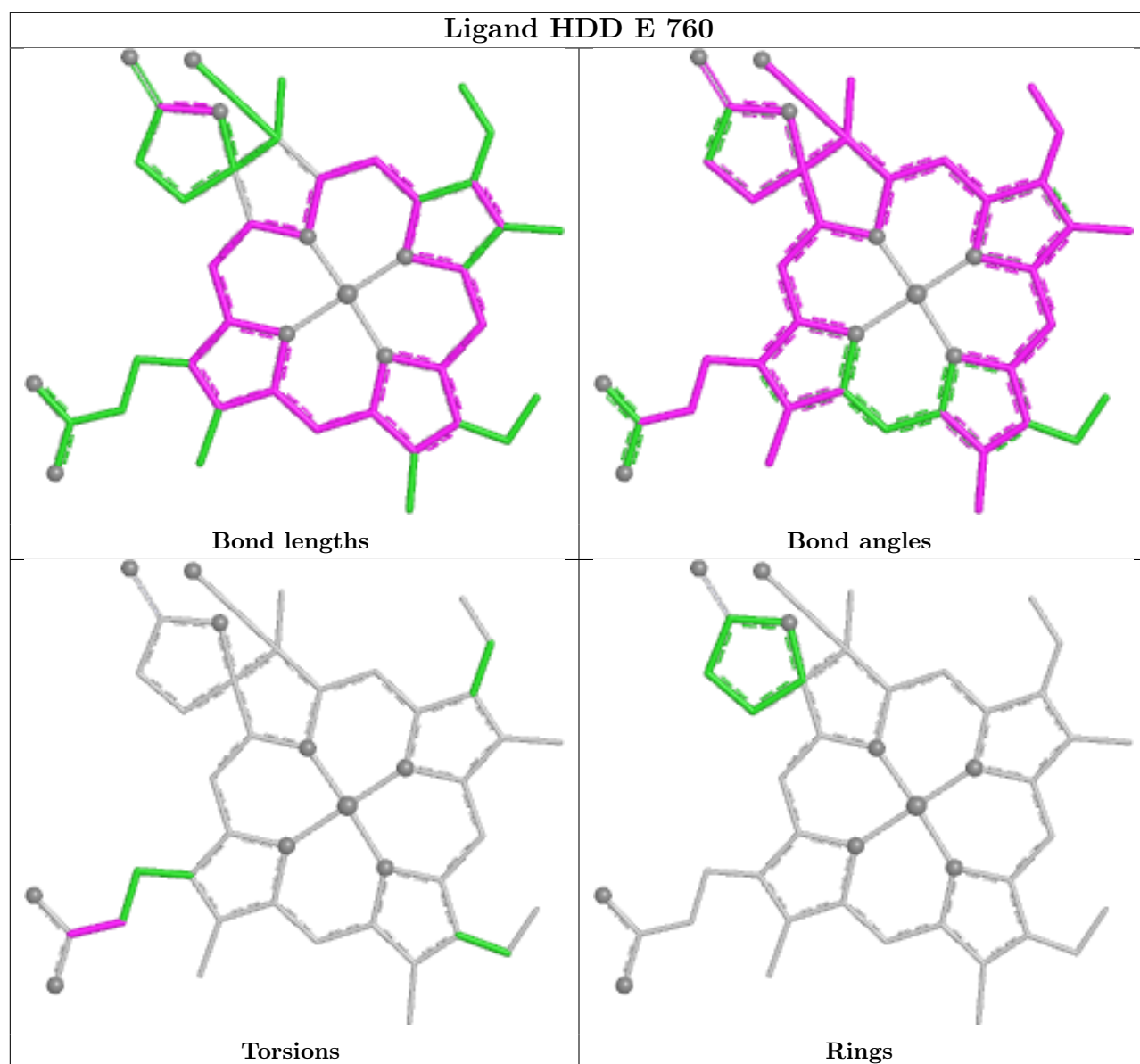
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

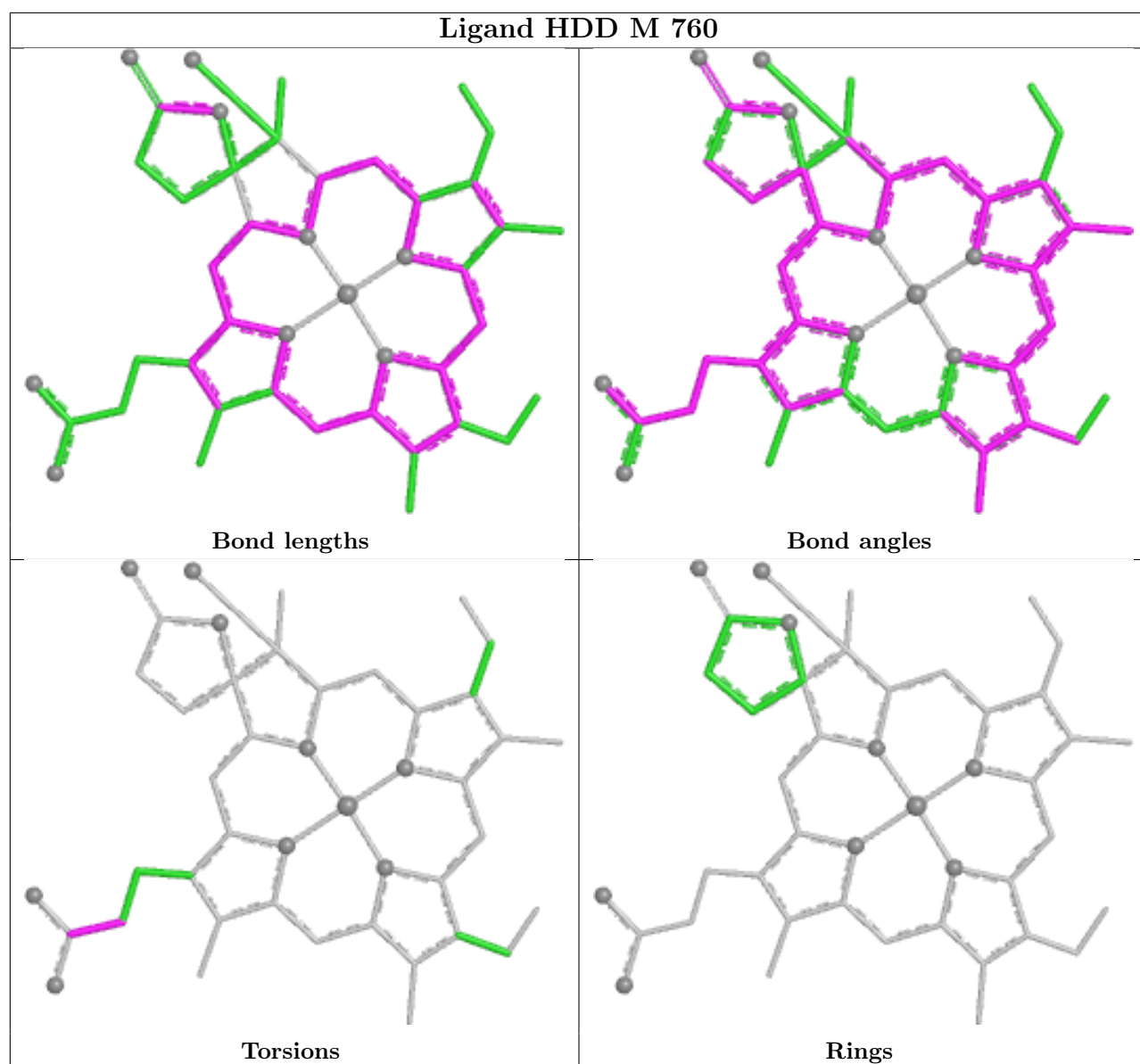


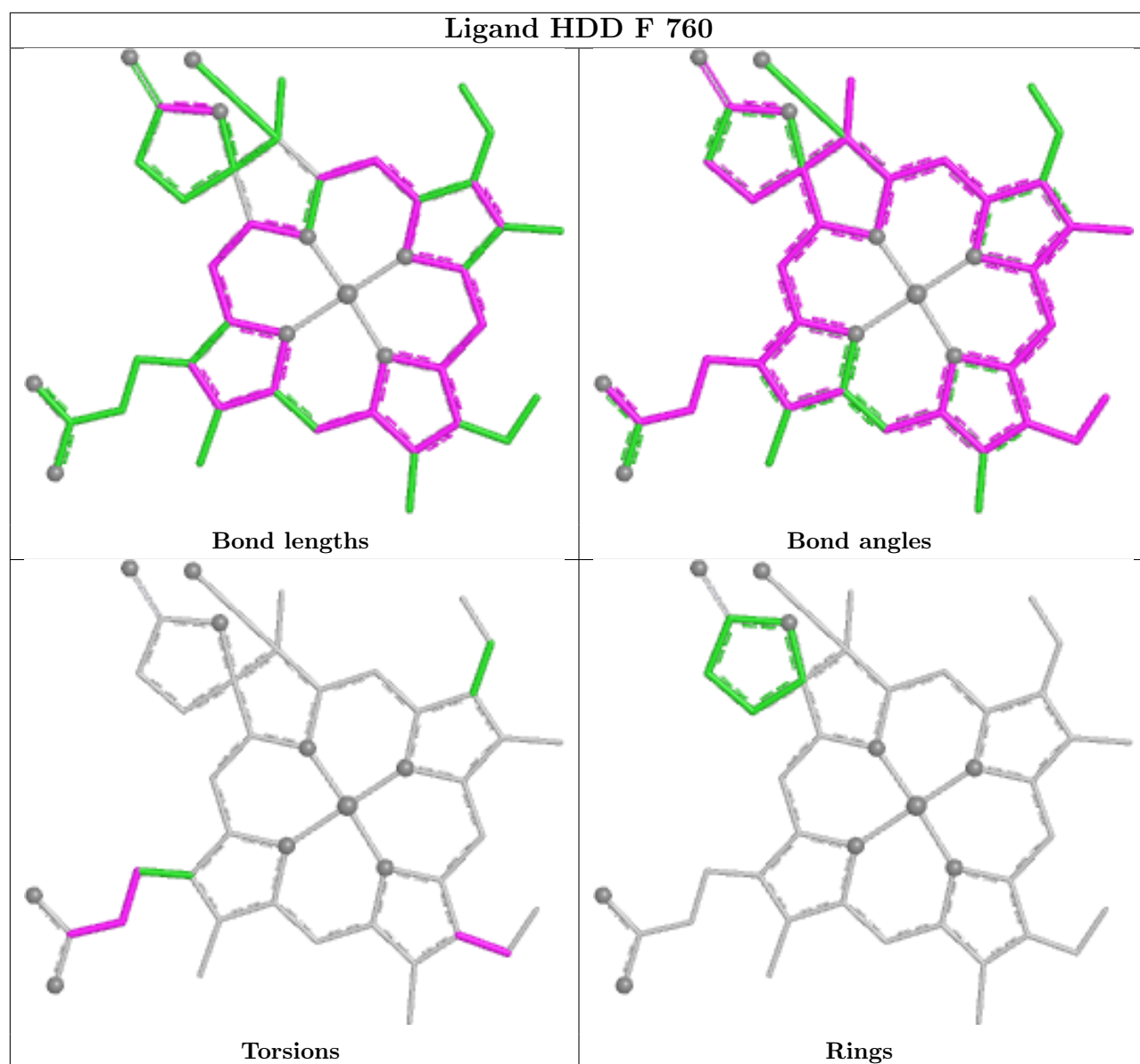


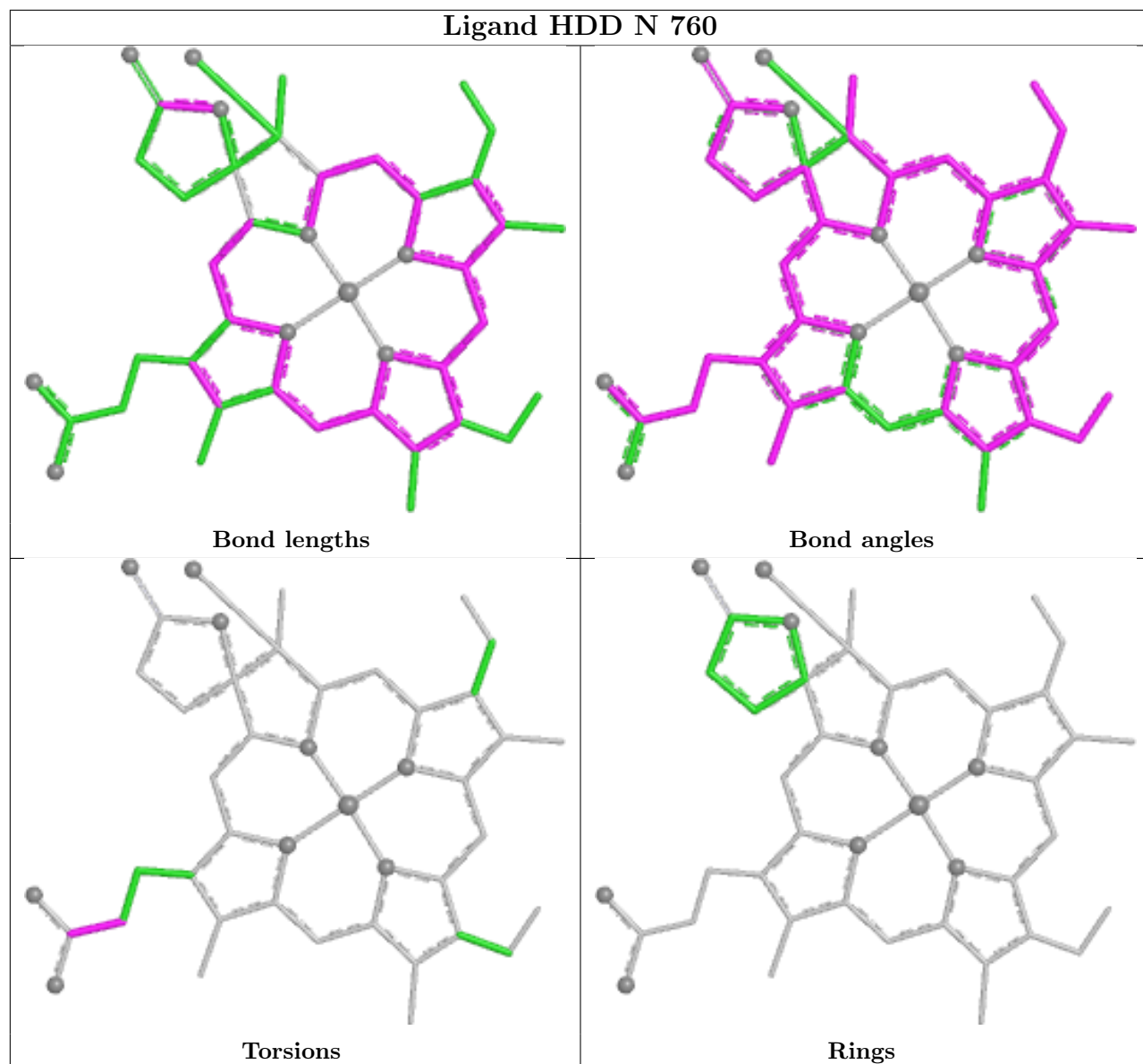


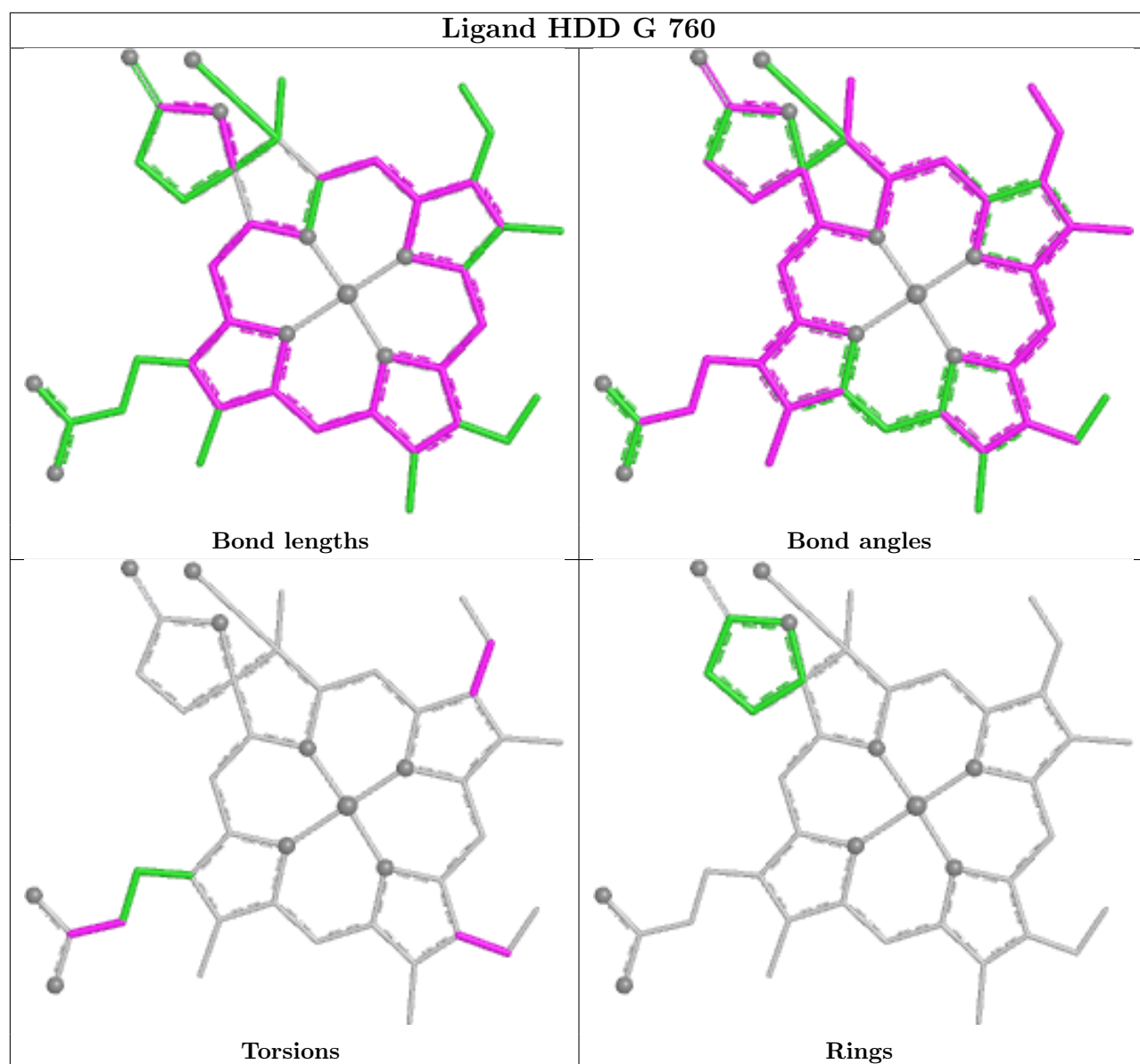












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 223/226 (98%)   | -0.14  | 1 (0%) 88 84  | 28, 40, 51, 80        | 0       |
| 1   | B     | 223/226 (98%)   | -0.27  | 0 100 100     | 26, 40, 51, 80        | 1 (0%)  |
| 1   | C     | 223/226 (98%)   | -0.21  | 3 (1%) 75 66  | 28, 40, 51, 80        | 1 (0%)  |
| 1   | D     | 223/226 (98%)   | -0.21  | 0 100 100     | 28, 40, 51, 80        | 1 (0%)  |
| 1   | I     | 223/226 (98%)   | -0.04  | 0 100 100     | 28, 41, 53, 80        | 0       |
| 1   | J     | 223/226 (98%)   | -0.18  | 2 (0%) 81 74  | 28, 41, 51, 80        | 0       |
| 1   | K     | 223/226 (98%)   | 0.07   | 3 (1%) 75 66  | 28, 41, 53, 80        | 0       |
| 1   | L     | 223/226 (98%)   | -0.17  | 2 (0%) 81 74  | 25, 40, 52, 80        | 1 (0%)  |
| 2   | E     | 256/259 (98%)   | -0.03  | 5 (1%) 65 56  | 14, 44, 61, 81        | 3 (1%)  |
| 2   | F     | 256/259 (98%)   | -0.08  | 4 (1%) 70 61  | 29, 45, 61, 81        | 0       |
| 2   | G     | 256/259 (98%)   | -0.05  | 1 (0%) 88 84  | 19, 45, 61, 81        | 2 (0%)  |
| 2   | H     | 256/259 (98%)   | -0.06  | 4 (1%) 70 61  | 19, 45, 61, 81        | 1 (0%)  |
| 2   | M     | 256/259 (98%)   | 0.07   | 4 (1%) 70 61  | 22, 45, 61, 81        | 1 (0%)  |
| 2   | N     | 256/259 (98%)   | -0.08  | 4 (1%) 70 61  | 20, 45, 61, 81        | 1 (0%)  |
| 2   | O     | 256/259 (98%)   | 0.15   | 5 (1%) 65 56  | 30, 46, 61, 81        | 0       |
| 2   | P     | 256/259 (98%)   | -0.00  | 4 (1%) 70 61  | 29, 45, 61, 81        | 0       |
| All | All   | 3832/3880 (98%) | -0.07  | 42 (1%) 78 70 | 14, 42, 59, 81        | 12 (0%) |

All (42) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 312 | GLY  | 4.2  |
| 1   | A     | 75  | SER  | 4.1  |
| 2   | E     | 311 | THR  | 4.1  |
| 2   | F     | 518 | PHE  | 4.0  |
| 1   | L     | 75  | SER  | 3.8  |

*Continued on next page...*

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 312 | GLY  | 3.7  |
| 2   | P     | 310 | LEU  | 3.6  |
| 2   | H     | 518 | PHE  | 3.4  |
| 2   | P     | 312 | GLY  | 3.3  |
| 2   | P     | 311 | THR  | 3.3  |
| 2   | H     | 312 | GLY  | 3.3  |
| 1   | K     | 75  | SER  | 3.3  |
| 2   | O     | 310 | LEU  | 3.2  |
| 2   | M     | 312 | GLY  | 3.2  |
| 1   | C     | 75  | SER  | 3.1  |
| 2   | F     | 310 | LEU  | 3.1  |
| 1   | C     | 297 | ALA  | 3.1  |
| 2   | F     | 311 | THR  | 3.0  |
| 2   | E     | 310 | LEU  | 3.0  |
| 2   | N     | 310 | LEU  | 2.9  |
| 2   | H     | 564 | ILE  | 2.7  |
| 2   | O     | 564 | ILE  | 2.7  |
| 1   | K     | 297 | ALA  | 2.7  |
| 1   | C     | 76  | GLU  | 2.7  |
| 2   | H     | 311 | THR  | 2.6  |
| 2   | O     | 518 | PHE  | 2.6  |
| 2   | M     | 309 | LYS  | 2.6  |
| 2   | M     | 310 | LEU  | 2.6  |
| 2   | E     | 309 | LYS  | 2.6  |
| 2   | P     | 518 | PHE  | 2.6  |
| 2   | E     | 312 | GLY  | 2.5  |
| 2   | N     | 502 | GLY  | 2.5  |
| 1   | L     | 76  | GLU  | 2.5  |
| 2   | M     | 311 | THR  | 2.5  |
| 2   | E     | 518 | PHE  | 2.4  |
| 1   | J     | 228 | ALA  | 2.4  |
| 1   | J     | 75  | SER  | 2.4  |
| 2   | O     | 311 | THR  | 2.4  |
| 1   | K     | 157 | ASN  | 2.1  |
| 2   | G     | 310 | LEU  | 2.1  |
| 2   | N     | 312 | GLY  | 2.1  |
| 2   | N     | 309 | LYS  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains

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



## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

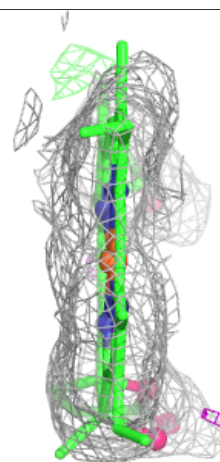
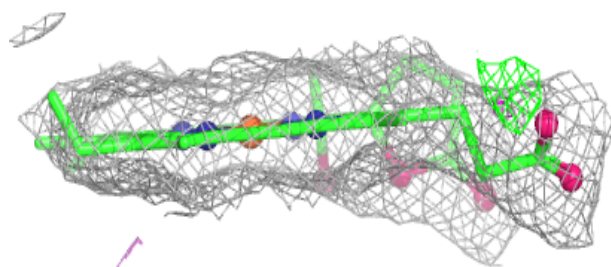
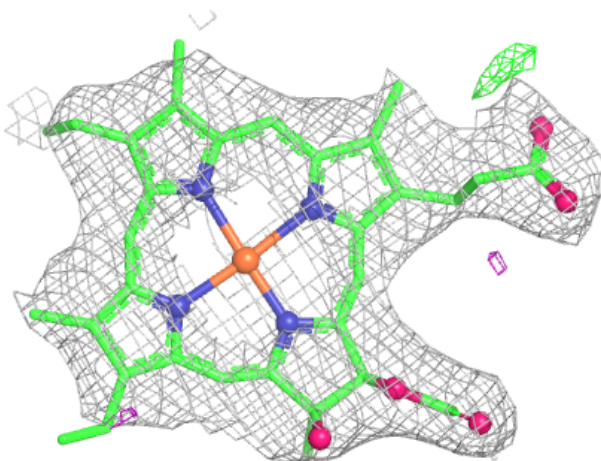
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HDD  | H     | 760 | 44/44 | 0.96 | 0.09 | 31,43,49,58                 | 0     |
| 3   | HDD  | M     | 760 | 44/44 | 0.96 | 0.10 | 24,52,64,66                 | 0     |
| 3   | HDD  | N     | 760 | 44/44 | 0.96 | 0.08 | 25,38,47,57                 | 0     |
| 3   | HDD  | O     | 760 | 44/44 | 0.96 | 0.09 | 32,53,62,63                 | 0     |
| 3   | HDD  | F     | 760 | 44/44 | 0.97 | 0.07 | 10,24,39,42                 | 0     |
| 3   | HDD  | G     | 760 | 44/44 | 0.97 | 0.08 | 24,35,48,55                 | 0     |
| 3   | HDD  | P     | 760 | 44/44 | 0.97 | 0.08 | 12,28,43,45                 | 0     |
| 3   | HDD  | E     | 760 | 44/44 | 0.98 | 0.07 | 10,23,34,42                 | 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.

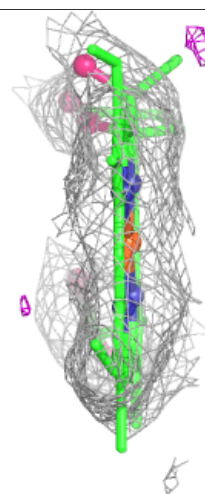
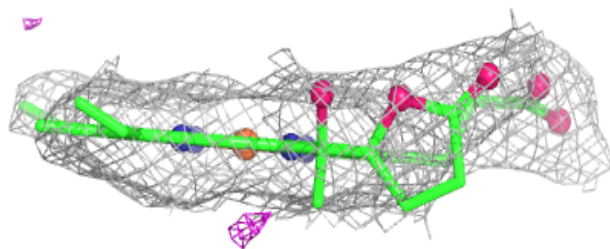
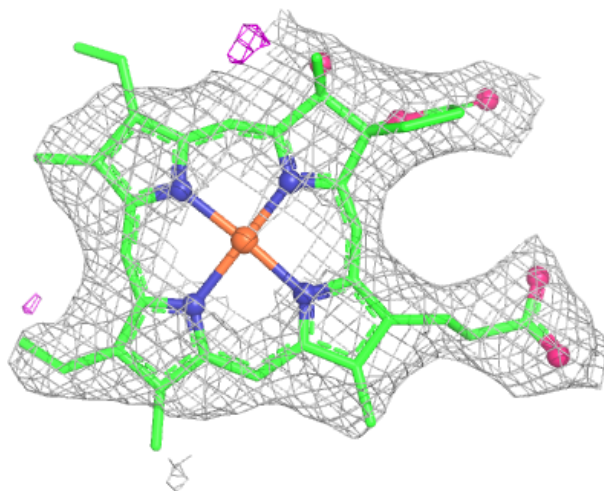
**Electron density around HDD H 760:**

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



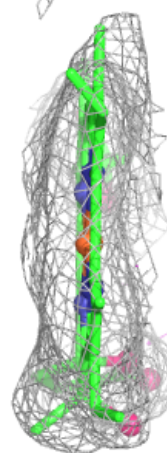
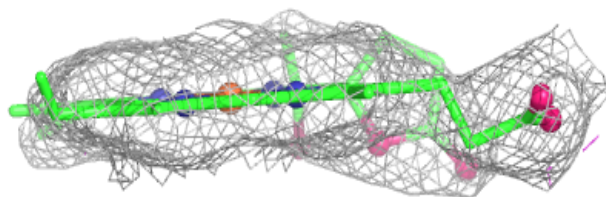
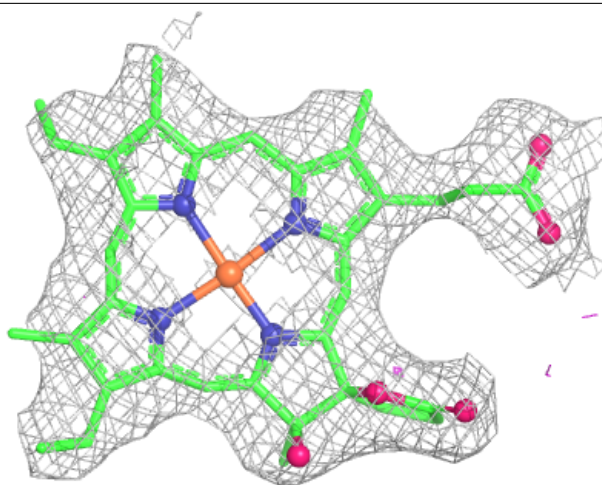
**Electron density around HDD M 760:**

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



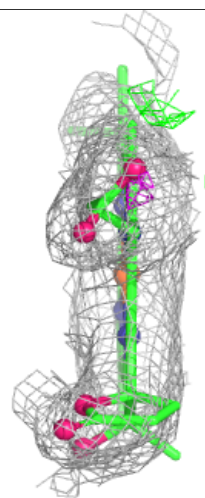
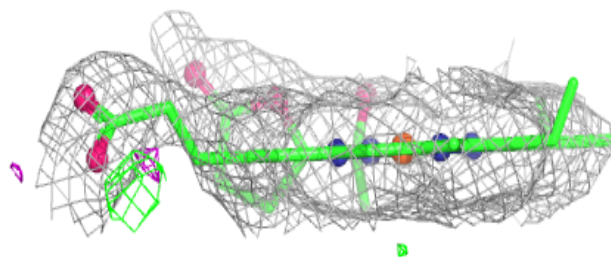
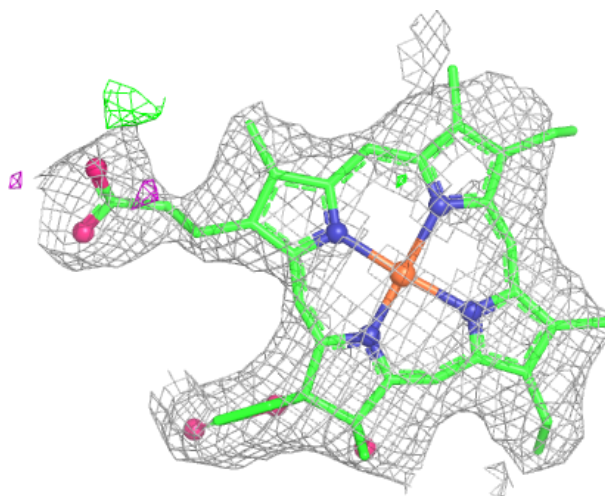
**Electron density around HDD N 760:**

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



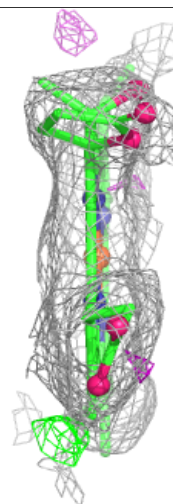
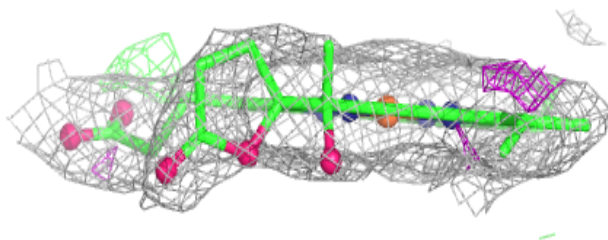
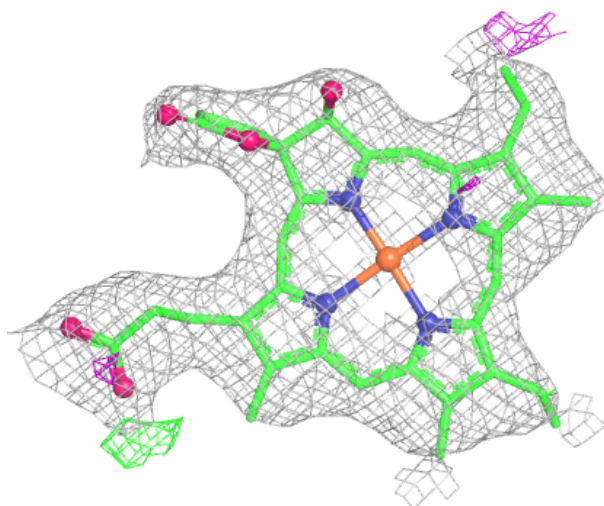
**Electron density around HDD O 760:**

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



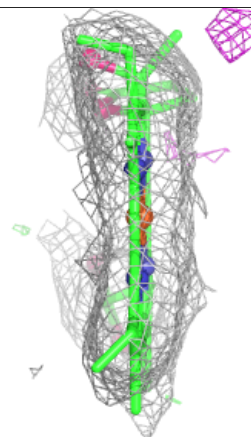
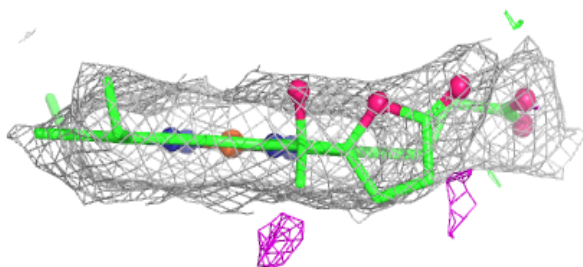
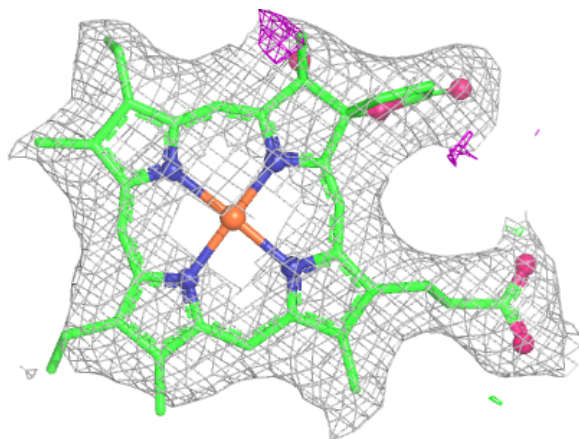
**Electron density around HDD F 760:**

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



**Electron density around HDD G 760:**

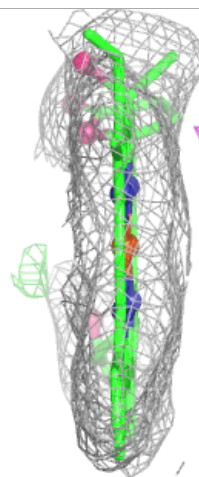
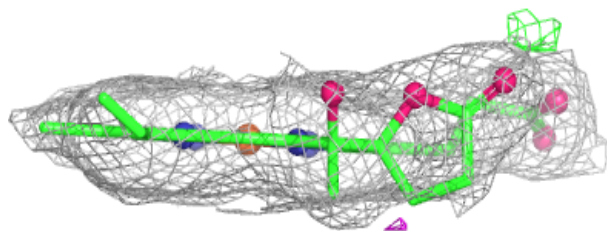
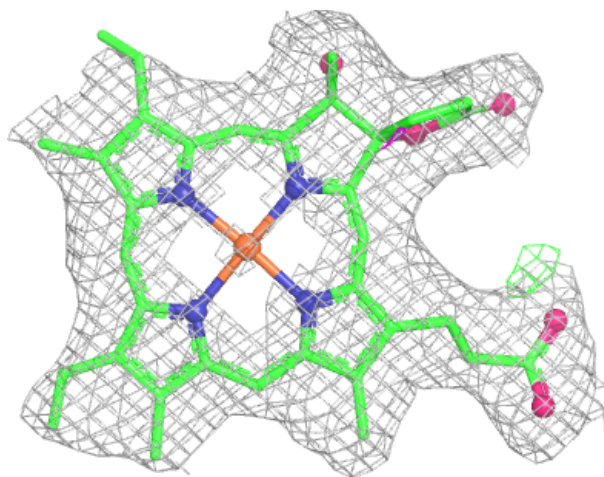
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



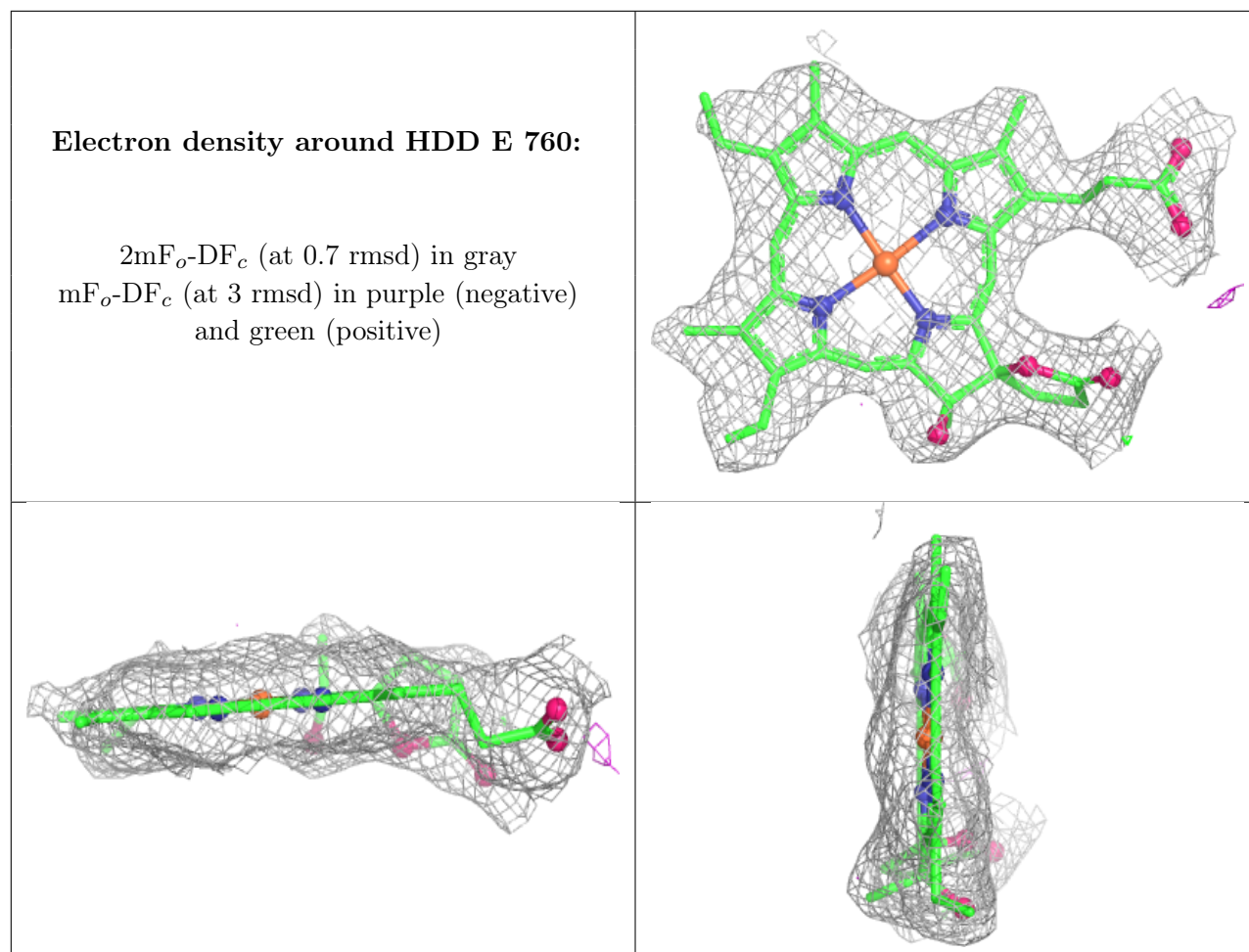


**Electron density around HDD P 760:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.