



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:02 AM EDT

PDB ID : 1KFY / pdb\_00001kfy  
Title : QUINOL-FUMARATE REDUCTASE WITH QUINOL INHIBITOR 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL  
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Deposited on : 2001-11-24  
Resolution : 3.60 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

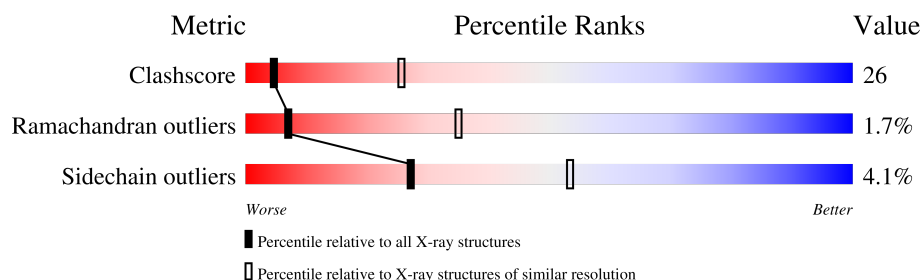
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |

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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 602    |                  |
| 1   | M     | 602    |                  |
| 2   | B     | 243    |                  |
| 2   | N     | 243    |                  |
| 3   | C     | 130    |                  |
| 3   | O     | 130    |                  |
| 4   | D     | 119    |                  |
| 4   | P     | 119    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 10  | BRS  | B     | 700 | -         | -        | X       | -                |
| 5   | OAA  | A     | 702 | -         | X        | -       | -                |
| 8   | F3S  | N     | 245 | -         | -        | X       | -                |
| 9   | SF4  | N     | 246 | -         | -        | X       | -                |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16957 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 FUMARATE REDUCTASE FLAVOPROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4448  | 2775 | 802 | 840 | 31 |         |         |       |
| 1   | M     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4448  | 2775 | 802 | 840 | 31 |         |         |       |

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1888  | 1189 | 323 | 357 | 19 |         |         |       |
| 2   | N     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1888  | 1189 | 323 | 357 | 19 |         |         |       |

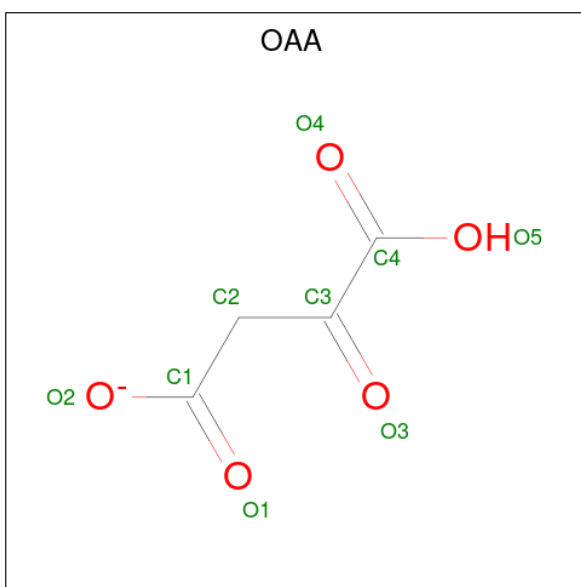
- Molecule 3 is a protein called FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 720 | 166 | 169 | 3 |         |         |       |
| 3   | O     | 130      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1058  | 720 | 166 | 169 | 3 |         |         |       |

- Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

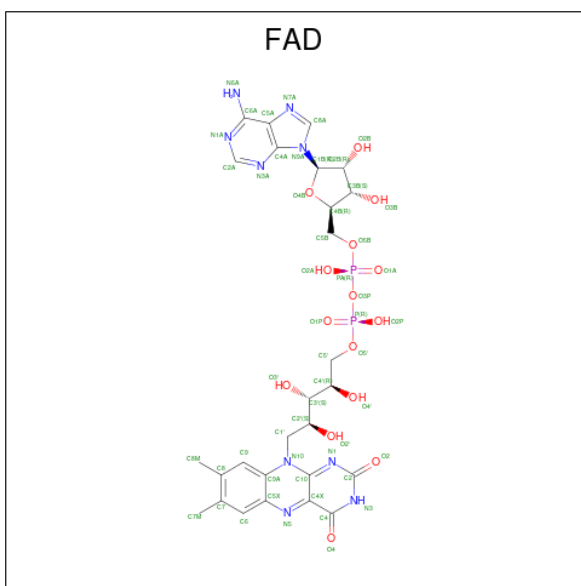
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 626 | 151 | 142 | 7 |         |         |       |
| 4   | P     | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 626 | 151 | 142 | 7 |         |         |       |

- Molecule 5 is OXALOACETATE ION (CCD ID: OAA) (formula:  $C_4H_3O_5$ ).



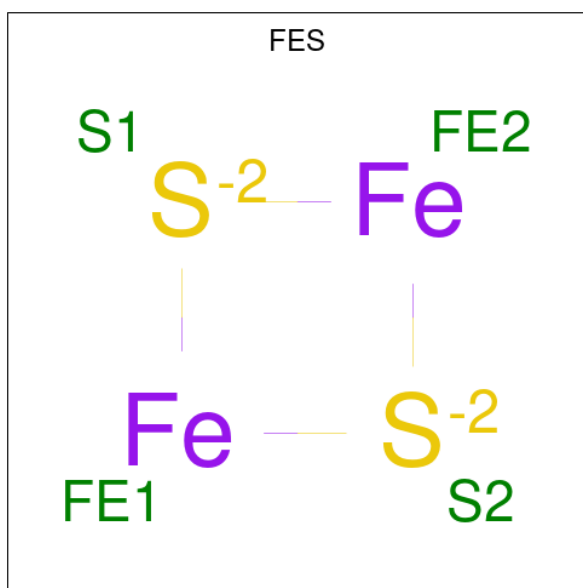
| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 1        | Total C O<br>9 4 5 | 0       | 0       |
| 5   | M     | 1        | Total C O<br>9 4 5 | 0       | 0       |

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



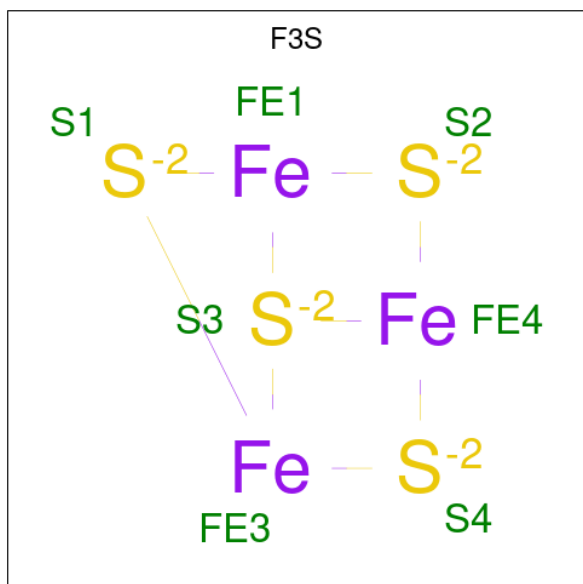
| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 6   | A     | 1        | Total<br>53 | C<br>27 | N<br>9 | O<br>15 | P<br>2 | 0       | 0       |
| 6   | M     | 1        | Total<br>53 | C<br>27 | N<br>9 | O<br>15 | P<br>2 | 0       | 0       |

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 7   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 7   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



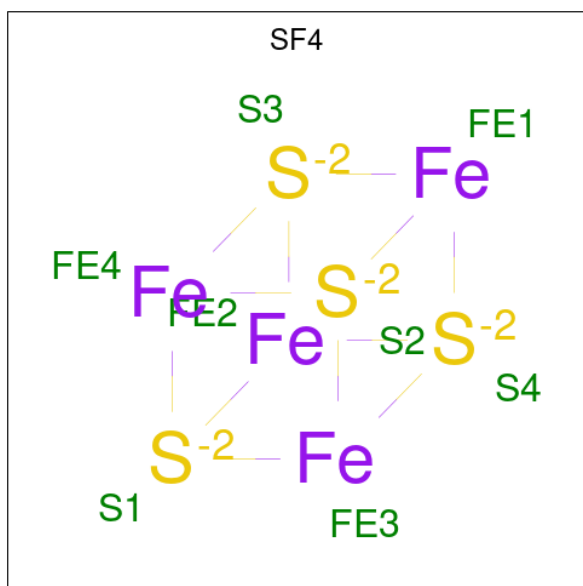
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |

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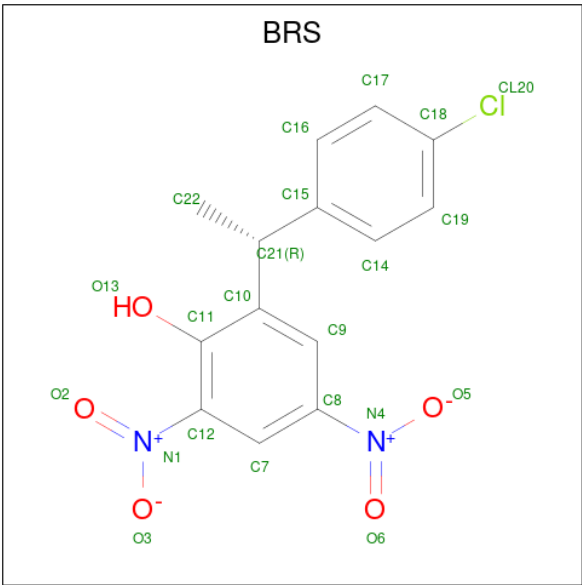
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 7     | 3  | 4 |         |         |

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



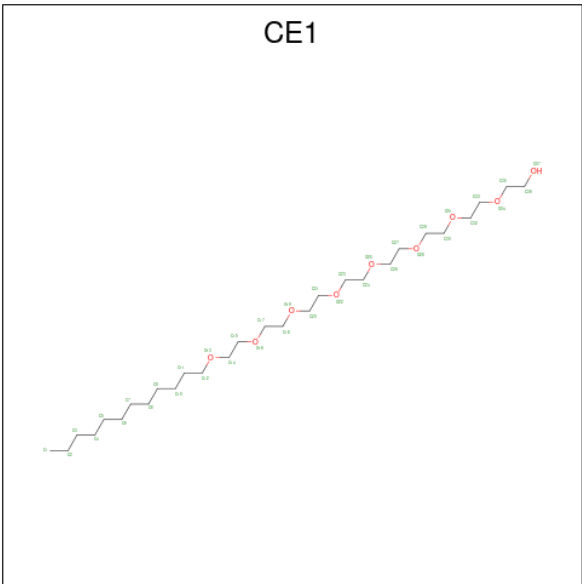
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 9   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 10 is 2-[1-(4-CHLORO-PHENYL)-ETHYL]-4,6-DINITRO-PHENOL (CCD ID: BRS) (formula:  $\text{C}_{14}\text{H}_{11}\text{ClN}_2\text{O}_5$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 10  | B     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 22    | 14 | 1  | 2 | 5 |         |         |
| 10  | N     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 22    | 14 | 1  | 2 | 5 |         |         |

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C<sub>28</sub>H<sub>58</sub>O<sub>9</sub>).



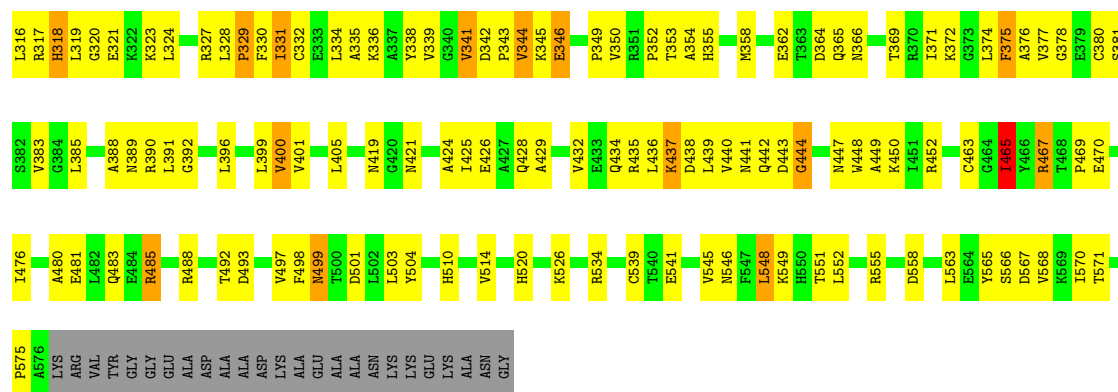
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |

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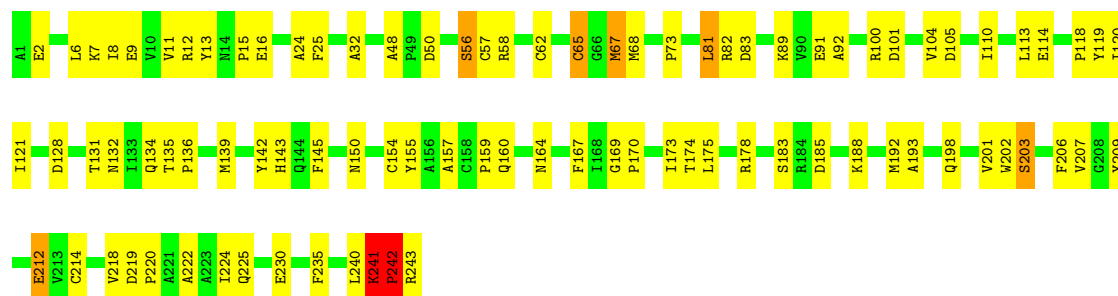
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 11  | O     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |
| 11  | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 28 | 9 |         |         |





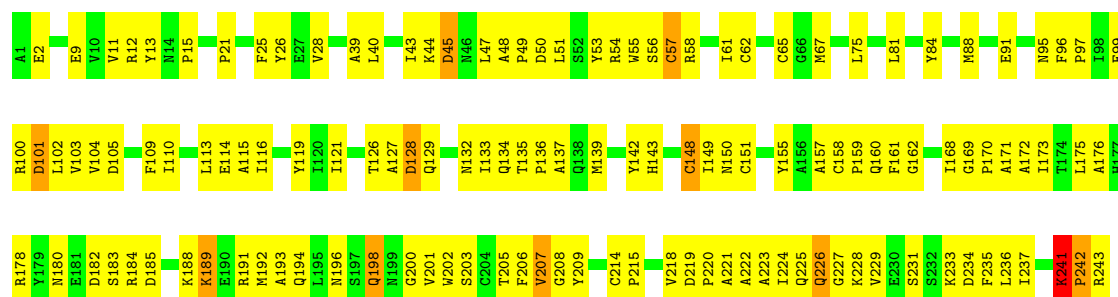
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain B: 63% 34%



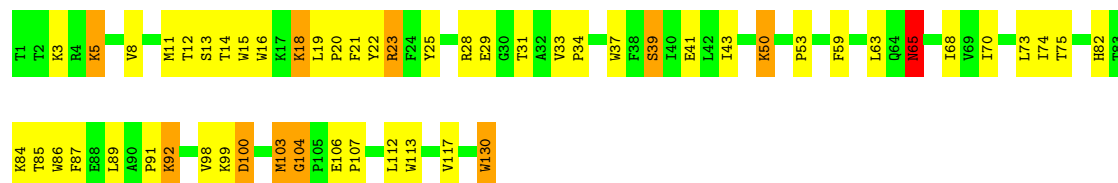
• Molecule 2: Fumarate reductase iron-sulfur protein

Chain N: 46% 49%



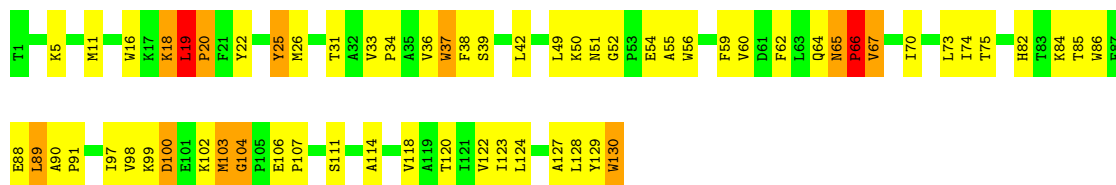
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain C: 58% 33% 8%



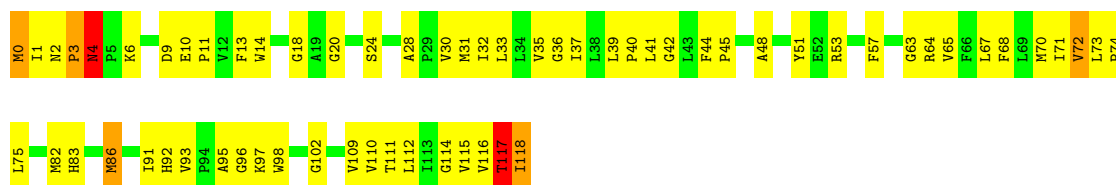
• Molecule 3: FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN

Chain O:  52% 38% 8% .

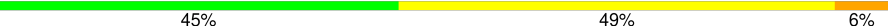


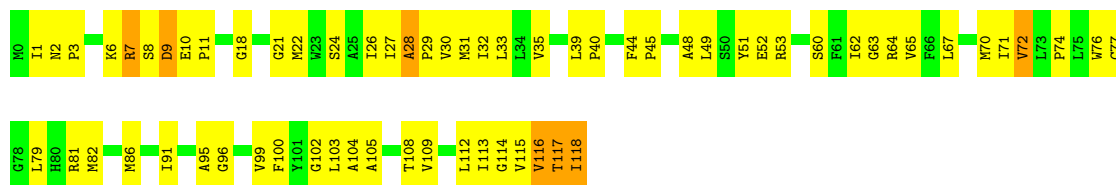
• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain D:  47% 47% . .



• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN

Chain P:  45% 49% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 96.15Å 137.81Å 270.99Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 50.00 – 3.60                                   | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (50.00-3.60)                   | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | 0.10                                           | Depositor |
| Refinement program                                       | CNS                                            | Depositor |
| R, $R_{free}$                                            | 0.264 , 0.301                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 16957                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 50.0                                           | wwPDB-VP  |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CE1, OAA, FAD, BRS, SF4, FES, F3S

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     | 0.87         | 3/4540 (0.1%)   | 1.15        | 26/6139 (0.4%)   |
| 1   | M     | 0.72         | 2/4540 (0.0%)   | 1.11        | 24/6139 (0.4%)   |
| 2   | B     | 0.80         | 1/1931 (0.1%)   | 1.16        | 9/2617 (0.3%)    |
| 2   | N     | 0.74         | 2/1931 (0.1%)   | 1.19        | 10/2617 (0.4%)   |
| 3   | C     | 0.96         | 3/1094 (0.3%)   | 1.19        | 9/1496 (0.6%)    |
| 3   | O     | 0.88         | 2/1094 (0.2%)   | 1.20        | 10/1496 (0.7%)   |
| 4   | D     | 1.00         | 3/956 (0.3%)    | 1.29        | 11/1303 (0.8%)   |
| 4   | P     | 0.91         | 3/956 (0.3%)    | 1.19        | 6/1303 (0.5%)    |
| All | All   | 0.83         | 19/17042 (0.1%) | 1.16        | 105/23110 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | O     | 0                   | 1                   |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4   | D     | 117 | THR  | CA-C  | -12.36 | 1.36        | 1.52     |
| 4   | P     | 117 | THR  | CA-C  | -10.53 | 1.38        | 1.52     |
| 4   | D     | 3   | PRO  | C-O   | -8.86  | 1.13        | 1.24     |
| 1   | A     | 135 | MET  | SD-CE | 8.80   | 2.01        | 1.79     |
| 3   | C     | 65  | ASN  | C-O   | -8.29  | 1.13        | 1.24     |
| 3   | C     | 104 | GLY  | C-O   | -7.85  | 1.13        | 1.24     |
| 3   | O     | 104 | GLY  | C-O   | -7.69  | 1.13        | 1.24     |
| 4   | P     | 3   | PRO  | C-O   | -7.61  | 1.15        | 1.23     |
| 2   | N     | 242 | PRO  | CA-C  | -7.24  | 1.42        | 1.52     |
| 1   | A     | 241 | ILE  | CA-CB | -7.22  | 1.46        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | D     | 117 | THR  | CA-CB | 6.68  | 1.64        | 1.53     |
| 3   | O     | 65  | ASN  | C-O   | -6.41 | 1.16        | 1.24     |
| 4   | P     | 31  | MET  | SD-CE | 6.39  | 1.95        | 1.79     |
| 1   | M     | 268 | MET  | SD-CE | 5.84  | 1.94        | 1.79     |
| 1   | M     | 465 | ILE  | CA-CB | 5.33  | 1.61        | 1.54     |
| 1   | A     | 243 | MET  | SD-CE | -5.14 | 1.66        | 1.79     |
| 3   | C     | 130 | TRP  | CB-CG | -5.12 | 1.34        | 1.50     |
| 2   | N     | 172 | ALA  | CA-CB | -5.10 | 1.45        | 1.53     |
| 2   | B     | 67  | MET  | SD-CE | -5.07 | 1.66        | 1.79     |

All (105) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | N     | 241 | LYS  | CA-C-N  | -12.81 | 103.83      | 119.84   |
| 2   | N     | 241 | LYS  | C-N-CA  | -12.81 | 103.83      | 119.84   |
| 4   | D     | 117 | THR  | N-CA-C  | 10.96  | 134.14      | 110.80   |
| 3   | C     | 65  | ASN  | N-CA-C  | 10.04  | 132.01      | 109.81   |
| 2   | N     | 65  | CYS  | N-CA-C  | 9.10   | 123.98      | 113.15   |
| 2   | B     | 65  | CYS  | N-CA-C  | 8.68   | 123.62      | 112.34   |
| 4   | D     | 72  | VAL  | N-CA-C  | 7.79   | 117.75      | 110.42   |
| 4   | D     | 117 | THR  | CA-C-N  | -7.70  | 107.83      | 121.70   |
| 4   | D     | 117 | THR  | C-N-CA  | -7.70  | 107.83      | 121.70   |
| 4   | P     | 116 | VAL  | N-CA-C  | -7.67  | 102.12      | 113.39   |
| 4   | D     | 117 | THR  | CB-CA-C | -7.66  | 95.18       | 110.42   |
| 1   | A     | 547 | PHE  | N-CA-C  | 7.39   | 122.02      | 112.41   |
| 4   | D     | 35  | VAL  | N-CA-C  | 7.38   | 117.47      | 110.53   |
| 1   | A     | 106 | ARG  | N-CA-C  | -7.37  | 100.49      | 110.36   |
| 1   | M     | 75  | TRP  | N-CA-C  | 7.35   | 121.58      | 112.47   |
| 1   | M     | 467 | ARG  | N-CA-C  | 7.27   | 120.78      | 109.07   |
| 1   | A     | 242 | LEU  | N-CA-C  | 7.22   | 120.79      | 109.96   |
| 2   | B     | 48  | ALA  | CA-C-N  | 7.21   | 126.91      | 119.56   |
| 2   | B     | 48  | ALA  | C-N-CA  | 7.21   | 126.91      | 119.56   |
| 3   | O     | 66  | PRO  | N-CA-C  | 7.17   | 127.25      | 112.47   |
| 3   | O     | 25  | TYR  | N-CA-C  | -7.09  | 103.16      | 111.03   |
| 1   | M     | 100 | GLY  | N-CA-C  | 6.95   | 121.93      | 113.79   |
| 1   | A     | 337 | ALA  | N-CA-C  | 6.87   | 118.84      | 111.36   |
| 2   | N     | 48  | ALA  | CA-C-N  | 6.81   | 126.51      | 119.56   |
| 2   | N     | 48  | ALA  | C-N-CA  | 6.81   | 126.51      | 119.56   |
| 1   | M     | 242 | LEU  | N-CA-C  | 6.57   | 120.21      | 109.76   |
| 1   | M     | 106 | ARG  | N-CA-C  | -6.57  | 100.54      | 110.39   |
| 3   | C     | 104 | GLY  | CA-C-O  | -6.47  | 112.27      | 121.52   |
| 4   | P     | 72  | VAL  | N-CA-C  | 6.42   | 116.56      | 110.53   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | M     | 400 | VAL  | CB-CA-C  | -6.38 | 103.70      | 112.24   |
| 2   | B     | 198 | GLN  | N-CA-C   | -6.34 | 104.80      | 112.54   |
| 4   | P     | 117 | THR  | CB-CA-C  | -6.34 | 97.79       | 110.42   |
| 1   | A     | 105 | ARG  | N-CA-C   | 6.33  | 119.85      | 109.85   |
| 1   | A     | 204 | ASN  | N-CA-C   | 6.29  | 119.83      | 110.52   |
| 3   | O     | 104 | GLY  | CA-C-O   | -6.26 | 112.57      | 121.52   |
| 1   | M     | 44  | HIS  | N-CA-C   | 6.25  | 120.00      | 112.38   |
| 1   | A     | 175 | MET  | N-CA-C   | 6.12  | 117.95      | 111.28   |
| 4   | P     | 100 | PHE  | N-CA-C   | 6.10  | 117.62      | 110.97   |
| 4   | D     | 2   | ASN  | CA-C-N   | 6.06  | 126.58      | 120.04   |
| 4   | D     | 2   | ASN  | C-N-CA   | 6.06  | 126.58      | 120.04   |
| 1   | A     | 100 | GLY  | N-CA-C   | 6.05  | 121.99      | 114.37   |
| 1   | A     | 339 | VAL  | N-CA-C   | -6.03 | 107.42      | 113.20   |
| 1   | A     | 285 | GLY  | CA-C-N   | 6.02  | 126.37      | 119.93   |
| 1   | A     | 285 | GLY  | C-N-CA   | 6.02  | 126.37      | 119.93   |
| 3   | O     | 65  | ASN  | CA-C-N   | -5.93 | 112.43      | 119.84   |
| 3   | O     | 65  | ASN  | C-N-CA   | -5.93 | 112.43      | 119.84   |
| 3   | C     | 65  | ASN  | CA-C-N   | 5.92  | 141.22      | 127.00   |
| 3   | C     | 65  | ASN  | C-N-CA   | 5.92  | 141.22      | 127.00   |
| 1   | A     | 312 | VAL  | N-CA-C   | -5.91 | 99.20       | 108.95   |
| 3   | O     | 130 | TRP  | CA-CB-CG | 5.90  | 124.82      | 113.60   |
| 1   | A     | 467 | ARG  | N-CA-C   | 5.90  | 119.09      | 109.59   |
| 3   | O     | 19  | LEU  | N-CA-C   | 5.88  | 117.48      | 110.07   |
| 1   | A     | 355 | HIS  | N-CA-C   | 5.84  | 123.25      | 110.80   |
| 2   | B     | 241 | LYS  | CA-C-N   | 5.71  | 126.98      | 119.84   |
| 2   | B     | 241 | LYS  | C-N-CA   | 5.71  | 126.98      | 119.84   |
| 2   | N     | 207 | VAL  | N-CA-C   | -5.70 | 104.80      | 110.62   |
| 1   | A     | 313 | TYR  | N-CA-C   | 5.69  | 118.51      | 109.24   |
| 1   | M     | 341 | VAL  | N-CA-C   | 5.68  | 116.29      | 108.12   |
| 1   | M     | 346 | GLU  | N-CA-C   | 5.68  | 114.67      | 108.14   |
| 1   | M     | 567 | ASP  | N-CA-C   | 5.67  | 118.67      | 110.28   |
| 1   | A     | 146 | PHE  | CA-C-N   | 5.66  | 125.34      | 119.56   |
| 1   | A     | 146 | PHE  | C-N-CA   | 5.66  | 125.34      | 119.56   |
| 1   | M     | 437 | LYS  | N-CA-C   | -5.63 | 105.22      | 111.36   |
| 2   | N     | 45  | ASP  | N-CA-C   | 5.61  | 117.20      | 111.14   |
| 1   | M     | 338 | TYR  | N-CA-C   | 5.61  | 120.25      | 112.45   |
| 1   | M     | 285 | GLY  | CA-C-N   | 5.60  | 126.84      | 119.84   |
| 1   | M     | 285 | GLY  | C-N-CA   | 5.60  | 126.84      | 119.84   |
| 3   | C     | 73  | LEU  | N-CA-C   | -5.60 | 105.26      | 111.36   |
| 1   | M     | 355 | HIS  | N-CA-C   | 5.53  | 122.58      | 110.80   |
| 1   | M     | 381 | SER  | N-CA-C   | 5.53  | 117.16      | 109.31   |
| 1   | A     | 75  | TRP  | N-CA-C   | 5.53  | 119.32      | 112.47   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 198 | GLN  | N-CA-C  | -5.49 | 105.84      | 112.54   |
| 3   | C     | 65  | ASN  | C-N-CD  | -5.49 | 108.53      | 120.60   |
| 1   | A     | 110 | SER  | N-CA-C  | -5.48 | 103.15      | 110.55   |
| 1   | M     | 110 | SER  | N-CA-C  | -5.47 | 103.16      | 110.55   |
| 4   | D     | 4   | ASN  | N-CA-C  | -5.47 | 100.89      | 108.76   |
| 1   | M     | 234 | THR  | N-CA-C  | 5.45  | 118.64      | 107.69   |
| 3   | O     | 67  | VAL  | N-CA-C  | 5.42  | 116.05      | 110.36   |
| 2   | N     | 57  | CYS  | N-CA-C  | 5.42  | 117.89      | 111.33   |
| 1   | A     | 386 | HIS  | N-CA-C  | 5.36  | 119.87      | 113.23   |
| 1   | M     | 419 | ASN  | N-CA-C  | 5.32  | 117.96      | 110.14   |
| 1   | M     | 0   | MET  | CA-C-N  | 5.29  | 131.64      | 121.54   |
| 1   | M     | 0   | MET  | C-N-CA  | 5.29  | 131.64      | 121.54   |
| 4   | P     | 28  | ALA  | N-CA-C  | 5.26  | 119.90      | 112.75   |
| 1   | A     | 234 | THR  | N-CA-C  | 5.25  | 118.83      | 107.49   |
| 4   | P     | 117 | THR  | N-CA-CB | 5.25  | 119.36      | 110.49   |
| 1   | A     | 138 | THR  | N-CA-C  | -5.25 | 105.46      | 111.07   |
| 1   | M     | 130 | LYS  | N-CA-C  | -5.24 | 105.97      | 114.09   |
| 1   | A     | 131 | THR  | N-CA-C  | 5.22  | 117.64      | 111.33   |
| 3   | O     | 52  | GLY  | CA-C-N  | 5.21  | 126.35      | 119.84   |
| 3   | O     | 52  | GLY  | C-N-CA  | 5.21  | 126.35      | 119.84   |
| 1   | A     | 126 | PHE  | N-CA-C  | 5.21  | 116.99      | 109.07   |
| 1   | M     | 92  | GLU  | N-CA-C  | 5.20  | 116.95      | 111.28   |
| 2   | B     | 135 | THR  | CA-C-N  | -5.16 | 113.33      | 119.05   |
| 2   | B     | 135 | THR  | C-N-CA  | -5.16 | 113.33      | 119.05   |
| 3   | C     | 5   | LYS  | CA-C-N  | 5.14  | 126.27      | 119.84   |
| 3   | C     | 5   | LYS  | C-N-CA  | 5.14  | 126.27      | 119.84   |
| 3   | C     | 65  | ASN  | CB-CA-C | -5.12 | 100.08      | 110.17   |
| 2   | B     | 24  | ALA  | N-CA-C  | -5.11 | 101.31      | 109.23   |
| 4   | D     | 45  | PRO  | N-CA-C  | 5.11  | 119.20      | 111.19   |
| 1   | A     | 1   | GLN  | N-CA-C  | -5.09 | 103.81      | 110.53   |
| 4   | D     | 65  | VAL  | CB-CA-C | -5.09 | 105.46      | 111.97   |
| 2   | N     | 242 | PRO  | O-C-N   | 5.07  | 129.49      | 122.64   |
| 1   | A     | 44  | HIS  | N-CA-C  | 5.04  | 118.69      | 112.54   |
| 1   | M     | 202 | ASN  | N-CA-C  | 5.02  | 115.67      | 108.74   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | O     | 129 | TYR  | Sidechain |

## 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     | 4448  | 0        | 4335     | 162     | 0            |
| 1   | M     | 4448  | 0        | 4335     | 284     | 0            |
| 2   | B     | 1888  | 0        | 1837     | 86      | 0            |
| 2   | N     | 1888  | 0        | 1837     | 130     | 0            |
| 3   | C     | 1058  | 0        | 1108     | 65      | 0            |
| 3   | O     | 1058  | 0        | 1108     | 69      | 0            |
| 4   | D     | 926   | 0        | 971      | 83      | 0            |
| 4   | P     | 926   | 0        | 971      | 78      | 0            |
| 5   | A     | 9     | 0        | 2        | 1       | 0            |
| 5   | M     | 9     | 0        | 2        | 2       | 0            |
| 6   | A     | 53    | 0        | 31       | 7       | 0            |
| 6   | M     | 53    | 0        | 31       | 11      | 0            |
| 7   | B     | 4     | 0        | 0        | 0       | 0            |
| 7   | N     | 4     | 0        | 0        | 0       | 0            |
| 8   | B     | 7     | 0        | 0        | 0       | 0            |
| 8   | N     | 7     | 0        | 0        | 2       | 0            |
| 9   | B     | 8     | 0        | 0        | 0       | 0            |
| 9   | N     | 8     | 0        | 0        | 7       | 0            |
| 10  | B     | 22    | 0        | 11       | 13      | 0            |
| 10  | N     | 22    | 0        | 11       | 5       | 0            |
| 11  | D     | 37    | 0        | 58       | 5       | 0            |
| 11  | O     | 37    | 0        | 58       | 1       | 0            |
| 11  | P     | 37    | 0        | 58       | 2       | 0            |
| All | All   | 16957 | 0        | 16764    | 872     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (872) 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:A:135:MET:SD | 1:A:135:MET:CE   | 2.01                     | 1.48              |
| 1:A:44:HIS:NE2 | 6:A:703:FAD:C8M  | 1.81                     | 1.41              |
| 1:M:44:HIS:NE2 | 6:M:803:FAD:C8M  | 1.83                     | 1.38              |
| 1:M:44:HIS:NE2 | 6:M:803:FAD:HM82 | 0.88                     | 1.21              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:44:HIS:NE2   | 6:A:703:FAD:HM82  | 0.85                     | 1.17              |
| 4:D:6:LYS:HG3    | 4:P:6:LYS:HB3     | 1.27                     | 1.16              |
| 2:B:225:GLN:NE2  | 10:B:700:BRS:H222 | 1.66                     | 1.09              |
| 1:M:190:MET:HE1  | 1:M:215:MET:HE3   | 1.26                     | 1.08              |
| 1:M:421:ASN:HD22 | 1:M:424:ALA:HB2   | 1.15                     | 1.08              |
| 2:B:225:GLN:HE21 | 10:B:700:BRS:C22  | 1.68                     | 1.06              |
| 1:A:44:HIS:CE1   | 6:A:703:FAD:HM82  | 1.92                     | 1.05              |
| 1:M:44:HIS:CD2   | 6:M:803:FAD:HM82  | 1.90                     | 1.05              |
| 1:M:44:HIS:CE1   | 6:M:803:FAD:HM82  | 1.92                     | 1.04              |
| 1:M:251:GLY:HA2  | 1:M:277:PRO:HG2   | 1.41                     | 1.03              |
| 1:A:358:MET:HE3  | 1:A:389:ASN:HA    | 1.38                     | 1.02              |
| 2:B:225:GLN:HE21 | 10:B:700:BRS:H222 | 0.88                     | 1.01              |
| 3:C:50:LYS:HD2   | 4:D:118:ILE:O     | 1.59                     | 1.01              |
| 1:A:44:HIS:CD2   | 6:A:703:FAD:HM82  | 1.95                     | 1.01              |
| 2:N:148:CYS:SG   | 9:N:246:SF4:S2    | 2.59                     | 0.99              |
| 9:N:246:SF4:S2   | 9:N:246:SF4:S4    | 2.60                     | 0.99              |
| 3:C:12:THR:HG22  | 3:C:14:THR:H      | 1.22                     | 0.99              |
| 1:M:469:PRO:HG3  | 1:M:534:ARG:HH21  | 1.28                     | 0.99              |
| 3:O:50:LYS:HG3   | 4:P:118:ILE:HA    | 1.39                     | 0.98              |
| 2:N:116:ILE:HG21 | 2:N:176:ALA:HB2   | 1.42                     | 0.98              |
| 3:C:50:LYS:HD2   | 4:D:118:ILE:C     | 1.87                     | 0.98              |
| 3:O:19:LEU:H     | 3:O:19:LEU:HD23   | 1.27                     | 0.97              |
| 1:M:421:ASN:HD22 | 1:M:424:ALA:CB    | 1.77                     | 0.97              |
| 2:N:54:ARG:HE    | 2:N:103:VAL:HG13  | 1.31                     | 0.96              |
| 1:M:316:LEU:HB3  | 1:M:319:LEU:HD12  | 1.48                     | 0.93              |
| 3:C:50:LYS:HD3   | 4:D:118:ILE:HG22  | 1.49                     | 0.91              |
| 1:M:447:ASN:HD21 | 1:M:449:ALA:HB3   | 1.34                     | 0.90              |
| 1:M:42:ARG:HH21  | 2:N:150:ASN:HB2   | 1.35                     | 0.90              |
| 4:P:117:THR:O    | 4:P:118:ILE:C     | 2.13                     | 0.90              |
| 4:P:117:THR:HG22 | 4:P:118:ILE:N     | 1.88                     | 0.89              |
| 3:O:50:LYS:CG    | 4:P:118:ILE:HA    | 2.02                     | 0.89              |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:HB2   | 1.34                     | 0.89              |
| 2:N:189:LYS:H    | 2:N:189:LYS:HD3   | 1.37                     | 0.88              |
| 3:C:99:LYS:O     | 3:C:100:ASP:HB2   | 1.74                     | 0.87              |
| 4:D:92:HIS:HB3   | 2:N:243:ARG:HB2   | 1.55                     | 0.87              |
| 2:N:225:GLN:NE2  | 10:N:800:BRS:H222 | 1.90                     | 0.87              |
| 2:B:241:LYS:O    | 2:B:243:ARG:N     | 2.08                     | 0.86              |
| 1:M:155:HIS:CD2  | 1:M:174:ASN:HA    | 2.10                     | 0.85              |
| 4:D:64:ARG:NH1   | 4:D:117:THR:HG23  | 1.92                     | 0.85              |
| 3:O:86:TRP:HE1   | 4:P:22:MET:HE2    | 1.42                     | 0.84              |
| 4:D:0:MET:HG2    | 4:D:1:ILE:H       | 1.39                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:437:LYS:HG2  | 1:M:441:ASN:HD21  | 1.42                     | 0.84              |
| 2:N:214:CYS:SG   | 2:N:218:VAL:HG23  | 2.16                     | 0.84              |
| 3:O:31:THR:HG21  | 3:O:82:HIS:HB2    | 1.58                     | 0.84              |
| 1:M:304:ILE:HD12 | 1:M:304:ILE:H     | 1.39                     | 0.84              |
| 1:M:197:ARG:HD2  | 1:M:206:GLY:HA2   | 1.58                     | 0.83              |
| 1:M:98:LEU:HD11  | 2:N:127:ALA:HA    | 1.60                     | 0.83              |
| 2:B:15:PRO:HB2   | 3:C:5:LYS:H       | 1.43                     | 0.81              |
| 1:A:356:TYR:CE2  | 1:A:390:ARG:HD3   | 2.14                     | 0.81              |
| 3:O:50:LYS:CD    | 4:P:118:ILE:HA    | 2.11                     | 0.81              |
| 1:A:7:LEU:HD21   | 1:A:32:ILE:HG12   | 1.61                     | 0.81              |
| 1:A:514:VAL:HG12 | 1:A:518:MET:HE3   | 1.62                     | 0.81              |
| 1:A:484:GLU:HG3  | 1:A:488:ARG:NH1   | 1.96                     | 0.80              |
| 2:N:11:VAL:HG21  | 2:N:91:GLU:HG2    | 1.63                     | 0.80              |
| 1:M:465:ILE:HD13 | 1:M:465:ILE:H     | 1.45                     | 0.80              |
| 3:O:33:VAL:HB    | 3:O:34:PRO:HD3    | 1.63                     | 0.80              |
| 1:M:425:ILE:O    | 1:M:428:GLN:HB2   | 1.83                     | 0.79              |
| 3:C:33:VAL:HB    | 3:C:34:PRO:HD3    | 1.63                     | 0.79              |
| 2:N:157:ALA:HB1  | 2:N:209:TYR:CD2   | 2.18                     | 0.79              |
| 1:A:413:ARG:HB2  | 1:A:413:ARG:NH1   | 1.96                     | 0.78              |
| 1:M:41:MET:HE2   | 2:N:150:ASN:ND2   | 1.97                     | 0.78              |
| 1:M:152:PHE:HB3  | 1:M:155:HIS:ND1   | 1.98                     | 0.78              |
| 3:O:128:LEU:HD22 | 4:P:44:PHE:HB2    | 1.66                     | 0.77              |
| 1:A:184:ARG:HG2  | 1:A:184:ARG:HH11  | 1.48                     | 0.77              |
| 3:C:50:LYS:CD    | 4:D:118:ILE:HG22  | 2.12                     | 0.77              |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:CB    | 1.97                     | 0.77              |
| 2:B:134:GLN:HE21 | 2:B:139:MET:HE3   | 1.49                     | 0.77              |
| 2:B:13:TYR:OH    | 3:C:5:LYS:O       | 2.01                     | 0.77              |
| 1:M:421:ASN:ND2  | 1:M:424:ALA:HB2   | 1.95                     | 0.77              |
| 1:M:549:LYS:HD2  | 1:M:565:TYR:HB3   | 1.67                     | 0.76              |
| 2:B:241:LYS:C    | 2:B:243:ARG:H     | 1.94                     | 0.76              |
| 4:D:92:HIS:HB3   | 2:N:243:ARG:CB    | 2.14                     | 0.76              |
| 1:M:316:LEU:HD22 | 1:M:319:LEU:HD11  | 1.68                     | 0.76              |
| 2:N:225:GLN:HE21 | 10:N:800:BRS:H222 | 1.51                     | 0.75              |
| 4:D:63:GLY:O     | 4:D:67:LEU:HD23   | 1.87                     | 0.75              |
| 1:M:102:PRO:HB2  | 2:N:139:MET:HE3   | 1.67                     | 0.75              |
| 2:N:159:PRO:HG2  | 2:N:207:VAL:HG21  | 1.68                     | 0.75              |
| 3:O:104:GLY:O    | 3:O:107:PRO:HD2   | 1.86                     | 0.75              |
| 3:O:50:LYS:HD2   | 4:P:117:THR:HG22  | 1.68                     | 0.74              |
| 2:N:116:ILE:HG21 | 2:N:176:ALA:CB    | 2.18                     | 0.74              |
| 1:M:488:ARG:NH1  | 1:M:488:ARG:HB3   | 2.03                     | 0.74              |
| 4:D:48:ALA:O     | 4:D:53:ARG:HD3    | 1.87                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:279:ASN:O     | 1:A:280:LYS:HB2  | 1.88                     | 0.74              |
| 4:D:64:ARG:HH22   | 4:D:117:THR:HG21 | 1.52                     | 0.74              |
| 1:A:192:THR:OG1   | 1:A:212:GLY:HA3  | 1.88                     | 0.73              |
| 1:M:311:VAL:HG11  | 1:M:349:PRO:HB2  | 1.71                     | 0.73              |
| 10:B:700:BRS:HC19 | 4:D:18:GLY:HA2   | 1.71                     | 0.72              |
| 1:M:447:ASN:ND2   | 1:M:449:ALA:HB3  | 2.04                     | 0.72              |
| 3:C:19:LEU:HD12   | 3:C:20:PRO:HD2   | 1.70                     | 0.72              |
| 1:M:331:ILE:HD12  | 1:M:331:ILE:H    | 1.53                     | 0.72              |
| 1:M:96:LEU:HD21   | 1:M:139:LEU:HD21 | 1.70                     | 0.72              |
| 1:A:0:MET:SD      | 1:A:182:GLN:HG3  | 2.29                     | 0.72              |
| 1:M:41:MET:HE2    | 2:N:150:ASN:HD22 | 1.52                     | 0.72              |
| 1:M:311:VAL:HG12  | 1:M:312:VAL:O    | 1.89                     | 0.72              |
| 4:D:64:ARG:NH2    | 4:D:117:THR:HG21 | 2.04                     | 0.72              |
| 4:D:0:MET:CG      | 4:D:1:ILE:H      | 2.00                     | 0.71              |
| 1:M:11:GLY:O      | 1:M:16:GLY:HA3   | 1.89                     | 0.71              |
| 1:M:469:PRO:HG3   | 1:M:534:ARG:NH2  | 2.05                     | 0.71              |
| 1:M:436:LEU:O     | 1:M:440:VAL:HG23 | 1.89                     | 0.71              |
| 2:N:222:ALA:O     | 2:N:226:GLN:NE2  | 2.24                     | 0.71              |
| 1:A:323:LYS:HG3   | 1:A:327:ARG:HH11 | 1.56                     | 0.71              |
| 1:A:103:TRP:O     | 2:B:139:MET:HE1  | 1.91                     | 0.70              |
| 1:M:48:ALA:HB3    | 1:M:132:GLY:HA3  | 1.73                     | 0.70              |
| 1:M:549:LYS:HA    | 1:M:568:VAL:HG23 | 1.73                     | 0.70              |
| 4:P:105:ALA:O     | 4:P:109:VAL:HG23 | 1.90                     | 0.70              |
| 3:O:97:ILE:HD13   | 3:O:102:LYS:HA   | 1.73                     | 0.70              |
| 1:M:497:VAL:HG21  | 2:N:15:PRO:HG2   | 1.73                     | 0.70              |
| 1:M:437:LYS:HG2   | 1:M:441:ASN:ND2  | 2.07                     | 0.70              |
| 1:M:510:HIS:O     | 1:M:514:VAL:HG23 | 1.91                     | 0.70              |
| 1:A:41:MET:HE2    | 2:B:150:ASN:HD22 | 1.57                     | 0.70              |
| 1:M:260:TYR:CE1   | 1:M:264:GLN:NE2  | 2.60                     | 0.70              |
| 3:O:19:LEU:H      | 3:O:19:LEU:CD2   | 2.02                     | 0.70              |
| 4:D:6:LYS:CG      | 4:P:6:LYS:HB3    | 2.14                     | 0.69              |
| 1:M:174:ASN:ND2   | 1:M:177:GLU:HG2  | 2.07                     | 0.69              |
| 1:M:174:ASN:HD22  | 1:M:177:GLU:H    | 1.40                     | 0.69              |
| 1:M:192:THR:OG1   | 1:M:212:GLY:HA3  | 1.91                     | 0.69              |
| 4:P:77:CYS:O      | 4:P:81:ARG:HG3   | 1.93                     | 0.69              |
| 1:M:358:MET:SD    | 1:M:390:ARG:N    | 2.65                     | 0.69              |
| 1:M:332:CYS:HA    | 1:M:343:PRO:HG2  | 1.74                     | 0.69              |
| 1:M:444:GLY:HA3   | 1:M:488:ARG:O    | 1.93                     | 0.69              |
| 3:O:130:TRP:O     | 4:P:53:ARG:NH2   | 2.26                     | 0.69              |
| 1:M:342:ASP:HB3   | 1:M:345:LYS:HB3  | 1.75                     | 0.68              |
| 3:O:75:THR:HG22   | 4:P:32:ILE:HD13  | 1.73                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:99:LYS:O      | 3:C:100:ASP:CB    | 2.35                     | 0.68              |
| 1:A:484:GLU:HG3   | 1:A:488:ARG:HH12  | 1.57                     | 0.68              |
| 1:M:10:VAL:HG13   | 1:M:157:VAL:HG21  | 1.75                     | 0.68              |
| 11:D:710:CE1:H211 | 11:D:710:CE1:H171 | 1.76                     | 0.67              |
| 1:A:7:LEU:CD2     | 1:A:32:ILE:HG12   | 2.23                     | 0.67              |
| 1:M:327:ARG:O     | 1:M:328:LEU:HD23  | 1.94                     | 0.67              |
| 4:D:13:PHE:HE2    | 4:D:97:LYS:HE2    | 1.58                     | 0.67              |
| 4:P:51:TYR:HD1    | 4:P:52:GLU:HG3    | 1.60                     | 0.67              |
| 1:M:182:GLN:NE2   | 1:M:429:ALA:HB1   | 2.10                     | 0.67              |
| 1:M:122:GLU:H     | 1:M:122:GLU:CD    | 2.03                     | 0.66              |
| 2:N:11:VAL:CG2    | 2:N:91:GLU:HG2    | 2.25                     | 0.66              |
| 1:A:372:LYS:HE3   | 1:A:413:ARG:HE    | 1.60                     | 0.66              |
| 1:A:324:LEU:CD1   | 1:A:344:VAL:HG22  | 2.26                     | 0.66              |
| 3:C:50:LYS:HB3    | 4:D:118:ILE:HG22  | 1.78                     | 0.66              |
| 1:M:162:VAL:HG13  | 1:M:166:HIS:O     | 1.96                     | 0.66              |
| 1:M:202:ASN:HA    | 1:M:353:THR:HG22  | 1.78                     | 0.66              |
| 4:D:0:MET:HG2     | 4:D:1:ILE:N       | 2.11                     | 0.65              |
| 3:O:50:LYS:HG3    | 4:P:118:ILE:CA    | 2.24                     | 0.65              |
| 4:P:86:MET:HE3    | 4:P:91:ILE:HB     | 1.77                     | 0.65              |
| 1:A:390:ARG:HH22  | 5:A:702:OAA:C4    | 2.09                     | 0.65              |
| 1:A:204:ASN:N     | 1:A:204:ASN:HD22  | 1.91                     | 0.65              |
| 1:M:444:GLY:HA3   | 1:M:488:ARG:C     | 2.22                     | 0.65              |
| 2:B:81:LEU:HD23   | 2:B:81:LEU:N      | 2.12                     | 0.65              |
| 1:M:93:MET:HB3    | 1:M:125:TRP:CE3   | 2.31                     | 0.65              |
| 1:M:304:ILE:HD12  | 1:M:304:ILE:N     | 2.11                     | 0.65              |
| 1:M:204:ASN:N     | 1:M:204:ASN:HD22  | 1.95                     | 0.64              |
| 1:M:217:LEU:HG    | 1:M:555:ARG:HB3   | 1.79                     | 0.64              |
| 1:A:232:HIS:CE1   | 1:A:242:LEU:HD11  | 2.33                     | 0.64              |
| 1:A:57:GLN:NE2    | 1:A:122:GLU:HG2   | 2.12                     | 0.64              |
| 1:M:41:MET:HB2    | 1:M:137:HIS:CE1   | 2.32                     | 0.64              |
| 2:N:135:THR:HG23  | 2:N:136:PRO:HD2   | 1.80                     | 0.64              |
| 4:P:24:SER:O      | 4:P:28:ALA:HB3    | 1.98                     | 0.64              |
| 1:M:168:ARG:HD3   | 1:M:425:ILE:CD1   | 2.28                     | 0.63              |
| 1:M:435:ARG:HH12  | 1:M:439:LEU:HD22  | 1.62                     | 0.63              |
| 2:N:81:LEU:N      | 2:N:81:LEU:HD12   | 2.12                     | 0.63              |
| 4:D:13:PHE:CE2    | 4:D:97:LYS:HE2    | 2.33                     | 0.63              |
| 10:N:800:BRG:HC19 | 4:P:18:GLY:HA2    | 1.80                     | 0.63              |
| 3:O:99:LYS:O      | 3:O:100:ASP:CG    | 2.41                     | 0.63              |
| 4:P:39:LEU:HD13   | 4:P:49:LEU:HB3    | 1.81                     | 0.63              |
| 1:A:250:GLU:CB    | 1:A:319:LEU:HD11  | 2.28                     | 0.63              |
| 2:B:15:PRO:CB     | 3:C:5:LYS:H       | 2.09                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:40:LEU:HB3   | 2:N:53:TYR:CE2   | 2.34                     | 0.63              |
| 2:N:54:ARG:NE    | 2:N:103:VAL:HG13 | 2.09                     | 0.63              |
| 3:C:87:PHE:O     | 3:C:91:PRO:HD3   | 1.99                     | 0.62              |
| 1:M:242:LEU:HD12 | 1:M:243:MET:N    | 2.14                     | 0.62              |
| 4:P:51:TYR:CD1   | 4:P:52:GLU:HG3   | 2.34                     | 0.62              |
| 1:A:27:ASN:ND2   | 1:A:30:ALA:HB2   | 2.15                     | 0.62              |
| 1:M:435:ARG:HA   | 1:M:438:ASP:OD2  | 1.99                     | 0.62              |
| 1:A:251:GLY:O    | 1:A:318:HIS:NE2  | 2.23                     | 0.62              |
| 2:B:6:LEU:HD23   | 2:B:81:LEU:HD13  | 1.82                     | 0.62              |
| 4:D:112:LEU:O    | 4:D:116:VAL:HG22 | 2.00                     | 0.62              |
| 2:N:57:CYS:HB3   | 2:N:62:CYS:HB3   | 1.79                     | 0.62              |
| 1:A:236:LEU:HD11 | 1:A:243:MET:HE3  | 1.81                     | 0.62              |
| 4:D:64:ARG:NH2   | 4:D:117:THR:CG2  | 2.62                     | 0.62              |
| 1:M:44:HIS:NE2   | 6:M:803:FAD:C8   | 2.61                     | 0.62              |
| 2:B:32:ALA:O     | 2:B:82:ARG:NH1   | 2.32                     | 0.62              |
| 1:M:51:GLY:HA2   | 1:M:131:THR:HG21 | 1.82                     | 0.62              |
| 4:P:60:SER:O     | 4:P:64:ARG:HG3   | 2.00                     | 0.62              |
| 1:M:168:ARG:HD3  | 1:M:425:ILE:HD11 | 1.80                     | 0.62              |
| 3:O:59:PHE:O     | 3:O:62:PHE:HB3   | 2.00                     | 0.62              |
| 1:M:399:LEU:HD11 | 6:M:803:FAD:H4'  | 1.80                     | 0.62              |
| 4:D:86:MET:HE3   | 4:D:86:MET:HA    | 1.79                     | 0.61              |
| 2:N:81:LEU:H     | 2:N:81:LEU:CD1   | 2.13                     | 0.61              |
| 1:A:253:ILE:HG13 | 1:A:315:ASP:HB3  | 1.82                     | 0.61              |
| 1:M:230:GLN:HB2  | 1:M:358:MET:HE2  | 1.80                     | 0.61              |
| 1:A:197:ARG:HD2  | 1:A:206:GLY:HA2  | 1.82                     | 0.61              |
| 4:D:36:GLY:C     | 4:D:37:ILE:HG13  | 2.24                     | 0.61              |
| 2:N:196:ASN:ND2  | 2:N:234:ASP:OD1  | 2.32                     | 0.61              |
| 3:O:106:GLU:H    | 3:O:106:GLU:CD   | 2.08                     | 0.61              |
| 1:M:156:PHE:CD2  | 1:M:503:LEU:HD22 | 2.36                     | 0.61              |
| 4:D:64:ARG:HH12  | 4:D:117:THR:HG23 | 1.61                     | 0.61              |
| 3:O:50:LYS:HD2   | 4:P:118:ILE:HA   | 1.81                     | 0.61              |
| 4:P:79:LEU:HD23  | 4:P:82:MET:HE3   | 1.81                     | 0.61              |
| 2:B:155:TYR:CE2  | 2:B:169:GLY:HA3  | 2.36                     | 0.61              |
| 3:O:86:TRP:HE1   | 4:P:22:MET:CE    | 2.11                     | 0.61              |
| 1:A:436:LEU:O    | 1:A:440:VAL:HG23 | 2.01                     | 0.61              |
| 4:D:64:ARG:CZ    | 4:D:117:THR:HG23 | 2.30                     | 0.61              |
| 1:M:390:ARG:NH1  | 1:M:392:GLY:HA2  | 2.15                     | 0.61              |
| 3:C:130:TRP:O    | 4:D:53:ARG:NH2   | 2.32                     | 0.60              |
| 1:M:448:TRP:CH2  | 1:M:504:TYR:HB3  | 2.36                     | 0.60              |
| 2:N:201:VAL:HG23 | 2:N:202:TRP:N    | 2.16                     | 0.60              |
| 2:N:39:ALA:O     | 2:N:43:ILE:HG12  | 2.02                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:155:TYR:CZ    | 2:B:169:GLY:HA3  | 2.37                     | 0.60              |
| 2:N:116:ILE:HG22  | 2:N:191:ARG:HD3  | 1.83                     | 0.60              |
| 1:A:157:VAL:HG12  | 1:A:215:MET:HE1  | 1.82                     | 0.60              |
| 1:M:21:ILE:HG21   | 1:M:99:TRP:CH2   | 2.36                     | 0.60              |
| 1:M:275:GLY:O     | 1:M:277:PRO:HD3  | 2.01                     | 0.60              |
| 2:N:169:GLY:O     | 2:N:173:ILE:HG13 | 2.02                     | 0.60              |
| 2:B:241:LYS:C     | 2:B:243:ARG:N    | 2.58                     | 0.60              |
| 1:A:321:GLU:OE1   | 1:A:321:GLU:HA   | 2.00                     | 0.60              |
| 4:P:64:ARG:HB3    | 4:P:115:VAL:HG22 | 1.84                     | 0.59              |
| 2:B:15:PRO:HB2    | 3:C:5:LYS:N      | 2.16                     | 0.59              |
| 1:M:447:ASN:HD22  | 1:M:450:LYS:HG2  | 1.66                     | 0.59              |
| 2:N:135:THR:HG22  | 2:N:137:ALA:H    | 1.66                     | 0.59              |
| 1:M:545:VAL:C     | 1:M:546:ASN:HD22 | 2.09                     | 0.59              |
| 2:N:162:GLY:HA3   | 3:O:11:MET:HE1   | 1.85                     | 0.59              |
| 1:A:42:ARG:HD2    | 1:A:42:ARG:N     | 2.18                     | 0.59              |
| 2:N:113:LEU:HD11  | 2:N:175:LEU:HD22 | 1.85                     | 0.59              |
| 1:A:11:GLY:O      | 1:A:16:GLY:HA3   | 2.03                     | 0.59              |
| 1:M:329:PRO:HG2   | 1:M:330:PHE:H    | 1.67                     | 0.59              |
| 1:M:396:LEU:HG    | 6:M:803:FAD:C2   | 2.32                     | 0.59              |
| 3:O:19:LEU:HD21   | 3:O:22:TYR:CE2   | 2.38                     | 0.59              |
| 1:A:324:LEU:HD12  | 1:A:344:VAL:HG22 | 1.84                     | 0.59              |
| 10:B:700:BRS:HO13 | 4:D:14:TRP:HE1   | 1.50                     | 0.59              |
| 4:D:73:LEU:HB2    | 4:D:74:PRO:HD3   | 1.85                     | 0.59              |
| 2:N:194:GLN:HE22  | 4:P:1:ILE:HG21   | 1.68                     | 0.59              |
| 4:D:64:ARG:HH22   | 4:D:117:THR:CG2  | 2.16                     | 0.58              |
| 1:M:236:LEU:HD22  | 1:M:339:VAL:HG11 | 1.84                     | 0.58              |
| 1:M:311:VAL:HG11  | 1:M:349:PRO:CB   | 2.33                     | 0.58              |
| 1:M:331:ILE:HD12  | 1:M:331:ILE:N    | 2.18                     | 0.58              |
| 1:M:331:ILE:H     | 1:M:331:ILE:CD1  | 2.15                     | 0.58              |
| 3:O:106:GLU:HB2   | 3:O:107:PRO:HD3  | 1.83                     | 0.58              |
| 1:A:323:LYS:HG3   | 1:A:327:ARG:NH1  | 2.18                     | 0.58              |
| 10:N:800:BRS:HC19 | 4:P:18:GLY:CA    | 2.33                     | 0.58              |
| 2:B:8:ILE:HD11    | 2:B:81:LEU:HD11  | 1.86                     | 0.58              |
| 4:D:67:LEU:O      | 4:D:71:ILE:HG13  | 2.04                     | 0.58              |
| 1:M:213:MET:HE2   | 1:M:380:CYS:HA   | 1.84                     | 0.58              |
| 2:N:225:GLN:NE2   | 2:N:228:LYS:HD2  | 2.18                     | 0.58              |
| 1:A:18:ARG:NH1    | 1:A:92:GLU:OE1   | 2.37                     | 0.58              |
| 1:M:82:VAL:HG22   | 1:M:385:LEU:HD12 | 1.84                     | 0.58              |
| 1:M:476:ILE:HG23  | 1:M:520:HIS:CE1  | 2.39                     | 0.58              |
| 1:M:499:ASN:HD21  | 1:M:501:ASP:HB3  | 1.68                     | 0.58              |
| 2:N:81:LEU:HD12   | 2:N:81:LEU:H     | 1.69                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:10:GLU:N     | 4:P:11:PRO:CD    | 2.67                     | 0.58              |
| 3:C:113:TRP:O    | 3:C:117:VAL:HG23 | 2.04                     | 0.58              |
| 4:P:39:LEU:N     | 4:P:40:PRO:HD2   | 2.18                     | 0.58              |
| 1:M:171:VAL:HB   | 1:M:432:VAL:HG11 | 1.86                     | 0.57              |
| 1:M:311:VAL:HG13 | 1:M:350:VAL:O    | 2.02                     | 0.57              |
| 1:M:296:HIS:ND1  | 1:M:299:ARG:NH2  | 2.52                     | 0.57              |
| 1:M:332:CYS:O    | 1:M:336:LYS:HG3  | 2.04                     | 0.57              |
| 2:B:57:CYS:HB3   | 2:B:62:CYS:HB3   | 1.86                     | 0.57              |
| 1:M:155:HIS:HD2  | 1:M:174:ASN:HA   | 1.66                     | 0.57              |
| 2:N:119:TYR:CE1  | 2:N:121:ILE:HD11 | 2.40                     | 0.57              |
| 1:A:527:GLU:OE1  | 1:A:529:ARG:HD2  | 2.05                     | 0.57              |
| 1:M:358:MET:SD   | 1:M:389:ASN:HA   | 2.44                     | 0.57              |
| 1:M:183:ILE:HD12 | 1:M:183:ILE:N    | 2.20                     | 0.57              |
| 3:O:36:VAL:HG23  | 3:O:37:TRP:N     | 2.20                     | 0.57              |
| 1:A:448:TRP:CH2  | 1:A:504:TYR:HB3  | 2.40                     | 0.56              |
| 1:M:545:VAL:HG12 | 1:M:546:ASN:ND2  | 2.19                     | 0.56              |
| 3:O:60:VAL:O     | 3:O:64:GLN:HG3   | 2.06                     | 0.56              |
| 3:C:130:TRP:N    | 3:C:130:TRP:CD1  | 2.69                     | 0.56              |
| 1:M:288:ASP:O    | 1:M:292:GLN:HG3  | 2.05                     | 0.56              |
| 1:M:435:ARG:O    | 1:M:438:ASP:HB2  | 2.05                     | 0.56              |
| 2:N:206:PHE:CE1  | 2:N:225:GLN:HG3  | 2.40                     | 0.56              |
| 1:A:28:PRO:HA    | 1:A:148:GLN:HE21 | 1.70                     | 0.56              |
| 1:A:141:GLN:HB3  | 2:B:118:PRO:O    | 2.06                     | 0.56              |
| 1:M:48:ALA:HB3   | 1:M:132:GLY:CA   | 2.36                     | 0.56              |
| 2:N:97:PRO:HG2   | 2:N:105:ASP:HB3  | 1.87                     | 0.56              |
| 3:C:50:LYS:CD    | 4:D:118:ILE:C    | 2.73                     | 0.56              |
| 4:D:83:HIS:O     | 4:D:86:MET:HB2   | 2.06                     | 0.56              |
| 2:N:12:ARG:NH2   | 2:N:101:ASP:OD1  | 2.38                     | 0.56              |
| 4:P:28:ALA:N     | 4:P:29:PRO:HD2   | 2.20                     | 0.56              |
| 3:O:33:VAL:O     | 3:O:36:VAL:HG22  | 2.06                     | 0.56              |
| 1:A:395:SER:OG   | 6:A:703:FAD:H2'  | 2.06                     | 0.56              |
| 1:M:162:VAL:HG22 | 1:M:167:VAL:HA   | 1.86                     | 0.56              |
| 1:M:213:MET:CE   | 1:M:380:CYS:HA   | 2.36                     | 0.56              |
| 3:O:65:ASN:O     | 3:O:66:PRO:C     | 2.47                     | 0.56              |
| 4:P:35:VAL:O     | 4:P:40:PRO:HD3   | 2.06                     | 0.56              |
| 2:N:155:TYR:CE2  | 2:N:169:GLY:HA3  | 2.41                     | 0.56              |
| 1:M:17:LEU:HD13  | 1:M:140:PHE:N    | 2.21                     | 0.55              |
| 1:M:217:LEU:HG   | 1:M:555:ARG:CB   | 2.37                     | 0.55              |
| 2:N:188:LYS:HE2  | 2:N:192:MET:HE2  | 1.88                     | 0.55              |
| 2:N:151:CYS:N    | 9:N:246:SF4:S4   | 2.79                     | 0.55              |
| 1:A:250:GLU:HB3  | 1:A:319:LEU:HD11 | 1.87                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:57:CYS:O      | 2:B:58:ARG:HB2   | 2.05                     | 0.55              |
| 1:M:174:ASN:ND2   | 1:M:177:GLU:CG   | 2.69                     | 0.55              |
| 1:M:476:ILE:HG23  | 1:M:520:HIS:HE1  | 1.71                     | 0.55              |
| 2:B:16:GLU:HG2    | 3:C:3:LYS:HB3    | 1.89                     | 0.55              |
| 3:C:75:THR:HG22   | 4:D:32:ILE:HD13  | 1.89                     | 0.55              |
| 1:M:113:VAL:HA    | 1:M:124:THR:O    | 2.06                     | 0.55              |
| 1:A:35:ILE:HG22   | 1:A:36:SER:N     | 2.20                     | 0.55              |
| 1:A:328:LEU:O     | 1:A:332:CYS:SG   | 2.49                     | 0.55              |
| 3:C:85:THR:O      | 3:C:89:LEU:HD12  | 2.05                     | 0.55              |
| 1:M:549:LYS:HD2   | 1:M:565:TYR:CB   | 2.37                     | 0.55              |
| 2:N:241:LYS:O     | 2:N:241:LYS:CD   | 2.55                     | 0.55              |
| 2:N:241:LYS:O     | 2:N:241:LYS:CG   | 2.55                     | 0.55              |
| 2:B:2:GLU:HA      | 2:B:2:GLU:OE2    | 2.05                     | 0.55              |
| 2:N:233:LYS:O     | 2:N:237:ILE:HD13 | 2.06                     | 0.55              |
| 3:O:18:LYS:HD2    | 3:O:19:LEU:HD22  | 1.87                     | 0.55              |
| 1:A:546:ASN:O     | 1:A:549:LYS:HE2  | 2.07                     | 0.55              |
| 3:O:70:ILE:O      | 3:O:73:LEU:HB2   | 2.07                     | 0.55              |
| 1:M:499:ASN:HD22  | 1:M:499:ASN:C    | 2.15                     | 0.54              |
| 2:N:175:LEU:O     | 2:N:178:ARG:HB3  | 2.06                     | 0.54              |
| 4:D:4:ASN:HD22    | 4:P:2:ASN:ND2    | 2.05                     | 0.54              |
| 1:M:323:LYS:HG2   | 1:M:327:ARG:HH21 | 1.71                     | 0.54              |
| 4:P:51:TYR:CD1    | 4:P:52:GLU:N     | 2.72                     | 0.54              |
| 2:B:81:LEU:HD23   | 2:B:81:LEU:H     | 1.72                     | 0.54              |
| 3:C:65:ASN:HB3    | 3:C:68:ILE:H     | 1.72                     | 0.54              |
| 1:M:76:LEU:HD12   | 1:M:388:ALA:HB2  | 1.89                     | 0.54              |
| 1:M:195:ALA:O     | 1:M:198:VAL:HG22 | 2.06                     | 0.54              |
| 1:A:170:LEU:C     | 1:A:170:LEU:HD12 | 2.31                     | 0.54              |
| 3:C:33:VAL:HA     | 4:D:82:MET:CE    | 2.37                     | 0.54              |
| 1:M:548:LEU:HD21  | 1:M:575:PRO:HG3  | 1.89                     | 0.54              |
| 1:M:42:ARG:HH21   | 2:N:150:ASN:CB   | 2.14                     | 0.54              |
| 1:M:239:SER:HB2   | 1:M:241:ILE:HG13 | 1.89                     | 0.54              |
| 1:M:499:ASN:O     | 1:M:503:LEU:HG   | 2.07                     | 0.54              |
| 2:N:157:ALA:HB1   | 2:N:209:TYR:HD2  | 1.71                     | 0.54              |
| 1:M:84:TYR:HE2    | 1:M:405:LEU:HD22 | 1.73                     | 0.54              |
| 4:D:10:GLU:N      | 4:D:11:PRO:HD2   | 2.22                     | 0.54              |
| 2:N:13:TYR:HB2    | 2:N:21:PRO:HB3   | 1.90                     | 0.54              |
| 2:B:56:SER:O      | 2:B:58:ARG:HG3   | 2.08                     | 0.54              |
| 11:D:710:CE1:H362 | 4:P:76:TRP:NE1   | 2.24                     | 0.54              |
| 1:M:84:TYR:CE2    | 1:M:405:LEU:HD22 | 2.43                     | 0.54              |
| 2:B:170:PRO:HA    | 2:B:224:ILE:HD11 | 1.90                     | 0.53              |
| 1:M:304:ILE:H     | 1:M:304:ILE:CD1  | 2.16                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:O:74:ILE:HA    | 11:O:811:CE1:H151 | 1.90                     | 0.53              |
| 4:P:64:ARG:O     | 4:P:115:VAL:HG21  | 2.08                     | 0.53              |
| 1:A:89:CYS:HB2   | 1:A:90:PRO:HD3    | 1.90                     | 0.53              |
| 1:A:232:HIS:HD2  | 1:A:234:THR:H     | 1.56                     | 0.53              |
| 2:B:110:ILE:O    | 2:B:114:GLU:HG3   | 2.08                     | 0.53              |
| 1:M:499:ASN:HA   | 2:N:100:ARG:HH21  | 1.73                     | 0.53              |
| 1:A:93:MET:HB3   | 1:A:125:TRP:CZ3   | 2.44                     | 0.53              |
| 1:A:556:ASP:HB2  | 1:A:558:ASP:OD2   | 2.08                     | 0.53              |
| 4:P:113:ILE:O    | 4:P:117:THR:N     | 2.41                     | 0.53              |
| 1:M:204:ASN:N    | 1:M:204:ASN:ND2   | 2.52                     | 0.53              |
| 1:A:469:PRO:HB3  | 1:A:523:MET:HE1   | 1.91                     | 0.53              |
| 1:M:44:HIS:CE1   | 1:M:204:ASN:HA    | 2.44                     | 0.53              |
| 1:A:18:ARG:HG2   | 1:A:400:VAL:HA    | 1.91                     | 0.53              |
| 1:A:395:SER:HB3  | 6:A:703:FAD:N1    | 2.24                     | 0.53              |
| 1:A:442:GLN:OE1  | 1:A:487:LYS:HA    | 2.08                     | 0.53              |
| 2:B:225:GLN:HE21 | 10:B:700:BRS:C21  | 2.20                     | 0.53              |
| 3:C:59:PHE:CE1   | 3:C:63:LEU:HD11   | 2.44                     | 0.53              |
| 2:N:220:PRO:O    | 2:N:223:ALA:N     | 2.41                     | 0.53              |
| 4:P:62:ILE:HG23  | 4:P:63:GLY:N      | 2.24                     | 0.53              |
| 1:A:159:ASP:OD2  | 1:A:160:ILE:N     | 2.42                     | 0.53              |
| 2:N:139:MET:HA   | 2:N:142:TYR:CE2   | 2.44                     | 0.53              |
| 3:C:50:LYS:CG    | 4:D:118:ILE:HG22  | 2.39                     | 0.53              |
| 1:M:190:MET:HE1  | 1:M:215:MET:CE    | 2.18                     | 0.53              |
| 1:M:279:ASN:O    | 1:M:280:LYS:HB2   | 2.09                     | 0.53              |
| 2:B:169:GLY:O    | 2:B:173:ILE:HG13  | 2.09                     | 0.53              |
| 1:M:36:SER:HA    | 6:M:803:FAD:N3A   | 2.24                     | 0.53              |
| 4:P:62:ILE:O     | 4:P:65:VAL:HG22   | 2.09                     | 0.53              |
| 1:A:157:VAL:CG1  | 1:A:215:MET:HE1   | 2.39                     | 0.52              |
| 1:A:204:ASN:N    | 1:A:204:ASN:ND2   | 2.52                     | 0.52              |
| 2:N:12:ARG:NH1   | 2:N:50:ASP:OD1    | 2.23                     | 0.52              |
| 2:N:225:GLN:O    | 2:N:229:VAL:HG23  | 2.09                     | 0.52              |
| 3:O:19:LEU:HD23  | 3:O:19:LEU:N      | 2.06                     | 0.52              |
| 1:M:209:THR:O    | 1:M:209:THR:HG22  | 2.09                     | 0.52              |
| 1:M:497:VAL:HG21 | 2:N:15:PRO:CG     | 2.38                     | 0.52              |
| 1:M:54:ALA:O     | 1:M:55:VAL:C      | 2.51                     | 0.52              |
| 2:N:81:LEU:N     | 2:N:81:LEU:CD1    | 2.71                     | 0.52              |
| 2:N:135:THR:CG2  | 2:N:136:PRO:HD2   | 2.40                     | 0.52              |
| 3:O:130:TRP:C    | 4:P:53:ARG:NH2    | 2.67                     | 0.52              |
| 2:B:207:VAL:HG22 | 3:C:25:TYR:CE1    | 2.45                     | 0.52              |
| 3:C:50:LYS:HE2   | 3:C:50:LYS:HA     | 1.91                     | 0.52              |
| 1:M:97:GLU:OE2   | 2:N:132:ASN:ND2   | 2.42                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:117:THR:O    | 4:P:118:ILE:OXT  | 2.27                     | 0.52              |
| 2:B:134:GLN:HE21 | 2:B:139:MET:CE   | 2.20                     | 0.52              |
| 1:M:66:PHE:HD1   | 1:M:82:VAL:HG12  | 1.74                     | 0.52              |
| 2:N:241:LYS:O    | 2:N:241:LYS:HD2  | 2.09                     | 0.52              |
| 1:A:142:THR:O    | 1:A:145:GLN:HG2  | 2.08                     | 0.52              |
| 2:B:157:ALA:HB1  | 2:B:209:TYR:CD2  | 2.45                     | 0.52              |
| 1:M:199:TYR:CE1  | 1:M:229:VAL:HG11 | 2.44                     | 0.52              |
| 1:A:342:ASP:C    | 1:A:344:VAL:H    | 2.18                     | 0.52              |
| 3:C:98:VAL:HG23  | 3:C:98:VAL:O     | 2.10                     | 0.52              |
| 1:M:58:ASP:C     | 1:M:60:ASP:H     | 2.18                     | 0.52              |
| 1:A:253:ILE:CG1  | 1:A:315:ASP:HB3  | 2.39                     | 0.52              |
| 1:M:390:ARG:HD2  | 1:M:391:LEU:O    | 2.10                     | 0.52              |
| 3:C:50:LYS:HB3   | 4:D:118:ILE:CG2  | 2.39                     | 0.52              |
| 1:M:10:VAL:CG1   | 1:M:157:VAL:HG21 | 2.40                     | 0.52              |
| 1:M:41:MET:CE    | 2:N:150:ASN:HD22 | 2.23                     | 0.52              |
| 2:B:120:ILE:HD13 | 2:B:185:ASP:HB2  | 1.92                     | 0.51              |
| 2:B:212:GLU:HG3  | 3:C:21:PHE:CE2   | 2.44                     | 0.51              |
| 4:D:24:SER:O     | 4:D:28:ALA:HB3   | 2.10                     | 0.51              |
| 1:M:105:ARG:HG3  | 2:N:134:GLN:O    | 2.10                     | 0.51              |
| 1:M:195:ALA:O    | 1:M:198:VAL:HG13 | 2.11                     | 0.51              |
| 3:O:120:THR:HG23 | 4:P:30:VAL:HB    | 1.92                     | 0.51              |
| 1:A:54:ALA:HB3   | 1:A:125:TRP:NE1  | 2.25                     | 0.51              |
| 1:A:184:ARG:HG2  | 1:A:184:ARG:NH1  | 2.21                     | 0.51              |
| 1:M:435:ARG:NH1  | 1:M:439:LEU:HB2  | 2.25                     | 0.51              |
| 1:M:103:TRP:HH2  | 1:M:135:MET:SD   | 2.33                     | 0.51              |
| 1:A:446:GLU:HB2  | 1:A:488:ARG:O    | 2.11                     | 0.51              |
| 1:A:462:GLY:HA3  | 1:A:475:THR:OG1  | 2.09                     | 0.51              |
| 3:C:87:PHE:CD2   | 3:C:112:LEU:HD13 | 2.46                     | 0.51              |
| 3:O:127:ALA:O    | 3:O:128:LEU:HD23 | 2.10                     | 0.51              |
| 1:A:200:ARG:HG3  | 1:A:457:LEU:HD23 | 1.93                     | 0.51              |
| 4:D:4:ASN:ND2    | 4:P:2:ASN:ND2    | 2.58                     | 0.51              |
| 4:D:114:GLY:O    | 4:D:117:THR:HA   | 2.11                     | 0.51              |
| 1:M:99:TRP:CD2   | 1:M:142:THR:HG21 | 2.45                     | 0.51              |
| 1:M:232:HIS:O    | 1:M:352:PRO:HA   | 2.10                     | 0.51              |
| 1:M:6:ASP:HB3    | 1:M:7:LEU:HD23   | 1.91                     | 0.51              |
| 2:N:225:GLN:HE21 | 10:N:800:BRS:C22 | 2.21                     | 0.51              |
| 3:O:97:ILE:CD1   | 3:O:102:LYS:HA   | 2.41                     | 0.51              |
| 1:M:199:TYR:OH   | 1:M:229:VAL:HG21 | 2.11                     | 0.51              |
| 2:N:2:GLU:OE1    | 2:N:2:GLU:HA     | 2.10                     | 0.51              |
| 2:B:113:LEU:HD23 | 2:B:113:LEU:O    | 2.09                     | 0.51              |
| 1:M:96:LEU:HD21  | 1:M:139:LEU:CD2  | 2.40                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:488:ARG:HB3  | 1:M:488:ARG:CZ   | 2.41                     | 0.51              |
| 2:N:155:TYR:CZ   | 2:N:169:GLY:HA3  | 2.46                     | 0.51              |
| 1:A:44:HIS:NE2   | 6:A:703:FAD:C8   | 2.68                     | 0.51              |
| 1:A:316:LEU:O    | 1:A:319:LEU:HB2  | 2.09                     | 0.51              |
| 2:B:145:PHE:HA   | 2:B:218:VAL:HG13 | 1.93                     | 0.51              |
| 1:M:130:LYS:O    | 1:M:133:PHE:HB3  | 2.11                     | 0.51              |
| 1:M:176:MET:O    | 1:M:497:VAL:HA   | 2.10                     | 0.51              |
| 1:M:222:PRO:CG   | 1:M:362:GLU:OE1  | 2.59                     | 0.51              |
| 1:M:162:VAL:HG13 | 1:M:166:HIS:C    | 2.36                     | 0.51              |
| 1:A:253:ILE:HA   | 1:A:283:GLU:HG2  | 1.92                     | 0.50              |
| 1:A:317:ARG:C    | 1:A:319:LEU:H    | 2.19                     | 0.50              |
| 2:B:192:MET:O    | 2:B:193:ALA:C    | 2.52                     | 0.50              |
| 1:M:213:MET:HB3  | 1:M:223:LEU:HD21 | 1.92                     | 0.50              |
| 1:A:184:ARG:HH11 | 1:A:184:ARG:CG   | 2.18                     | 0.50              |
| 3:C:104:GLY:HA2  | 3:C:107:PRO:HD2  | 1.92                     | 0.50              |
| 4:D:28:ALA:O     | 4:D:32:ILE:HG13  | 2.11                     | 0.50              |
| 1:M:233:PRO:HG2  | 1:M:248:ARG:HH22 | 1.76                     | 0.50              |
| 1:A:525:ARG:NH1  | 1:A:527:GLU:OE1  | 2.42                     | 0.50              |
| 1:M:400:VAL:HG23 | 1:M:401:VAL:N    | 2.26                     | 0.50              |
| 1:A:148:GLN:OE1  | 1:A:148:GLN:N    | 2.40                     | 0.50              |
| 3:C:11:MET:HE2   | 3:C:15:TRP:CD1   | 2.47                     | 0.50              |
| 1:M:435:ARG:O    | 1:M:435:ARG:HD2  | 2.11                     | 0.50              |
| 3:O:84:LYS:HE2   | 3:O:88:GLU:CD    | 2.36                     | 0.50              |
| 1:A:94:THR:HA    | 2:B:131:THR:HG22 | 1.92                     | 0.50              |
| 1:A:500:THR:HB   | 1:A:504:TYR:CZ   | 2.46                     | 0.50              |
| 3:C:82:HIS:HE1   | 3:C:86:TRP:CE3   | 2.30                     | 0.50              |
| 2:N:235:PHE:HE1  | 4:P:8:SER:O      | 1.95                     | 0.50              |
| 1:A:228:PHE:O    | 1:A:358:MET:HB2  | 2.12                     | 0.50              |
| 1:A:236:LEU:HD21 | 1:A:243:MET:HE3  | 1.92                     | 0.50              |
| 2:N:236:LEU:HD23 | 2:N:236:LEU:C    | 2.37                     | 0.50              |
| 4:P:117:THR:HG22 | 4:P:118:ILE:CA   | 2.41                     | 0.50              |
| 1:M:23:ALA:HB3   | 1:M:32:ILE:HD13  | 1.93                     | 0.50              |
| 1:M:98:LEU:HD11  | 2:N:127:ALA:CA   | 2.38                     | 0.50              |
| 1:M:488:ARG:NH1  | 1:M:488:ARG:CB   | 2.74                     | 0.50              |
| 2:N:9:GLU:HG3    | 2:N:25:PHE:CZ    | 2.47                     | 0.50              |
| 2:B:240:LEU:C    | 2:B:242:PRO:HD3  | 2.37                     | 0.50              |
| 2:B:241:LYS:O    | 2:B:241:LYS:HG3  | 2.11                     | 0.50              |
| 2:N:110:ILE:O    | 2:N:114:GLU:HG3  | 2.11                     | 0.50              |
| 1:M:452:ARG:NH2  | 2:N:45:ASP:OD2   | 2.45                     | 0.49              |
| 1:M:493:ASP:OD2  | 1:M:499:ASN:CG   | 2.55                     | 0.49              |
| 3:O:50:LYS:HD2   | 4:P:118:ILE:CA   | 2.41                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:336:LYS:O    | 1:A:340:GLY:HA2   | 2.11                     | 0.49              |
| 3:C:50:LYS:CB    | 4:D:118:ILE:HG22  | 2.42                     | 0.49              |
| 1:M:251:GLY:CA   | 1:M:277:PRO:HG2   | 2.29                     | 0.49              |
| 3:C:28:ARG:HD2   | 3:C:29:GLU:OE2    | 2.13                     | 0.49              |
| 3:O:84:LYS:HG3   | 3:O:85:THR:N      | 2.27                     | 0.49              |
| 1:A:244:THR:HG22 | 1:A:331:ILE:HG13  | 1.92                     | 0.49              |
| 2:N:96:PHE:HB3   | 2:N:104:VAL:HB    | 1.93                     | 0.49              |
| 1:A:390:ARG:HD2  | 1:A:395:SER:HB2   | 1.94                     | 0.49              |
| 4:D:0:MET:CG     | 4:D:1:ILE:N       | 2.72                     | 0.49              |
| 4:D:102:GLY:HA2  | 11:D:710:CE1:H62  | 1.93                     | 0.49              |
| 1:M:488:ARG:CB   | 1:M:488:ARG:HH11  | 2.25                     | 0.49              |
| 2:N:225:GLN:HE22 | 2:N:228:LYS:HD2   | 1.76                     | 0.49              |
| 4:P:30:VAL:O     | 4:P:33:LEU:HB3    | 2.12                     | 0.49              |
| 4:P:95:ALA:O     | 4:P:96:GLY:C      | 2.55                     | 0.49              |
| 1:M:1:GLN:HG2    | 1:M:2:THR:N       | 2.27                     | 0.49              |
| 1:M:324:LEU:O    | 1:M:328:LEU:N     | 2.42                     | 0.49              |
| 2:N:208:GLY:N    | 8:N:245:F3S:S1    | 2.81                     | 0.49              |
| 3:O:36:VAL:HG11  | 4:P:82:MET:CE     | 2.43                     | 0.49              |
| 1:A:288:ASP:O    | 1:A:292:GLN:HG3   | 2.13                     | 0.49              |
| 2:B:119:TYR:O    | 2:B:121:ILE:HG13  | 2.13                     | 0.49              |
| 1:M:222:PRO:HG3  | 1:M:362:GLU:OE1   | 2.12                     | 0.49              |
| 4:P:7:ARG:HG2    | 4:P:8:SER:N       | 2.28                     | 0.49              |
| 1:M:321:GLU:HA   | 1:M:324:LEU:HB3   | 1.95                     | 0.49              |
| 1:M:375:PHE:CD1  | 1:M:375:PHE:N     | 2.81                     | 0.49              |
| 1:M:421:ASN:ND2  | 1:M:424:ALA:CB    | 2.61                     | 0.49              |
| 1:A:391:LEU:O    | 1:A:394:ASN:HB2   | 2.13                     | 0.49              |
| 2:B:175:LEU:O    | 2:B:178:ARG:HB3   | 2.13                     | 0.49              |
| 3:C:106:GLU:HB2  | 3:C:107:PRO:HD3   | 1.95                     | 0.49              |
| 2:N:221:ALA:O    | 2:N:225:GLN:HG2   | 2.13                     | 0.49              |
| 3:O:31:THR:O     | 3:O:34:PRO:HD2    | 2.13                     | 0.49              |
| 3:O:103:MET:CG   | 3:O:104:GLY:N     | 2.76                     | 0.49              |
| 1:A:232:HIS:NE2  | 1:A:242:LEU:HD11  | 2.28                     | 0.49              |
| 2:B:222:ALA:HB2  | 3:C:92:LYS:HE3    | 1.95                     | 0.49              |
| 4:D:30:VAL:HG13  | 4:D:31:MET:N      | 2.27                     | 0.49              |
| 2:B:225:GLN:CG   | 10:B:700:BRS:H222 | 2.43                     | 0.48              |
| 3:C:31:THR:O     | 3:C:34:PRO:HD2    | 2.13                     | 0.48              |
| 1:M:40:PRO:HB2   | 1:M:140:PHE:CD1   | 2.48                     | 0.48              |
| 1:M:311:VAL:HG12 | 1:M:312:VAL:N     | 2.28                     | 0.48              |
| 3:C:106:GLU:CD   | 3:C:106:GLU:H     | 2.22                     | 0.48              |
| 1:A:85:PHE:CD2   | 1:A:385:LEU:HD11  | 2.49                     | 0.48              |
| 1:M:66:PHE:CD1   | 1:M:82:VAL:HG12   | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:72:VAL:HG11  | 4:P:108:THR:HG23 | 1.94                     | 0.48              |
| 4:D:93:VAL:N     | 2:N:243:ARG:O    | 2.40                     | 0.48              |
| 3:O:103:MET:HG2  | 3:O:104:GLY:N    | 2.28                     | 0.48              |
| 1:M:7:LEU:CD1    | 1:M:23:ALA:HB1   | 2.43                     | 0.48              |
| 3:O:85:THR:O     | 3:O:89:LEU:HD12  | 2.14                     | 0.48              |
| 1:A:184:ARG:NH1  | 1:A:184:ARG:CG   | 2.76                     | 0.48              |
| 1:A:469:PRO:CB   | 1:A:523:MET:HE1  | 2.43                     | 0.48              |
| 4:P:9:ASP:C      | 4:P:11:PRO:HD2   | 2.39                     | 0.48              |
| 3:C:12:THR:CG2   | 3:C:13:SER:N     | 2.77                     | 0.48              |
| 1:M:465:ILE:HD13 | 1:M:465:ILE:N    | 2.21                     | 0.48              |
| 1:A:127:ALA:HB3  | 1:A:131:THR:HA   | 1.96                     | 0.48              |
| 4:D:4:ASN:CG     | 4:D:4:ASN:O      | 2.56                     | 0.48              |
| 1:M:233:PRO:HG2  | 1:M:248:ARG:NH2  | 2.29                     | 0.48              |
| 1:M:448:TRP:CG   | 1:M:449:ALA:N    | 2.81                     | 0.48              |
| 1:A:308:ARG:HH12 | 1:A:339:VAL:HA   | 1.79                     | 0.48              |
| 4:D:86:MET:CE    | 4:D:91:ILE:HD12  | 2.43                     | 0.48              |
| 2:N:84:TYR:CD1   | 2:N:88:MET:HE3   | 2.49                     | 0.48              |
| 2:N:182:ASP:OD2  | 2:N:184:ARG:HD3  | 2.14                     | 0.48              |
| 1:M:175:MET:HE3  | 1:M:503:LEU:HD13 | 1.96                     | 0.47              |
| 1:M:463:CYS:HA   | 1:M:467:ARG:HE   | 1.78                     | 0.47              |
| 1:M:546:ASN:HD22 | 1:M:546:ASN:N    | 2.10                     | 0.47              |
| 1:M:548:LEU:CD2  | 1:M:575:PRO:HG3  | 2.44                     | 0.47              |
| 2:N:44:LYS:HD3   | 2:N:51:LEU:O     | 2.14                     | 0.47              |
| 3:O:65:ASN:O     | 3:O:65:ASN:OD1   | 2.32                     | 0.47              |
| 2:B:159:PRO:CG   | 2:B:207:VAL:HG21 | 2.44                     | 0.47              |
| 3:O:50:LYS:HD2   | 4:P:117:THR:CG2  | 2.41                     | 0.47              |
| 1:M:304:ILE:HG12 | 1:M:313:TYR:HE2  | 1.79                     | 0.47              |
| 2:N:241:LYS:O    | 2:N:241:LYS:HG3  | 2.14                     | 0.47              |
| 3:C:28:ARG:NH1   | 3:C:29:GLU:OE2   | 2.38                     | 0.47              |
| 4:D:92:HIS:HA    | 2:N:243:ARG:OXT  | 2.15                     | 0.47              |
| 4:D:95:ALA:O     | 4:D:96:GLY:C     | 2.57                     | 0.47              |
| 1:M:2:THR:HG22   | 1:M:3:PHE:N      | 2.29                     | 0.47              |
| 4:P:6:LYS:H      | 4:P:6:LYS:HG3    | 1.36                     | 0.47              |
| 2:N:201:VAL:CG2  | 2:N:202:TRP:N    | 2.77                     | 0.47              |
| 3:O:98:VAL:HG23  | 3:O:103:MET:HB2  | 1.96                     | 0.47              |
| 1:A:126:PHE:N    | 1:A:126:PHE:CD2  | 2.82                     | 0.47              |
| 2:B:81:LEU:N     | 2:B:81:LEU:CD2   | 2.77                     | 0.47              |
| 1:M:7:LEU:HD11   | 1:M:23:ALA:HB1   | 1.97                     | 0.47              |
| 1:M:358:MET:HE1  | 1:M:389:ASN:HA   | 1.96                     | 0.47              |
| 1:M:546:ASN:O    | 1:M:549:LYS:HE3  | 2.15                     | 0.47              |
| 1:A:250:GLU:HB2  | 1:A:319:LEU:HD11 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:7:LYS:HE2     | 2:B:25:PHE:CD2   | 2.50                     | 0.47              |
| 1:M:17:LEU:O      | 1:M:21:ILE:HG13  | 2.15                     | 0.47              |
| 1:M:421:ASN:ND2   | 1:M:424:ALA:H    | 2.13                     | 0.47              |
| 1:A:49:GLU:HG3    | 1:A:244:THR:HB   | 1.96                     | 0.47              |
| 1:A:408:GLU:O     | 1:A:411:THR:HB   | 2.15                     | 0.47              |
| 1:M:89:CYS:N      | 1:M:90:PRO:HD2   | 2.30                     | 0.47              |
| 1:M:159:ASP:OD2   | 1:M:160:ILE:N    | 2.48                     | 0.47              |
| 2:B:100:ARG:NE    | 2:B:101:ASP:OD2  | 2.43                     | 0.46              |
| 1:M:88:HIS:O      | 1:M:401:VAL:HG22 | 2.15                     | 0.46              |
| 1:M:100:GLY:C     | 2:N:184:ARG:HH22 | 2.24                     | 0.46              |
| 2:N:12:ARG:NE     | 2:N:101:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:247:CYS:SG    | 1:A:331:ILE:HG21 | 2.56                     | 0.46              |
| 2:B:11:VAL:HG21   | 2:B:91:GLU:HG2   | 1.97                     | 0.46              |
| 10:B:700:BRS:HC21 | 4:D:14:TRP:HZ2   | 1.80                     | 0.46              |
| 1:M:184:ARG:NH2   | 1:M:426:GLU:HG2  | 2.30                     | 0.46              |
| 1:M:251:GLY:HA2   | 1:M:277:PRO:CG   | 2.29                     | 0.46              |
| 3:O:22:TYR:O      | 3:O:25:TYR:HB3   | 2.15                     | 0.46              |
| 3:O:51:ASN:HB2    | 3:O:55:ALA:CB    | 2.45                     | 0.46              |
| 4:P:48:ALA:HA     | 4:P:53:ARG:HD3   | 1.97                     | 0.46              |
| 1:A:39:TYR:O      | 1:A:40:PRO:C     | 2.58                     | 0.46              |
| 1:A:182:GLN:OE1   | 1:A:184:ARG:NH1  | 2.46                     | 0.46              |
| 1:A:451:ILE:HG23  | 1:A:482:LEU:HD22 | 1.96                     | 0.46              |
| 1:A:466:TYR:CD2   | 1:A:535:LEU:HD21 | 2.51                     | 0.46              |
| 2:B:68:MET:HE1    | 2:B:73:PRO:HD3   | 1.96                     | 0.46              |
| 1:M:242:LEU:HD12  | 1:M:242:LEU:C    | 2.40                     | 0.46              |
| 2:N:28:VAL:HG22   | 2:N:43:ILE:HD11  | 1.97                     | 0.46              |
| 1:A:145:GLN:HB3   | 2:B:119:TYR:CZ   | 2.50                     | 0.46              |
| 4:D:53:ARG:HH11   | 4:D:53:ARG:HG2   | 1.81                     | 0.46              |
| 4:D:57:PHE:CZ     | 4:D:63:GLY:HA2   | 2.51                     | 0.46              |
| 1:M:316:LEU:O     | 1:M:317:ARG:C    | 2.58                     | 0.46              |
| 4:P:114:GLY:O     | 4:P:118:ILE:HG22 | 2.14                     | 0.46              |
| 1:M:219:HIS:O     | 1:M:371:ILE:HD11 | 2.15                     | 0.46              |
| 1:M:481:GLU:O     | 1:M:485:ARG:HG2  | 2.15                     | 0.46              |
| 1:A:55:VAL:HG21   | 1:A:62:PHE:CD2   | 2.51                     | 0.46              |
| 1:A:94:THR:HG23   | 2:B:131:THR:HG22 | 1.97                     | 0.46              |
| 1:A:556:ASP:OD2   | 1:A:562:ARG:NE   | 2.49                     | 0.46              |
| 1:M:342:ASP:OD1   | 1:M:344:VAL:HG22 | 2.16                     | 0.46              |
| 2:N:220:PRO:O     | 2:N:221:ALA:C    | 2.59                     | 0.46              |
| 2:B:188:LYS:NZ    | 2:B:230:GLU:HG3  | 2.30                     | 0.46              |
| 10:B:700:BRS:HC19 | 4:D:18:GLY:CA    | 2.43                     | 0.46              |
| 1:M:428:GLN:O     | 1:M:432:VAL:HG23 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:551:THR:HG23 | 1:M:563:LEU:HD22  | 1.98                     | 0.46              |
| 4:P:1:ILE:N      | 4:P:1:ILE:HD12    | 2.31                     | 0.46              |
| 4:P:26:ILE:HG22  | 4:P:27:ILE:HG13   | 1.96                     | 0.46              |
| 1:A:542:ARG:NH2  | 1:A:544:ASP:OD2   | 2.46                     | 0.46              |
| 3:C:33:VAL:HG22  | 4:D:82:MET:HE2    | 1.96                     | 0.46              |
| 1:M:100:GLY:O    | 1:M:101:CYS:C     | 2.58                     | 0.46              |
| 1:M:206:GLY:HA3  | 2:N:55:TRP:CZ3    | 2.51                     | 0.46              |
| 2:N:12:ARG:HH22  | 2:N:50:ASP:C      | 2.24                     | 0.46              |
| 1:A:304:ILE:HD12 | 1:A:304:ILE:H     | 1.80                     | 0.46              |
| 4:D:9:ASP:HB2    | 11:P:810:CE1:H242 | 1.98                     | 0.46              |
| 1:M:18:ARG:HG2   | 1:M:400:VAL:HA    | 1.98                     | 0.46              |
| 1:M:330:PHE:HB3  | 1:M:331:ILE:HD12  | 1.97                     | 0.46              |
| 1:M:421:ASN:O    | 1:M:425:ILE:HG13  | 2.17                     | 0.46              |
| 1:M:174:ASN:ND2  | 1:M:177:GLU:H     | 2.11                     | 0.45              |
| 3:O:18:LYS:HD2   | 3:O:19:LEU:CD2    | 2.46                     | 0.45              |
| 3:O:38:PHE:CE2   | 3:O:42:LEU:HD11   | 2.52                     | 0.45              |
| 3:C:8:VAL:O      | 3:C:8:VAL:HG12    | 2.14                     | 0.45              |
| 1:M:339:VAL:O    | 1:M:341:VAL:HG23  | 2.16                     | 0.45              |
| 2:N:109:PHE:CE2  | 2:N:113:LEU:HD22  | 2.51                     | 0.45              |
| 2:N:158:CYS:HA   | 8:N:245:F3S:S4    | 2.56                     | 0.45              |
| 3:O:128:LEU:O    | 4:P:45:PRO:HG2    | 2.17                     | 0.45              |
| 2:B:214:CYS:SG   | 2:B:218:VAL:HB    | 2.56                     | 0.45              |
| 3:C:98:VAL:HG22  | 3:C:103:MET:HB3   | 1.98                     | 0.45              |
| 4:D:117:THR:O    | 4:D:118:ILE:C     | 2.54                     | 0.45              |
| 2:N:28:VAL:CG2   | 2:N:43:ILE:HD11   | 2.46                     | 0.45              |
| 2:N:192:MET:O    | 2:N:193:ALA:C     | 2.58                     | 0.45              |
| 2:B:57:CYS:O     | 2:B:58:ARG:CB     | 2.63                     | 0.45              |
| 1:M:35:ILE:CD1   | 1:M:155:HIS:HB3   | 2.46                     | 0.45              |
| 1:A:250:GLU:O    | 1:A:319:LEU:HD11  | 2.17                     | 0.45              |
| 4:D:42:GLY:O     | 4:D:44:PHE:N      | 2.48                     | 0.45              |
| 1:M:151:ARG:NH1  | 1:M:153:ASP:OD2   | 2.49                     | 0.45              |
| 2:N:202:TRP:NE1  | 2:N:231:SER:OG    | 2.48                     | 0.45              |
| 4:P:51:TYR:HD1   | 4:P:52:GLU:H      | 1.55                     | 0.45              |
| 3:C:12:THR:HG22  | 3:C:13:SER:N      | 2.30                     | 0.45              |
| 1:M:92:GLU:HB3   | 1:M:400:VAL:HB    | 1.99                     | 0.45              |
| 1:M:184:ARG:HG3  | 1:M:184:ARG:HH11  | 1.82                     | 0.45              |
| 4:P:53:ARG:NH1   | 4:P:53:ARG:HG2    | 2.32                     | 0.45              |
| 3:C:70:ILE:O     | 3:C:74:ILE:HG13   | 2.16                     | 0.45              |
| 1:M:145:GLN:O    | 1:M:147:PRO:HD3   | 2.16                     | 0.45              |
| 1:M:299:ARG:HE   | 1:M:299:ARG:HB2   | 1.54                     | 0.45              |
| 2:N:168:ILE:HD11 | 2:N:173:ILE:HG12  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:492:THR:HG22 | 1:M:492:THR:O    | 2.16                     | 0.45              |
| 4:P:67:LEU:O     | 4:P:71:ILE:HG13  | 2.16                     | 0.45              |
| 4:P:102:GLY:O    | 4:P:103:LEU:C    | 2.60                     | 0.45              |
| 1:M:570:ILE:HG22 | 1:M:571:THR:N    | 2.31                     | 0.45              |
| 1:M:150:GLN:HG3  | 1:M:152:PHE:CE1  | 2.51                     | 0.44              |
| 1:M:341:VAL:HG13 | 1:M:346:GLU:HB2  | 1.99                     | 0.44              |
| 1:M:480:ALA:O    | 1:M:483:GLN:HB2  | 2.17                     | 0.44              |
| 1:M:1:GLN:HG2    | 1:M:2:THR:H      | 1.83                     | 0.44              |
| 1:M:105:ARG:NH1  | 2:N:134:GLN:H    | 2.15                     | 0.44              |
| 1:M:273:PRO:O    | 1:M:274:LEU:C    | 2.58                     | 0.44              |
| 1:M:443:ASP:CG   | 1:M:444:GLY:N    | 2.74                     | 0.44              |
| 2:N:198:GLN:O    | 2:N:203:SER:HB2  | 2.17                     | 0.44              |
| 2:N:214:CYS:SG   | 9:N:246:SF4:S1   | 3.15                     | 0.44              |
| 3:O:33:VAL:HB    | 3:O:34:PRO:CD    | 2.42                     | 0.44              |
| 1:A:282:MET:HB3  | 1:A:283:GLU:OE1  | 2.17                     | 0.44              |
| 3:C:39:SER:O     | 3:C:43:ILE:HG13  | 2.18                     | 0.44              |
| 4:D:39:LEU:HB3   | 4:D:40:PRO:CD    | 2.47                     | 0.44              |
| 4:D:117:THR:HB   | 4:D:118:ILE:O    | 2.17                     | 0.44              |
| 1:M:38:VAL:O     | 1:M:39:TYR:C     | 2.61                     | 0.44              |
| 1:M:377:VAL:HG22 | 1:M:378:GLY:N    | 2.33                     | 0.44              |
| 1:A:17:LEU:HD22  | 1:A:140:PHE:HA   | 1.99                     | 0.44              |
| 4:D:20:GLY:HA2   | 4:D:73:LEU:HB3   | 2.00                     | 0.44              |
| 4:D:30:VAL:CG1   | 4:D:31:MET:N     | 2.81                     | 0.44              |
| 4:D:72:VAL:O     | 4:D:75:LEU:HB2   | 2.18                     | 0.44              |
| 2:N:126:THR:OG1  | 2:N:129:GLN:HG3  | 2.18                     | 0.44              |
| 2:N:218:VAL:O    | 2:N:219:ASP:HB3  | 2.18                     | 0.44              |
| 4:P:112:LEU:O    | 4:P:116:VAL:HG22 | 2.18                     | 0.44              |
| 3:C:15:TRP:CD2   | 3:C:16:TRP:N     | 2.85                     | 0.44              |
| 2:N:170:PRO:HG2  | 2:N:171:ALA:H    | 1.82                     | 0.44              |
| 4:P:79:LEU:HD12  | 4:P:104:ALA:HB2  | 1.98                     | 0.44              |
| 1:A:2:THR:HA     | 1:A:182:GLN:O    | 2.18                     | 0.44              |
| 1:A:244:THR:HG22 | 1:A:331:ILE:CG1  | 2.47                     | 0.44              |
| 1:A:356:TYR:CZ   | 1:A:390:ARG:HD3  | 2.51                     | 0.44              |
| 2:B:206:PHE:CE1  | 2:B:225:GLN:HG3  | 2.53                     | 0.44              |
| 4:P:109:VAL:O    | 4:P:112:LEU:HB3  | 2.17                     | 0.44              |
| 2:B:142:TYR:O    | 2:B:143:HIS:C    | 2.57                     | 0.44              |
| 2:B:201:VAL:HG23 | 2:B:202:TRP:N    | 2.32                     | 0.44              |
| 1:M:127:ALA:C    | 1:M:128:ALA:O    | 2.60                     | 0.44              |
| 1:M:399:LEU:HD11 | 6:M:803:FAD:C4'  | 2.46                     | 0.44              |
| 1:A:151:ARG:NH1  | 1:A:153:ASP:OD2  | 2.49                     | 0.44              |
| 2:B:81:LEU:O     | 2:B:83:ASP:N     | 2.51                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:113:LEU:HD23 | 2:B:113:LEU:C     | 2.43                     | 0.44              |
| 2:B:160:GLN:OE1  | 2:B:160:GLN:HA    | 2.17                     | 0.44              |
| 4:D:40:PRO:O     | 4:D:41:LEU:HD23   | 2.18                     | 0.44              |
| 1:M:196:GLY:C    | 1:M:198:VAL:H     | 2.26                     | 0.44              |
| 1:A:386:HIS:ND1  | 1:A:390:ARG:HG3   | 2.33                     | 0.44              |
| 2:B:81:LEU:O     | 2:B:82:ARG:C      | 2.60                     | 0.44              |
| 4:D:64:ARG:NH1   | 4:D:115:VAL:O     | 2.51                     | 0.44              |
| 1:M:328:LEU:N    | 1:M:329:PRO:CD    | 2.81                     | 0.44              |
| 1:M:364:ASP:CG   | 1:M:366:ASN:H     | 2.26                     | 0.44              |
| 1:M:434:GLN:HA   | 1:M:434:GLN:NE2   | 2.33                     | 0.44              |
| 1:M:190:MET:O    | 1:M:376:ALA:HA    | 2.18                     | 0.43              |
| 1:M:203:THR:C    | 1:M:204:ASN:HD22  | 2.25                     | 0.43              |
| 1:M:435:ARG:HD2  | 1:M:435:ARG:C     | 2.43                     | 0.43              |
| 2:N:75:LEU:HD11  | 2:N:215:PRO:HG3   | 2.00                     | 0.43              |
| 3:O:49:LEU:HD13  | 3:O:56:TRP:CE3    | 2.53                     | 0.43              |
| 3:C:37:TRP:CZ2   | 3:C:41:GLU:OE1    | 2.71                     | 0.43              |
| 1:M:2:THR:CG2    | 1:M:3:PHE:N       | 2.81                     | 0.43              |
| 1:M:526:LYS:HA   | 1:M:534:ARG:NH1   | 2.33                     | 0.43              |
| 2:N:133:ILE:O    | 2:N:133:ILE:HG22  | 2.17                     | 0.43              |
| 3:O:111:SER:O    | 3:O:114:ALA:HB3   | 2.18                     | 0.43              |
| 3:O:124:LEU:HD23 | 3:O:124:LEU:HA    | 1.79                     | 0.43              |
| 1:A:304:ILE:HD12 | 1:A:304:ILE:N     | 2.33                     | 0.43              |
| 1:A:324:LEU:O    | 1:A:328:LEU:N     | 2.46                     | 0.43              |
| 4:D:70:MET:HE3   | 4:D:70:MET:O      | 2.17                     | 0.43              |
| 2:N:142:TYR:O    | 2:N:143:HIS:C     | 2.60                     | 0.43              |
| 2:N:159:PRO:CG   | 2:N:207:VAL:HG21  | 2.44                     | 0.43              |
| 1:A:40:PRO:HB2   | 1:A:140:PHE:CD1   | 2.53                     | 0.43              |
| 2:B:240:LEU:O    | 2:B:242:PRO:CD    | 2.66                     | 0.43              |
| 1:M:316:LEU:HD22 | 1:M:319:LEU:CD1   | 2.43                     | 0.43              |
| 1:A:273:PRO:O    | 1:A:274:LEU:C     | 2.59                     | 0.43              |
| 2:B:164:ASN:OD1  | 2:B:164:ASN:C     | 2.59                     | 0.43              |
| 3:O:65:ASN:O     | 3:O:67:VAL:N      | 2.51                     | 0.43              |
| 2:B:225:GLN:CD   | 10:B:700:BRS:H222 | 2.38                     | 0.43              |
| 1:M:35:ILE:CG1   | 1:M:36:SER:N      | 2.81                     | 0.43              |
| 1:M:274:LEU:HD22 | 1:M:318:HIS:CD2   | 2.53                     | 0.43              |
| 1:M:304:ILE:HG22 | 1:M:305:SER:N     | 2.34                     | 0.43              |
| 1:M:435:ARG:HH12 | 1:M:439:LEU:CD2   | 2.27                     | 0.43              |
| 3:O:86:TRP:CH2   | 4:P:21:GLY:HA3    | 2.54                     | 0.43              |
| 1:A:493:ASP:OD1  | 1:A:495:SER:OG    | 2.28                     | 0.43              |
| 2:B:136:PRO:HB2  | 3:C:100:ASP:OD1   | 2.18                     | 0.43              |
| 3:C:87:PHE:O     | 3:C:91:PRO:CD     | 2.67                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:86:MET:HA    | 4:D:86:MET:CE     | 2.44                     | 0.43              |
| 1:M:2:THR:HA     | 1:M:182:GLN:O     | 2.18                     | 0.43              |
| 2:N:44:LYS:NZ    | 2:N:49:PRO:O      | 2.42                     | 0.43              |
| 1:A:358:MET:HE3  | 1:A:389:ASN:CA    | 2.27                     | 0.43              |
| 2:B:167:PHE:CD1  | 2:B:203:SER:HB3   | 2.54                     | 0.43              |
| 4:D:109:VAL:O    | 4:D:110:VAL:C     | 2.62                     | 0.43              |
| 1:M:331:ILE:HA   | 1:M:334:LEU:HD12  | 2.01                     | 0.43              |
| 1:M:439:LEU:O    | 1:M:442:GLN:HB3   | 2.19                     | 0.43              |
| 2:N:149:ILE:HG12 | 9:N:246:SF4:S3    | 2.59                     | 0.43              |
| 1:A:83:ASP:O     | 1:A:87:HIS:HD2    | 2.02                     | 0.43              |
| 4:D:64:ARG:CZ    | 4:D:117:THR:CG2   | 2.96                     | 0.43              |
| 1:M:320:GLY:O    | 1:M:324:LEU:HB2   | 2.19                     | 0.43              |
| 1:A:311:VAL:HB   | 1:A:350:VAL:O     | 2.19                     | 0.43              |
| 1:M:449:ALA:HB1  | 2:N:45:ASP:OD2    | 2.18                     | 0.43              |
| 1:A:343:PRO:HG3  | 1:A:348:ILE:HD11  | 2.00                     | 0.42              |
| 1:A:377:VAL:HG21 | 1:A:403:GLY:HA2   | 2.01                     | 0.42              |
| 2:B:225:GLN:HG3  | 10:B:700:BRS:H222 | 2.00                     | 0.42              |
| 4:D:13:PHE:HZ    | 11:D:710:CE1:H102 | 1.83                     | 0.42              |
| 1:M:118:GLY:O    | 1:M:119:MET:C     | 2.62                     | 0.42              |
| 1:M:315:ASP:OD1  | 1:M:317:ARG:HG3   | 2.19                     | 0.42              |
| 3:O:73:LEU:HD23  | 3:O:73:LEU:HA     | 1.79                     | 0.42              |
| 3:O:90:ALA:N     | 3:O:91:PRO:HD2    | 2.33                     | 0.42              |
| 1:A:118:GLY:HA2  | 1:A:279:ASN:HD21  | 1.84                     | 0.42              |
| 1:M:112:ASN:C    | 1:M:126:PHE:HE2   | 2.27                     | 0.42              |
| 1:M:184:ARG:HG3  | 1:M:184:ARG:NH1   | 2.33                     | 0.42              |
| 4:D:98:TRP:NE1   | 11:D:710:CE1:H141 | 2.34                     | 0.42              |
| 1:M:66:PHE:O     | 1:M:70:VAL:HG23   | 2.18                     | 0.42              |
| 1:M:493:ASP:OD2  | 1:M:499:ASN:ND2   | 2.53                     | 0.42              |
| 3:O:118:VAL:O    | 3:O:122:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:274:LEU:HD23 | 1:A:274:LEU:HA    | 1.73                     | 0.42              |
| 2:B:6:LEU:CD2    | 2:B:81:LEU:HD13   | 2.48                     | 0.42              |
| 2:N:26:TYR:HB3   | 2:N:47:LEU:HD13   | 2.00                     | 0.42              |
| 1:A:84:TYR:OH    | 1:A:405:LEU:HD13  | 2.19                     | 0.42              |
| 1:A:135:MET:CE   | 1:A:135:MET:CG    | 2.94                     | 0.42              |
| 1:A:202:ASN:HA   | 1:A:353:THR:HG22  | 2.00                     | 0.42              |
| 4:D:48:ALA:HA    | 4:D:53:ARG:HD3    | 2.01                     | 0.42              |
| 1:A:281:TYR:O    | 1:A:282:MET:C     | 2.63                     | 0.42              |
| 1:M:105:ARG:HH12 | 2:N:134:GLN:H     | 1.68                     | 0.42              |
| 3:O:19:LEU:HA    | 3:O:20:PRO:HD3    | 1.90                     | 0.42              |
| 3:O:123:ILE:HD12 | 4:P:30:VAL:HG11   | 2.00                     | 0.42              |
| 2:B:188:LYS:HZ1  | 2:B:230:GLU:HG3   | 1.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:82:HIS:CE1    | 3:C:86:TRP:CE3    | 3.08                     | 0.42              |
| 2:N:58:ARG:HH11   | 2:N:58:ARG:HD2    | 1.66                     | 0.42              |
| 2:N:61:ILE:O      | 2:N:61:ILE:HG13   | 2.19                     | 0.42              |
| 2:N:67:MET:SD     | 2:N:102:LEU:HD13  | 2.60                     | 0.42              |
| 2:N:150:ASN:HA    | 9:N:246:SF4:S4    | 2.60                     | 0.42              |
| 1:A:196:GLY:HA3   | 1:A:204:ASN:OD1   | 2.20                     | 0.42              |
| 1:M:369:THR:HG23  | 1:M:374:LEU:O     | 2.19                     | 0.42              |
| 3:O:19:LEU:CD2    | 3:O:19:LEU:N      | 2.72                     | 0.42              |
| 3:O:36:VAL:HG11   | 4:P:82:MET:HE1    | 2.00                     | 0.42              |
| 2:B:154:CYS:SG    | 2:B:170:PRO:HG2   | 2.60                     | 0.42              |
| 10:B:700:BRS:O5   | 3:C:89:LEU:HB2    | 2.19                     | 0.42              |
| 3:C:15:TRP:CE3    | 3:C:16:TRP:N      | 2.88                     | 0.42              |
| 1:M:72:GLY:O      | 1:M:389:ASN:HB3   | 2.20                     | 0.42              |
| 1:M:127:ALA:O     | 1:M:128:ALA:C     | 2.63                     | 0.42              |
| 1:M:434:GLN:HA    | 1:M:434:GLN:HE21  | 1.84                     | 0.42              |
| 1:M:552:LEU:HD11  | 1:M:566:SER:OG    | 2.20                     | 0.42              |
| 3:O:16:TRP:CD1    | 3:O:26:MET:HE2    | 2.55                     | 0.42              |
| 4:P:22:MET:O      | 4:P:26:ILE:HD13   | 2.19                     | 0.42              |
| 1:A:181:VAL:HG12  | 1:A:182:GLN:N     | 2.34                     | 0.42              |
| 2:B:9:GLU:CD      | 2:B:89:LYS:HG3    | 2.45                     | 0.42              |
| 3:C:15:TRP:O      | 3:C:18:LYS:HG2    | 2.20                     | 0.42              |
| 1:M:498:PHE:CD2   | 2:N:103:VAL:HG21  | 2.55                     | 0.42              |
| 2:N:95:ASN:O      | 2:N:161:PHE:HE2   | 2.02                     | 0.42              |
| 3:O:36:VAL:CG2    | 3:O:37:TRP:N      | 2.82                     | 0.42              |
| 3:O:98:VAL:HG21   | 3:O:103:MET:HE3   | 2.02                     | 0.42              |
| 11:P:810:CE1:H171 | 11:P:810:CE1:H211 | 2.02                     | 0.42              |
| 3:C:33:VAL:HB     | 3:C:34:PRO:CD     | 2.43                     | 0.41              |
| 1:M:152:PHE:O     | 1:M:155:HIS:HB2   | 2.20                     | 0.41              |
| 1:A:200:ARG:NH1   | 1:A:457:LEU:HD21  | 2.35                     | 0.41              |
| 1:A:558:ASP:OD2   | 1:A:558:ASP:N     | 2.54                     | 0.41              |
| 2:B:105:ASP:OD1   | 2:B:105:ASP:C     | 2.63                     | 0.41              |
| 3:C:53:PRO:HD3    | 4:D:51:TYR:CZ     | 2.54                     | 0.41              |
| 4:D:67:LEU:N      | 4:D:67:LEU:HD22   | 2.34                     | 0.41              |
| 1:M:2:THR:HG23    | 1:M:184:ARG:HG2   | 2.01                     | 0.41              |
| 1:M:155:HIS:O     | 6:M:803:FAD:H2A   | 2.19                     | 0.41              |
| 1:M:222:PRO:HG2   | 1:M:362:GLU:OE1   | 2.20                     | 0.41              |
| 2:N:201:VAL:HG23  | 2:N:202:TRP:CD2   | 2.55                     | 0.41              |
| 4:P:24:SER:O      | 4:P:28:ALA:CB     | 2.67                     | 0.41              |
| 1:M:329:PRO:HG2   | 1:M:330:PHE:N     | 2.34                     | 0.41              |
| 1:A:62:PHE:CE2    | 1:A:90:PRO:HG2    | 2.55                     | 0.41              |
| 1:A:81:VAL:HG21   | 1:A:383:VAL:O     | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:413:ARG:HA   | 1:A:413:ARG:HD3  | 1.73                     | 0.41              |
| 2:B:67:MET:HE2   | 2:B:67:MET:HB3   | 1.85                     | 0.41              |
| 2:B:100:ARG:O    | 2:B:101:ASP:C    | 2.61                     | 0.41              |
| 2:B:174:THR:OG1  | 2:B:220:PRO:HA   | 2.19                     | 0.41              |
| 4:D:67:LEU:HD13  | 4:D:67:LEU:HA    | 1.88                     | 0.41              |
| 1:M:316:LEU:HB3  | 1:M:319:LEU:CD1  | 2.33                     | 0.41              |
| 4:P:70:MET:O     | 4:P:74:PRO:HG2   | 2.20                     | 0.41              |
| 1:A:198:VAL:O    | 1:A:456:GLY:HA2  | 2.21                     | 0.41              |
| 1:A:529:ARG:O    | 1:A:530:GLY:C    | 2.63                     | 0.41              |
| 1:M:119:MET:HE2  | 1:M:391:LEU:HG   | 2.02                     | 0.41              |
| 1:M:150:GLN:HG3  | 1:M:152:PHE:HE1  | 1.86                     | 0.41              |
| 1:M:263:LEU:CD1  | 1:M:283:GLU:HA   | 2.50                     | 0.41              |
| 1:M:390:ARG:HH22 | 5:M:802:OAA:C4   | 2.34                     | 0.41              |
| 2:N:116:ILE:HD11 | 2:N:168:ILE:HD12 | 2.01                     | 0.41              |
| 1:A:146:PHE:HA   | 1:A:147:PRO:HD2  | 1.88                     | 0.41              |
| 2:B:9:GLU:HG3    | 2:B:25:PHE:CZ    | 2.55                     | 0.41              |
| 10:B:700:BRS:O13 | 4:D:14:TRP:NE1   | 2.42                     | 0.41              |
| 3:C:23:ARG:HB3   | 3:C:23:ARG:HH11  | 1.86                     | 0.41              |
| 4:D:93:VAL:H     | 2:N:243:ARG:C    | 2.26                     | 0.41              |
| 1:M:375:PHE:N    | 1:M:375:PHE:HD1  | 2.19                     | 0.41              |
| 2:N:214:CYS:HB2  | 9:N:246:SF4:S1   | 2.60                     | 0.41              |
| 2:N:224:ILE:O    | 2:N:227:GLY:N    | 2.54                     | 0.41              |
| 4:P:79:LEU:HD23  | 4:P:82:MET:CE    | 2.49                     | 0.41              |
| 1:A:41:MET:HG2   | 1:A:42:ARG:HD2   | 2.02                     | 0.41              |
| 1:A:98:LEU:HD23  | 2:B:132:ASN:ND2  | 2.36                     | 0.41              |
| 1:A:195:ALA:O    | 1:A:198:VAL:HG22 | 2.20                     | 0.41              |
| 1:A:247:CYS:HB3  | 1:A:316:LEU:HD21 | 2.03                     | 0.41              |
| 4:D:42:GLY:HA2   | 4:D:44:PHE:CE2   | 2.56                     | 0.41              |
| 1:M:335:ALA:HA   | 1:M:339:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:54:ALA:O     | 1:A:55:VAL:C     | 2.64                     | 0.41              |
| 1:A:76:LEU:HD23  | 1:A:76:LEU:HA    | 1.79                     | 0.41              |
| 1:A:227:GLU:OE1  | 1:A:551:THR:OG1  | 2.26                     | 0.41              |
| 1:A:232:HIS:CD2  | 1:A:242:LEU:CD1  | 3.04                     | 0.41              |
| 2:B:235:PHE:CD2  | 2:B:235:PHE:C    | 2.99                     | 0.41              |
| 3:C:59:PHE:CZ    | 3:C:63:LEU:HD11  | 2.55                     | 0.41              |
| 4:D:68:PHE:HD1   | 4:D:111:THR:HG22 | 1.85                     | 0.41              |
| 1:M:80:ASP:OD2   | 1:M:365:GLN:HG2  | 2.21                     | 0.41              |
| 1:M:100:GLY:O    | 2:N:184:ARG:NH2  | 2.52                     | 0.41              |
| 1:M:329:PRO:CG   | 1:M:330:PHE:H    | 2.32                     | 0.41              |
| 1:M:534:ARG:HD3  | 1:M:539:CYS:HB3  | 2.03                     | 0.41              |
| 2:B:174:THR:O    | 2:B:175:LEU:C    | 2.62                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:212:GLU:HG3  | 3:C:21:PHE:HE2  | 1.85                     | 0.41              |
| 1:M:37:LYS:NZ    | 1:M:211:ASP:OD2 | 2.54                     | 0.41              |
| 1:M:100:GLY:C    | 2:N:184:ARG:NH2 | 2.79                     | 0.41              |
| 1:M:176:MET:SD   | 2:N:99:GLU:HG3  | 2.61                     | 0.41              |
| 1:M:279:ASN:O    | 1:M:280:LYS:CB  | 2.69                     | 0.41              |
| 1:A:232:HIS:CD2  | 1:A:234:THR:H   | 2.35                     | 0.41              |
| 1:A:236:LEU:CD1  | 1:A:243:MET:HE3 | 2.51                     | 0.41              |
| 3:C:65:ASN:O     | 3:C:65:ASN:CG   | 2.62                     | 0.41              |
| 1:M:81:VAL:HG21  | 1:M:383:VAL:O   | 2.20                     | 0.41              |
| 1:M:122:GLU:CD   | 1:M:122:GLU:N   | 2.77                     | 0.41              |
| 1:M:242:LEU:HD11 | 1:M:244:THR:HA  | 2.03                     | 0.41              |
| 1:A:157:VAL:HG12 | 1:A:215:MET:CE  | 2.49                     | 0.40              |
| 4:D:30:VAL:O     | 4:D:33:LEU:HB3  | 2.22                     | 0.40              |
| 1:M:105:ARG:NH1  | 1:M:109:GLY:O   | 2.53                     | 0.40              |
| 1:M:122:GLU:N    | 1:M:122:GLU:OE2 | 2.49                     | 0.40              |
| 1:M:353:THR:HG22 | 1:M:354:ALA:N   | 2.36                     | 0.40              |
| 2:N:155:TYR:HE1  | 2:N:171:ALA:CB  | 2.33                     | 0.40              |
| 2:N:226:GLN:HE21 | 2:N:226:GLN:HB2 | 1.60                     | 0.40              |
| 3:O:130:TRP:C    | 4:P:53:ARG:HH21 | 2.29                     | 0.40              |
| 1:A:230:GLN:HB2  | 1:A:358:MET:HE1 | 2.03                     | 0.40              |
| 1:A:321:GLU:OE1  | 1:A:321:GLU:CA  | 2.68                     | 0.40              |
| 2:B:92:ALA:HB1   | 2:B:104:VAL:CG1 | 2.51                     | 0.40              |
| 2:B:219:ASP:OD2  | 3:C:92:LYS:HE2  | 2.22                     | 0.40              |
| 1:M:62:PHE:HB3   | 1:M:86:VAL:HG23 | 2.02                     | 0.40              |
| 1:M:311:VAL:CG1  | 1:M:312:VAL:N   | 2.84                     | 0.40              |
| 2:N:180:ASN:OD1  | 2:N:188:LYS:HA  | 2.21                     | 0.40              |
| 4:P:72:VAL:HG12  | 4:P:76:TRP:CD1  | 2.56                     | 0.40              |
| 1:A:89:CYS:N     | 1:A:90:PRO:CD   | 2.84                     | 0.40              |
| 2:B:12:ARG:HH22  | 2:B:50:ASP:CG   | 2.29                     | 0.40              |
| 2:B:240:LEU:C    | 2:B:242:PRO:CD  | 2.94                     | 0.40              |
| 3:C:22:TYR:O     | 3:C:25:TYR:HB3  | 2.21                     | 0.40              |
| 1:M:126:PHE:CD2  | 1:M:126:PHE:N   | 2.89                     | 0.40              |
| 2:N:160:GLN:NE2  | 2:N:205:THR:CG2 | 2.84                     | 0.40              |
| 2:N:200:GLY:O    | 2:N:201:VAL:C   | 2.64                     | 0.40              |
| 4:P:62:ILE:HG23  | 4:P:63:GLY:H    | 1.85                     | 0.40              |
| 4:P:104:ALA:O    | 4:P:108:THR:OG1 | 2.31                     | 0.40              |
| 1:A:283:GLU:OE1  | 1:A:283:GLU:N   | 2.44                     | 0.40              |
| 1:M:56:ALA:HB2   | 1:M:125:TRP:HE1 | 1.86                     | 0.40              |
| 1:M:242:LEU:HD21 | 5:M:802:OAA:O1  | 2.22                     | 0.40              |
| 3:O:99:LYS:O     | 3:O:100:ASP:OD1 | 2.38                     | 0.40              |
| 4:P:53:ARG:HG2   | 4:P:53:ARG:HH11 | 1.87                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:45:THR:O     | 1:A:132:GLY:HA3 | 2.21                     | 0.40              |
| 1:A:79:GLN:HB2   | 1:A:569:LYS:O   | 2.22                     | 0.40              |
| 1:A:93:MET:HB3   | 1:A:125:TRP:CE3 | 2.57                     | 0.40              |
| 1:A:413:ARG:HH11 | 1:A:413:ARG:CA  | 2.34                     | 0.40              |
| 1:A:424:ALA:O    | 1:A:425:ILE:C   | 2.64                     | 0.40              |
| 4:D:75:LEU:HA    | 4:D:75:LEU:HD23 | 1.84                     | 0.40              |
| 1:M:44:HIS:CD2   | 6:M:803:FAD:C8M | 2.74                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 575/602 (96%)   | 525 (91%)  | 43 (8%)  | 7 (1%)   | 10          | 41 |
| 1   | M     | 575/602 (96%)   | 506 (88%)  | 59 (10%) | 10 (2%)  | 7           | 35 |
| 2   | B     | 241/243 (99%)   | 218 (90%)  | 19 (8%)  | 4 (2%)   | 7           | 35 |
| 2   | N     | 241/243 (99%)   | 212 (88%)  | 23 (10%) | 6 (2%)   | 4           | 28 |
| 3   | C     | 128/130 (98%)   | 116 (91%)  | 9 (7%)   | 3 (2%)   | 5           | 30 |
| 3   | O     | 128/130 (98%)   | 114 (89%)  | 10 (8%)  | 4 (3%)   | 3           | 25 |
| 4   | D     | 117/119 (98%)   | 103 (88%)  | 13 (11%) | 1 (1%)   | 14          | 46 |
| 4   | P     | 117/119 (98%)   | 106 (91%)  | 10 (8%)  | 1 (1%)   | 14          | 46 |
| All | All   | 2122/2188 (97%) | 1900 (90%) | 186 (9%) | 36 (2%)  | 7           | 35 |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 242 | PRO  |
| 1   | M     | 1   | GLN  |
| 1   | M     | 244 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | O     | 18  | LYS  |
| 1   | A     | 79  | GLN  |
| 1   | A     | 244 | THR  |
| 1   | A     | 321 | GLU  |
| 2   | B     | 56  | SER  |
| 3   | C     | 18  | LYS  |
| 1   | M     | 79  | GLN  |
| 2   | N     | 56  | SER  |
| 1   | A     | 318 | HIS  |
| 1   | M     | 128 | ALA  |
| 1   | M     | 318 | HIS  |
| 2   | N     | 128 | ASP  |
| 3   | O     | 66  | PRO  |
| 3   | O     | 100 | ASP  |
| 2   | B     | 183 | SER  |
| 2   | N     | 101 | ASP  |
| 2   | N     | 115 | ALA  |
| 2   | N     | 183 | SER  |
| 1   | A     | 282 | MET  |
| 3   | C     | 100 | ASP  |
| 1   | M     | 131 | THR  |
| 1   | M     | 329 | PRO  |
| 1   | M     | 344 | VAL  |
| 3   | O     | 103 | MET  |
| 1   | A     | 343 | PRO  |
| 2   | B     | 241 | LYS  |
| 4   | D     | 117 | THR  |
| 1   | M     | 282 | MET  |
| 3   | C     | 65  | ASN  |
| 1   | M     | 444 | GLY  |
| 2   | N     | 242 | PRO  |
| 4   | P     | 99  | VAL  |
| 1   | A     | 444 | GLY  |

### 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     | 460/475 (97%)   | 447 (97%)  | 13 (3%)  | 38          | 60 |
| 1   | M     | 460/475 (97%)   | 434 (94%)  | 26 (6%)  | 18          | 46 |
| 2   | B     | 205/205 (100%)  | 199 (97%)  | 6 (3%)   | 37          | 60 |
| 2   | N     | 205/205 (100%)  | 199 (97%)  | 6 (3%)   | 37          | 60 |
| 3   | C     | 111/111 (100%)  | 105 (95%)  | 6 (5%)   | 20          | 47 |
| 3   | O     | 111/111 (100%)  | 104 (94%)  | 7 (6%)   | 16          | 44 |
| 4   | D     | 97/97 (100%)    | 92 (95%)   | 5 (5%)   | 21          | 48 |
| 4   | P     | 97/97 (100%)    | 94 (97%)   | 3 (3%)   | 35          | 59 |
| All | All   | 1746/1776 (98%) | 1674 (96%) | 72 (4%)  | 27          | 53 |

All (72) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ARG  |
| 1   | A     | 74  | ASP  |
| 1   | A     | 122 | GLU  |
| 1   | A     | 184 | ARG  |
| 1   | A     | 197 | ARG  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 204 | ASN  |
| 1   | A     | 276 | GLU  |
| 1   | A     | 319 | LEU  |
| 1   | A     | 327 | ARG  |
| 1   | A     | 358 | MET  |
| 1   | A     | 413 | ARG  |
| 1   | A     | 560 | THR  |
| 2   | B     | 65  | CYS  |
| 2   | B     | 81  | LEU  |
| 2   | B     | 128 | ASP  |
| 2   | B     | 203 | SER  |
| 2   | B     | 212 | GLU  |
| 2   | B     | 242 | PRO  |
| 3   | C     | 23  | ARG  |
| 3   | C     | 39  | SER  |
| 3   | C     | 50  | LYS  |
| 3   | C     | 84  | LYS  |
| 3   | C     | 92  | LYS  |
| 3   | C     | 103 | MET  |
| 4   | D     | 0   | MET  |
| 4   | D     | 3   | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 4   | ASN  |
| 4   | D     | 86  | MET  |
| 4   | D     | 118 | ILE  |
| 1   | M     | 7   | LEU  |
| 1   | M     | 35  | ILE  |
| 1   | M     | 36  | SER  |
| 1   | M     | 93  | MET  |
| 1   | M     | 122 | GLU  |
| 1   | M     | 126 | PHE  |
| 1   | M     | 143 | SER  |
| 1   | M     | 155 | HIS  |
| 1   | M     | 163 | ASP  |
| 1   | M     | 164 | ASP  |
| 1   | M     | 197 | ARG  |
| 1   | M     | 204 | ASN  |
| 1   | M     | 227 | GLU  |
| 1   | M     | 242 | LEU  |
| 1   | M     | 243 | MET  |
| 1   | M     | 304 | ILE  |
| 1   | M     | 331 | ILE  |
| 1   | M     | 372 | LYS  |
| 1   | M     | 375 | PHE  |
| 1   | M     | 465 | ILE  |
| 1   | M     | 470 | GLU  |
| 1   | M     | 485 | ARG  |
| 1   | M     | 499 | ASN  |
| 1   | M     | 541 | GLU  |
| 1   | M     | 548 | LEU  |
| 1   | M     | 558 | ASP  |
| 2   | N     | 128 | ASP  |
| 2   | N     | 148 | CYS  |
| 2   | N     | 185 | ASP  |
| 2   | N     | 189 | LYS  |
| 2   | N     | 226 | GLN  |
| 2   | N     | 241 | LYS  |
| 3   | O     | 5   | LYS  |
| 3   | O     | 19  | LEU  |
| 3   | O     | 20  | PRO  |
| 3   | O     | 37  | TRP  |
| 3   | O     | 39  | SER  |
| 3   | O     | 54  | GLU  |
| 3   | O     | 89  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | P     | 7   | ARG  |
| 4   | P     | 9   | ASP  |
| 4   | P     | 118 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | HIS  |
| 1   | A     | 67  | HIS  |
| 1   | A     | 87  | HIS  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 141 | GLN  |
| 1   | A     | 155 | HIS  |
| 1   | A     | 204 | ASN  |
| 1   | A     | 232 | HIS  |
| 1   | A     | 279 | ASN  |
| 1   | A     | 428 | GLN  |
| 1   | A     | 434 | GLN  |
| 2   | B     | 134 | GLN  |
| 2   | B     | 150 | ASN  |
| 2   | B     | 194 | GLN  |
| 2   | B     | 196 | ASN  |
| 2   | B     | 225 | GLN  |
| 3   | C     | 51  | ASN  |
| 3   | C     | 64  | GLN  |
| 3   | C     | 72  | ASN  |
| 3   | C     | 82  | HIS  |
| 4   | D     | 4   | ASN  |
| 4   | D     | 59  | GLN  |
| 4   | D     | 92  | HIS  |
| 1   | M     | 1   | GLN  |
| 1   | M     | 27  | ASN  |
| 1   | M     | 57  | GLN  |
| 1   | M     | 137 | HIS  |
| 1   | M     | 174 | ASN  |
| 1   | M     | 182 | GLN  |
| 1   | M     | 186 | ASN  |
| 1   | M     | 204 | ASN  |
| 1   | M     | 230 | GLN  |
| 1   | M     | 264 | GLN  |
| 1   | M     | 292 | GLN  |
| 1   | M     | 366 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 409 | GLN  |
| 1   | M     | 421 | ASN  |
| 1   | M     | 434 | GLN  |
| 1   | M     | 441 | ASN  |
| 1   | M     | 447 | ASN  |
| 1   | M     | 499 | ASN  |
| 1   | M     | 520 | HIS  |
| 1   | M     | 546 | ASN  |
| 1   | M     | 550 | HIS  |
| 2   | N     | 95  | ASN  |
| 2   | N     | 150 | ASN  |
| 2   | N     | 160 | GLN  |
| 2   | N     | 225 | GLN  |
| 2   | N     | 226 | GLN  |
| 3   | O     | 65  | ASN  |
| 3   | O     | 72  | ASN  |
| 3   | O     | 95  | ASN  |
| 4   | P     | 2   | ASN  |
| 4   | P     | 4   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

15 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 | $\# Z  > 2$ |
| 10  | BRS  | N     | 800 | -    | 23,23,23     | 2.34 | 6 (26%)     | 26,33,33    | 1.57 | 6 (23%)     |
| 9   | SF4  | B     | 246 | 2    | 0,12,12      | -    | -           | -           | -    | -           |
| 5   | OAA  | A     | 702 | -    | 8,8,8        | 2.22 | 4 (50%)     | 8,10,10     | 2.21 | 3 (37%)     |
| 11  | CE1  | O     | 811 | -    | 36,36,36     | 1.10 | 0           | 35,35,35    | 1.60 | 10 (28%)    |
| 10  | BRS  | B     | 700 | -    | 23,23,23     | 2.54 | 10 (43%)    | 26,33,33    | 1.87 | 7 (26%)     |
| 11  | CE1  | D     | 710 | -    | 36,36,36     | 1.17 | 2 (5%)      | 35,35,35    | 1.56 | 8 (22%)     |
| 7   | FES  | B     | 244 | 2    | 0,4,4        | -    | -           | -           | -    | -           |
| 6   | FAD  | A     | 703 | -    | 58,58,58     | 2.24 | 12 (20%)    | 85,89,89    | 1.64 | 21 (24%)    |
| 6   | FAD  | M     | 803 | -    | 58,58,58     | 1.73 | 14 (24%)    | 85,89,89    | 1.54 | 14 (16%)    |
| 7   | FES  | N     | 244 | 2    | 0,4,4        | -    | -           | -           | -    | -           |
| 11  | CE1  | P     | 810 | -    | 36,36,36     | 1.10 | 3 (8%)      | 35,35,35    | 1.67 | 9 (25%)     |
| 8   | F3S  | N     | 245 | 2    | 0,9,9        | -    | -           | -           | -    | -           |
| 9   | SF4  | N     | 246 | 2    | 0,12,12      | -    | -           | -           | -    | -           |
| 5   | OAA  | M     | 802 | -    | 8,8,8        | 1.28 | 0           | 8,10,10     | 1.09 | 1 (12%)     |
| 8   | F3S  | B     | 245 | 2    | 0,9,9        | -    | -           | -           | -    | -           |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 10  | BRS  | N     | 800 | -    | -       | 5/12/16/16  | 0/2/2/2 |
| 9   | SF4  | B     | 246 | 2    | -       | -           | 0/6/5/5 |
| 5   | OAA  | A     | 702 | -    | -       | 4/8/8/8     | -       |
| 11  | CE1  | O     | 811 | -    | -       | 17/34/34/34 | -       |
| 10  | BRS  | B     | 700 | -    | -       | 6/12/16/16  | 0/2/2/2 |
| 11  | CE1  | D     | 710 | -    | -       | 17/34/34/34 | -       |
| 7   | FES  | B     | 244 | 2    | -       | -           | 0/1/1/1 |
| 6   | FAD  | A     | 703 | -    | -       | 7/34/50/50  | 0/6/6/6 |
| 6   | FAD  | M     | 803 | -    | -       | 5/34/50/50  | 0/6/6/6 |
| 11  | CE1  | P     | 810 | -    | -       | 14/34/34/34 | -       |
| 7   | FES  | N     | 244 | 2    | -       | -           | 0/1/1/1 |
| 8   | F3S  | N     | 245 | 2    | -       | -           | 0/3/3/3 |
| 9   | SF4  | N     | 246 | 2    | -       | -           | 0/6/5/5 |
| 5   | OAA  | M     | 802 | -    | -       | 4/8/8/8     | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 8   | F3S  | B     | 245 | 2    | -       | -        | 0/3/3/3 |

All (51) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | A     | 703 | FAD  | PA-O3P   | -9.33 | 1.49        | 1.59     |
| 6   | A     | 703 | FAD  | P-O3P    | -9.07 | 1.49        | 1.59     |
| 10  | N     | 800 | BRS  | C12-N1   | 6.60  | 1.57        | 1.45     |
| 6   | M     | 803 | FAD  | PA-O3P   | -5.79 | 1.53        | 1.59     |
| 10  | B     | 700 | BRS  | C17-C16  | 5.37  | 1.47        | 1.38     |
| 6   | M     | 803 | FAD  | P-O3P    | -4.79 | 1.54        | 1.59     |
| 10  | B     | 700 | BRS  | C12-N1   | 4.67  | 1.54        | 1.45     |
| 10  | B     | 700 | BRS  | C8-N4    | 3.98  | 1.54        | 1.45     |
| 10  | N     | 800 | BRS  | C12-C11  | 3.98  | 1.46        | 1.40     |
| 5   | A     | 702 | OAA  | C3-C4    | 3.94  | 1.59        | 1.53     |
| 10  | B     | 700 | BRS  | C17-C18  | 3.76  | 1.45        | 1.38     |
| 6   | A     | 703 | FAD  | C10-N10  | 3.76  | 1.45        | 1.37     |
| 10  | B     | 700 | BRS  | C15-C21  | 3.65  | 1.58        | 1.52     |
| 5   | A     | 702 | OAA  | O3-C3    | 3.52  | 1.30        | 1.23     |
| 10  | B     | 700 | BRS  | C12-C11  | 3.35  | 1.45        | 1.40     |
| 6   | A     | 703 | FAD  | P-O5'    | -3.34 | 1.46        | 1.59     |
| 10  | N     | 800 | BRS  | C15-C21  | 3.23  | 1.58        | 1.52     |
| 10  | B     | 700 | BRS  | C18-CL20 | 3.15  | 1.81        | 1.74     |
| 6   | M     | 803 | FAD  | C4A-N3A  | 2.99  | 1.40        | 1.34     |
| 10  | N     | 800 | BRS  | C8-N4    | 2.99  | 1.52        | 1.45     |
| 10  | N     | 800 | BRS  | C11-C10  | 2.83  | 1.43        | 1.39     |
| 10  | B     | 700 | BRS  | C19-C14  | 2.78  | 1.43        | 1.38     |
| 6   | A     | 703 | FAD  | C9-C9A   | 2.69  | 1.44        | 1.39     |
| 6   | M     | 803 | FAD  | O4B-C1B  | 2.69  | 1.48        | 1.42     |
| 6   | M     | 803 | FAD  | C10-N10  | 2.68  | 1.43        | 1.37     |
| 6   | M     | 803 | FAD  | P-O5'    | -2.66 | 1.49        | 1.59     |
| 6   | A     | 703 | FAD  | C4A-N9A  | -2.63 | 1.32        | 1.37     |
| 10  | N     | 800 | BRS  | C16-C15  | 2.61  | 1.43        | 1.39     |
| 11  | P     | 810 | CE1  | C30-C29  | 2.53  | 1.61        | 1.49     |
| 11  | D     | 710 | CE1  | C27-C26  | 2.53  | 1.61        | 1.49     |
| 11  | D     | 710 | CE1  | O25-C26  | 2.51  | 1.52        | 1.42     |
| 10  | B     | 700 | BRS  | C16-C15  | 2.50  | 1.43        | 1.39     |
| 6   | M     | 803 | FAD  | C5A-C4A  | 2.50  | 1.43        | 1.39     |
| 6   | M     | 803 | FAD  | C5A-N7A  | -2.49 | 1.34        | 1.39     |
| 6   | A     | 703 | FAD  | C5A-N7A  | -2.45 | 1.34        | 1.39     |
| 6   | A     | 703 | FAD  | C4A-N3A  | 2.34  | 1.38        | 1.34     |
| 6   | M     | 803 | FAD  | C9A-N10  | 2.29  | 1.45        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | A     | 702 | OAA  | O2-C1   | 2.28  | 1.38        | 1.30     |
| 6   | A     | 703 | FAD  | O4B-C1B | 2.28  | 1.47        | 1.42     |
| 6   | A     | 703 | FAD  | C4X-N5  | 2.27  | 1.35        | 1.30     |
| 11  | P     | 810 | CE1  | O28-C29 | 2.17  | 1.51        | 1.42     |
| 6   | M     | 803 | FAD  | C1'-C2' | 2.16  | 1.55        | 1.52     |
| 6   | A     | 703 | FAD  | C5A-C4A | 2.14  | 1.42        | 1.39     |
| 6   | M     | 803 | FAD  | C8A-N7A | 2.14  | 1.35        | 1.31     |
| 6   | A     | 703 | FAD  | O2'-C2' | -2.13 | 1.38        | 1.43     |
| 6   | M     | 803 | FAD  | C5X-N5  | -2.12 | 1.35        | 1.39     |
| 5   | A     | 702 | OAA  | O5-C4   | 2.11  | 1.36        | 1.30     |
| 10  | B     | 700 | BRS  | C14-C15 | 2.06  | 1.42        | 1.39     |
| 11  | P     | 810 | CE1  | C35-C36 | 2.05  | 1.60        | 1.49     |
| 6   | M     | 803 | FAD  | C1B-N9A | 2.03  | 1.51        | 1.46     |
| 6   | M     | 803 | FAD  | C9-C9A  | 2.01  | 1.42        | 1.39     |

All (79) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms        | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------------|-------|-------------|----------|
| 6   | A     | 703 | FAD  | N3A-C2A-N1A  | -5.36 | 120.47      | 128.58   |
| 6   | M     | 803 | FAD  | N3A-C2A-N1A  | -5.34 | 120.50      | 128.58   |
| 6   | A     | 703 | FAD  | N3A-C4A-N9A  | 4.00  | 133.98      | 127.17   |
| 6   | M     | 803 | FAD  | C4'-C3'-C2'  | -3.81 | 107.22      | 113.57   |
| 6   | M     | 803 | FAD  | N3A-C4A-N9A  | 3.71  | 133.48      | 127.17   |
| 6   | M     | 803 | FAD  | C5A-C4A-N3A  | -3.70 | 121.62      | 126.72   |
| 6   | A     | 703 | FAD  | C4A-N9A-C8A  | 3.68  | 109.60      | 105.74   |
| 5   | A     | 702 | OAA  | O4-C4-C3     | 3.65  | 126.35      | 121.81   |
| 5   | A     | 702 | OAA  | O3-C3-C2     | 3.62  | 125.97      | 120.41   |
| 6   | A     | 703 | FAD  | C5A-C4A-N3A  | -3.58 | 121.79      | 126.72   |
| 6   | M     | 803 | FAD  | C4-N3-C2     | -3.56 | 119.33      | 125.64   |
| 10  | N     | 800 | BRS  | C9-C10-C21   | -3.41 | 117.89      | 122.20   |
| 10  | B     | 700 | BRS  | C9-C10-C11   | 3.39  | 120.96      | 117.49   |
| 6   | A     | 703 | FAD  | C2A-N3A-C4A  | 3.38  | 120.08      | 111.83   |
| 6   | A     | 703 | FAD  | C5X-N5-C4X   | 3.29  | 123.42      | 118.09   |
| 6   | M     | 803 | FAD  | C2A-N3A-C4A  | 3.28  | 119.84      | 111.83   |
| 10  | B     | 700 | BRS  | C17-C18-CL20 | 3.27  | 124.19      | 119.36   |
| 6   | M     | 803 | FAD  | C5X-N5-C4X   | 3.02  | 122.98      | 118.09   |
| 11  | O     | 811 | CE1  | O16-C17-C18  | 2.99  | 124.00      | 110.35   |
| 10  | B     | 700 | BRS  | O2-N1-C12    | 2.99  | 124.14      | 119.03   |
| 10  | N     | 800 | BRS  | C7-C12-C11   | -2.98 | 118.51      | 121.54   |
| 6   | A     | 703 | FAD  | O4B-C1B-N9A  | 2.95  | 113.75      | 108.09   |
| 10  | B     | 700 | BRS  | C19-C18-C17  | -2.95 | 117.59      | 121.24   |
| 11  | P     | 810 | CE1  | O25-C26-C27  | 2.90  | 123.56      | 110.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | M     | 803 | FAD  | C4X-C4-N3   | 2.86  | 120.52      | 113.25   |
| 6   | A     | 703 | FAD  | C4-N3-C2    | -2.85 | 120.58      | 125.64   |
| 5   | A     | 702 | OAA  | O3-C3-C4    | 2.75  | 123.60      | 119.67   |
| 10  | B     | 700 | BRS  | C14-C19-C18 | 2.73  | 121.99      | 119.24   |
| 6   | A     | 703 | FAD  | C4'-C3'-C2' | -2.73 | 109.03      | 113.57   |
| 11  | P     | 810 | CE1  | O22-C23-C24 | 2.69  | 122.60      | 110.35   |
| 10  | N     | 800 | BRS  | O2-N1-C12   | 2.69  | 123.63      | 119.03   |
| 10  | N     | 800 | BRS  | C7-C8-N4    | 2.68  | 121.05      | 118.74   |
| 6   | M     | 803 | FAD  | C4A-N9A-C8A | 2.67  | 108.54      | 105.74   |
| 6   | M     | 803 | FAD  | O4-C4-C4X   | -2.65 | 119.53      | 126.53   |
| 10  | B     | 700 | BRS  | C22-C21-C10 | -2.52 | 107.86      | 112.21   |
| 11  | P     | 810 | CE1  | O22-C21-C20 | 2.51  | 121.77      | 110.35   |
| 11  | D     | 710 | CE1  | O16-C17-C18 | 2.49  | 121.71      | 110.35   |
| 11  | O     | 811 | CE1  | O19-C18-C17 | 2.49  | 121.69      | 110.35   |
| 10  | N     | 800 | BRS  | C9-C10-C11  | 2.45  | 119.99      | 117.49   |
| 6   | A     | 703 | FAD  | N9A-C8A-N7A | -2.44 | 110.48      | 113.94   |
| 6   | M     | 803 | FAD  | C10-N1-C2   | 2.43  | 122.12      | 116.85   |
| 11  | P     | 810 | CE1  | O28-C29-C30 | 2.43  | 121.44      | 110.35   |
| 6   | A     | 703 | FAD  | C4X-C4-N3   | 2.40  | 119.35      | 113.25   |
| 11  | D     | 710 | CE1  | O13-C14-C15 | 2.37  | 121.17      | 110.35   |
| 6   | M     | 803 | FAD  | C2A-N1A-C6A | 2.36  | 122.61      | 118.73   |
| 6   | A     | 703 | FAD  | C7M-C7-C6   | -2.34 | 115.45      | 119.57   |
| 6   | A     | 703 | FAD  | C5'-C4'-C3' | 2.34  | 116.63      | 112.22   |
| 6   | A     | 703 | FAD  | C10-C4X-N5  | -2.33 | 120.05      | 124.81   |
| 11  | O     | 811 | CE1  | O28-C27-C26 | 2.33  | 120.95      | 110.35   |
| 6   | A     | 703 | FAD  | C4X-C10-N1  | -2.32 | 118.89      | 124.59   |
| 6   | A     | 703 | FAD  | C10-N1-C2   | 2.30  | 121.83      | 116.85   |
| 11  | D     | 710 | CE1  | O22-C21-C20 | 2.28  | 120.73      | 110.35   |
| 11  | O     | 811 | CE1  | O22-C23-C24 | 2.25  | 120.61      | 110.35   |
| 11  | O     | 811 | CE1  | O25-C26-C27 | 2.25  | 120.59      | 110.35   |
| 11  | D     | 710 | CE1  | O13-C12-C11 | 2.24  | 122.07      | 110.32   |
| 6   | M     | 803 | FAD  | O4B-C1B-N9A | 2.23  | 112.38      | 108.09   |
| 11  | O     | 811 | CE1  | O16-C15-C14 | 2.23  | 120.54      | 110.35   |
| 6   | A     | 703 | FAD  | O4-C4-C4X   | -2.23 | 120.65      | 126.53   |
| 11  | O     | 811 | CE1  | O34-C35-C36 | 2.22  | 119.91      | 110.11   |
| 11  | D     | 710 | CE1  | O28-C29-C30 | 2.21  | 120.43      | 110.35   |
| 11  | P     | 810 | CE1  | O31-C32-C33 | 2.21  | 120.41      | 110.35   |
| 11  | D     | 710 | CE1  | O22-C23-C24 | 2.20  | 120.40      | 110.35   |
| 11  | P     | 810 | CE1  | O13-C12-C11 | 2.19  | 121.84      | 110.32   |
| 10  | N     | 800 | BRS  | C22-C21-C10 | -2.18 | 108.45      | 112.21   |
| 11  | O     | 811 | CE1  | O25-C24-C23 | 2.17  | 120.26      | 110.35   |
| 6   | A     | 703 | FAD  | O3P-P-O1P   | -2.17 | 104.18      | 110.70   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 11  | D     | 710 | CE1  | O31-C32-C33 | 2.14 | 120.09      | 110.35   |
| 11  | P     | 810 | CE1  | O16-C17-C18 | 2.14 | 120.09      | 110.35   |
| 6   | A     | 703 | FAD  | C4-C4X-N5   | 2.13 | 121.14      | 118.21   |
| 10  | B     | 700 | BRS  | C7-C8-N4    | 2.12 | 120.56      | 118.74   |
| 11  | P     | 810 | CE1  | O25-C24-C23 | 2.09 | 119.87      | 110.35   |
| 11  | O     | 811 | CE1  | O31-C30-C29 | 2.08 | 119.84      | 110.35   |
| 5   | M     | 802 | OAA  | O4-C4-C3    | 2.08 | 124.39      | 121.81   |
| 6   | M     | 803 | FAD  | C5'-C4'-C3' | 2.07 | 116.12      | 112.22   |
| 6   | A     | 703 | FAD  | O2P-P-O3P   | 2.06 | 112.84      | 107.27   |
| 11  | D     | 710 | CE1  | O19-C18-C17 | 2.06 | 119.72      | 110.35   |
| 11  | O     | 811 | CE1  | O13-C14-C15 | 2.06 | 119.72      | 110.35   |
| 6   | A     | 703 | FAD  | C7M-C7-C8   | 2.02 | 124.88      | 120.76   |
| 11  | P     | 810 | CE1  | O37-C36-C35 | 2.01 | 123.67      | 111.82   |

There are no chirality outliers.

All (79) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 702 | OAA  | O3-C3-C4-O4     |
| 5   | A     | 702 | OAA  | O3-C3-C4-O5     |
| 5   | A     | 702 | OAA  | C2-C3-C4-O5     |
| 5   | M     | 802 | OAA  | O3-C3-C4-O4     |
| 5   | M     | 802 | OAA  | O3-C3-C4-O5     |
| 5   | M     | 802 | OAA  | C2-C3-C4-O5     |
| 6   | A     | 703 | FAD  | N10-C1'-C2'-O2' |
| 6   | A     | 703 | FAD  | N10-C1'-C2'-C3' |
| 6   | A     | 703 | FAD  | PA-O3P-P-O5'    |
| 6   | M     | 803 | FAD  | N10-C1'-C2'-O2' |
| 6   | M     | 803 | FAD  | N10-C1'-C2'-C3' |
| 6   | M     | 803 | FAD  | PA-O3P-P-O5'    |
| 11  | P     | 810 | CE1  | O13-C14-C15-O16 |
| 11  | P     | 810 | CE1  | O28-C29-C30-O31 |
| 11  | O     | 811 | CE1  | C17-C18-O19-C20 |
| 11  | D     | 710 | CE1  | O28-C29-C30-O31 |
| 11  | D     | 710 | CE1  | O34-C35-C36-O37 |
| 11  | D     | 710 | CE1  | O25-C26-C27-O28 |
| 11  | D     | 710 | CE1  | O13-C14-C15-O16 |
| 11  | P     | 810 | CE1  | O22-C23-C24-O25 |
| 11  | P     | 810 | CE1  | O34-C35-C36-O37 |
| 11  | P     | 810 | CE1  | C11-C10-C9-C8   |
| 11  | O     | 811 | CE1  | O25-C26-C27-O28 |
| 11  | P     | 810 | CE1  | O25-C26-C27-O28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | O     | 811 | CE1  | C7-C8-C9-C10    |
| 11  | D     | 710 | CE1  | C2-C3-C4-C5     |
| 11  | D     | 710 | CE1  | C6-C7-C8-C9     |
| 11  | O     | 811 | CE1  | C6-C7-C8-C9     |
| 11  | O     | 811 | CE1  | O34-C35-C36-O37 |
| 11  | O     | 811 | CE1  | C36-C35-O34-C33 |
| 11  | P     | 810 | CE1  | C36-C35-O34-C33 |
| 5   | A     | 702 | OAA  | C2-C3-C4-O4     |
| 5   | M     | 802 | OAA  | C2-C3-C4-O4     |
| 11  | D     | 710 | CE1  | C36-C35-O34-C33 |
| 11  | P     | 810 | CE1  | C33-C32-O31-C30 |
| 11  | O     | 811 | CE1  | C3-C4-C5-C6     |
| 11  | O     | 811 | CE1  | C32-C33-O34-C35 |
| 11  | D     | 710 | CE1  | C11-C12-O13-C14 |
| 10  | B     | 700 | BRS  | C11-C10-C21-C15 |
| 6   | A     | 703 | FAD  | C5B-O5B-PA-O1A  |
| 6   | M     | 803 | FAD  | C5B-O5B-PA-O1A  |
| 11  | D     | 710 | CE1  | C24-C23-O22-C21 |
| 11  | O     | 811 | CE1  | C20-C21-O22-C23 |
| 11  | O     | 811 | CE1  | O28-C29-C30-O31 |
| 11  | D     | 710 | CE1  | C11-C10-C9-C8   |
| 10  | N     | 800 | BRS  | C11-C10-C21-C15 |
| 11  | D     | 710 | CE1  | C14-C15-O16-C17 |
| 11  | P     | 810 | CE1  | C24-C23-O22-C21 |
| 11  | P     | 810 | CE1  | C4-C5-C6-C7     |
| 11  | D     | 710 | CE1  | C18-C17-O16-C15 |
| 10  | B     | 700 | BRS  | C11-C10-C21-C22 |
| 11  | P     | 810 | CE1  | C6-C7-C8-C9     |
| 11  | D     | 710 | CE1  | O22-C23-C24-O25 |
| 11  | D     | 710 | CE1  | O16-C17-C18-O19 |
| 11  | P     | 810 | CE1  | O16-C17-C18-O19 |
| 10  | N     | 800 | BRS  | C11-C10-C21-C22 |
| 6   | M     | 803 | FAD  | O4B-C4B-C5B-O5B |
| 11  | O     | 811 | CE1  | C11-C12-O13-C14 |
| 11  | O     | 811 | CE1  | C24-C23-O22-C21 |
| 6   | A     | 703 | FAD  | O4B-C4B-C5B-O5B |
| 10  | N     | 800 | BRS  | C16-C15-C21-C22 |
| 10  | N     | 800 | BRS  | C9-C10-C21-C15  |
| 10  | B     | 700 | BRS  | C9-C10-C21-C15  |
| 11  | D     | 710 | CE1  | C30-C29-O28-C27 |
| 10  | B     | 700 | BRS  | C9-C10-C21-C22  |
| 11  | O     | 811 | CE1  | O16-C17-C18-O19 |

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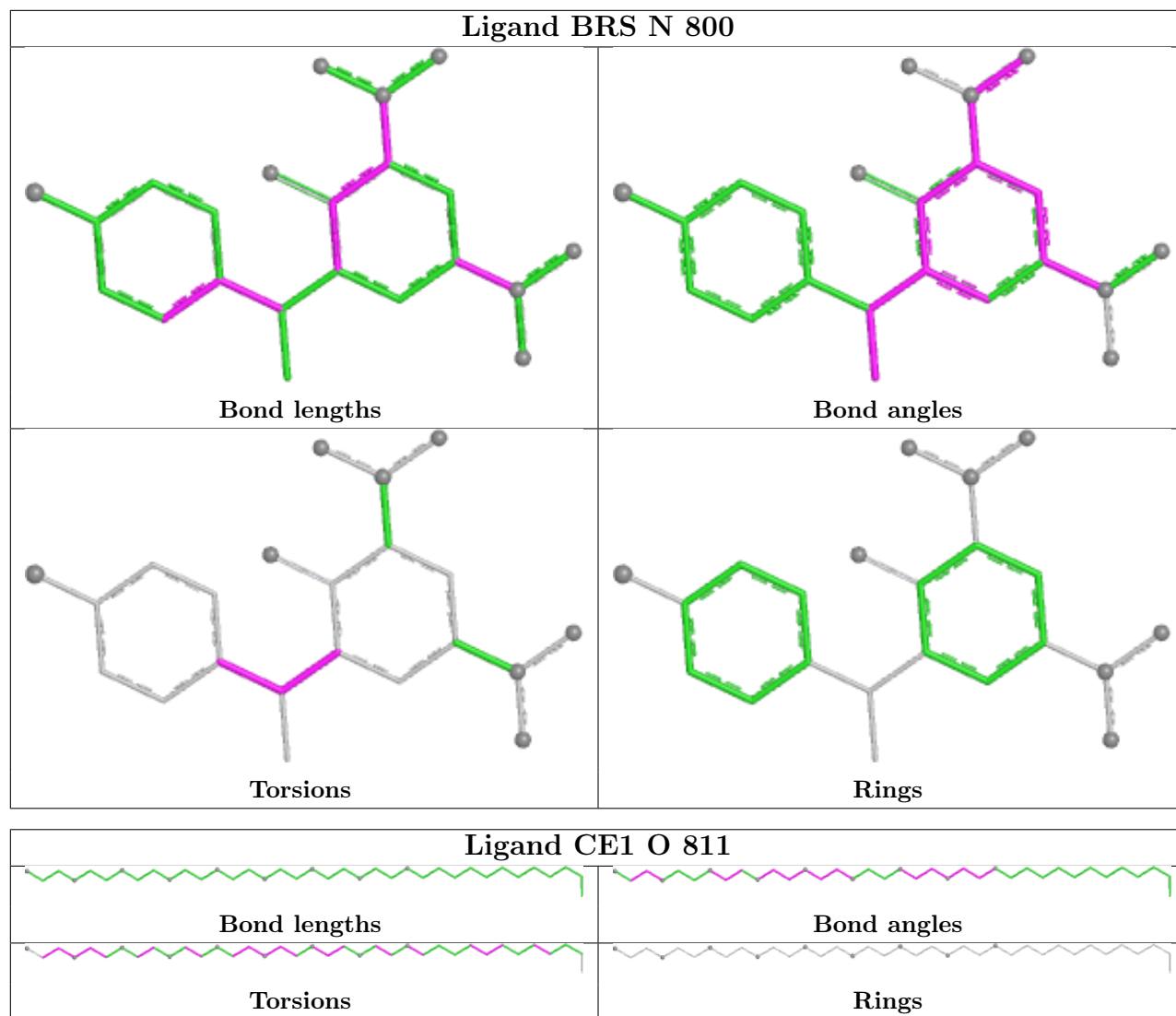
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | B     | 700 | BRS  | C14-C15-C21-C22 |
| 10  | B     | 700 | BRS  | C16-C15-C21-C22 |
| 10  | N     | 800 | BRS  | C14-C15-C21-C22 |
| 11  | P     | 810 | CE1  | C11-C12-O13-C14 |
| 11  | O     | 811 | CE1  | O22-C23-C24-O25 |
| 11  | D     | 710 | CE1  | O19-C20-C21-O22 |
| 11  | O     | 811 | CE1  | O19-C20-C21-O22 |
| 11  | O     | 811 | CE1  | O31-C32-C33-O34 |
| 11  | P     | 810 | CE1  | O19-C20-C21-O22 |
| 11  | D     | 710 | CE1  | C23-C24-O25-C26 |
| 11  | O     | 811 | CE1  | O13-C14-C15-O16 |
| 6   | A     | 703 | FAD  | PA-O3P-P-O1P    |
| 6   | A     | 703 | FAD  | PA-O3P-P-O2P    |

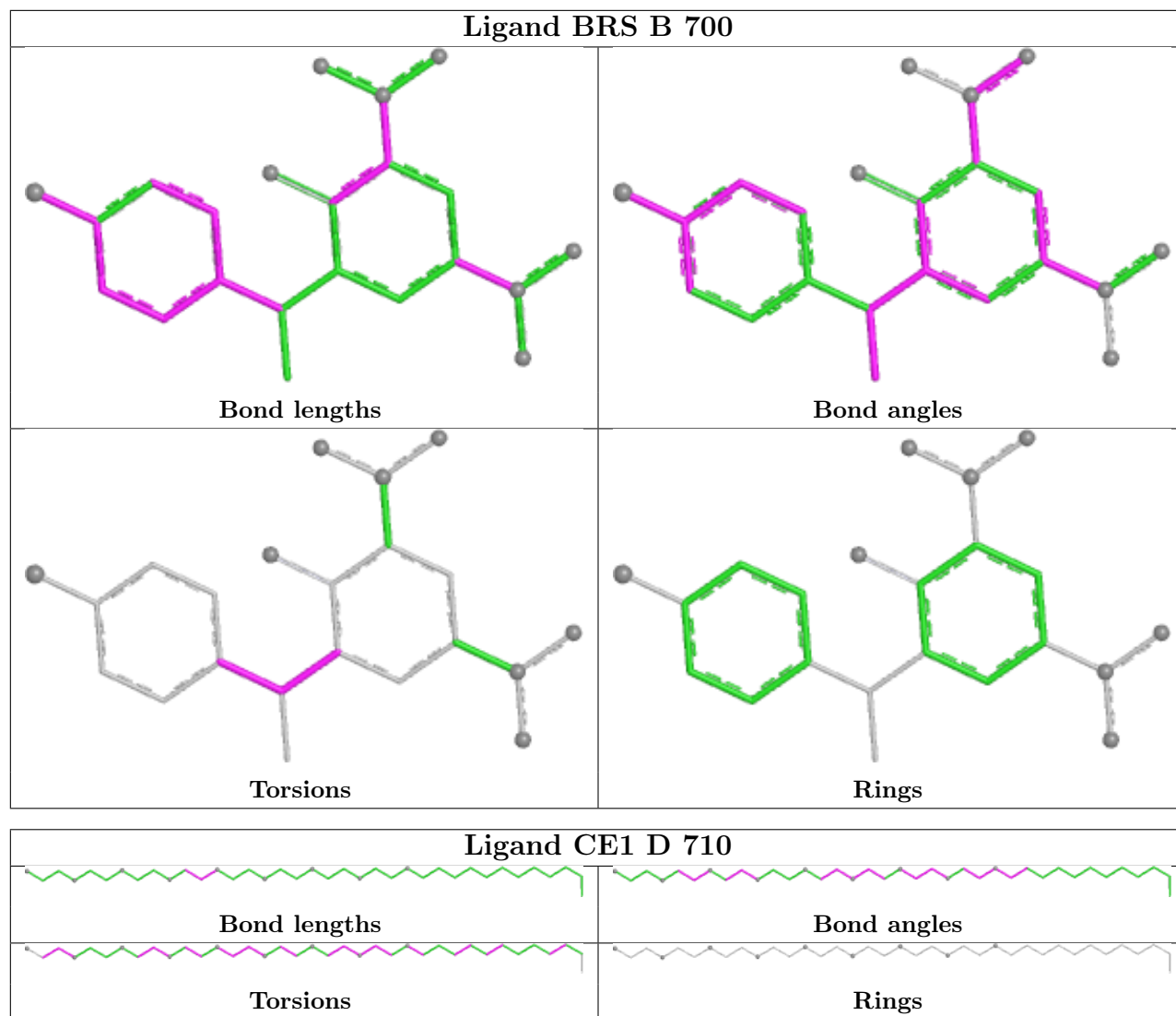
There are no ring outliers.

11 monomers are involved in 56 short contacts:

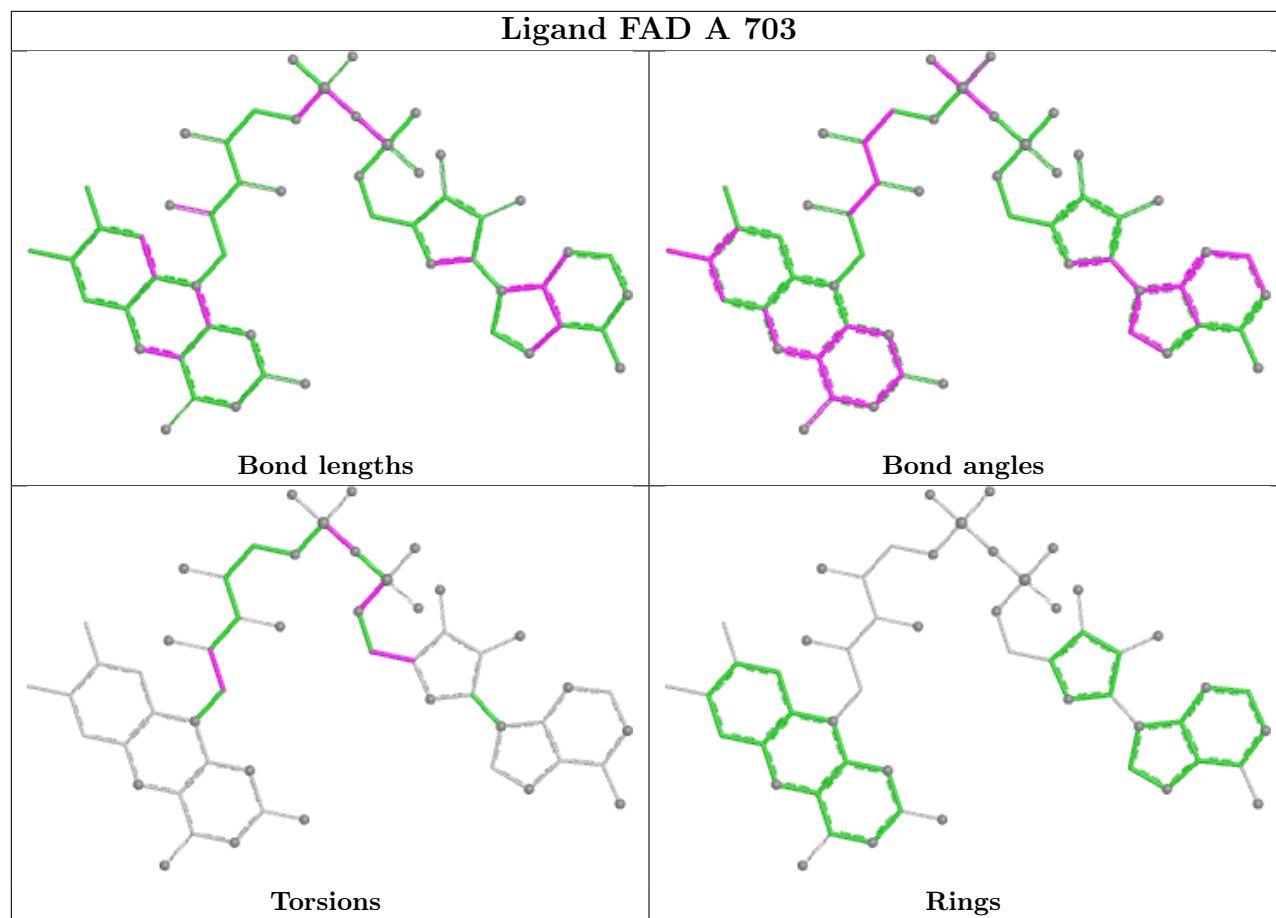
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10  | N     | 800 | BRS  | 5       | 0            |
| 5   | A     | 702 | OAA  | 1       | 0            |
| 11  | O     | 811 | CE1  | 1       | 0            |
| 10  | B     | 700 | BRS  | 13      | 0            |
| 11  | D     | 710 | CE1  | 5       | 0            |
| 6   | A     | 703 | FAD  | 7       | 0            |
| 6   | M     | 803 | FAD  | 11      | 0            |
| 11  | P     | 810 | CE1  | 2       | 0            |
| 8   | N     | 245 | F3S  | 2       | 0            |
| 9   | N     | 246 | SF4  | 7       | 0            |
| 5   | M     | 802 | OAA  | 2       | 0            |

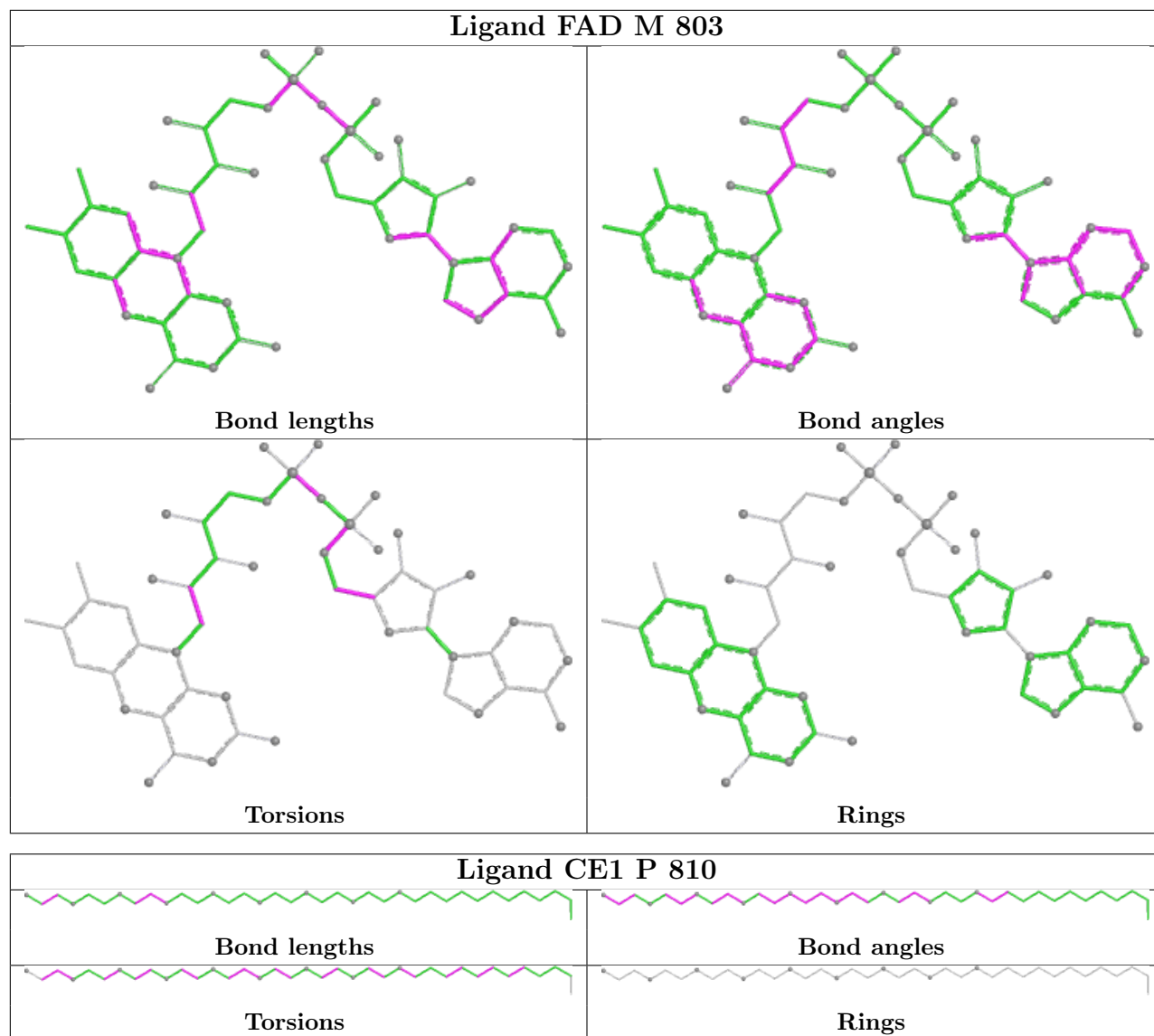
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





## Ligand FAD A 703





## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.