



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:33 PM EDT

PDB ID : 1YCG / pdb\_00001ycg  
Title : X-ray Structures of Moorella thermoacetica FprA. Novel Diiron Site Structure and Mechanistic Insights into a Scavenging Nitric Oxide Reductase  
Authors : Silaghi-Dumitrescu, R.; Kurtz, D.M.; Lanzilotta, W.N.  
Deposited on : 2004-12-22  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

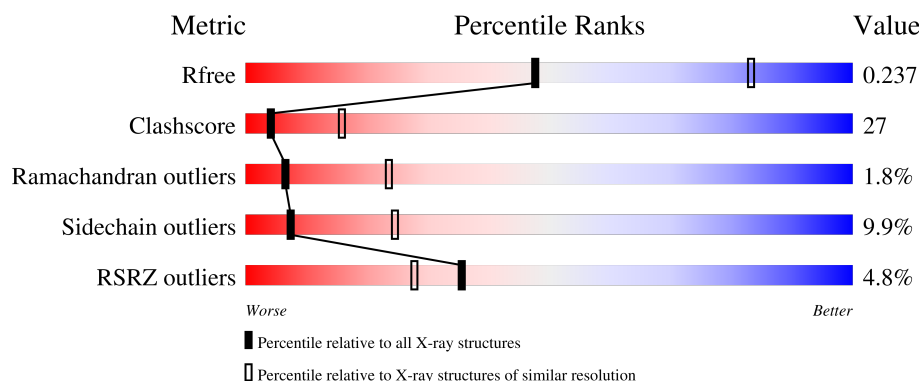
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

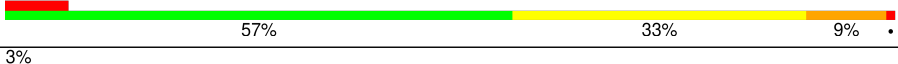
The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 398    |  |
| 1   | B     | 398    |  |
| 1   | C     | 398    |  |
| 1   | D     | 398    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | FEO  | A     | 501 | -         | -        | X       | -                |
| 3   | FEO  | B     | 511 | -         | -        | X       | -                |
| 3   | FEO  | D     | 531 | -         | -        | X       | -                |
| 4   | EDO  | A     | 602 | -         | -        | X       | -                |
| 4   | EDO  | B     | 612 | -         | -        | X       | -                |
| 4   | EDO  | C     | 622 | -         | -        | X       | -                |
| 4   | EDO  | D     | 632 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12758 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.

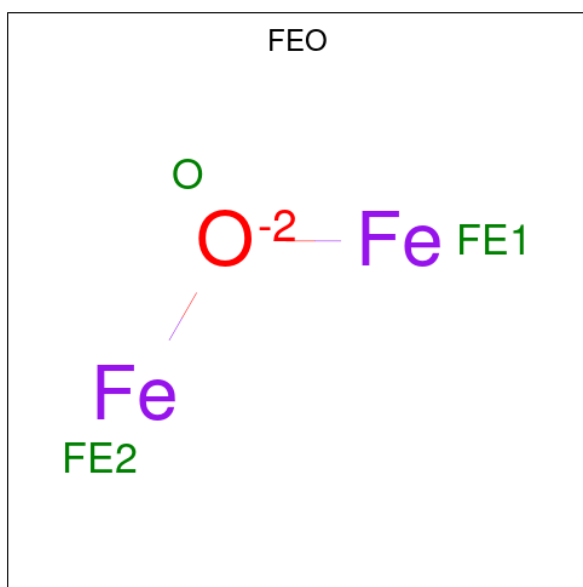
- Molecule 1 is a protein called Nitric oxide reductase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 398      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3115  | 2006 | 525 | 572 | 12 |         |         |       |
| 1   | B     | 398      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3115  | 2006 | 525 | 572 | 12 |         |         |       |
| 1   | C     | 398      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3115  | 2006 | 525 | 572 | 12 |         |         |       |
| 1   | D     | 398      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3115  | 2006 | 525 | 572 | 12 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

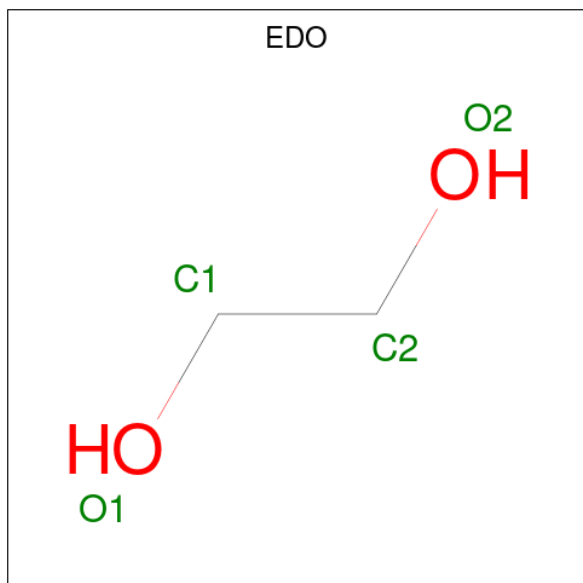
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 4        | Total | Zn | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 2   | B     | 4        | Total | Zn | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 2   | C     | 3        | Total | Zn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | D     | 3        | Total | Zn | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe<sub>2</sub>O).



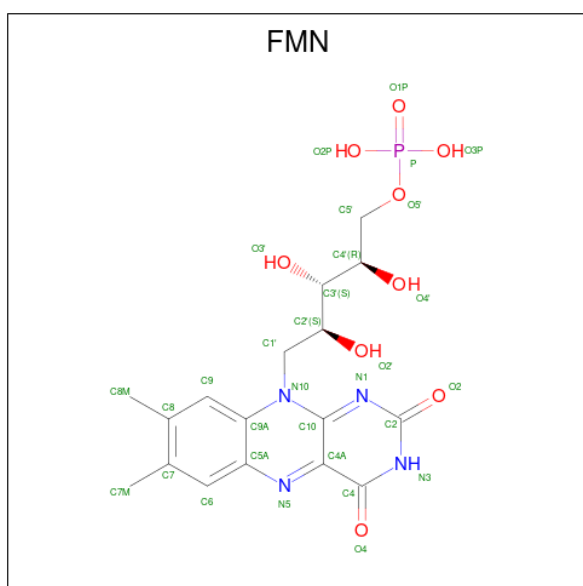
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | Fe | O | 0       | 0       |
|     |       |          | 3     | 2  | 1 |         |         |
| 3   | B     | 1        | Total | Fe | O | 0       | 0       |
|     |       |          | 3     | 2  | 1 |         |         |
| 3   | C     | 1        | Total | Fe | O | 0       | 0       |
|     |       |          | 3     | 2  | 1 |         |         |
| 3   | D     | 1        | Total | Fe | O | 0       | 0       |
|     |       |          | 3     | 2  | 1 |         |         |

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | C     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | D     | 1        | Total C O<br>4 2 2 | 0       | 0       |

- Molecule 5 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



| Mol | Chain | Residues | Atoms                        | ZeroOcc | AltConf |
|-----|-------|----------|------------------------------|---------|---------|
| 5   | A     | 1        | Total C N O P<br>31 17 4 9 1 | 0       | 0       |
| 5   | B     | 1        | Total C N O P<br>31 17 4 9 1 | 0       | 0       |
| 5   | C     | 1        | Total C N O P<br>31 17 4 9 1 | 0       | 0       |
| 5   | D     | 1        | Total C N O P<br>31 17 4 9 1 | 0       | 0       |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 6   | A     | 31       | Total O<br>31 31 | 0       | 0       |
| 6   | B     | 26       | Total O<br>26 26 | 0       | 0       |

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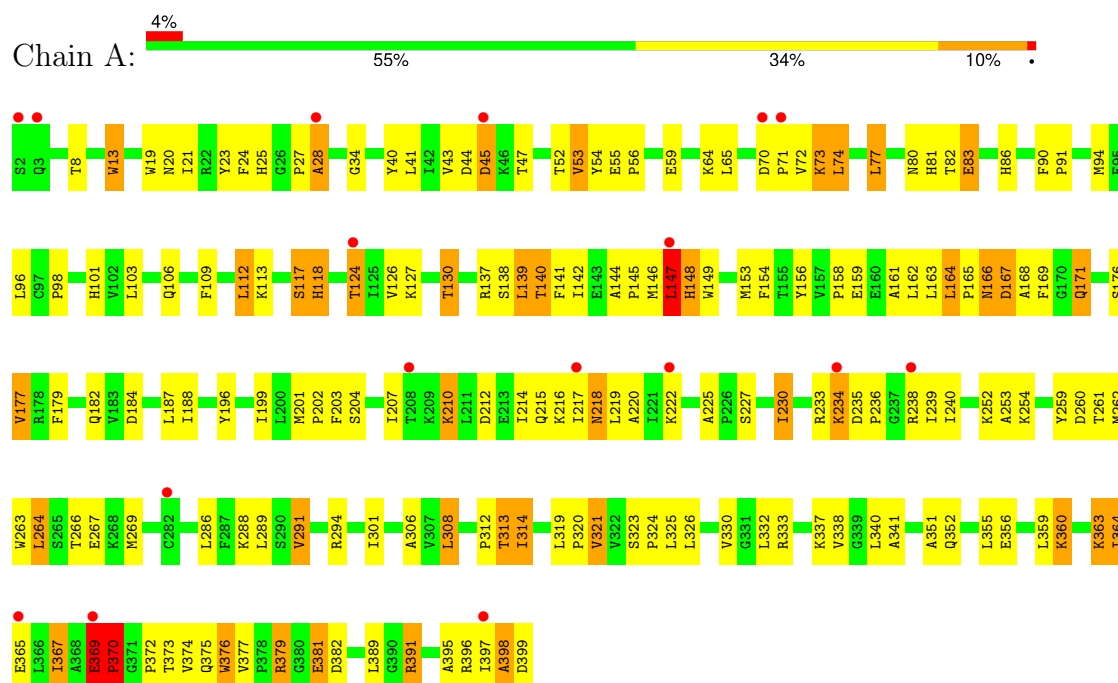
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | C     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 6   | D     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |

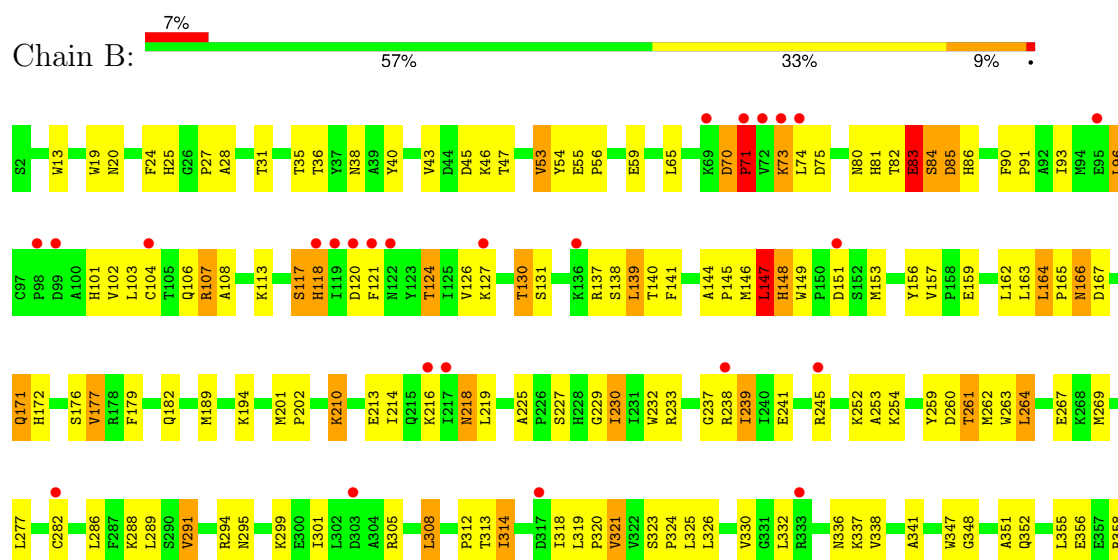
### 3 Residue-property plots

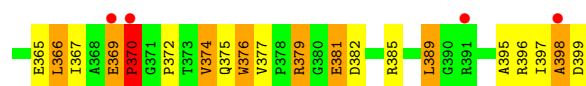
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Nitric oxide reductase

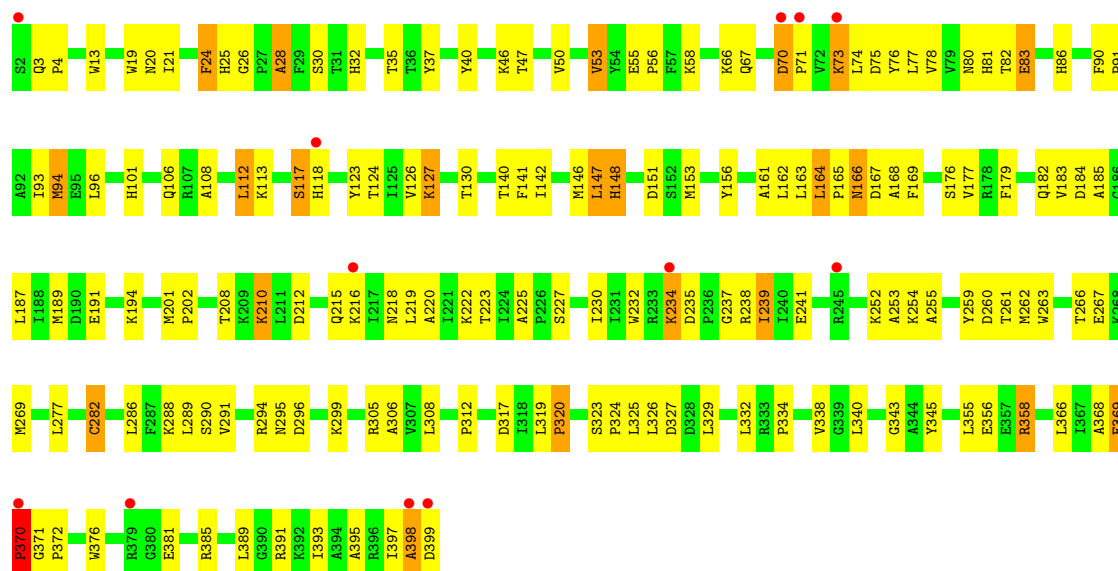


#### • Molecule 1: Nitric oxide reductase

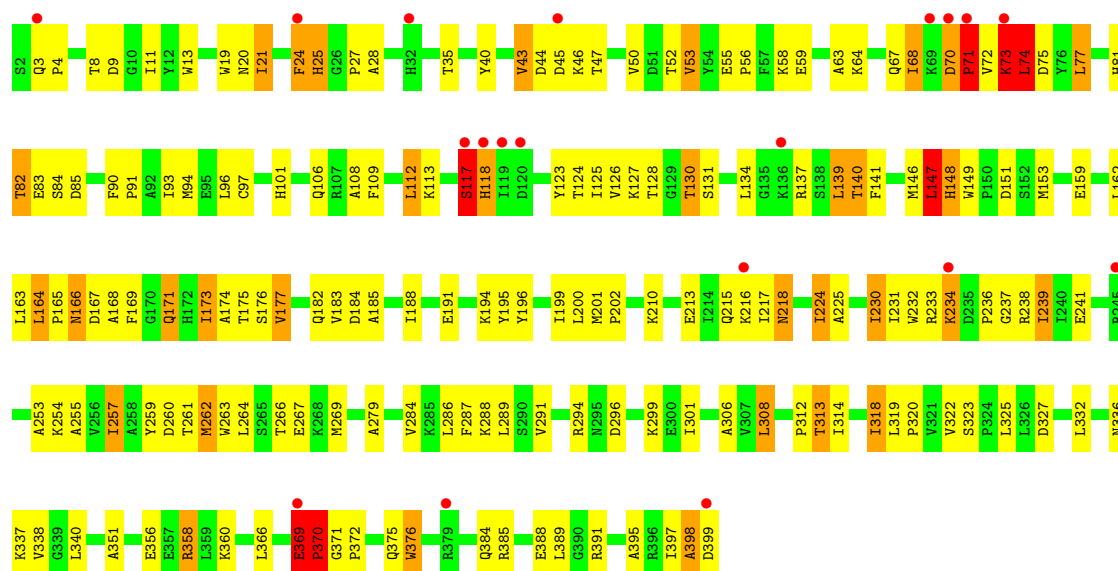




● Molecule 1: Nitric oxide reductase



● Molecule 1: Nitric oxide reductase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 159.68Å 159.68Å 278.14Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.71 – 2.80<br>49.71 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.71-2.80)<br>99.9 (49.71-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.94 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.245<br>0.221 , 0.237                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4459 reflections (5.02%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 63.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.075                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 20.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 12758                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FMN, FEO, EDO

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     | 0.68         | 4/3189 (0.1%)  | 1.20        | 31/4335 (0.7%)   |
| 1   | B     | 0.60         | 1/3189 (0.0%)  | 1.43        | 29/4335 (0.7%)   |
| 1   | C     | 0.61         | 0/3189         | 1.57        | 40/4335 (0.9%)   |
| 1   | D     | 0.67         | 2/3189 (0.1%)  | 1.41        | 37/4335 (0.9%)   |
| All | All   | 0.64         | 7/12756 (0.1%) | 1.41        | 137/17340 (0.8%) |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 118 | HIS  | C-O   | -13.47 | 1.09        | 1.24     |
| 1   | A     | 117 | SER  | C-N   | -12.10 | 1.13        | 1.34     |
| 1   | D     | 73  | LYS  | C-O   | -11.76 | 1.08        | 1.24     |
| 1   | A     | 118 | HIS  | C-N   | 8.09   | 1.43        | 1.33     |
| 1   | B     | 83  | GLU  | C-O   | -6.03  | 1.16        | 1.24     |
| 1   | A     | 73  | LYS  | C-O   | -5.49  | 1.18        | 1.23     |
| 1   | D     | 257 | ILE  | CA-CB | 5.34   | 1.60        | 1.54     |

All (137) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | C     | 70  | ASP  | CA-C-N | 47.81  | 179.60      | 119.84   |
| 1   | C     | 70  | ASP  | C-N-CA | 47.81  | 179.60      | 119.84   |
| 1   | B     | 70  | ASP  | CA-C-N | 39.57  | 169.30      | 119.84   |
| 1   | B     | 70  | ASP  | C-N-CA | 39.57  | 169.30      | 119.84   |
| 1   | D     | 70  | ASP  | CA-C-N | 34.99  | 163.58      | 119.84   |
| 1   | D     | 70  | ASP  | C-N-CA | 34.99  | 163.58      | 119.84   |
| 1   | A     | 70  | ASP  | C-N-CD | -12.88 | 92.27       | 120.60   |
| 1   | A     | 70  | ASP  | CA-C-N | 12.82  | 157.76      | 127.00   |
| 1   | A     | 70  | ASP  | C-N-CA | 12.82  | 157.76      | 127.00   |
| 1   | C     | 369 | GLU  | CA-C-N | 12.74  | 135.77      | 119.84   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 369 | GLU  | C-N-CA     | 12.74  | 135.77      | 119.84   |
| 1   | D     | 70  | ASP  | C-N-CD     | -12.73 | 72.82       | 125.00   |
| 1   | B     | 70  | ASP  | C-N-CD     | -12.66 | 73.09       | 125.00   |
| 1   | A     | 118 | HIS  | CA-C-O     | 12.58  | 132.29      | 119.08   |
| 1   | C     | 70  | ASP  | C-N-CD     | -12.39 | 74.22       | 125.00   |
| 1   | B     | 118 | HIS  | N-CA-C     | -10.39 | 98.66       | 113.21   |
| 1   | A     | 117 | SER  | N-CA-C     | 10.25  | 125.18      | 112.47   |
| 1   | C     | 369 | GLU  | C-N-CD     | -10.18 | 83.25       | 125.00   |
| 1   | B     | 117 | SER  | N-CA-C     | 10.16  | 125.31      | 111.90   |
| 1   | C     | 106 | GLN  | OE1-CD-NE2 | -10.05 | 112.55      | 122.60   |
| 1   | D     | 106 | GLN  | OE1-CD-NE2 | -9.91  | 112.69      | 122.60   |
| 1   | B     | 106 | GLN  | OE1-CD-NE2 | -9.50  | 113.10      | 122.60   |
| 1   | D     | 369 | GLU  | N-CA-C     | -9.46  | 96.69       | 109.84   |
| 1   | A     | 369 | GLU  | N-CA-C     | -9.38  | 96.80       | 109.84   |
| 1   | D     | 74  | LEU  | N-CA-C     | 9.34   | 124.06      | 110.42   |
| 1   | D     | 147 | LEU  | N-CA-C     | -9.13  | 98.00       | 110.68   |
| 1   | B     | 147 | LEU  | N-CA-C     | -9.11  | 98.01       | 110.68   |
| 1   | A     | 147 | LEU  | N-CA-C     | -9.09  | 98.04       | 110.68   |
| 1   | B     | 71  | PRO  | CA-N-CD    | -9.06  | 99.31       | 112.00   |
| 1   | A     | 106 | GLN  | OE1-CD-NE2 | -8.94  | 113.66      | 122.60   |
| 1   | A     | 164 | LEU  | CA-C-N     | 8.87   | 128.60      | 119.56   |
| 1   | A     | 164 | LEU  | C-N-CA     | 8.87   | 128.60      | 119.56   |
| 1   | D     | 118 | HIS  | N-CA-C     | -8.86  | 100.80      | 113.21   |
| 1   | D     | 289 | LEU  | N-CA-C     | 7.88   | 120.87      | 111.33   |
| 1   | C     | 289 | LEU  | N-CA-C     | 7.86   | 120.75      | 111.71   |
| 1   | A     | 289 | LEU  | N-CA-C     | 7.86   | 120.83      | 111.33   |
| 1   | B     | 164 | LEU  | CA-C-N     | 7.82   | 127.49      | 119.82   |
| 1   | B     | 164 | LEU  | C-N-CA     | 7.82   | 127.49      | 119.82   |
| 1   | B     | 289 | LEU  | N-CA-C     | 7.66   | 120.59      | 111.33   |
| 1   | A     | 117 | SER  | CA-C-N     | 7.61   | 132.93      | 120.23   |
| 1   | A     | 117 | SER  | C-N-CA     | 7.61   | 132.93      | 120.23   |
| 1   | C     | 147 | LEU  | N-CA-C     | -7.41  | 98.50       | 109.62   |
| 1   | C     | 369 | GLU  | N-CA-C     | -7.35  | 99.93       | 110.08   |
| 1   | C     | 370 | PRO  | N-CA-C     | -7.29  | 97.46       | 112.47   |
| 1   | C     | 369 | GLU  | CB-CA-C    | 7.01   | 120.56      | 109.27   |
| 1   | C     | 176 | SER  | N-CA-C     | -6.88  | 104.70      | 113.23   |
| 1   | B     | 176 | SER  | N-CA-C     | -6.78  | 105.01      | 113.28   |
| 1   | A     | 369 | GLU  | C-N-CD     | -6.68  | 97.62       | 125.00   |
| 1   | D     | 73  | LYS  | O-C-N      | -6.64  | 114.18      | 122.35   |
| 1   | C     | 106 | GLN  | CG-CD-NE2  | 6.63   | 126.35      | 116.40   |
| 1   | A     | 106 | GLN  | CG-CD-NE2  | 6.47   | 126.11      | 116.40   |
| 1   | D     | 70  | ASP  | N-CA-C     | 6.43   | 122.32      | 109.01   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 288 | LYS  | N-CA-C    | -6.40 | 98.10       | 108.41   |
| 1   | B     | 106 | GLN  | CG-CD-NE2 | 6.39  | 125.98      | 116.40   |
| 1   | B     | 84  | SER  | N-CA-CB   | -6.39 | 102.40      | 110.90   |
| 1   | D     | 176 | SER  | N-CA-C    | -6.37 | 105.33      | 113.23   |
| 1   | A     | 19  | TRP  | N-CA-C    | 6.30  | 118.23      | 111.36   |
| 1   | D     | 164 | LEU  | CA-C-N    | 6.29  | 126.41      | 119.87   |
| 1   | D     | 164 | LEU  | C-N-CA    | 6.29  | 126.41      | 119.87   |
| 1   | C     | 117 | SER  | N-CA-C    | 6.29  | 124.19      | 110.80   |
| 1   | D     | 167 | ASP  | N-CA-C    | 6.28  | 118.12      | 111.28   |
| 1   | D     | 71  | PRO  | N-CA-C    | -6.26 | 99.58       | 112.47   |
| 1   | B     | 19  | TRP  | N-CA-C    | 6.25  | 118.09      | 111.28   |
| 1   | C     | 164 | LEU  | CA-C-N    | 6.24  | 126.36      | 119.87   |
| 1   | C     | 164 | LEU  | C-N-CA    | 6.24  | 126.36      | 119.87   |
| 1   | D     | 288 | LYS  | N-CA-C    | -6.24 | 98.37       | 108.41   |
| 1   | D     | 106 | GLN  | CG-CD-NE2 | 6.22  | 125.73      | 116.40   |
| 1   | D     | 369 | GLU  | C-N-CD    | -6.21 | 99.52       | 125.00   |
| 1   | B     | 288 | LYS  | N-CA-C    | -6.17 | 98.48       | 108.41   |
| 1   | D     | 118 | HIS  | CA-CB-CG  | 6.04  | 119.84      | 113.80   |
| 1   | C     | 167 | ASP  | N-CA-C    | 6.01  | 117.83      | 111.28   |
| 1   | B     | 167 | ASP  | N-CA-C    | 6.01  | 117.83      | 111.28   |
| 1   | A     | 83  | GLU  | N-CA-C    | -6.00 | 102.59      | 110.33   |
| 1   | D     | 371 | GLY  | CA-C-N    | 5.98  | 126.33      | 119.93   |
| 1   | D     | 371 | GLY  | C-N-CA    | 5.98  | 126.33      | 119.93   |
| 1   | D     | 20  | ASN  | N-CA-C    | 5.94  | 120.53      | 113.28   |
| 1   | C     | 370 | PRO  | CA-N-CD   | -5.90 | 103.74      | 112.00   |
| 1   | A     | 28  | ALA  | N-CA-C    | 5.89  | 121.02      | 111.37   |
| 1   | C     | 19  | TRP  | N-CA-C    | 5.89  | 117.70      | 111.28   |
| 1   | C     | 235 | ASP  | N-CA-C    | 5.89  | 117.23      | 108.76   |
| 1   | B     | 20  | ASN  | N-CA-C    | 5.88  | 120.45      | 113.28   |
| 1   | C     | 83  | GLU  | N-CA-C    | -5.88 | 102.75      | 110.33   |
| 1   | B     | 117 | SER  | CB-CA-C   | -5.82 | 102.53      | 111.66   |
| 1   | C     | 118 | HIS  | N-CA-C    | -5.80 | 103.78      | 112.54   |
| 1   | D     | 19  | TRP  | N-CA-C    | 5.78  | 117.58      | 111.28   |
| 1   | D     | 71  | PRO  | CA-N-CD   | -5.78 | 103.91      | 112.00   |
| 1   | C     | 28  | ALA  | N-CA-C    | 5.76  | 120.82      | 111.37   |
| 1   | A     | 288 | LYS  | N-CA-C    | -5.76 | 99.13       | 108.41   |
| 1   | D     | 25  | HIS  | CB-CA-C   | -5.69 | 104.23      | 111.86   |
| 1   | A     | 262 | MET  | N-CA-C    | -5.63 | 106.45      | 113.55   |
| 1   | A     | 176 | SER  | N-CA-C    | -5.59 | 106.45      | 113.28   |
| 1   | A     | 179 | PHE  | N-CA-C    | 5.59  | 118.66      | 109.72   |
| 1   | C     | 20  | ASN  | N-CA-C    | 5.54  | 120.04      | 113.28   |
| 1   | D     | 262 | MET  | N-CA-C    | -5.52 | 106.59      | 113.55   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 70  | ASP  | CB-CA-C  | -5.51 | 104.70      | 110.33   |
| 1   | C     | 369 | GLU  | CA-CB-CG | -5.50 | 103.09      | 114.10   |
| 1   | A     | 118 | HIS  | O-C-N    | 5.49  | 128.37      | 122.05   |
| 1   | B     | 369 | GLU  | N-CA-C   | -5.48 | 97.69       | 109.81   |
| 1   | D     | 370 | PRO  | CA-N-CD  | -5.48 | 104.33      | 112.00   |
| 1   | A     | 199 | ILE  | N-CA-C   | 5.45  | 115.93      | 111.62   |
| 1   | A     | 20  | ASN  | N-CA-C   | 5.44  | 119.90      | 113.16   |
| 1   | B     | 13  | TRP  | N-CA-C   | -5.43 | 100.45      | 109.46   |
| 1   | B     | 264 | LEU  | N-CA-C   | 5.43  | 121.76      | 113.51   |
| 1   | D     | 45  | ASP  | N-CA-C   | -5.41 | 104.83      | 111.75   |
| 1   | C     | 179 | PHE  | N-CA-C   | 5.36  | 118.30      | 109.72   |
| 1   | B     | 85  | ASP  | N-CA-C   | -5.35 | 106.71      | 113.18   |
| 1   | C     | 320 | PRO  | N-CA-C   | 5.34  | 121.55      | 113.81   |
| 1   | D     | 13  | TRP  | N-CA-C   | -5.31 | 100.64      | 109.46   |
| 1   | A     | 52  | THR  | CB-CA-C  | -5.28 | 108.76      | 116.53   |
| 1   | A     | 167 | ASP  | N-CA-C   | 5.28  | 117.03      | 111.28   |
| 1   | B     | 157 | VAL  | CA-C-N   | 5.28  | 126.44      | 119.84   |
| 1   | B     | 157 | VAL  | C-N-CA   | 5.28  | 126.44      | 119.84   |
| 1   | C     | 262 | MET  | N-CA-C   | -5.27 | 106.90      | 113.55   |
| 1   | A     | 45  | ASP  | N-CA-C   | -5.25 | 104.98      | 111.33   |
| 1   | C     | 123 | TYR  | N-CA-C   | 5.24  | 115.97      | 108.74   |
| 1   | C     | 13  | TRP  | N-CA-C   | -5.21 | 100.81      | 109.46   |
| 1   | A     | 264 | LEU  | N-CA-C   | 5.21  | 121.42      | 113.51   |
| 1   | C     | 26  | GLY  | CA-C-N   | 5.20  | 126.35      | 119.84   |
| 1   | C     | 26  | GLY  | C-N-CA   | 5.20  | 126.35      | 119.84   |
| 1   | B     | 45  | ASP  | N-CA-C   | -5.19 | 105.11      | 111.75   |
| 1   | B     | 179 | PHE  | N-CA-C   | 5.18  | 118.00      | 109.72   |
| 1   | C     | 368 | ALA  | CA-C-N   | -5.18 | 112.81      | 120.68   |
| 1   | C     | 368 | ALA  | C-N-CA   | -5.18 | 112.81      | 120.68   |
| 1   | A     | 13  | TRP  | N-CA-C   | -5.16 | 100.90      | 109.46   |
| 1   | D     | 123 | TYR  | N-CA-C   | 5.14  | 115.84      | 108.74   |
| 1   | B     | 264 | LEU  | N-CA-CB  | -5.14 | 108.96      | 114.10   |
| 1   | C     | 4   | PRO  | N-CA-C   | -5.13 | 103.72      | 111.41   |
| 1   | A     | 370 | PRO  | CA-N-CD  | -5.12 | 104.83      | 112.00   |
| 1   | D     | 147 | LEU  | CA-C-N   | 5.09  | 131.27      | 121.54   |
| 1   | D     | 147 | LEU  | C-N-CA   | 5.09  | 131.27      | 121.54   |
| 1   | B     | 229 | GLY  | N-CA-C   | 5.07  | 121.05      | 112.22   |
| 1   | D     | 369 | GLU  | CA-C-N   | 5.03  | 126.13      | 119.84   |
| 1   | D     | 369 | GLU  | C-N-CA   | 5.03  | 126.13      | 119.84   |
| 1   | D     | 117 | SER  | N-CA-C   | 5.02  | 121.49      | 110.80   |
| 1   | C     | 371 | GLY  | CA-C-N   | 5.01  | 125.29      | 119.93   |
| 1   | C     | 371 | GLY  | C-N-CA   | 5.01  | 125.29      | 119.93   |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | C     | 369 | GLU  | N-CA-CB | 5.01 | 117.42      | 110.11   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3115  | 0        | 3130     | 194     | 0            |
| 1   | B     | 3115  | 0        | 3131     | 176     | 0            |
| 1   | C     | 3115  | 0        | 3131     | 150     | 0            |
| 1   | D     | 3115  | 0        | 3131     | 192     | 0            |
| 2   | A     | 4     | 0        | 0        | 1       | 0            |
| 2   | B     | 4     | 0        | 0        | 0       | 0            |
| 2   | C     | 3     | 0        | 0        | 0       | 0            |
| 2   | D     | 3     | 0        | 0        | 0       | 0            |
| 3   | A     | 3     | 0        | 0        | 4       | 0            |
| 3   | B     | 3     | 0        | 0        | 5       | 0            |
| 3   | C     | 3     | 0        | 0        | 1       | 0            |
| 3   | D     | 3     | 0        | 0        | 2       | 0            |
| 4   | A     | 4     | 0        | 6        | 9       | 0            |
| 4   | B     | 4     | 0        | 6        | 12      | 0            |
| 4   | C     | 4     | 0        | 6        | 11      | 0            |
| 4   | D     | 4     | 0        | 6        | 13      | 0            |
| 5   | A     | 31    | 0        | 19       | 0       | 0            |
| 5   | B     | 31    | 0        | 19       | 2       | 0            |
| 5   | C     | 31    | 0        | 19       | 2       | 0            |
| 5   | D     | 31    | 0        | 19       | 0       | 0            |
| 6   | A     | 31    | 0        | 0        | 4       | 0            |
| 6   | B     | 26    | 0        | 0        | 6       | 0            |
| 6   | C     | 40    | 0        | 0        | 6       | 3            |
| 6   | D     | 35    | 0        | 0        | 5       | 1            |
| All | All   | 12758 | 0        | 12623    | 691     | 3            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (691) 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:B:24:PHE:CE1   | 4:B:612:EDO:H11  | 1.50                     | 1.44              |
| 1:A:24:PHE:CE1   | 4:A:602:EDO:H11  | 1.56                     | 1.40              |
| 1:B:24:PHE:HE1   | 4:B:612:EDO:C1   | 1.53                     | 1.21              |
| 1:A:25:HIS:NE2   | 4:A:602:EDO:O1   | 1.74                     | 1.17              |
| 1:A:261:THR:HG22 | 1:A:266:THR:HB   | 1.18                     | 1.12              |
| 1:B:381:GLU:CD   | 1:B:381:GLU:H    | 1.59                     | 1.11              |
| 1:A:24:PHE:HE1   | 4:A:602:EDO:C1   | 1.65                     | 1.09              |
| 1:D:83:GLU:OE1   | 4:D:632:EDO:O1   | 1.68                     | 1.08              |
| 1:A:369:GLU:HB3  | 1:A:370:PRO:HD2  | 1.28                     | 1.08              |
| 1:D:85:ASP:CG    | 4:D:632:EDO:H12  | 1.77                     | 1.07              |
| 1:A:234:LYS:HE3  | 1:A:234:LYS:HA   | 1.38                     | 1.06              |
| 1:A:314:ILE:HD11 | 1:A:319:LEU:HA   | 1.37                     | 1.05              |
| 1:A:381:GLU:H    | 1:A:381:GLU:CD   | 1.66                     | 1.03              |
| 1:C:83:GLU:OE1   | 4:C:622:EDO:O1   | 1.76                     | 1.02              |
| 1:B:314:ILE:HD11 | 1:B:319:LEU:HA   | 1.41                     | 1.01              |
| 1:C:234:LYS:HE3  | 1:C:234:LYS:HA   | 1.44                     | 0.97              |
| 1:B:171:GLN:HE22 | 1:B:230:ILE:H    | 0.98                     | 0.96              |
| 1:A:83:GLU:OE1   | 4:A:602:EDO:O1   | 1.81                     | 0.96              |
| 1:A:379:ARG:HG3  | 1:A:381:GLU:OE2  | 1.67                     | 0.95              |
| 1:B:369:GLU:HG3  | 1:B:370:PRO:HD2  | 1.49                     | 0.95              |
| 1:C:56:PRO:HA    | 6:C:759:HOH:O    | 1.67                     | 0.94              |
| 1:A:369:GLU:CB   | 1:A:370:PRO:HD2  | 1.96                     | 0.94              |
| 1:D:101:HIS:HE1  | 1:D:124:THR:OG1  | 1.51                     | 0.93              |
| 1:A:333:ARG:HH11 | 1:A:363:LYS:HZ3  | 0.96                     | 0.93              |
| 1:A:171:GLN:HE22 | 1:A:230:ILE:H    | 1.14                     | 0.93              |
| 1:D:261:THR:HG22 | 1:D:266:THR:HB   | 1.49                     | 0.92              |
| 1:D:259:TYR:HE2  | 1:D:286:LEU:HD21 | 1.31                     | 0.92              |
| 1:A:294:ARG:NH1  | 1:B:320:PRO:HB2  | 1.85                     | 0.92              |
| 1:D:369:GLU:HB3  | 1:D:370:PRO:HD2  | 1.52                     | 0.91              |
| 1:D:24:PHE:CE1   | 4:D:632:EDO:H11  | 2.05                     | 0.91              |
| 1:B:43:VAL:HA    | 1:B:47:THR:HG22  | 1.51                     | 0.91              |
| 1:A:127:LYS:O    | 1:A:130:THR:HG23 | 1.72                     | 0.90              |
| 1:C:127:LYS:O    | 1:C:130:THR:HG22 | 1.72                     | 0.90              |
| 1:C:25:HIS:HB3   | 1:D:262:MET:HE2  | 1.54                     | 0.89              |
| 1:A:77:LEU:HD12  | 1:A:94:MET:HE1   | 1.51                     | 0.89              |
| 1:A:320:PRO:HG2  | 1:B:294:ARG:HH12 | 1.36                     | 0.89              |
| 1:D:171:GLN:HE22 | 1:D:230:ILE:H    | 0.94                     | 0.88              |
| 1:D:171:GLN:HE22 | 1:D:230:ILE:N    | 1.72                     | 0.87              |
| 1:B:202:PRO:HG3  | 1:B:332:LEU:HA   | 1.53                     | 0.87              |
| 1:A:391:ARG:HG3  | 1:A:391:ARG:HH11 | 1.38                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:318:ILE:CD1  | 1:D:322:VAL:HB   | 2.05                     | 0.87              |
| 1:A:320:PRO:HG2  | 1:B:294:ARG:NH1  | 1.90                     | 0.86              |
| 1:D:85:ASP:OD1   | 4:D:632:EDO:H12  | 1.76                     | 0.85              |
| 1:C:261:THR:CG2  | 1:C:266:THR:HB   | 2.07                     | 0.84              |
| 1:B:305:ARG:HB3  | 1:B:397:ILE:HD12 | 1.59                     | 0.84              |
| 1:C:320:PRO:HB2  | 1:D:294:ARG:NH1  | 1.92                     | 0.84              |
| 1:D:109:PHE:CE2  | 1:D:113:LYS:HE2  | 2.11                     | 0.84              |
| 1:D:306:ALA:HB2  | 1:D:397:ILE:HD11 | 1.58                     | 0.84              |
| 1:D:369:GLU:CB   | 1:D:370:PRO:HD2  | 2.06                     | 0.84              |
| 1:A:25:HIS:HB3   | 1:B:262:MET:HE3  | 1.60                     | 0.84              |
| 1:D:127:LYS:O    | 1:D:130:THR:HG23 | 1.78                     | 0.83              |
| 1:C:3:GLN:HE22   | 1:C:67:GLN:HE22  | 1.27                     | 0.83              |
| 1:C:58:LYS:HE2   | 6:C:760:HOH:O    | 1.79                     | 0.82              |
| 1:A:24:PHE:CE1   | 4:A:602:EDO:C1   | 2.51                     | 0.82              |
| 1:A:261:THR:CG2  | 1:A:266:THR:HB   | 2.07                     | 0.82              |
| 1:B:127:LYS:H    | 1:B:130:THR:CG2  | 1.93                     | 0.82              |
| 1:B:381:GLU:CD   | 1:B:381:GLU:N    | 2.29                     | 0.82              |
| 1:B:314:ILE:HD11 | 1:B:319:LEU:CA   | 2.09                     | 0.81              |
| 1:D:118:HIS:NE2  | 6:D:762:HOH:O    | 1.87                     | 0.81              |
| 1:D:259:TYR:CE2  | 1:D:286:LEU:HD21 | 2.14                     | 0.81              |
| 1:D:306:ALA:CB   | 1:D:397:ILE:HD11 | 2.11                     | 0.80              |
| 1:C:3:GLN:NE2    | 1:C:67:GLN:HE22  | 1.80                     | 0.80              |
| 3:A:501:FEO:O    | 4:A:602:EDO:H12  | 1.81                     | 0.79              |
| 1:A:314:ILE:HD11 | 1:A:319:LEU:CA   | 2.12                     | 0.79              |
| 1:D:171:GLN:NE2  | 1:D:230:ILE:H    | 1.77                     | 0.79              |
| 1:A:333:ARG:HH11 | 1:A:363:LYS:NZ   | 1.80                     | 0.79              |
| 1:B:313:THR:HG22 | 1:B:351:ALA:CB   | 2.13                     | 0.78              |
| 1:A:259:TYR:HE2  | 1:A:286:LEU:HD21 | 1.48                     | 0.78              |
| 1:C:83:GLU:CD    | 4:C:622:EDO:O1   | 2.26                     | 0.78              |
| 1:A:202:PRO:HG3  | 1:A:332:LEU:HA   | 1.64                     | 0.78              |
| 1:D:188:ILE:HD11 | 1:D:230:ILE:HB   | 1.66                     | 0.78              |
| 1:C:259:TYR:HE2  | 1:C:286:LEU:HD21 | 1.47                     | 0.77              |
| 1:A:308:LEU:HD13 | 1:A:340:LEU:HB3  | 1.64                     | 0.77              |
| 1:A:381:GLU:CD   | 1:A:381:GLU:N    | 2.41                     | 0.77              |
| 1:D:8:THR:HG23   | 1:D:11:ILE:HD13  | 1.67                     | 0.77              |
| 1:D:318:ILE:HD13 | 1:D:319:LEU:N    | 2.00                     | 0.77              |
| 1:B:171:GLN:HE22 | 1:B:230:ILE:N    | 1.80                     | 0.77              |
| 1:D:318:ILE:HD11 | 1:D:322:VAL:HB   | 1.66                     | 0.76              |
| 1:C:294:ARG:NH1  | 1:D:320:PRO:HB2  | 2.01                     | 0.76              |
| 1:D:266:THR:HA   | 1:D:269:MET:HE3  | 1.67                     | 0.76              |
| 3:C:521:FEO:O    | 4:C:622:EDO:H12  | 1.85                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:101:HIS:HE1  | 1:C:124:THR:OG1  | 1.68                     | 0.75              |
| 1:C:202:PRO:HG3  | 1:C:332:LEU:HA   | 1.68                     | 0.75              |
| 1:D:234:LYS:HE3  | 1:D:234:LYS:HA   | 1.67                     | 0.75              |
| 1:A:90:PHE:HB3   | 1:A:91:PRO:HD3   | 1.68                     | 0.74              |
| 1:D:261:THR:CG2  | 1:D:266:THR:HB   | 2.16                     | 0.74              |
| 1:D:43:VAL:HA    | 1:D:47:THR:HG22  | 1.68                     | 0.74              |
| 1:B:313:THR:HG22 | 1:B:351:ALA:HB3  | 1.68                     | 0.74              |
| 1:C:126:VAL:HG13 | 1:C:130:THR:CG2  | 2.18                     | 0.74              |
| 1:D:308:LEU:HD13 | 1:D:340:LEU:HB3  | 1.70                     | 0.73              |
| 1:C:77:LEU:HD13  | 1:C:94:MET:HE1   | 1.70                     | 0.73              |
| 1:D:201:MET:HE2  | 1:D:332:LEU:HB3  | 1.69                     | 0.73              |
| 1:C:372:PRO:HG3  | 1:C:389:LEU:HD12 | 1.70                     | 0.73              |
| 1:D:173:ILE:CD1  | 1:D:175:THR:HG23 | 2.19                     | 0.73              |
| 1:B:83:GLU:OE1   | 4:B:612:EDO:O1   | 2.08                     | 0.72              |
| 1:B:103:LEU:HD23 | 1:B:124:THR:HG23 | 1.71                     | 0.72              |
| 1:B:82:THR:O     | 1:B:83:GLU:O     | 2.06                     | 0.72              |
| 1:A:127:LYS:H    | 1:A:130:THR:CG2  | 2.02                     | 0.72              |
| 1:B:24:PHE:CE1   | 4:B:612:EDO:C1   | 2.43                     | 0.72              |
| 1:A:98:PRO:HB2   | 1:D:279:ALA:O    | 1.89                     | 0.72              |
| 1:B:372:PRO:HG3  | 1:B:389:LEU:CD1  | 2.20                     | 0.72              |
| 1:C:266:THR:HA   | 1:C:269:MET:HE3  | 1.71                     | 0.71              |
| 1:C:320:PRO:CB   | 1:D:294:ARG:NH1  | 2.54                     | 0.71              |
| 1:D:113:LYS:O    | 1:D:117:SER:HB3  | 1.91                     | 0.71              |
| 1:D:25:HIS:HB2   | 1:D:28:ALA:HB3   | 1.72                     | 0.71              |
| 1:B:127:LYS:O    | 1:B:130:THR:HG23 | 1.90                     | 0.70              |
| 1:C:237:GLY:O    | 1:C:241:GLU:HG3  | 1.92                     | 0.70              |
| 1:A:113:LYS:O    | 1:A:117:SER:HB3  | 1.92                     | 0.70              |
| 1:A:127:LYS:H    | 1:A:130:THR:HG21 | 1.57                     | 0.70              |
| 1:D:128:THR:O    | 6:D:734:HOH:O    | 2.09                     | 0.70              |
| 1:C:369:GLU:HB3  | 1:C:370:PRO:HD2  | 1.75                     | 0.69              |
| 1:C:381:GLU:OE1  | 1:C:381:GLU:N    | 2.22                     | 0.69              |
| 1:A:25:HIS:CD2   | 4:A:602:EDO:O1   | 2.46                     | 0.69              |
| 1:D:82:THR:HG22  | 1:D:112:LEU:HD13 | 1.74                     | 0.68              |
| 1:B:113:LYS:O    | 1:B:117:SER:HB3  | 1.93                     | 0.68              |
| 1:C:90:PHE:HB3   | 1:C:91:PRO:HD3   | 1.76                     | 0.68              |
| 1:A:379:ARG:CG   | 1:A:381:GLU:OE2  | 2.41                     | 0.68              |
| 1:B:127:LYS:H    | 1:B:130:THR:HG21 | 1.56                     | 0.68              |
| 1:C:177:VAL:HG22 | 1:C:182:GLN:OE1  | 1.94                     | 0.68              |
| 1:B:80:ASN:HD22  | 1:B:153:MET:HG3  | 1.59                     | 0.68              |
| 1:B:107:ARG:HB3  | 1:B:107:ARG:NH1  | 2.09                     | 0.68              |
| 1:A:369:GLU:HB3  | 1:A:370:PRO:CD   | 2.16                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:73:LYS:CD    | 1:D:73:LYS:O     | 2.42                     | 0.67              |
| 1:D:372:PRO:HG3  | 1:D:389:LEU:CD1  | 2.24                     | 0.67              |
| 1:D:262:MET:HE1  | 1:D:314:ILE:HD12 | 1.76                     | 0.67              |
| 1:A:72:VAL:HB    | 1:A:96:LEU:HD11  | 1.77                     | 0.67              |
| 1:B:117:SER:O    | 1:B:118:HIS:HD2  | 1.77                     | 0.67              |
| 1:C:261:THR:HG23 | 1:C:266:THR:HB   | 1.76                     | 0.67              |
| 1:A:379:ARG:HG2  | 1:A:382:ASP:OD2  | 1.94                     | 0.66              |
| 1:D:127:LYS:H    | 1:D:130:THR:CG2  | 2.09                     | 0.66              |
| 1:A:118:HIS:CE1  | 6:A:729:HOH:O    | 2.47                     | 0.66              |
| 1:C:269:MET:HE1  | 1:C:343:GLY:C    | 2.20                     | 0.66              |
| 1:A:359:LEU:HD22 | 1:A:364:ILE:HG21 | 1.76                     | 0.66              |
| 2:A:404:ZN:ZN    | 6:A:732:HOH:O    | 1.43                     | 0.66              |
| 1:A:367:ILE:O    | 1:A:367:ILE:HD12 | 1.96                     | 0.66              |
| 1:D:82:THR:CG2   | 1:D:112:LEU:HD13 | 2.26                     | 0.65              |
| 1:A:294:ARG:HH12 | 1:B:320:PRO:HB2  | 1.55                     | 0.65              |
| 1:C:261:THR:HG22 | 1:C:266:THR:HB   | 1.76                     | 0.65              |
| 3:D:531:FEO:O    | 4:D:632:EDO:C2   | 2.44                     | 0.65              |
| 1:A:398:ALA:O    | 1:A:399:ASP:CB   | 2.43                     | 0.65              |
| 1:C:185:ALA:HB1  | 1:C:238:ARG:NH1  | 2.12                     | 0.65              |
| 1:D:259:TYR:HE2  | 1:D:286:LEU:CD2  | 2.06                     | 0.65              |
| 1:C:372:PRO:HG3  | 1:C:389:LEU:CD1  | 2.27                     | 0.65              |
| 1:C:391:ARG:HG3  | 1:C:391:ARG:HH11 | 1.61                     | 0.65              |
| 1:B:372:PRO:HG3  | 1:B:389:LEU:HD13 | 1.78                     | 0.65              |
| 3:B:511:FEO:O    | 4:B:612:EDO:H12  | 1.96                     | 0.65              |
| 1:C:296:ASP:OD2  | 6:C:723:HOH:O    | 2.15                     | 0.65              |
| 1:C:47:THR:HG23  | 6:C:724:HOH:O    | 1.96                     | 0.64              |
| 1:C:113:LYS:O    | 1:C:117:SER:HB3  | 1.96                     | 0.64              |
| 1:A:365:GLU:OE2  | 1:A:396:ARG:NH2  | 2.31                     | 0.64              |
| 1:A:259:TYR:CE2  | 1:A:286:LEU:HD21 | 2.31                     | 0.64              |
| 1:D:202:PRO:HG3  | 1:D:332:LEU:HA   | 1.79                     | 0.64              |
| 3:D:531:FEO:O    | 4:D:632:EDO:H22  | 1.98                     | 0.64              |
| 1:B:59:GLU:OE2   | 6:B:736:HOH:O    | 2.15                     | 0.64              |
| 1:B:82:THR:C     | 1:B:83:GLU:O     | 2.40                     | 0.64              |
| 1:D:164:LEU:HD23 | 1:D:225:ALA:HB3  | 1.80                     | 0.64              |
| 1:B:85:ASP:OD2   | 4:B:612:EDO:H12  | 1.97                     | 0.63              |
| 1:B:366:LEU:N    | 1:B:366:LEU:HD23 | 2.12                     | 0.63              |
| 3:B:511:FEO:O    | 4:B:612:EDO:C1   | 2.45                     | 0.63              |
| 1:C:261:THR:HG22 | 5:C:721:FMN:O1P  | 1.97                     | 0.63              |
| 1:B:338:VAL:HG11 | 1:B:367:ILE:HD13 | 1.81                     | 0.63              |
| 1:A:391:ARG:HG3  | 1:A:391:ARG:NH1  | 2.04                     | 0.63              |
| 1:B:263:TRP:O    | 1:B:264:LEU:HB2  | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:PHE:CE1   | 1:C:94:MET:HE3   | 2.34                     | 0.63              |
| 1:D:55:GLU:HB3   | 1:D:56:PRO:HD3   | 1.80                     | 0.63              |
| 1:B:90:PHE:HB3   | 1:B:91:PRO:HD3   | 1.80                     | 0.63              |
| 1:B:259:TYR:HE2  | 1:B:286:LEU:HD21 | 1.63                     | 0.63              |
| 1:B:372:PRO:CG   | 1:B:389:LEU:HD13 | 2.29                     | 0.63              |
| 1:A:25:HIS:CB    | 1:B:262:MET:HE3  | 2.28                     | 0.63              |
| 1:B:313:THR:CG2  | 1:B:351:ALA:H    | 2.12                     | 0.63              |
| 1:A:372:PRO:HG3  | 1:A:389:LEU:CD1  | 2.28                     | 0.62              |
| 1:C:294:ARG:NH1  | 1:D:320:PRO:CB   | 2.62                     | 0.62              |
| 1:D:24:PHE:CE1   | 4:D:632:EDO:C1   | 2.79                     | 0.62              |
| 1:A:72:VAL:CG1   | 1:A:74:LEU:HD13  | 2.29                     | 0.62              |
| 1:A:340:LEU:HD11 | 1:A:372:PRO:HD3  | 1.82                     | 0.62              |
| 1:C:127:LYS:H    | 1:C:130:THR:CG2  | 2.12                     | 0.62              |
| 1:B:381:GLU:HG2  | 1:B:385:ARG:HH21 | 1.65                     | 0.62              |
| 1:C:185:ALA:HB1  | 1:C:238:ARG:HH12 | 1.64                     | 0.62              |
| 1:B:171:GLN:NE2  | 1:B:230:ILE:H    | 1.83                     | 0.62              |
| 1:C:320:PRO:HB2  | 1:D:294:ARG:HH12 | 1.65                     | 0.62              |
| 3:A:501:FEO:O    | 4:A:602:EDO:C1   | 2.48                     | 0.62              |
| 1:C:164:LEU:HD23 | 1:C:225:ALA:HB3  | 1.82                     | 0.62              |
| 1:C:25:HIS:HB2   | 1:C:28:ALA:HB3   | 1.81                     | 0.61              |
| 1:D:356:GLU:HG2  | 1:D:366:LEU:HD13 | 1.81                     | 0.61              |
| 1:A:81:HIS:HE1   | 1:A:149:TRP:HB2  | 1.66                     | 0.61              |
| 1:C:259:TYR:CE2  | 1:C:286:LEU:HD21 | 2.33                     | 0.61              |
| 1:D:3:GLN:HE22   | 1:D:67:GLN:HE22  | 1.47                     | 0.61              |
| 1:D:262:MET:CE   | 1:D:314:ILE:HD12 | 2.30                     | 0.61              |
| 1:B:70:ASP:OD1   | 1:B:71:PRO:HD3   | 2.01                     | 0.61              |
| 1:B:365:GLU:OE2  | 1:B:396:ARG:NH2  | 2.32                     | 0.61              |
| 1:C:369:GLU:CB   | 1:C:370:PRO:HD2  | 2.27                     | 0.60              |
| 1:D:3:GLN:NE2    | 1:D:67:GLN:HE22  | 1.98                     | 0.60              |
| 1:B:126:VAL:HG11 | 1:B:141:PHE:CG   | 2.36                     | 0.60              |
| 1:B:201:MET:HB3  | 1:B:202:PRO:HD3  | 1.83                     | 0.60              |
| 1:C:127:LYS:H    | 1:C:130:THR:HG21 | 1.66                     | 0.60              |
| 1:D:108:ALA:HB2  | 1:D:151:ASP:HB2  | 1.83                     | 0.60              |
| 1:C:305:ARG:HB2  | 1:C:397:ILE:HG23 | 1.83                     | 0.60              |
| 1:D:126:VAL:HG11 | 1:D:141:PHE:CG   | 2.37                     | 0.60              |
| 1:A:372:PRO:HG3  | 1:A:389:LEU:HD13 | 1.83                     | 0.60              |
| 1:D:96:LEU:O     | 1:D:96:LEU:HD13  | 2.01                     | 0.60              |
| 1:B:141:PHE:HB3  | 1:B:153:MET:CE   | 2.31                     | 0.60              |
| 1:C:3:GLN:HE22   | 1:C:67:GLN:NE2   | 1.97                     | 0.60              |
| 1:C:126:VAL:HG13 | 1:C:130:THR:HG23 | 1.83                     | 0.60              |
| 1:D:90:PHE:HB3   | 1:D:91:PRO:HD3   | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:117:SER:O    | 1:B:118:HIS:CD2  | 2.55                     | 0.60              |
| 1:C:305:ARG:HB3  | 1:C:397:ILE:HD12 | 1.82                     | 0.60              |
| 1:A:139:LEU:HD13 | 1:A:141:PHE:CZ   | 2.37                     | 0.59              |
| 1:D:11:ILE:HD11  | 1:D:137:ARG:CZ   | 2.31                     | 0.59              |
| 1:A:81:HIS:CE1   | 1:A:149:TRP:HB2  | 2.38                     | 0.59              |
| 1:A:86:HIS:CE1   | 1:A:227:SER:HB2  | 2.37                     | 0.59              |
| 1:D:318:ILE:HD11 | 1:D:322:VAL:CB   | 2.32                     | 0.59              |
| 1:C:126:VAL:HG11 | 1:C:141:PHE:CG   | 2.38                     | 0.59              |
| 1:B:369:GLU:CG   | 1:B:370:PRO:HD2  | 2.27                     | 0.59              |
| 1:A:40:TYR:CZ    | 1:A:225:ALA:HB1  | 2.37                     | 0.59              |
| 1:A:177:VAL:HG11 | 1:A:182:GLN:HB2  | 1.85                     | 0.59              |
| 1:A:171:GLN:NE2  | 1:A:230:ILE:H    | 1.95                     | 0.59              |
| 1:D:312:PRO:HD2  | 1:D:319:LEU:HD22 | 1.84                     | 0.59              |
| 1:A:72:VAL:CB    | 1:A:96:LEU:HD11  | 2.32                     | 0.59              |
| 1:D:194:LYS:HB2  | 1:D:299:LYS:HD3  | 1.84                     | 0.59              |
| 1:C:369:GLU:HG2  | 1:C:370:PRO:HD3  | 1.85                     | 0.58              |
| 1:D:73:LYS:O     | 1:D:73:LYS:HD3   | 2.02                     | 0.58              |
| 1:A:126:VAL:HG13 | 1:A:130:THR:OG1  | 2.03                     | 0.58              |
| 1:C:80:ASN:ND2   | 1:C:153:MET:HE3  | 2.18                     | 0.58              |
| 1:D:72:VAL:HB    | 1:D:96:LEU:CD1   | 2.34                     | 0.58              |
| 1:B:46:LYS:HA    | 1:B:75:ASP:OD2   | 2.02                     | 0.58              |
| 1:A:294:ARG:NH1  | 1:B:320:PRO:CB   | 2.64                     | 0.58              |
| 1:B:202:PRO:HG3  | 1:B:332:LEU:CA   | 2.31                     | 0.58              |
| 1:D:56:PRO:HA    | 6:D:766:HOH:O    | 2.02                     | 0.58              |
| 1:A:146:MET:C    | 1:A:148:HIS:H    | 2.12                     | 0.58              |
| 1:A:177:VAL:CG1  | 1:A:182:GLN:HB2  | 2.34                     | 0.58              |
| 1:C:83:GLU:CD    | 4:C:622:EDO:HO1  | 2.09                     | 0.58              |
| 1:A:118:HIS:HD1  | 1:D:388:GLU:CD   | 2.11                     | 0.58              |
| 1:C:66:LYS:HE2   | 6:C:730:HOH:O    | 2.03                     | 0.57              |
| 1:A:263:TRP:O    | 1:A:264:LEU:HB2  | 2.03                     | 0.57              |
| 1:A:313:THR:HG22 | 1:A:351:ALA:HB3  | 1.87                     | 0.57              |
| 1:A:101:HIS:NE2  | 1:A:124:THR:HG22 | 2.19                     | 0.57              |
| 1:A:103:LEU:HD23 | 1:A:124:THR:HG23 | 1.86                     | 0.57              |
| 1:A:234:LYS:HA   | 1:A:234:LYS:CE   | 2.21                     | 0.57              |
| 1:B:25:HIS:HB2   | 1:B:28:ALA:HB3   | 1.86                     | 0.57              |
| 1:B:120:ASP:OD1  | 6:B:732:HOH:O    | 2.17                     | 0.57              |
| 1:D:25:HIS:CB    | 1:D:28:ALA:HB3   | 2.34                     | 0.57              |
| 1:D:146:MET:C    | 1:D:148:HIS:H    | 2.13                     | 0.57              |
| 1:D:232:TRP:CZ2  | 1:D:239:ILE:HG13 | 2.39                     | 0.57              |
| 1:B:146:MET:C    | 1:B:148:HIS:H    | 2.13                     | 0.56              |
| 1:C:177:VAL:HG21 | 1:C:182:GLN:HB3  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:252:LYS:O    | 1:C:305:ARG:HG3  | 2.05                     | 0.56              |
| 1:A:333:ARG:NH1  | 1:A:363:LYS:HZ3  | 1.82                     | 0.56              |
| 1:B:286:LEU:HD23 | 1:B:286:LEU:C    | 2.30                     | 0.56              |
| 1:C:146:MET:C    | 1:C:148:HIS:H    | 2.12                     | 0.56              |
| 1:A:109:PHE:O    | 1:A:113:LYS:HG2  | 2.05                     | 0.56              |
| 1:B:28:ALA:O     | 1:B:294:ARG:NH2  | 2.38                     | 0.56              |
| 1:B:308:LEU:N    | 1:B:308:LEU:HD23 | 2.19                     | 0.56              |
| 1:B:314:ILE:CD1  | 1:B:319:LEU:HA   | 2.27                     | 0.56              |
| 1:B:313:THR:HG22 | 1:B:351:ALA:H    | 1.69                     | 0.56              |
| 1:A:261:THR:HG21 | 1:A:267:GLU:H    | 1.71                     | 0.56              |
| 1:D:127:LYS:H    | 1:D:130:THR:HG21 | 1.70                     | 0.56              |
| 1:A:149:TRP:CZ2  | 6:B:730:HOH:O    | 2.59                     | 0.56              |
| 1:C:55:GLU:HB3   | 1:C:56:PRO:HD3   | 1.86                     | 0.56              |
| 1:C:210:LYS:HE3  | 1:C:210:LYS:HA   | 1.87                     | 0.56              |
| 1:D:3:GLN:CD     | 1:D:67:GLN:HE22  | 2.14                     | 0.56              |
| 1:A:21:ILE:HG23  | 1:A:34:GLY:HA2   | 1.86                     | 0.56              |
| 1:D:213:GLU:HA   | 1:D:216:LYS:HE3  | 1.87                     | 0.56              |
| 1:C:369:GLU:CB   | 1:C:370:PRO:CD   | 2.82                     | 0.56              |
| 1:B:237:GLY:O    | 1:B:241:GLU:HG3  | 2.06                     | 0.55              |
| 1:B:305:ARG:CB   | 1:B:397:ILE:HD12 | 2.32                     | 0.55              |
| 1:C:381:GLU:HG2  | 1:C:385:ARG:NH2  | 2.22                     | 0.55              |
| 1:B:101:HIS:NE2  | 1:B:124:THR:HG22 | 2.21                     | 0.55              |
| 1:C:232:TRP:CZ2  | 1:C:239:ILE:HG13 | 2.42                     | 0.55              |
| 1:C:323:SER:HB3  | 1:D:323:SER:HB3  | 1.87                     | 0.55              |
| 1:B:305:ARG:HB2  | 1:B:397:ILE:HG23 | 1.87                     | 0.55              |
| 1:D:85:ASP:OD2   | 4:D:632:EDO:H12  | 2.06                     | 0.55              |
| 1:D:188:ILE:HD11 | 1:D:230:ILE:CB   | 2.35                     | 0.55              |
| 1:D:191:GLU:OE1  | 1:D:191:GLU:HA   | 2.07                     | 0.55              |
| 1:D:318:ILE:HD13 | 1:D:319:LEU:H    | 1.70                     | 0.55              |
| 1:A:333:ARG:HD2  | 1:A:363:LYS:CE   | 2.36                     | 0.55              |
| 1:B:137:ARG:HA   | 1:B:159:GLU:CD   | 2.32                     | 0.55              |
| 1:D:101:HIS:CE1  | 1:D:124:THR:OG1  | 2.44                     | 0.55              |
| 1:C:24:PHE:CE1   | 4:C:622:EDO:H11  | 2.41                     | 0.55              |
| 1:C:156:TYR:CE2  | 1:C:219:LEU:HD22 | 2.42                     | 0.55              |
| 1:A:269:MET:HE2  | 1:A:374:VAL:HB   | 1.88                     | 0.55              |
| 1:A:314:ILE:HG12 | 1:A:319:LEU:CD1  | 2.37                     | 0.55              |
| 1:C:80:ASN:HD22  | 1:C:153:MET:HE3  | 1.71                     | 0.55              |
| 1:A:55:GLU:HB3   | 1:A:56:PRO:HD3   | 1.89                     | 0.55              |
| 1:A:306:ALA:HB2  | 1:A:397:ILE:HD11 | 1.89                     | 0.55              |
| 1:D:177:VAL:HG22 | 1:D:182:GLN:CD   | 2.32                     | 0.55              |
| 1:C:163:LEU:HG   | 1:C:165:PRO:HG3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:171:GLN:HE22 | 1:A:230:ILE:N    | 1.95                     | 0.54              |
| 1:B:214:ILE:HG23 | 1:B:219:LEU:HD12 | 1.88                     | 0.54              |
| 1:B:301:ILE:O    | 1:B:337:LYS:HE3  | 2.07                     | 0.54              |
| 1:A:379:ARG:HH11 | 1:A:382:ASP:CG   | 2.15                     | 0.54              |
| 1:B:126:VAL:HG13 | 1:B:130:THR:HG23 | 1.90                     | 0.54              |
| 1:D:398:ALA:O    | 1:D:399:ASP:CB   | 2.55                     | 0.54              |
| 1:B:326:LEU:HD11 | 1:B:355:LEU:HD23 | 1.89                     | 0.54              |
| 1:D:8:THR:CG2    | 1:D:11:ILE:HD13  | 2.37                     | 0.54              |
| 1:D:63:ALA:O     | 1:D:67:GLN:HG3   | 2.08                     | 0.54              |
| 1:B:338:VAL:CG1  | 1:B:367:ILE:HD13 | 2.37                     | 0.54              |
| 1:D:72:VAL:HB    | 1:D:96:LEU:HD11  | 1.89                     | 0.54              |
| 1:A:161:ALA:HB1  | 1:A:220:ALA:O    | 2.08                     | 0.54              |
| 1:D:173:ILE:C    | 1:D:173:ILE:HD13 | 2.33                     | 0.54              |
| 1:B:367:ILE:HD11 | 1:B:396:ARG:HD3  | 1.88                     | 0.54              |
| 1:C:398:ALA:O    | 1:C:399:ASP:CB   | 2.56                     | 0.54              |
| 1:D:173:ILE:HD13 | 1:D:174:ALA:N    | 2.23                     | 0.54              |
| 1:A:365:GLU:CD   | 1:A:396:ARG:HH22 | 2.17                     | 0.53              |
| 1:B:356:GLU:HG2  | 1:B:366:LEU:CD1  | 2.38                     | 0.53              |
| 1:D:113:LYS:O    | 1:D:117:SER:CB   | 2.56                     | 0.53              |
| 1:B:70:ASP:OD1   | 1:B:71:PRO:CD    | 2.57                     | 0.53              |
| 1:C:81:HIS:CD2   | 1:C:166:ASN:HD21 | 2.25                     | 0.53              |
| 1:C:189:MET:HE3  | 1:C:238:ARG:NE   | 2.23                     | 0.53              |
| 1:A:25:HIS:HE2   | 4:A:602:EDO:C1   | 2.13                     | 0.53              |
| 1:A:77:LEU:HD12  | 1:A:94:MET:CE    | 2.32                     | 0.53              |
| 1:B:347:TRP:CD1  | 1:B:348:GLY:H    | 2.26                     | 0.53              |
| 1:C:254:LYS:HG2  | 1:C:255:ALA:N    | 2.23                     | 0.53              |
| 1:A:165:PRO:O    | 1:A:166:ASN:HB3  | 2.08                     | 0.53              |
| 1:B:210:LYS:HE2  | 1:B:213:GLU:OE2  | 2.09                     | 0.53              |
| 1:C:40:TYR:CZ    | 1:C:225:ALA:HB1  | 2.44                     | 0.53              |
| 1:C:312:PRO:HD2  | 1:C:319:LEU:HD22 | 1.89                     | 0.53              |
| 1:D:44:ASP:H     | 1:D:47:THR:HG22  | 1.73                     | 0.53              |
| 1:B:127:LYS:O    | 1:B:130:THR:CG2  | 2.55                     | 0.53              |
| 1:D:73:LYS:HB2   | 1:D:73:LYS:NZ    | 2.24                     | 0.53              |
| 1:B:141:PHE:HD2  | 1:B:153:MET:HE2  | 1.74                     | 0.53              |
| 1:C:28:ALA:O     | 1:C:294:ARG:NH2  | 2.42                     | 0.53              |
| 1:C:25:HIS:NE2   | 4:C:622:EDO:O2   | 2.41                     | 0.52              |
| 1:D:177:VAL:HG21 | 1:D:182:GLN:HB3  | 1.91                     | 0.52              |
| 1:D:286:LEU:HD23 | 1:D:287:PHE:N    | 2.24                     | 0.52              |
| 1:D:257:ILE:HD13 | 1:D:284:VAL:HG13 | 1.91                     | 0.52              |
| 1:D:82:THR:C     | 1:D:83:GLU:O     | 2.52                     | 0.52              |
| 1:D:372:PRO:HG3  | 1:D:389:LEU:HD12 | 1.89                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:146:MET:C    | 1:A:148:HIS:N    | 2.66                     | 0.52              |
| 1:A:210:LYS:HE3  | 1:A:210:LYS:HA   | 1.92                     | 0.52              |
| 1:C:329:LEU:HD22 | 1:C:334:PRO:HG2  | 1.92                     | 0.52              |
| 1:D:24:PHE:CE1   | 4:D:632:EDO:H21  | 2.45                     | 0.52              |
| 1:B:189:MET:HE3  | 1:B:238:ARG:HD3  | 1.92                     | 0.52              |
| 1:B:259:TYR:CE2  | 1:B:286:LEU:HD21 | 2.43                     | 0.52              |
| 1:A:320:PRO:CG   | 1:B:294:ARG:NH1  | 2.67                     | 0.52              |
| 1:A:398:ALA:O    | 1:A:399:ASP:HB2  | 2.07                     | 0.52              |
| 1:C:21:ILE:HG21  | 1:C:35:THR:HG22  | 1.92                     | 0.52              |
| 1:D:71:PRO:HD2   | 1:D:71:PRO:O     | 2.08                     | 0.52              |
| 1:D:85:ASP:OD2   | 4:D:632:EDO:H22  | 2.10                     | 0.52              |
| 1:A:259:TYR:HE2  | 1:A:286:LEU:CD2  | 2.20                     | 0.52              |
| 1:A:321:VAL:HG21 | 1:B:27:PRO:CB    | 2.38                     | 0.52              |
| 1:C:340:LEU:HD11 | 1:C:372:PRO:HD3  | 1.92                     | 0.52              |
| 1:D:173:ILE:HD11 | 1:D:175:THR:HG23 | 1.91                     | 0.52              |
| 1:D:318:ILE:HD12 | 1:D:322:VAL:HB   | 1.88                     | 0.52              |
| 1:A:323:SER:HB3  | 1:B:323:SER:HB3  | 1.91                     | 0.52              |
| 1:B:102:VAL:HG12 | 1:B:104:CYS:SG   | 2.49                     | 0.52              |
| 1:B:262:MET:HE1  | 5:B:711:FMN:C8M  | 2.39                     | 0.52              |
| 1:C:216:LYS:C    | 1:C:218:ASN:N    | 2.67                     | 0.52              |
| 1:C:77:LEU:HD13  | 1:C:94:MET:CE    | 2.39                     | 0.52              |
| 1:C:146:MET:C    | 1:C:148:HIS:N    | 2.67                     | 0.52              |
| 1:C:308:LEU:HD22 | 1:C:340:LEU:HB3  | 1.92                     | 0.52              |
| 1:D:215:GLN:OE1  | 1:D:215:GLN:HA   | 2.10                     | 0.52              |
| 1:B:81:HIS:CE1   | 1:B:149:TRP:HB2  | 2.45                     | 0.52              |
| 1:A:164:LEU:HD23 | 1:A:225:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:214:ILE:HG23 | 1:A:219:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:296:ASP:OD2  | 6:D:741:HOH:O    | 2.18                     | 0.51              |
| 1:A:326:LEU:HD11 | 1:A:355:LEU:HD23 | 1.92                     | 0.51              |
| 1:C:46:LYS:HA    | 1:C:75:ASP:OD2   | 2.10                     | 0.51              |
| 1:D:391:ARG:HG3  | 1:D:391:ARG:HH11 | 1.76                     | 0.51              |
| 1:B:85:ASP:CG    | 4:B:612:EDO:H12  | 2.35                     | 0.51              |
| 1:B:379:ARG:HG3  | 1:B:382:ASP:OD2  | 2.11                     | 0.51              |
| 1:B:156:TYR:CZ   | 1:B:219:LEU:HD22 | 2.44                     | 0.51              |
| 1:C:194:LYS:HB2  | 1:C:299:LYS:HD3  | 1.91                     | 0.51              |
| 1:D:21:ILE:HG21  | 1:D:35:THR:HG22  | 1.91                     | 0.51              |
| 1:D:185:ALA:HB1  | 1:D:238:ARG:NH1  | 2.25                     | 0.51              |
| 1:D:257:ILE:CD1  | 1:D:284:VAL:HG13 | 2.41                     | 0.51              |
| 1:B:146:MET:C    | 1:B:148:HIS:N    | 2.67                     | 0.51              |
| 1:B:261:THR:HG21 | 1:B:267:GLU:HB2  | 1.92                     | 0.51              |
| 1:D:40:TYR:CZ    | 1:D:225:ALA:HB1  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:3:GLN:OE1    | 1:C:67:GLN:NE2   | 2.43                     | 0.51              |
| 1:C:70:ASP:OD2   | 1:C:70:ASP:C     | 2.54                     | 0.51              |
| 1:D:259:TYR:CD1  | 1:D:260:ASP:N    | 2.78                     | 0.51              |
| 1:B:194:LYS:HB2  | 1:B:299:LYS:HD3  | 1.92                     | 0.51              |
| 1:B:395:ALA:O    | 1:B:398:ALA:HB2  | 2.10                     | 0.51              |
| 1:C:398:ALA:O    | 1:C:399:ASP:HB3  | 2.10                     | 0.51              |
| 1:B:269:MET:HE2  | 1:B:374:VAL:HB   | 1.93                     | 0.51              |
| 1:A:137:ARG:HA   | 1:A:159:GLU:HG2  | 1.93                     | 0.51              |
| 1:A:375:GLN:O    | 1:A:376:TRP:HB2  | 2.10                     | 0.51              |
| 1:B:277:LEU:O    | 1:B:282:CYS:HB3  | 2.10                     | 0.51              |
| 1:C:25:HIS:NE2   | 4:C:622:EDO:O1   | 2.41                     | 0.51              |
| 1:A:72:VAL:HB    | 1:A:96:LEU:CD1   | 2.41                     | 0.50              |
| 1:A:118:HIS:ND1  | 1:D:388:GLU:OE1  | 2.42                     | 0.50              |
| 1:D:77:LEU:HD12  | 1:D:94:MET:HE1   | 1.92                     | 0.50              |
| 1:A:306:ALA:CB   | 1:A:397:ILE:HD11 | 2.40                     | 0.50              |
| 1:C:358:ARG:NH2  | 1:D:327:ASP:OD2  | 2.44                     | 0.50              |
| 1:A:166:ASN:ND2  | 1:A:167:ASP:H    | 2.08                     | 0.50              |
| 1:D:384:GLN:O    | 1:D:388:GLU:HG3  | 2.12                     | 0.50              |
| 1:A:90:PHE:CE1   | 1:A:94:MET:HE3   | 2.46                     | 0.50              |
| 1:B:120:ASP:CG   | 6:B:732:HOH:O    | 2.54                     | 0.50              |
| 1:D:46:LYS:HA    | 1:D:75:ASP:OD2   | 2.12                     | 0.50              |
| 1:D:73:LYS:O     | 1:D:73:LYS:CG    | 2.59                     | 0.50              |
| 1:D:127:LYS:H    | 1:D:130:THR:HG23 | 1.75                     | 0.50              |
| 1:D:257:ILE:HD13 | 1:D:284:VAL:CG1  | 2.42                     | 0.50              |
| 1:B:381:GLU:HG2  | 1:B:385:ARG:NH2  | 2.27                     | 0.50              |
| 1:C:305:ARG:CB   | 1:C:397:ILE:HD12 | 2.41                     | 0.50              |
| 1:D:146:MET:C    | 1:D:148:HIS:N    | 2.68                     | 0.50              |
| 1:D:131:SER:OG   | 1:D:140:THR:HB   | 2.12                     | 0.50              |
| 1:A:203:PHE:O    | 1:A:207:ILE:HG12 | 2.11                     | 0.50              |
| 3:B:511:FEO:O    | 4:B:612:EDO:C2   | 2.60                     | 0.50              |
| 1:D:398:ALA:O    | 1:D:399:ASP:HB3  | 2.12                     | 0.50              |
| 1:A:291:VAL:O    | 1:A:291:VAL:CG1  | 2.60                     | 0.50              |
| 1:C:73:LYS:HE2   | 1:C:73:LYS:HA    | 1.94                     | 0.50              |
| 1:D:11:ILE:HD12  | 1:D:11:ILE:N     | 2.27                     | 0.49              |
| 1:D:306:ALA:HB3  | 1:D:397:ILE:HD11 | 1.92                     | 0.49              |
| 1:D:24:PHE:CZ    | 4:D:632:EDO:H11  | 2.47                     | 0.49              |
| 1:D:224:ILE:HG13 | 1:D:236:PRO:HB3  | 1.94                     | 0.49              |
| 1:A:59:GLU:CD    | 1:A:59:GLU:H     | 2.20                     | 0.49              |
| 1:D:366:LEU:HD12 | 1:D:369:GLU:OE1  | 2.12                     | 0.49              |
| 1:D:24:PHE:HE1   | 4:D:632:EDO:H21  | 1.77                     | 0.49              |
| 1:B:81:HIS:HE1   | 1:B:149:TRP:HB2  | 1.78                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:356:GLU:HG2  | 1:D:366:LEU:CD1  | 2.43                     | 0.49              |
| 1:A:159:GLU:CD   | 1:A:159:GLU:H    | 2.21                     | 0.49              |
| 1:D:159:GLU:H    | 1:D:159:GLU:CD   | 2.20                     | 0.49              |
| 1:A:216:LYS:C    | 1:A:218:ASN:H    | 2.20                     | 0.49              |
| 1:A:330:VAL:O    | 1:A:333:ARG:NE   | 2.46                     | 0.49              |
| 1:B:164:LEU:HD23 | 1:B:225:ALA:HB3  | 1.93                     | 0.49              |
| 1:D:301:ILE:O    | 1:D:337:LYS:HE3  | 2.13                     | 0.49              |
| 1:B:126:VAL:HG13 | 1:B:130:THR:CG2  | 2.43                     | 0.49              |
| 1:B:177:VAL:HG22 | 1:B:182:GLN:CD   | 2.38                     | 0.49              |
| 1:D:3:GLN:OE1    | 1:D:67:GLN:NE2   | 2.46                     | 0.49              |
| 1:B:25:HIS:CB    | 1:B:28:ALA:HB3   | 2.43                     | 0.49              |
| 1:C:108:ALA:HB2  | 1:C:151:ASP:HB2  | 1.93                     | 0.49              |
| 1:A:142:ILE:HD11 | 1:A:219:LEU:HD11 | 1.95                     | 0.49              |
| 1:A:216:LYS:C    | 1:A:218:ASN:N    | 2.69                     | 0.49              |
| 1:B:216:LYS:C    | 1:B:218:ASN:N    | 2.68                     | 0.49              |
| 1:D:183:VAL:HG12 | 1:D:184:ASP:N    | 2.28                     | 0.49              |
| 1:D:261:THR:HG21 | 1:D:267:GLU:H    | 1.78                     | 0.49              |
| 1:A:80:ASN:HD22  | 1:A:153:MET:CG   | 2.25                     | 0.48              |
| 1:C:294:ARG:HH11 | 1:D:320:PRO:CB   | 2.24                     | 0.48              |
| 1:A:83:GLU:CD    | 3:A:501:FEO:O    | 2.56                     | 0.48              |
| 1:B:341:ALA:HB3  | 1:B:352:GLN:NE2  | 2.28                     | 0.48              |
| 1:C:86:HIS:CE1   | 1:C:227:SER:HB2  | 2.49                     | 0.48              |
| 1:A:83:GLU:OE2   | 3:A:501:FEO:O    | 2.30                     | 0.48              |
| 1:A:139:LEU:HD13 | 1:A:141:PHE:HZ   | 1.79                     | 0.48              |
| 1:B:163:LEU:HG   | 1:B:165:PRO:HG3  | 1.96                     | 0.48              |
| 1:A:72:VAL:CG2   | 1:A:96:LEU:HD11  | 2.43                     | 0.48              |
| 1:A:25:HIS:HB2   | 1:A:28:ALA:HB3   | 1.94                     | 0.48              |
| 1:A:184:ASP:CG   | 1:A:187:LEU:HD13 | 2.38                     | 0.48              |
| 1:A:261:THR:HG21 | 1:A:267:GLU:N    | 2.28                     | 0.48              |
| 1:A:372:PRO:CG   | 1:A:389:LEU:HD13 | 2.41                     | 0.48              |
| 1:C:3:GLN:CD     | 1:C:67:GLN:HE22  | 2.22                     | 0.48              |
| 1:D:58:LYS:HE2   | 6:D:763:HOH:O    | 2.14                     | 0.48              |
| 1:A:140:THR:HG23 | 1:A:156:TYR:HB3  | 1.96                     | 0.48              |
| 1:A:163:LEU:O    | 1:A:165:PRO:HD3  | 2.13                     | 0.48              |
| 1:A:333:ARG:HD2  | 1:A:363:LYS:HG3  | 1.95                     | 0.48              |
| 1:B:101:HIS:CD2  | 1:B:124:THR:HG22 | 2.48                     | 0.48              |
| 1:C:216:LYS:C    | 1:C:218:ASN:H    | 2.21                     | 0.48              |
| 1:C:306:ALA:HA   | 1:C:338:VAL:O    | 2.14                     | 0.48              |
| 1:B:305:ARG:HD2  | 1:B:397:ILE:HG23 | 1.96                     | 0.48              |
| 1:D:188:ILE:HD13 | 1:D:230:ILE:HG21 | 1.96                     | 0.48              |
| 1:C:25:HIS:CE1   | 4:C:622:EDO:O2   | 2.67                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:301:ILE:O    | 1:A:337:LYS:HE3  | 2.14                     | 0.48              |
| 1:B:216:LYS:C    | 1:B:218:ASN:H    | 2.22                     | 0.48              |
| 1:B:365:GLU:CD   | 1:B:396:ARG:HH22 | 2.21                     | 0.48              |
| 1:C:261:THR:HG21 | 1:C:267:GLU:H    | 1.79                     | 0.48              |
| 1:D:216:LYS:C    | 1:D:218:ASN:N    | 2.71                     | 0.48              |
| 1:B:398:ALA:O    | 1:B:399:ASP:CB   | 2.61                     | 0.47              |
| 1:D:77:LEU:HD12  | 1:D:94:MET:CE    | 2.44                     | 0.47              |
| 1:B:144:ALA:N    | 1:B:145:PRO:HD3  | 2.29                     | 0.47              |
| 1:B:263:TRP:O    | 1:B:264:LEU:CB   | 2.62                     | 0.47              |
| 1:C:259:TYR:HE2  | 1:C:286:LEU:CD2  | 2.22                     | 0.47              |
| 1:C:294:ARG:HH12 | 1:D:320:PRO:HB2  | 1.78                     | 0.47              |
| 1:D:70:ASP:C     | 1:D:70:ASP:OD1   | 2.57                     | 0.47              |
| 1:D:237:GLY:O    | 1:D:241:GLU:HG3  | 2.15                     | 0.47              |
| 1:D:385:ARG:HA   | 1:D:385:ARG:HD2  | 1.81                     | 0.47              |
| 1:B:294:ARG:HH21 | 1:B:295:ASN:HD21 | 1.62                     | 0.47              |
| 1:D:81:HIS:CE1   | 1:D:149:TRP:HB2  | 2.49                     | 0.47              |
| 1:B:141:PHE:CD2  | 1:B:153:MET:CE   | 2.97                     | 0.47              |
| 1:B:291:VAL:O    | 1:B:291:VAL:CG1  | 2.63                     | 0.47              |
| 1:B:326:LEU:O    | 1:B:330:VAL:HG23 | 2.14                     | 0.47              |
| 1:C:286:LEU:C    | 1:C:286:LEU:HD23 | 2.40                     | 0.47              |
| 1:D:163:LEU:HG   | 1:D:165:PRO:HG3  | 1.96                     | 0.47              |
| 1:A:263:TRP:O    | 1:A:264:LEU:CB   | 2.63                     | 0.47              |
| 1:B:31:THR:HG22  | 1:B:172:HIS:HB3  | 1.97                     | 0.47              |
| 1:B:232:TRP:CZ2  | 1:B:239:ILE:HG12 | 2.50                     | 0.47              |
| 1:D:147:LEU:HA   | 1:D:147:LEU:HD12 | 1.44                     | 0.47              |
| 1:C:393:ILE:O    | 1:C:397:ILE:HG12 | 2.15                     | 0.46              |
| 1:A:291:VAL:O    | 1:A:291:VAL:HG13 | 2.15                     | 0.46              |
| 1:B:323:SER:HB2  | 1:B:324:PRO:HD3  | 1.98                     | 0.46              |
| 1:A:314:ILE:CD1  | 1:A:319:LEU:HA   | 2.28                     | 0.46              |
| 1:C:82:THR:HG22  | 1:C:112:LEU:HD13 | 1.98                     | 0.46              |
| 1:D:286:LEU:HD23 | 1:D:286:LEU:C    | 2.41                     | 0.46              |
| 1:A:72:VAL:HG21  | 1:A:96:LEU:HD11  | 1.97                     | 0.46              |
| 1:A:321:VAL:HG21 | 1:B:27:PRO:HB2   | 1.98                     | 0.46              |
| 1:A:391:ARG:NH1  | 1:A:391:ARG:CG   | 2.76                     | 0.46              |
| 1:B:55:GLU:HB3   | 1:B:56:PRO:HD3   | 1.97                     | 0.46              |
| 1:B:102:VAL:HG21 | 1:B:121:PHE:CD2  | 2.51                     | 0.46              |
| 1:B:314:ILE:CD1  | 1:B:318:ILE:O    | 2.64                     | 0.46              |
| 1:B:83:GLU:CD    | 4:B:612:EDO:O1   | 2.58                     | 0.46              |
| 1:C:212:ASP:O    | 1:C:215:GLN:HB3  | 2.15                     | 0.46              |
| 1:B:139:LEU:HD13 | 1:B:141:PHE:CZ   | 2.50                     | 0.46              |
| 1:B:253:ALA:HB2  | 1:B:399:ASP:HB2  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:252:LYS:O    | 1:B:254:LYS:N    | 2.47                     | 0.46              |
| 1:C:25:HIS:CB    | 1:C:28:ALA:HB3   | 2.46                     | 0.46              |
| 1:A:163:LEU:HG   | 1:A:165:PRO:HG3  | 1.98                     | 0.46              |
| 1:B:141:PHE:HB3  | 1:B:153:MET:HE2  | 1.96                     | 0.46              |
| 1:A:163:LEU:C    | 1:A:165:PRO:HD3  | 2.40                     | 0.46              |
| 1:A:235:ASP:CG   | 1:A:238:ARG:HG3  | 2.41                     | 0.46              |
| 1:C:177:VAL:HG22 | 1:C:182:GLN:CD   | 2.41                     | 0.46              |
| 1:D:196:TYR:HA   | 1:D:200:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:103:LEU:CD2  | 1:A:124:THR:HG23 | 2.47                     | 0.45              |
| 1:B:24:PHE:HE1   | 4:B:612:EDO:H11  | 0.58                     | 0.45              |
| 1:C:25:HIS:HE2   | 4:C:622:EDO:C1   | 2.29                     | 0.45              |
| 1:C:30:SER:H     | 1:C:295:ASN:ND2  | 2.13                     | 0.45              |
| 1:C:253:ALA:HB2  | 1:C:399:ASP:HB2  | 1.98                     | 0.45              |
| 1:D:254:LYS:HG2  | 1:D:255:ALA:N    | 2.31                     | 0.45              |
| 1:B:96:LEU:HD13  | 1:B:96:LEU:O     | 2.16                     | 0.45              |
| 1:B:336:ASN:O    | 1:B:336:ASN:CG   | 2.59                     | 0.45              |
| 1:C:76:TYR:CD1   | 1:C:101:HIS:HB3  | 2.51                     | 0.45              |
| 1:B:35:THR:OG1   | 1:B:36:THR:N     | 2.49                     | 0.45              |
| 1:B:138:SER:N    | 1:B:159:GLU:OE1  | 2.40                     | 0.45              |
| 1:C:82:THR:CG2   | 1:C:112:LEU:HD13 | 2.46                     | 0.45              |
| 1:C:323:SER:HB2  | 1:C:324:PRO:HD3  | 1.99                     | 0.45              |
| 1:D:3:GLN:HE22   | 1:D:67:GLN:NE2   | 2.15                     | 0.45              |
| 1:A:113:LYS:NZ   | 6:A:705:HOH:O    | 2.50                     | 0.45              |
| 1:B:40:TYR:CZ    | 1:B:225:ALA:HB1  | 2.51                     | 0.45              |
| 1:D:188:ILE:CD1  | 1:D:230:ILE:HG21 | 2.46                     | 0.45              |
| 1:D:372:PRO:CG   | 1:D:389:LEU:CD1  | 2.95                     | 0.45              |
| 1:A:27:PRO:HG2   | 1:B:321:VAL:HG21 | 1.99                     | 0.45              |
| 1:D:90:PHE:CE1   | 1:D:94:MET:HE3   | 2.52                     | 0.45              |
| 1:D:294:ARG:HE   | 1:D:294:ARG:HB3  | 1.46                     | 0.45              |
| 1:D:81:HIS:HE1   | 1:D:149:TRP:HB2  | 1.82                     | 0.45              |
| 1:A:269:MET:CE   | 1:A:374:VAL:HB   | 2.47                     | 0.45              |
| 1:B:107:ARG:HH11 | 1:B:107:ARG:HA   | 1.81                     | 0.45              |
| 1:B:314:ILE:HD11 | 1:B:319:LEU:N    | 2.31                     | 0.45              |
| 1:A:13:TRP:CZ3   | 1:A:64:LYS:HE2   | 2.52                     | 0.44              |
| 1:A:188:ILE:HD12 | 1:A:188:ILE:HA   | 1.87                     | 0.44              |
| 1:A:259:TYR:CD1  | 1:A:260:ASP:N    | 2.85                     | 0.44              |
| 1:A:306:ALA:HA   | 1:A:338:VAL:O    | 2.17                     | 0.44              |
| 1:B:38:ASN:HB2   | 1:B:227:SER:HA   | 1.99                     | 0.44              |
| 1:B:85:ASP:OD1   | 3:B:511:FEO:O    | 2.36                     | 0.44              |
| 1:B:375:GLN:O    | 1:B:376:TRP:HB2  | 2.16                     | 0.44              |
| 1:D:201:MET:N    | 1:D:202:PRO:CD   | 2.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:127:LYS:H    | 1:A:130:THR:HG23 | 1.79                     | 0.44              |
| 1:B:54:TYR:CD2   | 1:B:56:PRO:HD2   | 2.53                     | 0.44              |
| 1:B:107:ARG:HB3  | 1:B:107:ARG:HH11 | 1.82                     | 0.44              |
| 1:C:326:LEU:HD11 | 1:C:355:LEU:HD23 | 2.00                     | 0.44              |
| 1:D:261:THR:HG22 | 1:D:266:THR:CB   | 2.33                     | 0.44              |
| 1:A:147:LEU:HA   | 1:A:147:LEU:HD12 | 1.49                     | 0.44              |
| 1:A:341:ALA:C    | 1:A:352:GLN:HE22 | 2.26                     | 0.44              |
| 1:B:53:VAL:CG1   | 1:B:54:TYR:N     | 2.80                     | 0.44              |
| 1:A:308:LEU:CD1  | 1:A:340:LEU:HB3  | 2.40                     | 0.44              |
| 1:A:333:ARG:HD3  | 1:A:333:ARG:HA   | 1.75                     | 0.44              |
| 1:B:73:LYS:HA    | 1:B:73:LYS:HE2   | 1.99                     | 0.44              |
| 1:B:367:ILE:CD1  | 1:B:396:ARG:HH11 | 2.30                     | 0.44              |
| 1:D:168:ALA:O    | 1:D:169:PHE:HB2  | 2.17                     | 0.44              |
| 1:D:397:ILE:O    | 1:D:397:ILE:HG22 | 2.15                     | 0.44              |
| 1:A:53:VAL:CG1   | 1:A:54:TYR:N     | 2.81                     | 0.44              |
| 1:A:72:VAL:HG12  | 1:A:74:LEU:HD13  | 1.99                     | 0.44              |
| 1:A:333:ARG:HD2  | 1:A:363:LYS:HE2  | 1.99                     | 0.44              |
| 1:C:184:ASP:OD2  | 1:C:187:LEU:HD13 | 2.18                     | 0.44              |
| 1:A:149:TRP:CH2  | 6:B:730:HOH:O    | 2.56                     | 0.44              |
| 1:A:140:THR:HG22 | 1:A:158:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:379:ARG:NH1  | 1:A:382:ASP:OD1  | 2.51                     | 0.44              |
| 1:B:83:GLU:HG2   | 1:B:84:SER:H     | 1.83                     | 0.44              |
| 1:B:165:PRO:O    | 1:B:166:ASN:HB3  | 2.17                     | 0.44              |
| 1:B:379:ARG:HB2  | 1:B:381:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:82:THR:C     | 1:A:83:GLU:O     | 2.58                     | 0.44              |
| 1:A:156:TYR:CE2  | 1:A:219:LEU:HD22 | 2.53                     | 0.44              |
| 1:A:395:ALA:O    | 1:A:398:ALA:HB2  | 2.18                     | 0.44              |
| 1:B:347:TRP:CD1  | 1:B:348:GLY:N    | 2.86                     | 0.44              |
| 1:C:77:LEU:HD11  | 1:C:93:ILE:HG21  | 1.99                     | 0.44              |
| 1:D:216:LYS:C    | 1:D:218:ASN:H    | 2.26                     | 0.44              |
| 1:B:291:VAL:O    | 1:B:291:VAL:HG13 | 2.17                     | 0.44              |
| 1:C:32:HIS:NE2   | 6:C:723:HOH:O    | 2.36                     | 0.44              |
| 1:C:177:VAL:HG21 | 1:C:182:GLN:CB   | 2.47                     | 0.44              |
| 1:D:163:LEU:C    | 1:D:165:PRO:HD3  | 2.43                     | 0.44              |
| 1:D:232:TRP:CZ2  | 1:D:239:ILE:CG1  | 3.01                     | 0.44              |
| 1:D:395:ALA:O    | 1:D:398:ALA:HB2  | 2.17                     | 0.44              |
| 1:C:320:PRO:CB   | 1:D:294:ARG:HH12 | 2.24                     | 0.43              |
| 1:D:217:ILE:O    | 1:D:217:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:234:LYS:HE3  | 1:A:234:LYS:CA   | 2.28                     | 0.43              |
| 1:A:252:LYS:O    | 1:A:254:LYS:N    | 2.49                     | 0.43              |
| 1:C:261:THR:HG22 | 1:C:266:THR:CB   | 2.44                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:73:LYS:O     | 1:D:73:LYS:HE3   | 2.18                     | 0.43              |
| 1:D:306:ALA:HA   | 1:D:338:VAL:O    | 2.18                     | 0.43              |
| 1:A:81:HIS:HE1   | 1:A:149:TRP:CG   | 2.36                     | 0.43              |
| 1:A:101:HIS:CD2  | 1:A:124:THR:HG22 | 2.53                     | 0.43              |
| 1:D:24:PHE:CE1   | 4:D:632:EDO:C2   | 3.01                     | 0.43              |
| 1:D:73:LYS:O     | 1:D:74:LEU:C     | 2.60                     | 0.43              |
| 1:D:183:VAL:CG1  | 1:D:184:ASP:N    | 2.81                     | 0.43              |
| 1:C:82:THR:C     | 1:C:83:GLU:O     | 2.57                     | 0.43              |
| 1:C:201:MET:N    | 1:C:202:PRO:CD   | 2.81                     | 0.43              |
| 1:D:134:LEU:HD11 | 1:D:139:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:241:GLU:O    | 1:B:245:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:312:PRO:HD2  | 1:B:319:LEU:HD22 | 1.99                     | 0.43              |
| 1:C:183:VAL:HG12 | 1:C:184:ASP:N    | 2.34                     | 0.43              |
| 1:C:277:LEU:O    | 1:C:282:CYS:HB2  | 2.19                     | 0.43              |
| 1:D:52:THR:OG1   | 1:D:53:VAL:N     | 2.52                     | 0.43              |
| 1:D:165:PRO:O    | 1:D:166:ASN:HB3  | 2.18                     | 0.43              |
| 1:A:126:VAL:HG12 | 1:A:127:LYS:N    | 2.33                     | 0.43              |
| 1:C:24:PHE:HE1   | 4:C:622:EDO:H11  | 1.83                     | 0.43              |
| 1:C:127:LYS:H    | 1:C:130:THR:HG22 | 1.84                     | 0.43              |
| 1:D:308:LEU:CD1  | 1:D:340:LEU:HB3  | 2.44                     | 0.43              |
| 1:A:41:LEU:HD13  | 1:A:65:LEU:CD2   | 2.49                     | 0.43              |
| 1:A:391:ARG:NH1  | 6:A:720:HOH:O    | 2.50                     | 0.43              |
| 1:C:77:LEU:CD1   | 1:C:93:ILE:HG21  | 2.49                     | 0.43              |
| 1:B:189:MET:HE3  | 1:B:238:ARG:HG2  | 1.99                     | 0.43              |
| 1:C:391:ARG:HG3  | 1:C:391:ARG:NH1  | 2.28                     | 0.43              |
| 1:C:222:LYS:O    | 1:C:223:THR:HG22 | 2.19                     | 0.43              |
| 1:C:263:TRP:CE3  | 1:D:84:SER:OG    | 2.72                     | 0.43              |
| 1:C:327:ASP:OD2  | 1:D:358:ARG:NH2  | 2.52                     | 0.43              |
| 1:D:4:PRO:HG3    | 1:D:64:LYS:HB3   | 2.00                     | 0.43              |
| 1:A:43:VAL:HG13  | 1:A:47:THR:HG22  | 2.01                     | 0.43              |
| 1:B:141:PHE:CD2  | 1:B:153:MET:HE2  | 2.52                     | 0.43              |
| 1:A:44:ASP:O     | 1:A:45:ASP:C     | 2.62                     | 0.42              |
| 1:B:43:VAL:CA    | 1:B:47:THR:HG22  | 2.36                     | 0.42              |
| 1:B:260:ASP:HB3  | 1:B:319:LEU:HD23 | 2.01                     | 0.42              |
| 1:D:313:THR:HG22 | 1:D:351:ALA:HB3  | 2.01                     | 0.42              |
| 1:A:236:PRO:O    | 1:A:240:ILE:HG13 | 2.19                     | 0.42              |
| 1:D:336:ASN:O    | 1:D:336:ASN:CG   | 2.62                     | 0.42              |
| 1:A:54:TYR:CG    | 1:A:56:PRO:HD2   | 2.55                     | 0.42              |
| 1:A:80:ASN:HD22  | 1:A:153:MET:HG2  | 1.84                     | 0.42              |
| 1:A:126:VAL:HG11 | 1:A:141:PHE:CG   | 2.54                     | 0.42              |
| 1:C:191:GLU:HA   | 1:C:191:GLU:OE1  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:149:TRP:HH2  | 6:B:730:HOH:O    | 2.01                     | 0.42              |
| 1:A:196:TYR:C    | 1:A:196:TYR:CD2  | 2.97                     | 0.42              |
| 1:B:147:LEU:HA   | 1:B:147:LEU:HD12 | 1.44                     | 0.42              |
| 1:B:341:ALA:C    | 1:B:352:GLN:HE22 | 2.27                     | 0.42              |
| 1:A:90:PHE:CZ    | 1:A:94:MET:HE3   | 2.54                     | 0.42              |
| 1:A:379:ARG:CB   | 1:A:381:GLU:OE2  | 2.67                     | 0.42              |
| 1:B:46:LYS:CA    | 1:B:75:ASP:OD2   | 2.68                     | 0.42              |
| 1:B:144:ALA:HB1  | 1:B:147:LEU:HB2  | 2.02                     | 0.42              |
| 1:C:356:GLU:HG2  | 1:C:366:LEU:HD13 | 2.00                     | 0.42              |
| 1:D:163:LEU:O    | 1:D:165:PRO:HD3  | 2.20                     | 0.42              |
| 1:D:253:ALA:HA   | 1:D:397:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:168:ALA:O    | 1:A:169:PHE:HB2  | 2.19                     | 0.42              |
| 1:C:37:TYR:HB2   | 1:C:53:VAL:HG22  | 2.02                     | 0.42              |
| 1:C:50:VAL:HA    | 1:C:78:VAL:HB    | 2.02                     | 0.42              |
| 1:A:147:LEU:HD23 | 1:A:154:PHE:HZ   | 1.84                     | 0.42              |
| 1:A:314:ILE:HG12 | 1:A:319:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:65:LEU:HD23  | 1:B:65:LEU:HA    | 1.84                     | 0.42              |
| 3:B:511:FEO:O    | 4:B:612:EDO:H22  | 2.20                     | 0.42              |
| 1:A:379:ARG:HG2  | 1:A:379:ARG:H    | 1.63                     | 0.42              |
| 1:B:314:ILE:HD11 | 1:B:318:ILE:C    | 2.45                     | 0.42              |
| 1:A:201:MET:N    | 1:A:202:PRO:CD   | 2.82                     | 0.41              |
| 1:A:260:ASP:O    | 1:A:312:PRO:HD3  | 2.20                     | 0.41              |
| 1:C:81:HIS:CB    | 1:C:166:ASN:ND2  | 2.83                     | 0.41              |
| 1:C:140:THR:HG23 | 1:C:156:TYR:HB3  | 2.02                     | 0.41              |
| 1:D:24:PHE:O     | 1:D:25:HIS:HB2   | 2.19                     | 0.41              |
| 1:C:260:ASP:O    | 1:C:312:PRO:HD3  | 2.20                     | 0.41              |
| 1:D:3:GLN:HA     | 1:D:4:PRO:HD3    | 1.94                     | 0.41              |
| 1:D:68:ILE:HD13  | 1:D:68:ILE:N     | 2.34                     | 0.41              |
| 1:D:375:GLN:O    | 1:D:376:TRP:HB2  | 2.19                     | 0.41              |
| 1:A:323:SER:HB2  | 1:A:324:PRO:HD3  | 2.02                     | 0.41              |
| 1:B:144:ALA:N    | 1:B:145:PRO:CD   | 2.84                     | 0.41              |
| 1:B:202:PRO:CG   | 1:B:332:LEU:HA   | 2.36                     | 0.41              |
| 1:C:165:PRO:O    | 1:C:166:ASN:HB3  | 2.20                     | 0.41              |
| 1:C:168:ALA:O    | 1:C:169:PHE:HB2  | 2.20                     | 0.41              |
| 1:C:294:ARG:NH1  | 1:D:320:PRO:HG2  | 2.36                     | 0.41              |
| 1:D:263:TRP:O    | 1:D:264:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:165:PRO:O    | 1:A:166:ASN:CB   | 2.69                     | 0.41              |
| 1:A:235:ASP:OD1  | 1:A:238:ARG:HG3  | 2.20                     | 0.41              |
| 1:C:83:GLU:OE2   | 4:C:622:EDO:O1   | 2.37                     | 0.41              |
| 1:A:144:ALA:N    | 1:A:145:PRO:HD3  | 2.36                     | 0.41              |
| 1:A:217:ILE:O    | 1:A:217:ILE:HG22 | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:290:SER:HB3  | 1:D:27:PRO:CG    | 2.51                     | 0.41              |
| 1:D:188:ILE:HD11 | 1:D:230:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:112:LEU:HD12 | 1:A:112:LEU:HA   | 1.83                     | 0.41              |
| 1:B:86:HIS:CE1   | 1:B:227:SER:HB2  | 2.55                     | 0.41              |
| 1:C:259:TYR:CD1  | 1:C:260:ASP:N    | 2.89                     | 0.41              |
| 1:C:372:PRO:CG   | 1:C:389:LEU:CD1  | 2.95                     | 0.41              |
| 1:A:126:VAL:HG11 | 1:A:141:PHE:CD1  | 2.55                     | 0.41              |
| 1:B:107:ARG:HH11 | 1:B:107:ARG:CB   | 2.34                     | 0.41              |
| 1:D:43:VAL:HG22  | 1:D:47:THR:HG21  | 2.02                     | 0.41              |
| 1:D:59:GLU:H     | 1:D:59:GLU:CD    | 2.29                     | 0.41              |
| 1:D:81:HIS:HE1   | 1:D:149:TRP:CG   | 2.39                     | 0.41              |
| 1:A:138:SER:N    | 1:A:159:GLU:OE1  | 2.49                     | 0.41              |
| 1:A:359:LEU:HD23 | 1:A:359:LEU:HA   | 1.95                     | 0.41              |
| 1:B:113:LYS:HA   | 1:B:113:LYS:HD2  | 1.89                     | 0.41              |
| 1:B:262:MET:HE1  | 5:B:711:FMN:HM83 | 2.03                     | 0.41              |
| 1:C:142:ILE:HD11 | 1:C:219:LEU:HD11 | 2.02                     | 0.41              |
| 1:C:161:ALA:HB1  | 1:C:220:ALA:O    | 2.21                     | 0.41              |
| 1:D:195:TYR:O    | 1:D:199:ILE:HD12 | 2.21                     | 0.41              |
| 1:B:108:ALA:CA   | 1:B:151:ASP:HB2  | 2.51                     | 0.41              |
| 1:C:395:ALA:O    | 1:C:398:ALA:HB2  | 2.21                     | 0.41              |
| 1:A:81:HIS:HE1   | 1:A:149:TRP:CB   | 2.33                     | 0.40              |
| 1:A:21:ILE:HD11  | 1:A:23:TYR:O     | 2.21                     | 0.40              |
| 1:A:253:ALA:HB2  | 1:A:399:ASP:HB2  | 2.03                     | 0.40              |
| 1:A:356:GLU:O    | 1:A:360:LYS:HD3  | 2.21                     | 0.40              |
| 1:B:396:ARG:C    | 1:B:398:ALA:H    | 2.30                     | 0.40              |
| 1:C:381:GLU:HG2  | 1:C:385:ARG:HH21 | 1.86                     | 0.40              |
| 1:D:81:HIS:CB    | 1:D:166:ASN:ND2  | 2.84                     | 0.40              |
| 1:A:212:ASP:O    | 1:A:215:GLN:HB3  | 2.21                     | 0.40              |
| 1:D:40:TYR:OH    | 1:D:231:ILE:HD11 | 2.21                     | 0.40              |
| 1:B:93:ILE:HA    | 1:B:93:ILE:HD13  | 1.89                     | 0.40              |
| 1:B:216:LYS:O    | 1:B:218:ASN:N    | 2.54                     | 0.40              |
| 1:C:345:TYR:HA   | 5:C:721:FMN:O2'  | 2.22                     | 0.40              |
| 1:D:376:TRP:HA   | 1:D:376:TRP:CE3  | 2.57                     | 0.40              |
| 1:A:25:HIS:O     | 1:B:262:MET:HG2  | 2.21                     | 0.40              |
| 1:A:333:ARG:HD2  | 1:A:363:LYS:CG   | 2.50                     | 0.40              |
| 1:B:397:ILE:O    | 1:B:397:ILE:HG22 | 2.21                     | 0.40              |

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

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 6:C:730:HOH:O | 6:C:730:HOH:O[8_663] | 1.95                     | 0.25              |
| 6:C:735:HOH:O | 6:C:735:HOH:O[8_663] | 2.04                     | 0.16              |
| 6:C:740:HOH:O | 6:D:745:HOH:O[3_544] | 2.05                     | 0.15              |

## 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     | 396/398 (100%)   | 360 (91%)  | 29 (7%)  | 7 (2%)   | 6           | 23 |
| 1   | B     | 396/398 (100%)   | 361 (91%)  | 27 (7%)  | 8 (2%)   | 6           | 21 |
| 1   | C     | 396/398 (100%)   | 364 (92%)  | 25 (6%)  | 7 (2%)   | 6           | 23 |
| 1   | D     | 396/398 (100%)   | 362 (91%)  | 27 (7%)  | 7 (2%)   | 6           | 23 |
| All | All   | 1584/1592 (100%) | 1447 (91%) | 108 (7%) | 29 (2%)  | 6           | 23 |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | HIS  |
| 1   | A     | 370 | PRO  |
| 1   | A     | 398 | ALA  |
| 1   | B     | 71  | PRO  |
| 1   | B     | 83  | GLU  |
| 1   | B     | 148 | HIS  |
| 1   | B     | 370 | PRO  |
| 1   | B     | 398 | ALA  |
| 1   | C     | 71  | PRO  |
| 1   | C     | 148 | HIS  |
| 1   | C     | 370 | PRO  |
| 1   | C     | 398 | ALA  |
| 1   | D     | 71  | PRO  |
| 1   | D     | 148 | HIS  |
| 1   | D     | 370 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 398 | ALA  |
| 1   | A     | 74  | LEU  |
| 1   | C     | 74  | LEU  |
| 1   | D     | 117 | SER  |
| 1   | A     | 376 | TRP  |
| 1   | B     | 74  | LEU  |
| 1   | A     | 71  | PRO  |
| 1   | A     | 166 | ASN  |
| 1   | B     | 376 | TRP  |
| 1   | C     | 376 | TRP  |
| 1   | D     | 376 | TRP  |
| 1   | D     | 166 | ASN  |
| 1   | B     | 166 | ASN  |
| 1   | C     | 166 | ASN  |

### 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     | 329/329 (100%)   | 292 (89%)  | 37 (11%)  | 6           | 19 |
| 1   | B     | 329/329 (100%)   | 296 (90%)  | 33 (10%)  | 7           | 24 |
| 1   | C     | 329/329 (100%)   | 309 (94%)  | 20 (6%)   | 17          | 46 |
| 1   | D     | 329/329 (100%)   | 289 (88%)  | 40 (12%)  | 5           | 16 |
| All | All   | 1316/1316 (100%) | 1186 (90%) | 130 (10%) | 7           | 24 |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | THR  |
| 1   | A     | 53  | VAL  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 77  | LEU  |
| 1   | A     | 112 | LEU  |
| 1   | A     | 124 | THR  |
| 1   | A     | 130 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 139 | LEU  |
| 1   | A     | 140 | THR  |
| 1   | A     | 147 | LEU  |
| 1   | A     | 162 | LEU  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 177 | VAL  |
| 1   | A     | 204 | SER  |
| 1   | A     | 210 | LYS  |
| 1   | A     | 218 | ASN  |
| 1   | A     | 222 | LYS  |
| 1   | A     | 230 | ILE  |
| 1   | A     | 233 | ARG  |
| 1   | A     | 234 | LYS  |
| 1   | A     | 239 | ILE  |
| 1   | A     | 291 | VAL  |
| 1   | A     | 308 | LEU  |
| 1   | A     | 313 | THR  |
| 1   | A     | 314 | ILE  |
| 1   | A     | 321 | VAL  |
| 1   | A     | 325 | LEU  |
| 1   | A     | 360 | LYS  |
| 1   | A     | 363 | LYS  |
| 1   | A     | 364 | ILE  |
| 1   | A     | 367 | ILE  |
| 1   | A     | 369 | GLU  |
| 1   | A     | 373 | THR  |
| 1   | A     | 377 | VAL  |
| 1   | A     | 379 | ARG  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 391 | ARG  |
| 1   | B     | 53  | VAL  |
| 1   | B     | 71  | PRO  |
| 1   | B     | 73  | LYS  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 107 | ARG  |
| 1   | B     | 124 | THR  |
| 1   | B     | 130 | THR  |
| 1   | B     | 131 | SER  |
| 1   | B     | 139 | LEU  |
| 1   | B     | 140 | THR  |
| 1   | B     | 147 | LEU  |
| 1   | B     | 162 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 171 | GLN  |
| 1   | B     | 177 | VAL  |
| 1   | B     | 210 | LYS  |
| 1   | B     | 218 | ASN  |
| 1   | B     | 230 | ILE  |
| 1   | B     | 233 | ARG  |
| 1   | B     | 239 | ILE  |
| 1   | B     | 261 | THR  |
| 1   | B     | 291 | VAL  |
| 1   | B     | 308 | LEU  |
| 1   | B     | 314 | ILE  |
| 1   | B     | 321 | VAL  |
| 1   | B     | 325 | LEU  |
| 1   | B     | 358 | ARG  |
| 1   | B     | 366 | LEU  |
| 1   | B     | 370 | PRO  |
| 1   | B     | 374 | VAL  |
| 1   | B     | 377 | VAL  |
| 1   | B     | 379 | ARG  |
| 1   | B     | 381 | GLU  |
| 1   | B     | 389 | LEU  |
| 1   | C     | 24  | PHE  |
| 1   | C     | 53  | VAL  |
| 1   | C     | 73  | LYS  |
| 1   | C     | 94  | MET  |
| 1   | C     | 96  | LEU  |
| 1   | C     | 112 | LEU  |
| 1   | C     | 127 | LYS  |
| 1   | C     | 147 | LEU  |
| 1   | C     | 162 | LEU  |
| 1   | C     | 208 | THR  |
| 1   | C     | 210 | LYS  |
| 1   | C     | 230 | ILE  |
| 1   | C     | 234 | LYS  |
| 1   | C     | 239 | ILE  |
| 1   | C     | 282 | CYS  |
| 1   | C     | 291 | VAL  |
| 1   | C     | 317 | ASP  |
| 1   | C     | 325 | LEU  |
| 1   | C     | 358 | ARG  |
| 1   | C     | 370 | PRO  |
| 1   | D     | 9   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 21  | ILE  |
| 1   | D     | 24  | PHE  |
| 1   | D     | 43  | VAL  |
| 1   | D     | 50  | VAL  |
| 1   | D     | 53  | VAL  |
| 1   | D     | 68  | ILE  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 74  | LEU  |
| 1   | D     | 77  | LEU  |
| 1   | D     | 82  | THR  |
| 1   | D     | 93  | ILE  |
| 1   | D     | 97  | CYS  |
| 1   | D     | 112 | LEU  |
| 1   | D     | 125 | ILE  |
| 1   | D     | 130 | THR  |
| 1   | D     | 139 | LEU  |
| 1   | D     | 140 | THR  |
| 1   | D     | 147 | LEU  |
| 1   | D     | 153 | MET  |
| 1   | D     | 162 | LEU  |
| 1   | D     | 171 | GLN  |
| 1   | D     | 173 | ILE  |
| 1   | D     | 177 | VAL  |
| 1   | D     | 210 | LYS  |
| 1   | D     | 218 | ASN  |
| 1   | D     | 224 | ILE  |
| 1   | D     | 230 | ILE  |
| 1   | D     | 233 | ARG  |
| 1   | D     | 234 | LYS  |
| 1   | D     | 239 | ILE  |
| 1   | D     | 291 | VAL  |
| 1   | D     | 308 | LEU  |
| 1   | D     | 313 | THR  |
| 1   | D     | 318 | ILE  |
| 1   | D     | 325 | LEU  |
| 1   | D     | 358 | ARG  |
| 1   | D     | 360 | LYS  |
| 1   | D     | 369 | GLU  |
| 1   | D     | 370 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | GLN  |
| 1   | A     | 80  | ASN  |
| 1   | A     | 166 | ASN  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 218 | ASN  |
| 1   | A     | 295 | ASN  |
| 1   | A     | 352 | GLN  |
| 1   | A     | 375 | GLN  |
| 1   | B     | 80  | ASN  |
| 1   | B     | 118 | HIS  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 171 | GLN  |
| 1   | B     | 198 | ASN  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 295 | ASN  |
| 1   | B     | 352 | GLN  |
| 1   | B     | 375 | GLN  |
| 1   | C     | 3   | GLN  |
| 1   | C     | 67  | GLN  |
| 1   | C     | 80  | ASN  |
| 1   | C     | 86  | HIS  |
| 1   | C     | 101 | HIS  |
| 1   | C     | 122 | ASN  |
| 1   | C     | 166 | ASN  |
| 1   | C     | 218 | ASN  |
| 1   | C     | 295 | ASN  |
| 1   | C     | 315 | ASN  |
| 1   | C     | 375 | GLN  |
| 1   | D     | 3   | GLN  |
| 1   | D     | 67  | GLN  |
| 1   | D     | 80  | ASN  |
| 1   | D     | 101 | HIS  |
| 1   | D     | 115 | HIS  |
| 1   | D     | 118 | HIS  |
| 1   | D     | 122 | ASN  |
| 1   | D     | 166 | ASN  |
| 1   | D     | 171 | GLN  |
| 1   | D     | 218 | ASN  |
| 1   | D     | 295 | ASN  |
| 1   | D     | 375 | GLN  |

### 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 ⓘ

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | FMN  | B     | 711 | -    | 33,33,33     | 3.01 | 12 (36%)    | 48,50,50    | 2.47 | 17 (35%)    |
| 3   | FEO  | C     | 521 | 1    | 0,2,2        | -    | -           | -           |      |             |
| 3   | FEO  | B     | 511 | 1    | 0,2,2        | -    | -           | -           |      |             |
| 5   | FMN  | A     | 701 | -    | 33,33,33     | 3.09 | 13 (39%)    | 48,50,50    | 2.51 | 18 (37%)    |
| 3   | FEO  | D     | 531 | 1    | 0,2,2        | -    | -           | -           |      |             |
| 4   | EDO  | A     | 602 | -    | 3,3,3        | 0.34 | 0           | 2,2,2       | 0.52 | 0           |
| 4   | EDO  | C     | 622 | -    | 3,3,3        | 0.42 | 0           | 2,2,2       | 0.36 | 0           |
| 5   | FMN  | D     | 731 | -    | 33,33,33     | 3.00 | 15 (45%)    | 48,50,50    | 2.44 | 16 (33%)    |
| 4   | EDO  | D     | 632 | -    | 3,3,3        | 0.53 | 0           | 2,2,2       | 0.27 | 0           |
| 3   | FEO  | A     | 501 | 1    | 0,2,2        | -    | -           | -           |      |             |
| 5   | FMN  | C     | 721 | -    | 33,33,33     | 2.87 | 15 (45%)    | 48,50,50    | 2.49 | 17 (35%)    |
| 4   | EDO  | B     | 612 | -    | 3,3,3        | 0.58 | 0           | 2,2,2       | 0.27 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | FMN  | B     | 711 | -    | -       | 2/18/18/18 | 0/3/3/3 |
| 5   | FMN  | A     | 701 | -    | -       | 0/18/18/18 | 0/3/3/3 |
| 4   | EDO  | C     | 622 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | A     | 602 | -    | -       | 1/1/1/1    | -       |
| 5   | FMN  | D     | 731 | -    | -       | 0/18/18/18 | 0/3/3/3 |
| 4   | EDO  | D     | 632 | -    | -       | 1/1/1/1    | -       |
| 5   | FMN  | C     | 721 | -    | -       | 0/18/18/18 | 0/3/3/3 |
| 4   | EDO  | B     | 612 | -    | -       | 1/1/1/1    | -       |

All (55) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | A     | 701 | FMN  | C9-C9A  | 7.74 | 1.52        | 1.39     |
| 5   | B     | 711 | FMN  | C9-C9A  | 7.60 | 1.51        | 1.39     |
| 5   | D     | 731 | FMN  | C9A-C5A | 7.50 | 1.53        | 1.41     |
| 5   | D     | 731 | FMN  | C9-C9A  | 7.36 | 1.51        | 1.39     |
| 5   | A     | 701 | FMN  | C6-C7   | 7.07 | 1.49        | 1.39     |
| 5   | C     | 721 | FMN  | C9A-C5A | 7.01 | 1.52        | 1.41     |
| 5   | A     | 701 | FMN  | C9A-C5A | 6.97 | 1.52        | 1.41     |
| 5   | B     | 711 | FMN  | C9A-C5A | 6.96 | 1.52        | 1.41     |
| 5   | C     | 721 | FMN  | C9-C9A  | 6.84 | 1.50        | 1.39     |
| 5   | D     | 731 | FMN  | C6-C7   | 6.75 | 1.48        | 1.39     |
| 5   | B     | 711 | FMN  | C6-C7   | 6.73 | 1.48        | 1.39     |
| 5   | B     | 711 | FMN  | C2-N3   | 5.39 | 1.50        | 1.39     |
| 5   | C     | 721 | FMN  | C6-C7   | 5.27 | 1.46        | 1.39     |
| 5   | A     | 701 | FMN  | C2-N3   | 5.10 | 1.50        | 1.39     |
| 5   | D     | 731 | FMN  | C2-N3   | 5.06 | 1.50        | 1.39     |
| 5   | C     | 721 | FMN  | C2-N3   | 4.68 | 1.49        | 1.39     |
| 5   | B     | 711 | FMN  | C4A-C10 | 4.62 | 1.57        | 1.44     |
| 5   | D     | 731 | FMN  | C4A-C10 | 4.41 | 1.57        | 1.44     |
| 5   | A     | 701 | FMN  | C4A-C10 | 4.36 | 1.57        | 1.44     |
| 5   | C     | 721 | FMN  | C4A-C10 | 4.32 | 1.56        | 1.44     |
| 5   | C     | 721 | FMN  | C4-N3   | 4.11 | 1.46        | 1.38     |
| 5   | B     | 711 | FMN  | C4-N3   | 4.10 | 1.46        | 1.38     |
| 5   | A     | 701 | FMN  | C6-C5A  | 3.94 | 1.46        | 1.40     |
| 5   | B     | 711 | FMN  | C6-C5A  | 3.82 | 1.45        | 1.40     |
| 5   | C     | 721 | FMN  | C6-C5A  | 3.82 | 1.45        | 1.40     |
| 5   | A     | 701 | FMN  | C4-N3   | 3.81 | 1.46        | 1.38     |
| 5   | A     | 701 | FMN  | C5A-N5  | 3.79 | 1.46        | 1.39     |
| 5   | C     | 721 | FMN  | C5A-N5  | 3.77 | 1.46        | 1.39     |
| 5   | D     | 731 | FMN  | C4-N3   | 3.73 | 1.45        | 1.38     |
| 5   | A     | 701 | FMN  | C5'-C4' | 3.44 | 1.56        | 1.51     |
| 5   | D     | 731 | FMN  | C6-C5A  | 3.40 | 1.45        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | D     | 731 | FMN  | C5A-N5  | 3.38  | 1.45        | 1.39     |
| 5   | D     | 731 | FMN  | C5'-C4' | 3.20  | 1.56        | 1.51     |
| 5   | C     | 721 | FMN  | C5'-C4' | 3.19  | 1.56        | 1.51     |
| 5   | B     | 711 | FMN  | C5A-N5  | 3.17  | 1.45        | 1.39     |
| 5   | D     | 731 | FMN  | C8-C7   | 3.17  | 1.48        | 1.40     |
| 5   | B     | 711 | FMN  | C8-C7   | 3.16  | 1.48        | 1.40     |
| 5   | A     | 701 | FMN  | C8-C7   | 3.12  | 1.48        | 1.40     |
| 5   | C     | 721 | FMN  | C8-C7   | 3.11  | 1.48        | 1.40     |
| 5   | A     | 701 | FMN  | C2'-C3' | -2.99 | 1.48        | 1.53     |
| 5   | B     | 711 | FMN  | C5'-C4' | 2.95  | 1.55        | 1.51     |
| 5   | C     | 721 | FMN  | C2'-C3' | -2.62 | 1.48        | 1.53     |
| 5   | A     | 701 | FMN  | O3'-C3' | 2.61  | 1.49        | 1.43     |
| 5   | D     | 731 | FMN  | O3'-C3' | 2.53  | 1.49        | 1.43     |
| 5   | B     | 711 | FMN  | C10-N10 | 2.27  | 1.42        | 1.37     |
| 5   | D     | 731 | FMN  | C10-N1  | 2.18  | 1.37        | 1.33     |
| 5   | C     | 721 | FMN  | O4-C4   | 2.12  | 1.27        | 1.23     |
| 5   | B     | 711 | FMN  | C10-N1  | 2.09  | 1.37        | 1.33     |
| 5   | C     | 721 | FMN  | C10-N10 | 2.06  | 1.41        | 1.37     |
| 5   | C     | 721 | FMN  | P-O2P   | -2.06 | 1.47        | 1.54     |
| 5   | D     | 731 | FMN  | C2'-C3' | -2.05 | 1.49        | 1.53     |
| 5   | C     | 721 | FMN  | O3'-C3' | 2.04  | 1.48        | 1.43     |
| 5   | A     | 701 | FMN  | P-O1P   | 2.04  | 1.56        | 1.50     |
| 5   | D     | 731 | FMN  | C8M-C8  | -2.03 | 1.47        | 1.51     |
| 5   | D     | 731 | FMN  | C10-N10 | 2.01  | 1.41        | 1.37     |

All (68) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | A     | 701 | FMN  | C5A-C9A-N10 | 6.94  | 124.24      | 117.97   |
| 5   | B     | 711 | FMN  | C5A-C9A-N10 | 6.94  | 124.24      | 117.97   |
| 5   | C     | 721 | FMN  | C5A-C9A-N10 | 6.91  | 124.21      | 117.97   |
| 5   | D     | 731 | FMN  | C5A-C9A-N10 | 6.81  | 124.12      | 117.97   |
| 5   | C     | 721 | FMN  | C7M-C7-C6   | -6.34 | 108.41      | 119.57   |
| 5   | A     | 701 | FMN  | C7M-C7-C6   | -6.13 | 108.77      | 119.57   |
| 5   | B     | 711 | FMN  | C7M-C7-C6   | -6.03 | 108.95      | 119.57   |
| 5   | D     | 731 | FMN  | C7M-C7-C6   | -6.03 | 108.95      | 119.57   |
| 5   | A     | 701 | FMN  | C9A-C5A-N5  | -5.65 | 116.46      | 122.45   |
| 5   | C     | 721 | FMN  | C9A-C5A-N5  | -5.50 | 116.62      | 122.45   |
| 5   | B     | 711 | FMN  | C9A-C5A-N5  | -5.46 | 116.66      | 122.45   |
| 5   | D     | 731 | FMN  | C9A-C5A-N5  | -5.32 | 116.81      | 122.45   |
| 5   | C     | 721 | FMN  | C7M-C7-C8   | 5.14  | 131.25      | 120.76   |
| 5   | A     | 701 | FMN  | C7M-C7-C8   | 5.00  | 130.97      | 120.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | B     | 711 | FMN  | C7M-C7-C8   | 5.00  | 130.97      | 120.76   |
| 5   | D     | 731 | FMN  | C7M-C7-C8   | 4.88  | 130.73      | 120.76   |
| 5   | A     | 701 | FMN  | O2-C2-N1    | 4.42  | 129.14      | 121.80   |
| 5   | C     | 721 | FMN  | O2-C2-N1    | 4.41  | 129.12      | 121.80   |
| 5   | B     | 711 | FMN  | O2-C2-N1    | 4.29  | 128.92      | 121.80   |
| 5   | D     | 731 | FMN  | O2-C2-N1    | 4.19  | 128.76      | 121.80   |
| 5   | C     | 721 | FMN  | C10-N1-C2   | 4.13  | 125.79      | 116.85   |
| 5   | A     | 701 | FMN  | C10-N1-C2   | 3.99  | 125.49      | 116.85   |
| 5   | D     | 731 | FMN  | C10-N1-C2   | 3.96  | 125.42      | 116.85   |
| 5   | B     | 711 | FMN  | C10-N1-C2   | 3.90  | 125.30      | 116.85   |
| 5   | A     | 701 | FMN  | C6-C5A-N5   | 3.45  | 124.17      | 118.44   |
| 5   | A     | 701 | FMN  | O4-C4-N3    | -3.40 | 113.71      | 120.11   |
| 5   | D     | 731 | FMN  | O4-C4-N3    | -3.32 | 113.87      | 120.11   |
| 5   | C     | 721 | FMN  | O4-C4-N3    | -3.25 | 114.00      | 120.11   |
| 5   | C     | 721 | FMN  | C4A-C10-N10 | 3.25  | 121.13      | 116.48   |
| 5   | D     | 731 | FMN  | C4A-C10-N10 | 3.17  | 121.02      | 116.48   |
| 5   | D     | 731 | FMN  | C9A-N10-C10 | -3.14 | 115.96      | 120.75   |
| 5   | B     | 711 | FMN  | C4'-C3'-C2' | 3.12  | 118.77      | 113.57   |
| 5   | B     | 711 | FMN  | C9A-N10-C10 | -3.11 | 116.01      | 120.75   |
| 5   | C     | 721 | FMN  | C6-C5A-N5   | 3.10  | 123.58      | 118.44   |
| 5   | C     | 721 | FMN  | C1'-N10-C9A | 3.09  | 126.64      | 120.63   |
| 5   | C     | 721 | FMN  | C9A-N10-C10 | -3.08 | 116.06      | 120.75   |
| 5   | D     | 731 | FMN  | C1'-N10-C9A | 3.07  | 126.60      | 120.63   |
| 5   | D     | 731 | FMN  | C6-C5A-N5   | 3.04  | 123.48      | 118.44   |
| 5   | A     | 701 | FMN  | C4A-C10-N10 | 3.00  | 120.78      | 116.48   |
| 5   | B     | 711 | FMN  | C6-C5A-N5   | 2.99  | 123.40      | 118.44   |
| 5   | B     | 711 | FMN  | O4-C4-N3    | -2.96 | 114.55      | 120.11   |
| 5   | B     | 711 | FMN  | C1'-N10-C9A | 2.88  | 126.23      | 120.63   |
| 5   | A     | 701 | FMN  | C1'-N10-C9A | 2.87  | 126.21      | 120.63   |
| 5   | D     | 731 | FMN  | C4A-C10-N1  | -2.84 | 117.63      | 124.59   |
| 5   | A     | 701 | FMN  | C4'-C3'-C2' | 2.83  | 118.28      | 113.57   |
| 5   | C     | 721 | FMN  | C4A-C10-N1  | -2.83 | 117.66      | 124.59   |
| 5   | B     | 711 | FMN  | C4A-C10-N1  | -2.78 | 117.78      | 124.59   |
| 5   | B     | 711 | FMN  | C4A-C10-N10 | 2.75  | 120.42      | 116.48   |
| 5   | D     | 731 | FMN  | O3'-C3'-C4' | -2.74 | 102.69      | 108.93   |
| 5   | A     | 701 | FMN  | C9A-N10-C10 | -2.74 | 116.57      | 120.75   |
| 5   | A     | 701 | FMN  | C4A-C10-N1  | -2.67 | 118.04      | 124.59   |
| 5   | B     | 711 | FMN  | O3'-C3'-C4' | -2.67 | 102.87      | 108.93   |
| 5   | C     | 721 | FMN  | O2-C2-N3    | -2.55 | 113.69      | 118.58   |
| 5   | B     | 711 | FMN  | O2-C2-N3    | -2.50 | 113.78      | 118.58   |
| 5   | D     | 731 | FMN  | O2-C2-N3    | -2.38 | 114.01      | 118.58   |
| 5   | A     | 701 | FMN  | O2-C2-N3    | -2.38 | 114.03      | 118.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | C     | 721 | FMN  | O3'-C3'-C4' | -2.35 | 103.60      | 108.93   |
| 5   | A     | 701 | FMN  | O3'-C3'-C4' | -2.32 | 103.67      | 108.93   |
| 5   | B     | 711 | FMN  | C5A-N5-C4A  | 2.32  | 121.84      | 118.09   |
| 5   | A     | 701 | FMN  | C9-C9A-N10  | -2.32 | 118.74      | 121.85   |
| 5   | D     | 731 | FMN  | C4'-C3'-C2' | 2.22  | 117.27      | 113.57   |
| 5   | D     | 731 | FMN  | C9-C9A-N10  | -2.21 | 118.88      | 121.85   |
| 5   | C     | 721 | FMN  | C10-C4A-N5  | -2.11 | 120.50      | 124.81   |
| 5   | C     | 721 | FMN  | C5A-N5-C4A  | 2.09  | 121.47      | 118.09   |
| 5   | A     | 701 | FMN  | C5'-C4'-C3' | 2.08  | 116.15      | 112.22   |
| 5   | A     | 701 | FMN  | C10-C4A-N5  | -2.05 | 120.62      | 124.81   |
| 5   | B     | 711 | FMN  | C9-C9A-N10  | -2.04 | 119.11      | 121.85   |
| 5   | C     | 721 | FMN  | C9-C9A-C5A  | -2.02 | 116.46      | 120.03   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | A     | 602 | EDO  | O1-C1-C2-O2     |
| 4   | B     | 612 | EDO  | O1-C1-C2-O2     |
| 4   | C     | 622 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 632 | EDO  | O1-C1-C2-O2     |
| 5   | B     | 711 | FMN  | C3'-C4'-C5'-O5' |
| 5   | B     | 711 | FMN  | O4'-C4'-C5'-O5' |

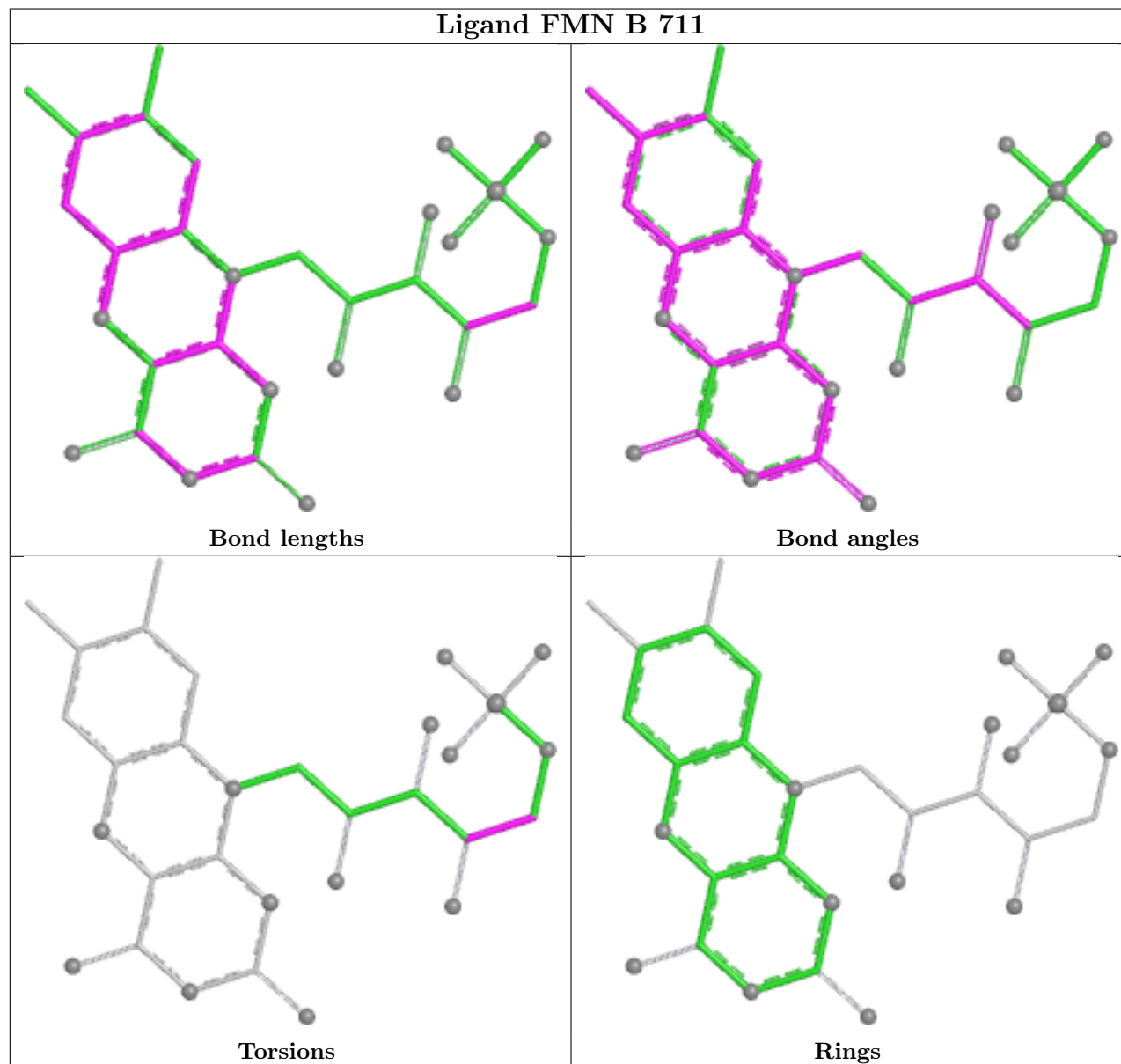
There are no ring outliers.

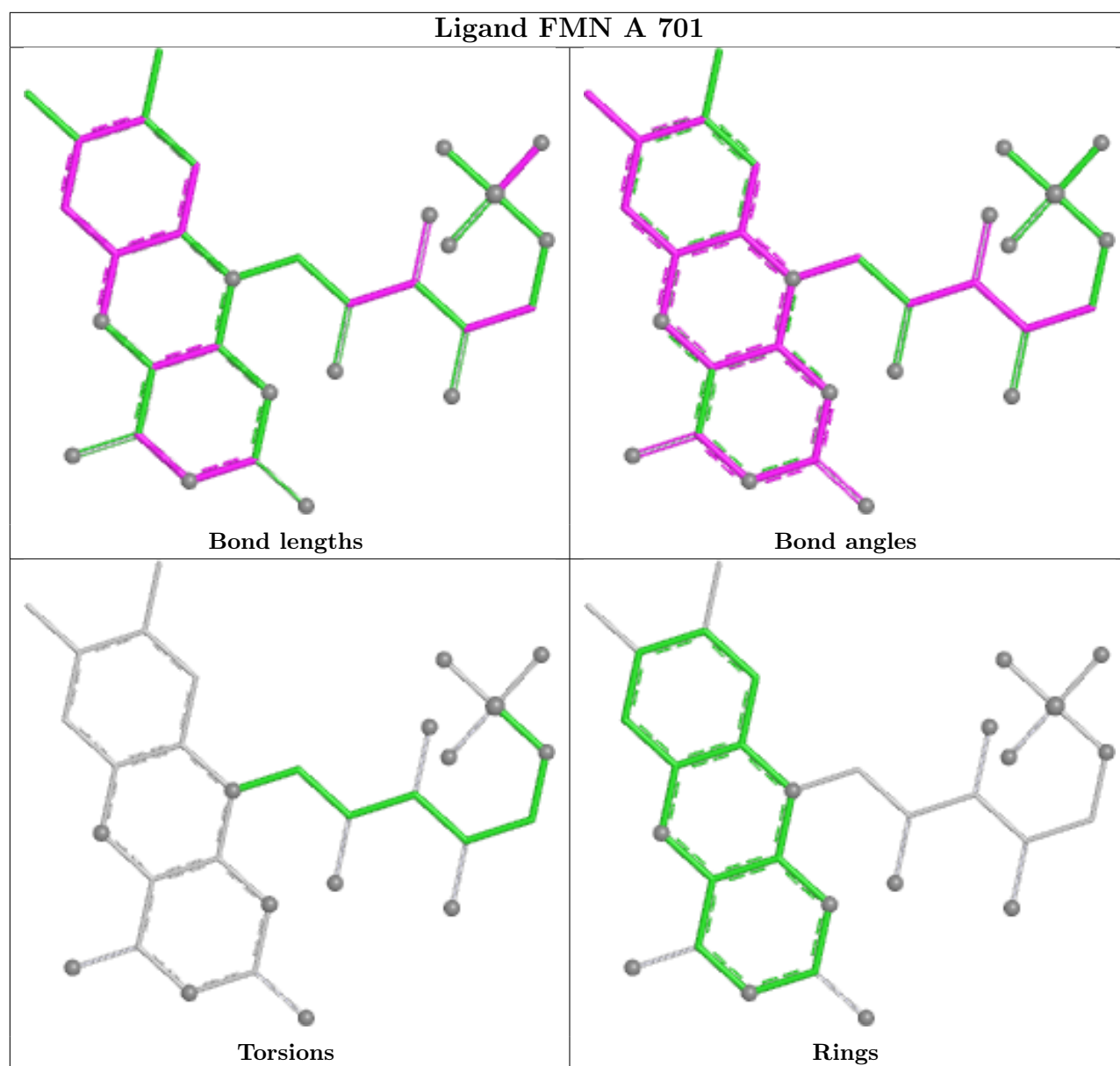
10 monomers are involved in 52 short contacts:

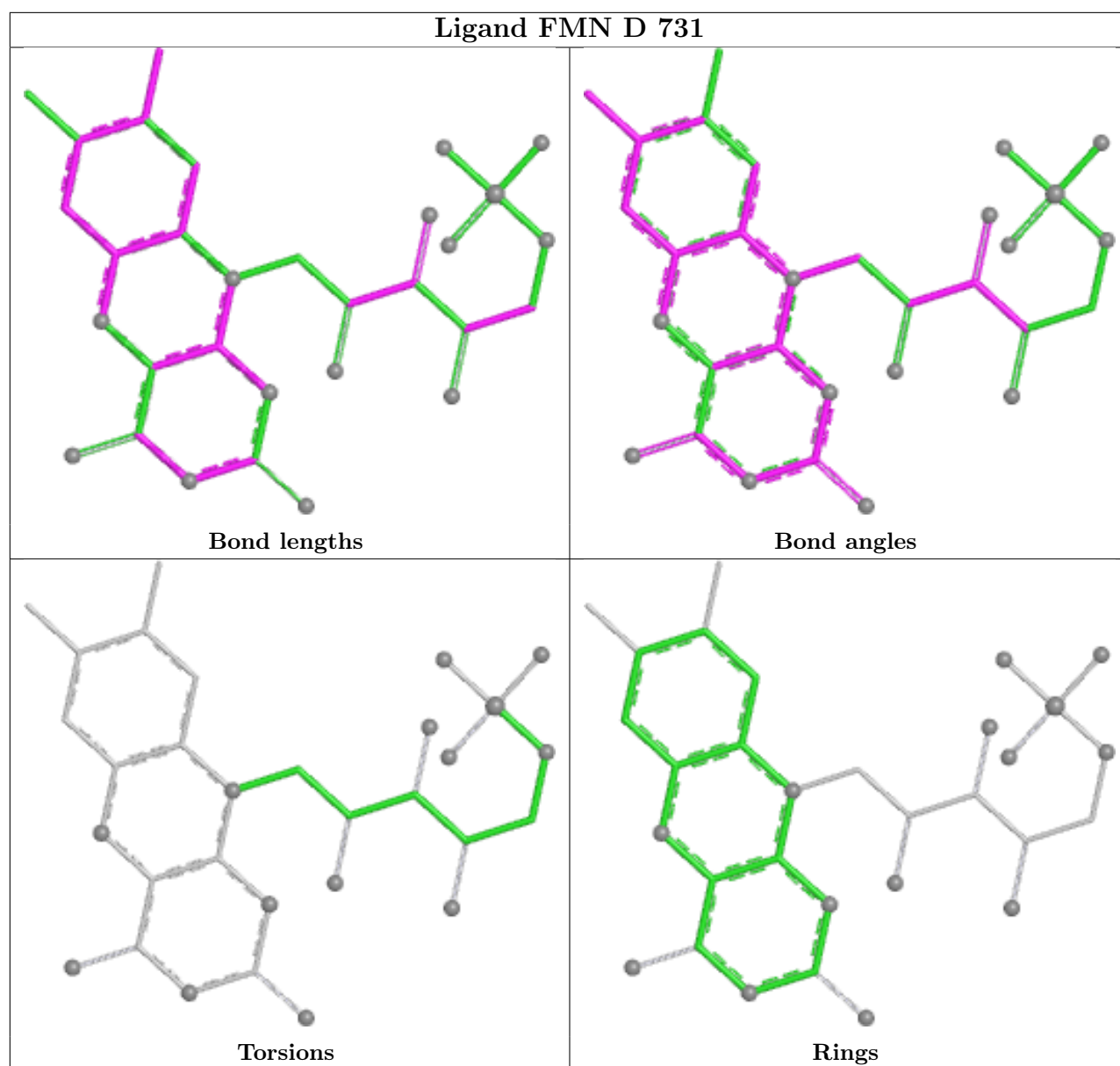
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | B     | 711 | FMN  | 2       | 0            |
| 3   | C     | 521 | FEO  | 1       | 0            |
| 3   | B     | 511 | FEO  | 5       | 0            |
| 3   | D     | 531 | FEO  | 2       | 0            |
| 4   | A     | 602 | EDO  | 9       | 0            |
| 4   | C     | 622 | EDO  | 11      | 0            |
| 4   | D     | 632 | EDO  | 13      | 0            |
| 3   | A     | 501 | FEO  | 4       | 0            |
| 5   | C     | 721 | FMN  | 2       | 0            |
| 4   | B     | 612 | EDO  | 12      | 0            |

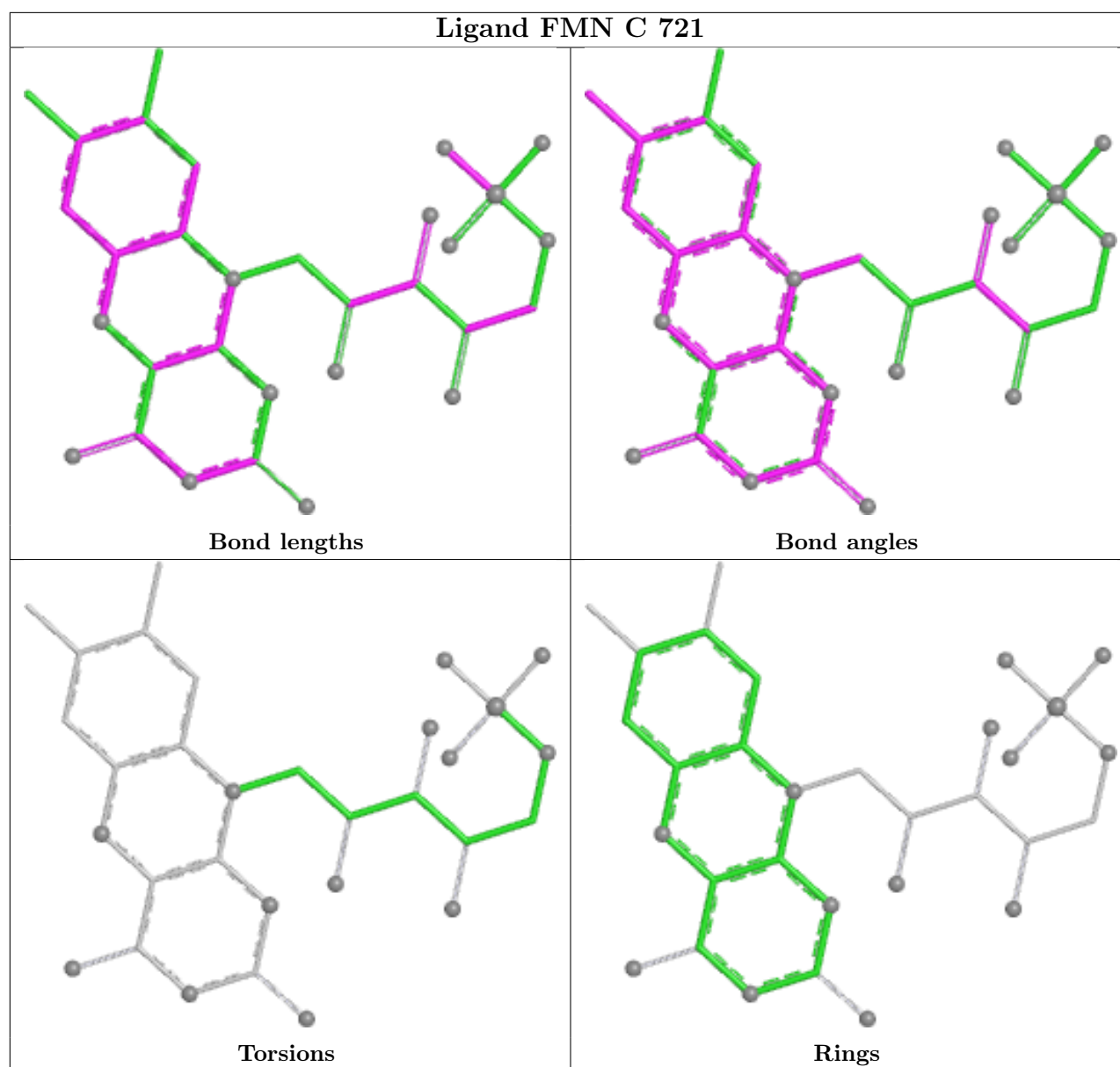
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 117:SER   | C      | 118:HIS   | N      | 1.13         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|------------------|--------|-----------|----|----|-----------------------|---------|
| 1   | A     | 398/398 (100%)   | 0.41   | 17 (4%)   | 40 | 31 | 37, 58, 77, 90        | 0       |
| 1   | B     | 398/398 (100%)   | 0.49   | 29 (7%)   | 21 | 15 | 39, 60, 84, 96        | 0       |
| 1   | C     | 398/398 (100%)   | 0.18   | 12 (3%)   | 52 | 42 | 36, 50, 70, 85        | 0       |
| 1   | D     | 398/398 (100%)   | 0.24   | 19 (4%)   | 35 | 28 | 37, 50, 71, 87        | 0       |
| All | All   | 1592/1592 (100%) | 0.33   | 77 (4%)   | 35 | 28 | 36, 54, 77, 96        | 0       |

All (77) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 45  | ASP  | 4.3  |
| 1   | A     | 70  | ASP  | 4.2  |
| 1   | D     | 71  | PRO  | 4.0  |
| 1   | A     | 238 | ARG  | 3.8  |
| 1   | D     | 117 | SER  | 3.7  |
| 1   | D     | 118 | HIS  | 3.7  |
| 1   | C     | 245 | ARG  | 3.6  |
| 1   | C     | 118 | HIS  | 3.5  |
| 1   | C     | 71  | PRO  | 3.4  |
| 1   | D     | 73  | LYS  | 3.3  |
| 1   | C     | 70  | ASP  | 3.3  |
| 1   | C     | 398 | ALA  | 3.2  |
| 1   | D     | 399 | ASP  | 3.2  |
| 1   | A     | 217 | ILE  | 3.1  |
| 1   | B     | 369 | GLU  | 3.0  |
| 1   | C     | 370 | PRO  | 3.0  |
| 1   | D     | 45  | ASP  | 3.0  |
| 1   | B     | 74  | LEU  | 2.9  |
| 1   | A     | 365 | GLU  | 2.9  |
| 1   | B     | 69  | LYS  | 2.9  |
| 1   | D     | 379 | ARG  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 245 | ARG  | 2.8  |
| 1   | D     | 32  | HIS  | 2.8  |
| 1   | B     | 104 | CYS  | 2.8  |
| 1   | B     | 391 | ARG  | 2.7  |
| 1   | B     | 73  | LYS  | 2.7  |
| 1   | D     | 24  | PHE  | 2.6  |
| 1   | D     | 120 | ASP  | 2.6  |
| 1   | B     | 98  | PRO  | 2.6  |
| 1   | A     | 3   | GLN  | 2.6  |
| 1   | B     | 398 | ALA  | 2.6  |
| 1   | D     | 70  | ASP  | 2.6  |
| 1   | B     | 238 | ARG  | 2.5  |
| 1   | B     | 136 | LYS  | 2.5  |
| 1   | B     | 217 | ILE  | 2.5  |
| 1   | A     | 208 | THR  | 2.4  |
| 1   | B     | 120 | ASP  | 2.4  |
| 1   | B     | 118 | HIS  | 2.4  |
| 1   | A     | 71  | PRO  | 2.3  |
| 1   | C     | 73  | LYS  | 2.3  |
| 1   | D     | 136 | LYS  | 2.3  |
| 1   | B     | 245 | ARG  | 2.3  |
| 1   | B     | 127 | LYS  | 2.3  |
| 1   | C     | 216 | LYS  | 2.3  |
| 1   | B     | 317 | ASP  | 2.3  |
| 1   | B     | 72  | VAL  | 2.3  |
| 1   | D     | 369 | GLU  | 2.3  |
| 1   | A     | 147 | LEU  | 2.3  |
| 1   | C     | 234 | LYS  | 2.3  |
| 1   | A     | 222 | LYS  | 2.2  |
| 1   | C     | 399 | ASP  | 2.2  |
| 1   | A     | 28  | ALA  | 2.2  |
| 1   | D     | 216 | LYS  | 2.2  |
| 1   | B     | 119 | ILE  | 2.2  |
| 1   | B     | 99  | ASP  | 2.2  |
| 1   | A     | 282 | CYS  | 2.2  |
| 1   | B     | 370 | PRO  | 2.2  |
| 1   | D     | 119 | ILE  | 2.1  |
| 1   | B     | 151 | ASP  | 2.1  |
| 1   | A     | 369 | GLU  | 2.1  |
| 1   | A     | 397 | ILE  | 2.1  |
| 1   | B     | 95  | GLU  | 2.1  |
| 1   | B     | 122 | ASN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 379 | ARG  | 2.1  |
| 1   | B     | 282 | CYS  | 2.1  |
| 1   | B     | 216 | LYS  | 2.1  |
| 1   | D     | 69  | LYS  | 2.1  |
| 1   | B     | 71  | PRO  | 2.1  |
| 1   | B     | 121 | PHE  | 2.1  |
| 1   | A     | 2   | SER  | 2.0  |
| 1   | A     | 124 | THR  | 2.0  |
| 1   | B     | 303 | ASP  | 2.0  |
| 1   | A     | 234 | LYS  | 2.0  |
| 1   | C     | 2   | SER  | 2.0  |
| 1   | D     | 3   | GLN  | 2.0  |
| 1   | B     | 333 | ARG  | 2.0  |
| 1   | D     | 234 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | EDO  | C     | 622 | 4/4   | 0.69 | 0.34 | 40,45,48,59                | 0     |
| 4   | EDO  | D     | 632 | 4/4   | 0.69 | 0.28 | 58,61,61,63                | 0     |
| 4   | EDO  | A     | 602 | 4/4   | 0.76 | 0.25 | 52,56,58,63                | 0     |
| 4   | EDO  | B     | 612 | 4/4   | 0.80 | 0.21 | 57,62,63,65                | 0     |
| 2   | ZN   | C     | 423 | 1/1   | 0.90 | 0.14 | 200,200,200,200            | 0     |
| 2   | ZN   | D     | 433 | 1/1   | 0.90 | 0.12 | 199,199,199,199            | 0     |
| 2   | ZN   | B     | 413 | 1/1   | 0.90 | 0.10 | 200,200,200,200            | 0     |
| 2   | ZN   | A     | 404 | 1/1   | 0.93 | 0.10 | 161,161,161,161            | 0     |
| 3   | FEO  | C     | 521 | 3/3   | 0.93 | 0.10 | 43,43,45,46                | 0     |

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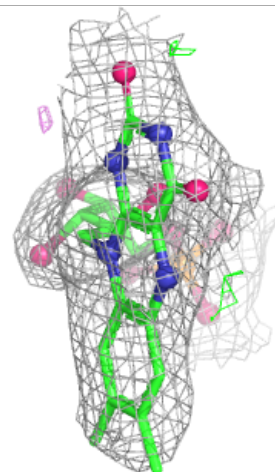
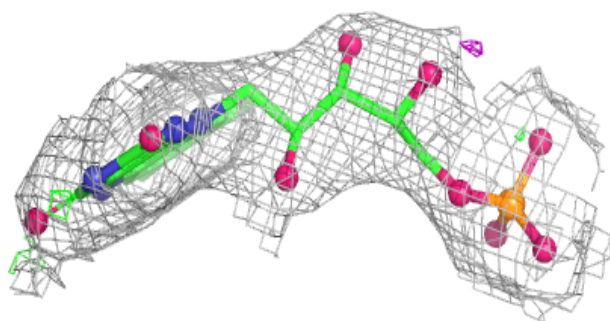
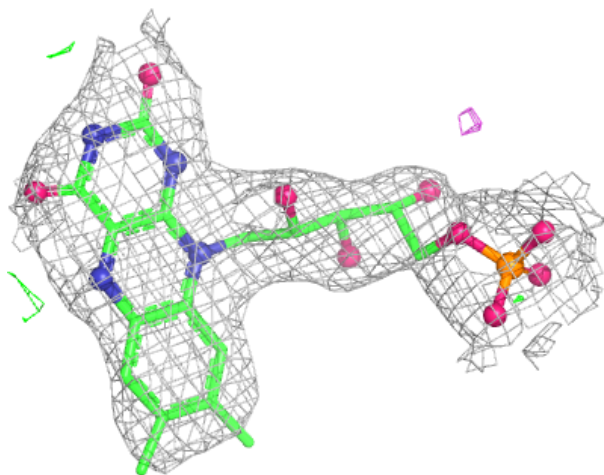
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | ZN   | B     | 414 | 1/1   | 0.94 | 0.08 | 130,130,130,130             | 0     |
| 2   | ZN   | A     | 403 | 1/1   | 0.94 | 0.07 | 106,106,106,106             | 0     |
| 3   | FEO  | B     | 511 | 3/3   | 0.95 | 0.08 | 54,54,55,56                 | 0     |
| 3   | FEO  | A     | 501 | 3/3   | 0.95 | 0.09 | 52,52,56,56                 | 0     |
| 3   | FEO  | D     | 531 | 3/3   | 0.96 | 0.07 | 42,42,46,46                 | 0     |
| 5   | FMN  | A     | 701 | 31/31 | 0.96 | 0.09 | 50,60,63,64                 | 0     |
| 5   | FMN  | D     | 731 | 31/31 | 0.96 | 0.08 | 41,43,47,47                 | 0     |
| 5   | FMN  | C     | 721 | 31/31 | 0.97 | 0.08 | 39,43,46,47                 | 0     |
| 5   | FMN  | B     | 711 | 31/31 | 0.97 | 0.08 | 45,59,63,64                 | 0     |
| 2   | ZN   | B     | 411 | 1/1   | 0.98 | 0.05 | 92,92,92,92                 | 0     |
| 2   | ZN   | C     | 422 | 1/1   | 0.98 | 0.09 | 96,96,96,96                 | 0     |
| 2   | ZN   | A     | 402 | 1/1   | 0.99 | 0.06 | 87,87,87,87                 | 0     |
| 2   | ZN   | B     | 412 | 1/1   | 0.99 | 0.06 | 91,91,91,91                 | 0     |
| 2   | ZN   | D     | 432 | 1/1   | 0.99 | 0.04 | 97,97,97,97                 | 0     |
| 2   | ZN   | C     | 421 | 1/1   | 0.99 | 0.06 | 77,77,77,77                 | 0     |
| 2   | ZN   | A     | 401 | 1/1   | 1.00 | 0.04 | 81,81,81,81                 | 0     |
| 2   | ZN   | D     | 431 | 1/1   | 1.00 | 0.03 | 78,78,78,78                 | 0     |

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

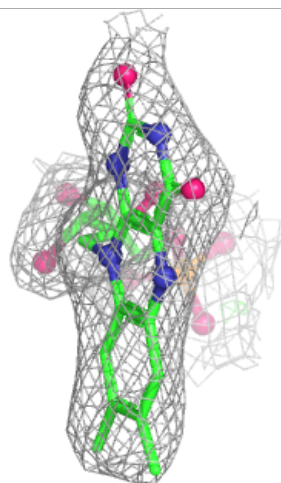
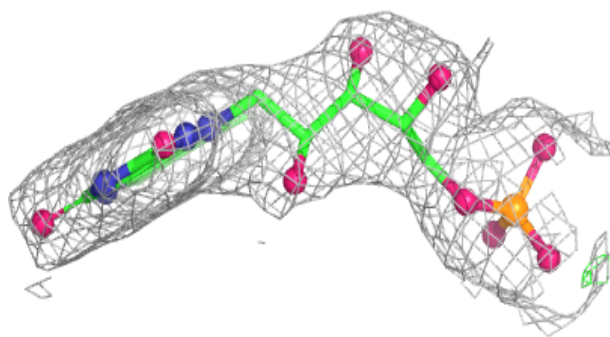
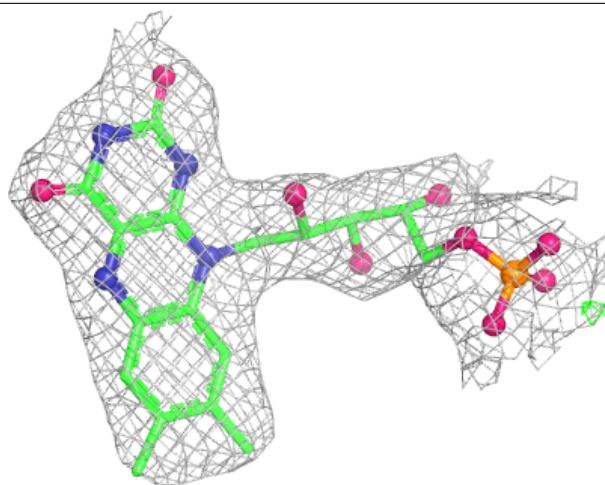
**Electron density around FMN A 701:**

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



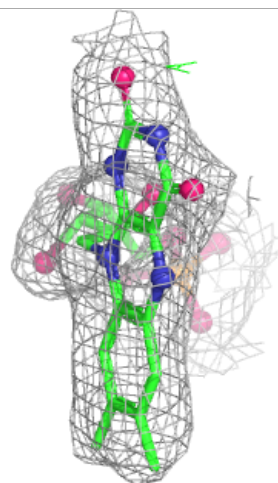
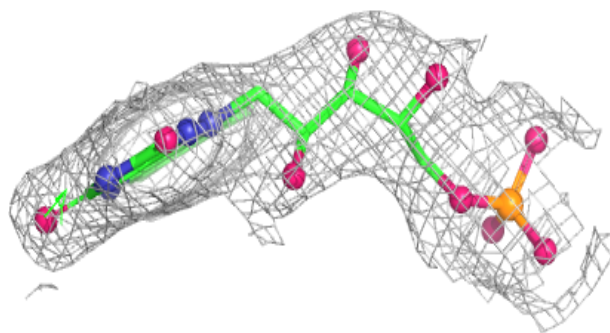
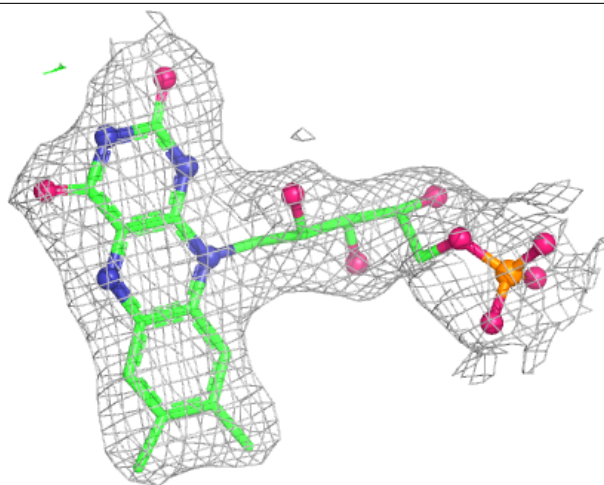
**Electron density around FMN D 731:**

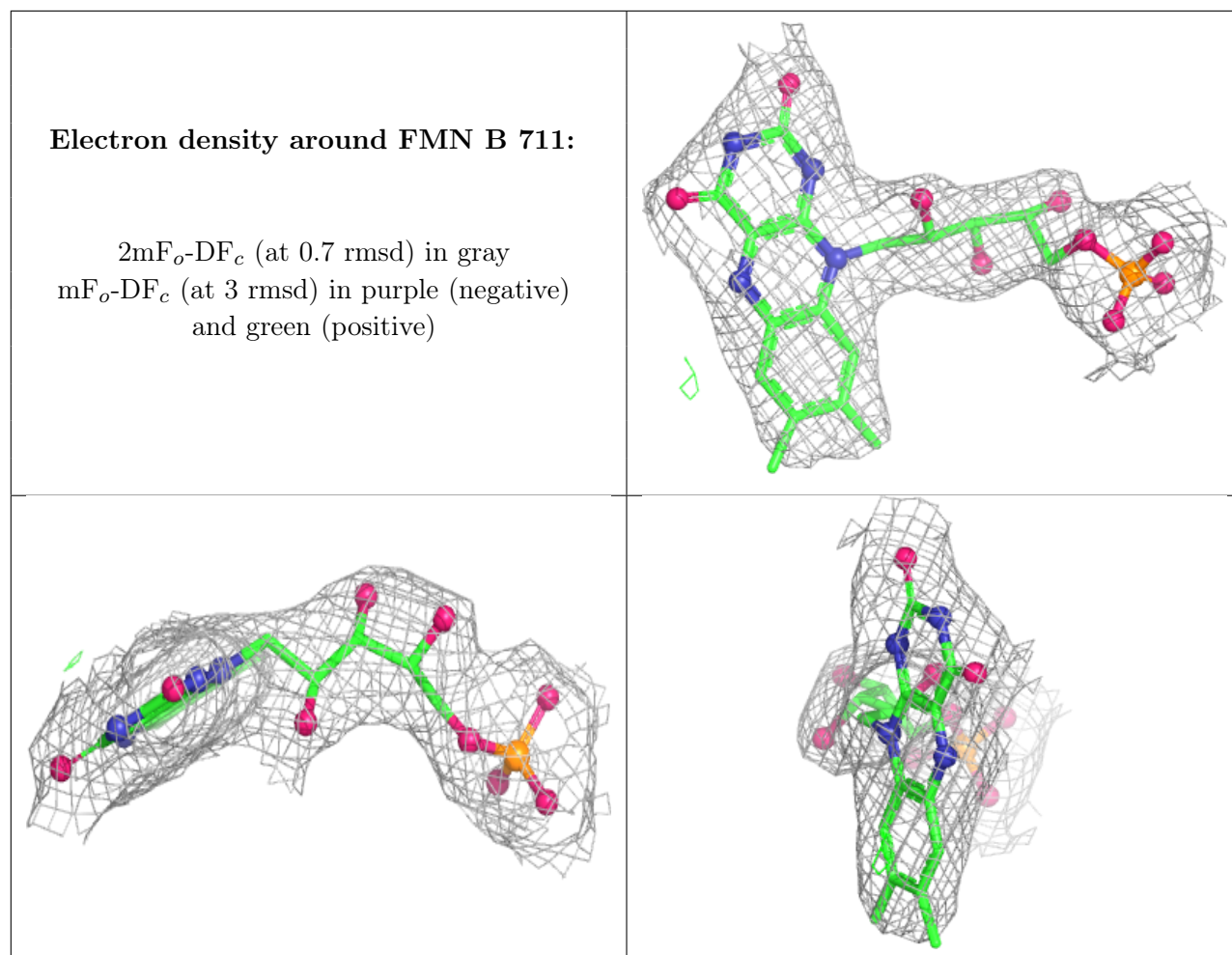
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN C 721:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.