



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:02 PM UTC

PDB ID : 1EFL / pdb\_00001efl  
Title : HUMAN MALIC ENZYME IN A QUATERNARY COMPLEX WITH NAD,  
MG, AND TARTRONATE  
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.  
Deposited on : 2000-02-09  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

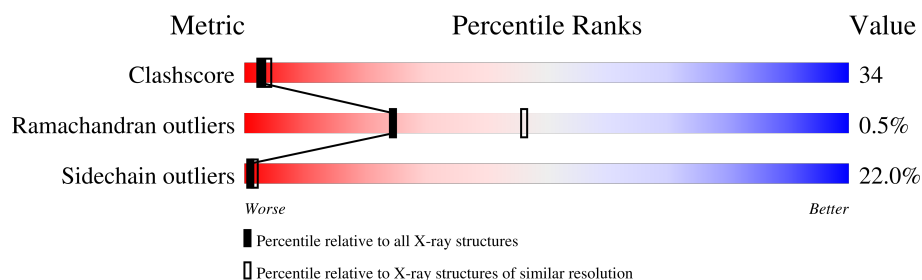
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 584    |                  |
| 1   | B     | 584    |                  |
| 1   | C     | 584    |                  |
| 1   | D     | 584    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17947 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 MALIC ENZYME.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 553      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 4367  | 2796 | 744 | 804 | 9 | 14 |         |         |       |
| 1   | B     | 553      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 4367  | 2796 | 744 | 804 | 9 | 14 |         |         |       |
| 1   | C     | 553      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 4367  | 2796 | 744 | 804 | 9 | 14 |         |         |       |
| 1   | D     | 553      | Total | C    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 4367  | 2796 | 744 | 804 | 9 | 14 |         |         |       |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 29      | MSE      | MET    | modified residue | UNP P23368 |
| A     | 38      | MSE      | MET    | modified residue | UNP P23368 |
| A     | 47      | MSE      | MET    | modified residue | UNP P23368 |
| A     | 75      | MSE      | MET    | modified residue | UNP P23368 |
| A     | 86      | MSE      | MET    | modified residue | UNP P23368 |
| A     | 108     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 177     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 219     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 239     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 325     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 327     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 343     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 407     | MSE      | MET    | modified residue | UNP P23368 |
| A     | 539     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 29      | MSE      | MET    | modified residue | UNP P23368 |
| B     | 38      | MSE      | MET    | modified residue | UNP P23368 |
| B     | 47      | MSE      | MET    | modified residue | UNP P23368 |
| B     | 75      | MSE      | MET    | modified residue | UNP P23368 |
| B     | 86      | MSE      | MET    | modified residue | UNP P23368 |
| B     | 108     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 177     | MSE      | MET    | modified residue | UNP P23368 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| B     | 219     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 239     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 325     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 327     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 343     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 407     | MSE      | MET    | modified residue | UNP P23368 |
| B     | 539     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 29      | MSE      | MET    | modified residue | UNP P23368 |
| C     | 38      | MSE      | MET    | modified residue | UNP P23368 |
| C     | 47      | MSE      | MET    | modified residue | UNP P23368 |
| C     | 75      | MSE      | MET    | modified residue | UNP P23368 |
| C     | 86      | MSE      | MET    | modified residue | UNP P23368 |
| C     | 108     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 177     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 219     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 239     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 325     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 327     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 343     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 407     | MSE      | MET    | modified residue | UNP P23368 |
| C     | 539     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 29      | MSE      | MET    | modified residue | UNP P23368 |
| D     | 38      | MSE      | MET    | modified residue | UNP P23368 |
| D     | 47      | MSE      | MET    | modified residue | UNP P23368 |
| D     | 75      | MSE      | MET    | modified residue | UNP P23368 |
| D     | 86      | MSE      | MET    | modified residue | UNP P23368 |
| D     | 108     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 177     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 219     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 239     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 325     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 327     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 343     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 407     | MSE      | MET    | modified residue | UNP P23368 |
| D     | 539     | MSE      | MET    | modified residue | UNP P23368 |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

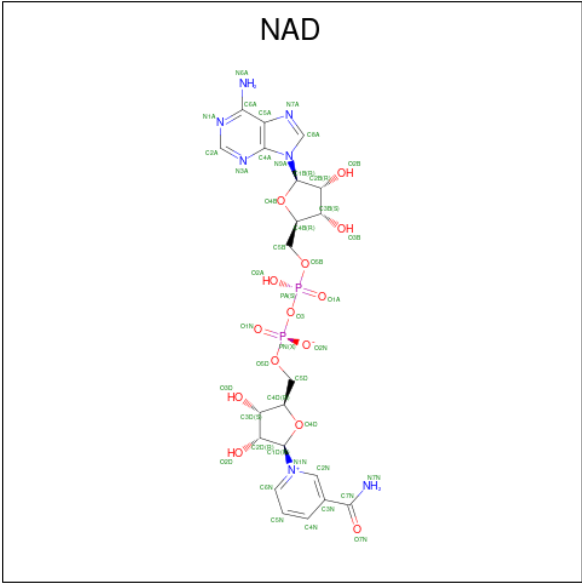
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Mg<br>1 1 | 0       | 0       |

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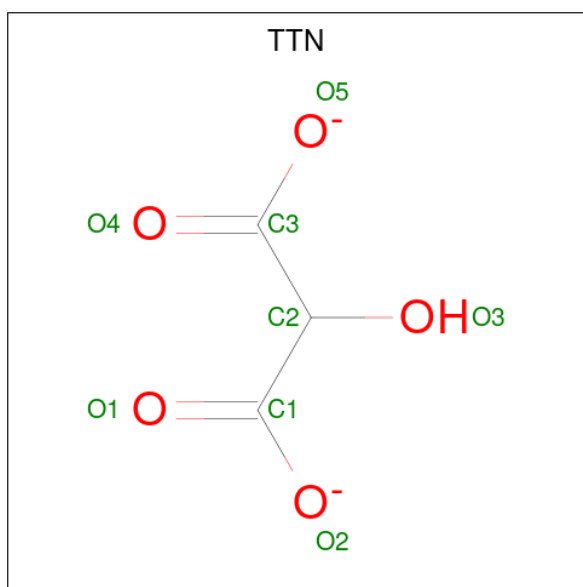
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | A     | 1        | Total | C  | N | O  | P | 9       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 9       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 9       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 9       | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |         |

- Molecule 4 is TARTRONATE (CCD ID: TTN) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 1        | Total C O<br>8 3 5 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>8 3 5 | 0       | 0       |
| 4   | C     | 1        | Total C O<br>8 3 5 | 0       | 0       |
| 4   | D     | 1        | Total C O<br>8 3 5 | 0       | 0       |

- Molecule 5 is water.

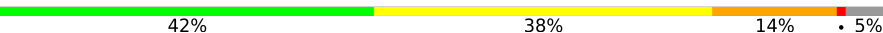
| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 24       | Total O<br>24 24 | 0       | 0       |
| 5   | B     | 17       | Total O<br>17 17 | 0       | 0       |
| 5   | C     | 23       | Total O<br>23 23 | 0       | 0       |
| 5   | D     | 27       | Total O<br>27 27 | 0       | 0       |

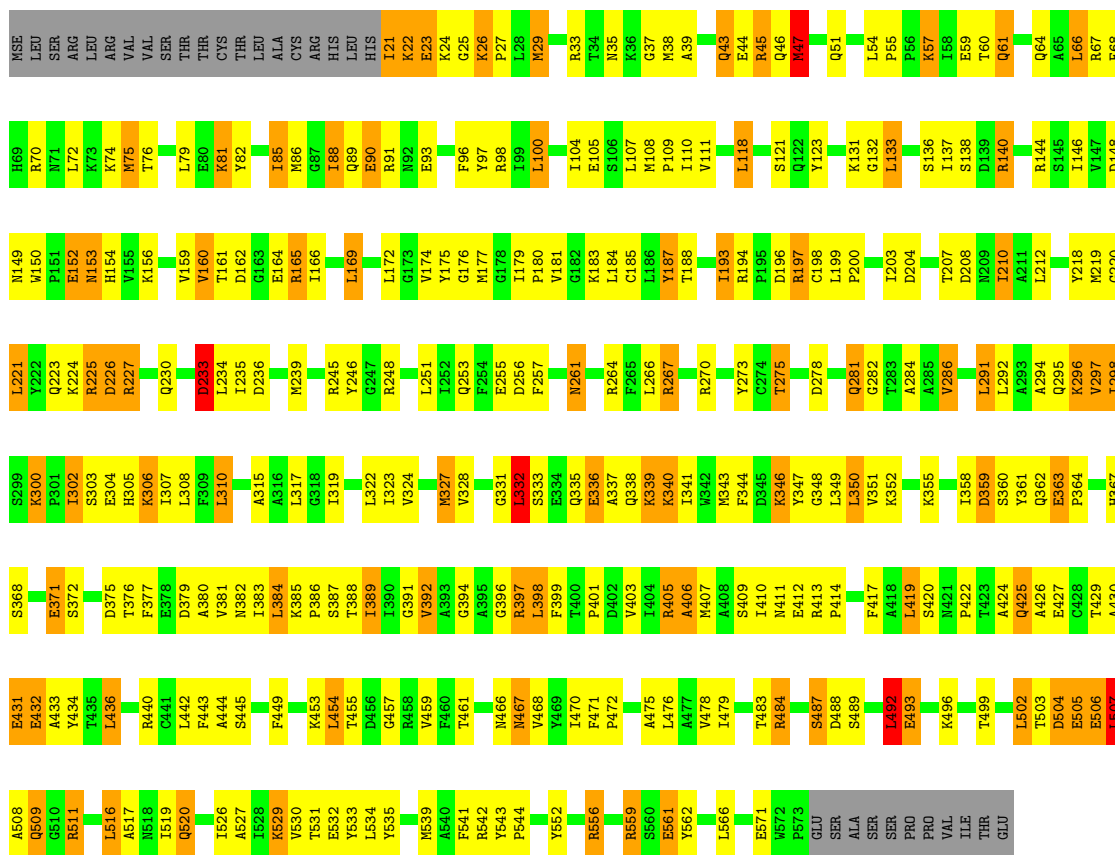
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

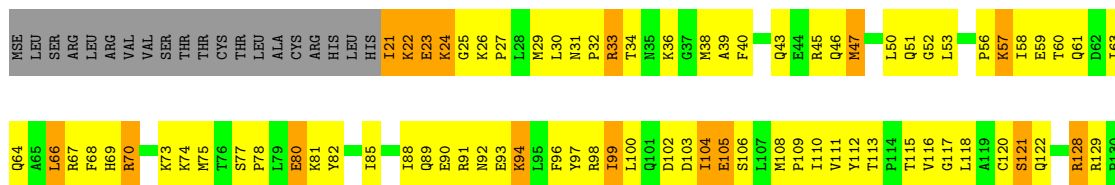
#### • Molecule 1: MALIC ENZYME

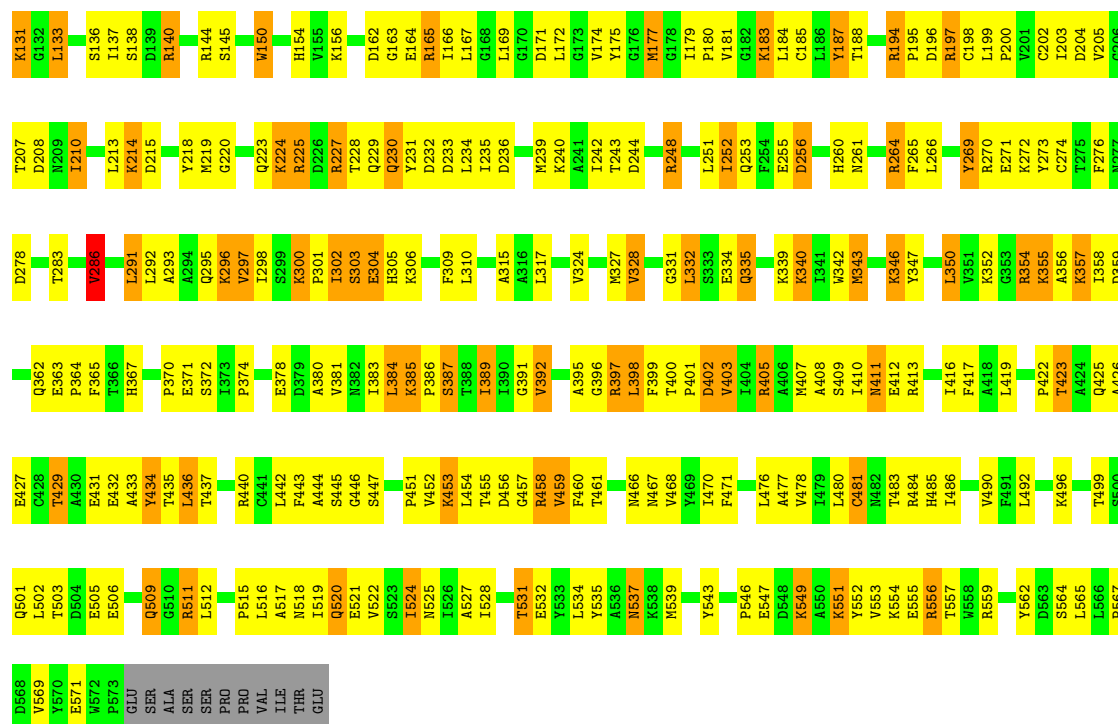
Chain A: 



#### • Molecule 1: MALIC ENZYME

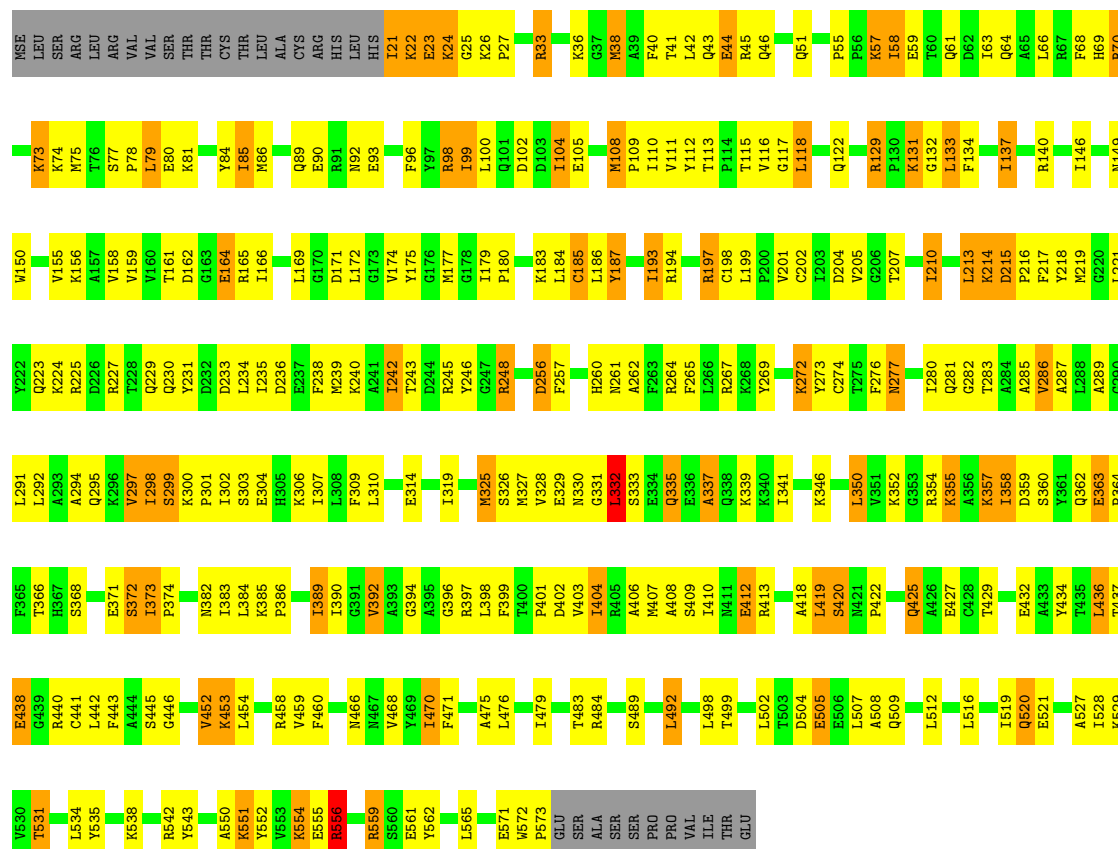
Chain B: 





### • Molecule 1: MALIC ENZYME

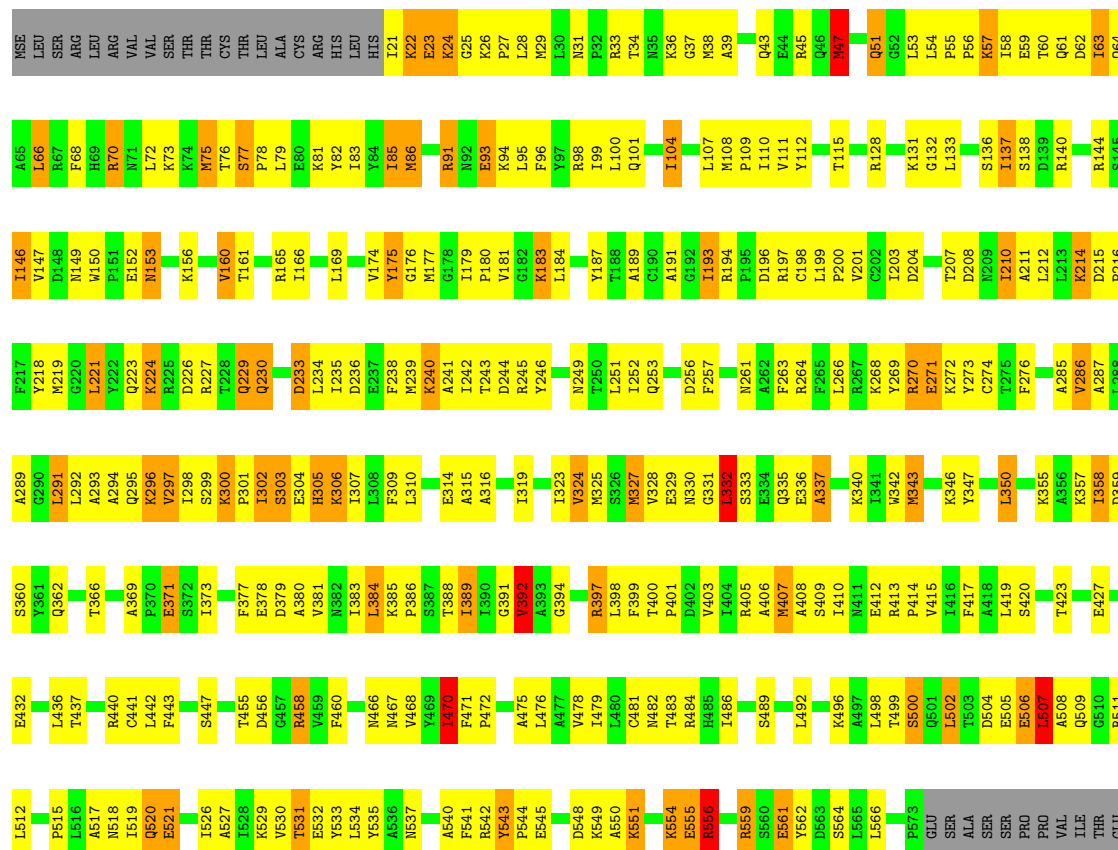
Chain C: 44% 39% 12% 5%





● Molecule 1: MALIC ENZYME

Chain D: 40% 43% 11% 5%



## 4 Data and refinement statistics

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

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | C 1 2 1                                          | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 228.80Å 117.00Å 114.30Å<br>90.00° 109.20° 90.00° | Depositor |
| Resolution (Å)                                           | 20.00 – 2.60                                     | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (20.00-2.60)                     | Depositor |
| $R_{merge}$                                              | 0.07                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | X-PLOR 3.851                                     | Depositor |
| R, $R_{free}$                                            | 0.206 , 0.285                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 17947                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 21.0                                             | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTN, NAD

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     | 0.56         | 0/4447      | 0.99        | 23/5998 (0.4%)  |
| 1   | B     | 0.56         | 0/4447      | 1.01        | 17/5998 (0.3%)  |
| 1   | C     | 0.55         | 0/4447      | 1.01        | 21/5998 (0.4%)  |
| 1   | D     | 0.56         | 0/4447      | 1.01        | 19/5998 (0.3%)  |
| All | All   | 0.56         | 0/17788     | 1.01        | 80/23992 (0.3%) |

There are no bond length outliers.

All (80) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 470 | ILE  | N-CA-C | 9.47  | 119.10      | 111.62   |
| 1   | A     | 430 | ALA  | N-CA-C | -7.35 | 103.27      | 111.28   |
| 1   | C     | 337 | ALA  | N-CA-C | -7.30 | 102.92      | 111.03   |
| 1   | D     | 419 | LEU  | N-CA-C | 7.25  | 121.97      | 113.20   |
| 1   | B     | 470 | ILE  | N-CA-C | 7.23  | 118.28      | 111.48   |
| 1   | A     | 419 | LEU  | N-CA-C | 7.15  | 122.03      | 113.16   |
| 1   | B     | 98  | ARG  | N-CA-C | -7.02 | 103.55      | 111.14   |
| 1   | D     | 532 | GLU  | N-CA-C | -6.97 | 103.68      | 111.28   |
| 1   | C     | 470 | ILE  | N-CA-C | 6.93  | 117.52      | 111.56   |
| 1   | C     | 98  | ARG  | N-CA-C | -6.63 | 103.98      | 111.07   |
| 1   | C     | 403 | VAL  | N-CA-C | -6.48 | 104.01      | 110.62   |
| 1   | D     | 77  | SER  | CA-C-N | 6.47  | 126.40      | 119.28   |
| 1   | D     | 77  | SER  | C-N-CA | 6.47  | 126.40      | 119.28   |
| 1   | D     | 268 | LYS  | N-CA-C | 6.46  | 118.40      | 111.36   |
| 1   | C     | 187 | TYR  | N-CA-C | -6.43 | 103.55      | 111.40   |
| 1   | B     | 59  | GLU  | N-CA-C | 6.41  | 118.30      | 110.41   |
| 1   | A     | 233 | ASP  | N-CA-C | -6.26 | 104.37      | 111.07   |
| 1   | D     | 187 | TYR  | N-CA-C | -6.24 | 104.40      | 111.14   |
| 1   | B     | 145 | SER  | N-CA-C | -6.14 | 104.67      | 111.36   |
| 1   | C     | 358 | ILE  | N-CA-C | -6.13 | 99.41       | 108.85   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 93  | GLU  | N-CA-C  | 6.01  | 117.50      | 111.07   |
| 1   | B     | 187 | TYR  | N-CA-C  | -6.00 | 104.67      | 112.23   |
| 1   | A     | 406 | ALA  | N-CA-C  | -5.98 | 104.45      | 110.97   |
| 1   | C     | 419 | LEU  | N-CA-C  | 5.95  | 120.54      | 113.28   |
| 1   | A     | 261 | ASN  | N-CA-C  | 5.94  | 117.84      | 111.36   |
| 1   | D     | 160 | VAL  | N-CA-C  | 5.92  | 117.11      | 108.53   |
| 1   | D     | 507 | LEU  | N-CA-C  | -5.87 | 104.79      | 111.07   |
| 1   | C     | 185 | CYS  | N-CA-C  | -5.81 | 105.03      | 111.36   |
| 1   | C     | 443 | PHE  | N-CA-C  | 5.79  | 119.50      | 110.17   |
| 1   | A     | 387 | SER  | N-CA-C  | -5.78 | 106.39      | 113.50   |
| 1   | D     | 181 | VAL  | N-CA-C  | -5.74 | 105.14      | 110.53   |
| 1   | C     | 512 | LEU  | N-CA-C  | -5.68 | 105.93      | 112.92   |
| 1   | B     | 162 | ASP  | N-CA-C  | -5.67 | 104.56      | 113.02   |
| 1   | B     | 387 | SER  | N-CA-C  | -5.66 | 105.09      | 112.23   |
| 1   | A     | 310 | LEU  | N-CA-C  | -5.63 | 98.02       | 107.99   |
| 1   | A     | 506 | GLU  | N-CA-C  | -5.58 | 105.28      | 111.36   |
| 1   | D     | 369 | ALA  | N-CA-C  | 5.55  | 115.99      | 109.60   |
| 1   | A     | 160 | VAL  | N-CA-C  | 5.55  | 117.33      | 108.89   |
| 1   | B     | 286 | VAL  | CB-CA-C | -5.51 | 104.91      | 111.97   |
| 1   | D     | 512 | LEU  | N-CA-C  | -5.47 | 106.38      | 113.16   |
| 1   | A     | 461 | THR  | CA-C-N  | 5.47  | 125.23      | 119.76   |
| 1   | A     | 461 | THR  | C-N-CA  | 5.47  | 125.23      | 119.76   |
| 1   | A     | 492 | LEU  | N-CA-C  | -5.46 | 105.41      | 111.36   |
| 1   | B     | 256 | ASP  | N-CA-C  | 5.45  | 118.92      | 111.39   |
| 1   | B     | 167 | LEU  | CB-CA-C | -5.45 | 110.31      | 116.63   |
| 1   | B     | 150 | TRP  | CA-C-N  | 5.43  | 124.89      | 119.24   |
| 1   | B     | 150 | TRP  | C-N-CA  | 5.43  | 124.89      | 119.24   |
| 1   | A     | 88  | ILE  | N-CA-C  | -5.41 | 105.45      | 110.53   |
| 1   | B     | 269 | TYR  | N-CA-C  | 5.40  | 120.14      | 113.50   |
| 1   | C     | 256 | ASP  | N-CA-C  | 5.39  | 118.83      | 111.39   |
| 1   | D     | 175 | TYR  | N-CA-C  | -5.39 | 106.78      | 113.19   |
| 1   | C     | 77  | SER  | CA-C-N  | 5.37  | 124.70      | 118.85   |
| 1   | C     | 77  | SER  | C-N-CA  | 5.37  | 124.70      | 118.85   |
| 1   | D     | 47  | MSE  | N-CA-C  | 5.34  | 117.19      | 111.36   |
| 1   | B     | 403 | VAL  | N-CA-C  | -5.33 | 105.18      | 110.62   |
| 1   | D     | 337 | ALA  | N-CA-C  | -5.33 | 105.11      | 111.03   |
| 1   | C     | 215 | ASP  | CA-C-N  | 5.30  | 124.97      | 119.56   |
| 1   | C     | 215 | ASP  | C-N-CA  | 5.30  | 124.97      | 119.56   |
| 1   | A     | 193 | ILE  | N-CA-C  | -5.29 | 102.25      | 109.55   |
| 1   | A     | 368 | SER  | N-CA-C  | -5.29 | 102.56      | 110.23   |
| 1   | C     | 383 | ILE  | N-CA-C  | -5.29 | 105.69      | 110.82   |
| 1   | A     | 162 | ASP  | N-CA-C  | -5.28 | 105.15      | 113.02   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 310 | LEU  | N-CA-C  | -5.25 | 97.27       | 107.62   |
| 1   | A     | 470 | ILE  | N-CA-C  | 5.24  | 116.41      | 111.48   |
| 1   | A     | 470 | ILE  | CB-CA-C | -5.20 | 107.29      | 111.71   |
| 1   | C     | 44  | GLU  | N-CA-C  | -5.20 | 105.61      | 111.28   |
| 1   | D     | 556 | ARG  | N-CA-C  | 5.18  | 119.30      | 112.25   |
| 1   | C     | 63  | ILE  | CB-CA-C | -5.15 | 105.11      | 112.22   |
| 1   | A     | 61  | GLN  | N-CA-C  | -5.15 | 105.79      | 111.71   |
| 1   | A     | 507 | LEU  | N-CA-C  | -5.14 | 105.67      | 111.28   |
| 1   | B     | 434 | TYR  | N-CA-C  | 5.13  | 116.88      | 111.28   |
| 1   | A     | 47  | MSE  | N-CA-C  | 5.08  | 116.62      | 111.14   |
| 1   | B     | 411 | ASN  | N-CA-C  | 5.08  | 117.84      | 109.72   |
| 1   | C     | 162 | ASP  | N-CA-C  | -5.06 | 105.81      | 112.94   |
| 1   | D     | 323 | ILE  | N-CA-C  | -5.03 | 105.59      | 110.42   |
| 1   | D     | 257 | PHE  | N-CA-C  | -5.03 | 102.75      | 110.14   |
| 1   | C     | 556 | ARG  | N-CA-C  | 5.02  | 118.48      | 111.30   |
| 1   | A     | 187 | TYR  | N-CA-C  | -5.02 | 105.70      | 111.07   |
| 1   | A     | 281 | GLN  | N-CA-C  | 5.01  | 117.85      | 111.69   |
| 1   | B     | 490 | VAL  | N-CA-C  | -5.01 | 105.66      | 110.72   |

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     | 4367  | 0        | 4407     | 344     | 0            |
| 1   | B     | 4367  | 0        | 4407     | 335     | 0            |
| 1   | C     | 4367  | 0        | 4407     | 253     | 0            |
| 1   | D     | 4367  | 0        | 4407     | 324     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 88    | 0        | 52       | 6       | 0            |
| 3   | B     | 88    | 0        | 52       | 2       | 0            |
| 3   | C     | 88    | 0        | 52       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 88    | 0        | 52       | 4       | 0            |
| 4   | A     | 8     | 0        | 1        | 0       | 0            |
| 4   | B     | 8     | 0        | 1        | 1       | 0            |
| 4   | C     | 8     | 0        | 1        | 2       | 0            |
| 4   | D     | 8     | 0        | 2        | 1       | 0            |
| 5   | A     | 24    | 0        | 0        | 6       | 0            |
| 5   | B     | 17    | 0        | 0        | 9       | 0            |
| 5   | C     | 23    | 0        | 0        | 5       | 0            |
| 5   | D     | 27    | 0        | 0        | 4       | 0            |
| All | All   | 17947 | 0        | 17841    | 1210    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:227:ARG:HH11  | 1:A:227:ARG:HG2  | 1.03                     | 1.11              |
| 1:D:520:GLN:HE22  | 1:D:521:GLU:HG2  | 1.13                     | 1.07              |
| 1:A:511:ARG:HH11  | 1:A:511:ARG:HB3  | 1.20                     | 1.02              |
| 1:C:355:LYS:HA    | 1:C:355:LYS:HE2  | 1.42                     | 1.01              |
| 1:B:227:ARG:HG2   | 1:B:227:ARG:HH11 | 1.24                     | 1.00              |
| 1:D:520:GLN:NE2   | 1:D:521:GLU:HG2  | 1.75                     | 1.00              |
| 1:D:298:ILE:HG22  | 1:D:300:LYS:H    | 1.27                     | 0.99              |
| 1:A:327:MSE:HE3   | 1:A:337:ALA:HB1  | 1.45                     | 0.97              |
| 1:A:108:MSE:HE3   | 1:A:516:LEU:HD11 | 1.46                     | 0.97              |
| 1:C:327:MSE:HE3   | 1:C:337:ALA:HB1  | 1.45                     | 0.96              |
| 3:B:1602:NAD:H51N | 5:C:4090:HOH:O   | 1.64                     | 0.96              |
| 1:A:324:VAL:HA    | 1:A:327:MSE:HE2  | 1.48                     | 0.95              |
| 1:D:481:CYS:SG    | 1:D:531:THR:HB   | 2.08                     | 0.94              |
| 1:D:520:GLN:NE2   | 1:D:521:GLU:H    | 1.66                     | 0.94              |
| 1:B:527:ALA:O     | 1:B:531:THR:HG22 | 1.66                     | 0.94              |
| 1:D:211:ALA:HA    | 1:D:214:LYS:HE2  | 1.51                     | 0.93              |
| 1:A:371:GLU:H     | 1:A:371:GLU:CD   | 1.75                     | 0.92              |
| 1:C:184:LEU:HD13  | 1:C:198:CYS:HB3  | 1.50                     | 0.92              |
| 1:C:197:ARG:HG3   | 1:C:197:ARG:HH11 | 1.35                     | 0.92              |
| 1:D:327:MSE:HE3   | 1:D:337:ALA:HB1  | 1.52                     | 0.92              |
| 1:A:425:GLN:HE21  | 1:A:425:GLN:N    | 1.67                     | 0.91              |
| 1:C:325:MSE:HE2   | 1:C:492:LEU:HD12 | 1.53                     | 0.91              |
| 1:C:194:ARG:HB2   | 1:C:197:ARG:HG2  | 1.51                     | 0.91              |
| 1:A:468:VAL:HA    | 1:A:471:PHE:CE2  | 2.06                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:47:MSE:HE3   | 1:D:566:LEU:HD22 | 1.53                     | 0.91              |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:HA   | 1.53                     | 0.90              |
| 1:A:405:ARG:HH11 | 1:A:405:ARG:HB2  | 1.34                     | 0.90              |
| 1:B:184:LEU:HD22 | 1:B:198:CYS:HB3  | 1.53                     | 0.90              |
| 1:A:397:ARG:HG3  | 1:A:397:ARG:HH11 | 1.36                     | 0.89              |
| 1:B:47:MSE:HE2   | 1:B:567:PRO:HG2  | 1.54                     | 0.87              |
| 1:B:61:GLN:HA    | 1:B:64:GLN:HE21  | 1.38                     | 0.87              |
| 1:A:227:ARG:HG2  | 1:A:227:ARG:NH1  | 1.82                     | 0.86              |
| 1:C:85:ILE:HD12  | 1:C:96:PHE:HE1   | 1.39                     | 0.86              |
| 1:B:453:LYS:HG2  | 1:B:459:VAL:HG12 | 1.57                     | 0.86              |
| 1:D:381:VAL:HG13 | 1:D:407:MSE:HE1  | 1.58                     | 0.86              |
| 1:A:220:GLY:HA2  | 1:B:56:PRO:HG2   | 1.58                     | 0.85              |
| 1:A:520:GLN:HE21 | 1:A:520:GLN:H    | 1.24                     | 0.85              |
| 1:D:315:ALA:O    | 1:D:319:ILE:HG13 | 1.77                     | 0.85              |
| 1:B:453:LYS:HE3  | 1:B:457:GLY:HA2  | 1.58                     | 0.84              |
| 1:A:23:GLU:HA    | 1:A:23:GLU:OE1   | 1.76                     | 0.83              |
| 1:B:378:GLU:O    | 1:B:381:VAL:HG12 | 1.77                     | 0.83              |
| 1:A:108:MSE:HB3  | 1:A:109:PRO:HD3  | 1.58                     | 0.83              |
| 1:A:286:VAL:HG21 | 1:A:467:ASN:HA   | 1.59                     | 0.83              |
| 1:B:29:MSE:HE1   | 1:B:53:LEU:HB2   | 1.59                     | 0.83              |
| 1:B:371:GLU:CD   | 1:B:371:GLU:H    | 1.87                     | 0.83              |
| 1:B:422:PRO:HD2  | 1:B:425:GLN:CG   | 2.09                     | 0.83              |
| 1:A:166:ILE:HD12 | 1:A:179:ILE:HG13 | 1.61                     | 0.82              |
| 1:B:397:ARG:NH2  | 1:B:423:THR:O    | 2.12                     | 0.82              |
| 1:B:300:LYS:NZ   | 1:B:300:LYS:HB3  | 1.93                     | 0.82              |
| 1:A:47:MSE:HE3   | 1:A:566:LEU:HD22 | 1.62                     | 0.82              |
| 1:B:532:GLU:HG2  | 1:B:549:LYS:HG2  | 1.62                     | 0.82              |
| 1:D:23:GLU:OE2   | 1:D:23:GLU:HA    | 1.80                     | 0.82              |
| 1:D:107:LEU:O    | 1:D:111:VAL:HG12 | 1.78                     | 0.81              |
| 1:D:286:VAL:HG22 | 1:D:470:ILE:HG13 | 1.61                     | 0.81              |
| 1:D:509:GLN:HB2  | 5:D:4058:HOH:O   | 1.80                     | 0.81              |
| 1:A:381:VAL:HG13 | 1:A:407:MSE:HE3  | 1.60                     | 0.81              |
| 1:D:261:ASN:ND2  | 1:D:264:ARG:HH21 | 1.78                     | 0.81              |
| 1:B:77:SER:O     | 1:B:81:LYS:HG3   | 1.80                     | 0.81              |
| 1:D:144:ARG:HD2  | 1:D:147:VAL:CG2  | 2.11                     | 0.81              |
| 1:D:300:LYS:HE3  | 1:D:305:HIS:ND1  | 1.95                     | 0.81              |
| 1:A:38:MSE:HE3   | 1:A:59:GLU:CD    | 2.07                     | 0.80              |
| 1:B:67:ARG:HD2   | 5:B:4079:HOH:O   | 1.80                     | 0.80              |
| 1:D:22:LYS:HD2   | 1:D:22:LYS:O     | 1.81                     | 0.80              |
| 1:A:487:SER:HB3  | 1:A:539:MSE:HE1  | 1.61                     | 0.80              |
| 1:D:559:ARG:HG3  | 1:D:561:GLU:OE1  | 1.80                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:425:GLN:HE21 | 1:A:425:GLN:H    | 1.27                     | 0.80              |
| 1:D:184:LEU:HD22 | 1:D:198:CYS:HB3  | 1.64                     | 0.80              |
| 1:B:306:LYS:HG2  | 1:B:386:PRO:HA   | 1.64                     | 0.80              |
| 1:A:407:MSE:HA   | 1:A:407:MSE:HE2  | 1.63                     | 0.79              |
| 1:A:425:GLN:N    | 1:A:425:GLN:NE2  | 2.31                     | 0.79              |
| 1:A:335:GLN:O    | 1:A:339:LYS:HD2  | 1.83                     | 0.79              |
| 1:D:43:GLN:HG2   | 1:D:566:LEU:HD11 | 1.64                     | 0.79              |
| 1:D:328:VAL:HA   | 1:D:332:LEU:O    | 1.83                     | 0.79              |
| 1:B:108:MSE:HE3  | 1:B:516:LEU:HD11 | 1.64                     | 0.78              |
| 1:B:422:PRO:HD2  | 1:B:425:GLN:HG3  | 1.65                     | 0.78              |
| 1:A:511:ARG:HB3  | 1:A:511:ARG:NH1  | 1.98                     | 0.78              |
| 1:D:177:MSE:HE1  | 1:D:180:PRO:HB2  | 1.66                     | 0.78              |
| 1:D:194:ARG:HE   | 1:D:197:ARG:NE   | 1.82                     | 0.78              |
| 1:B:343:MSE:HE3  | 1:B:350:LEU:HD12 | 1.66                     | 0.77              |
| 1:A:21:ILE:N     | 1:A:21:ILE:HD13  | 1.99                     | 0.77              |
| 1:B:29:MSE:HE2   | 1:B:50:LEU:HD22  | 1.64                     | 0.77              |
| 1:B:483:THR:HG21 | 1:B:534:LEU:HD13 | 1.67                     | 0.77              |
| 1:D:310:LEU:HB3  | 1:D:391:GLY:HA2  | 1.65                     | 0.77              |
| 1:D:324:VAL:HA   | 1:D:327:MSE:HE2  | 1.67                     | 0.77              |
| 1:B:431:GLU:O    | 1:B:435:THR:HG23 | 1.85                     | 0.77              |
| 1:A:24:LYS:HE2   | 1:C:22:LYS:HD2   | 1.67                     | 0.77              |
| 1:C:179:ILE:HB   | 1:C:180:PRO:HD3  | 1.66                     | 0.76              |
| 1:D:466:ASN:HB3  | 1:D:468:VAL:HG12 | 1.68                     | 0.76              |
| 1:B:29:MSE:HE2   | 1:B:50:LEU:HB3   | 1.65                     | 0.76              |
| 1:A:175:TYR:CD2  | 1:A:219:MSE:HE2  | 2.19                     | 0.76              |
| 1:A:511:ARG:HH11 | 1:A:511:ARG:CB   | 1.99                     | 0.76              |
| 1:A:543:TYR:OH   | 5:A:4080:HOH:O   | 2.03                     | 0.76              |
| 1:B:335:GLN:O    | 1:B:339:LYS:HG3  | 1.85                     | 0.76              |
| 1:C:85:ILE:HG13  | 1:C:86:MSE:N     | 1.98                     | 0.76              |
| 1:B:395:ALA:HB3  | 1:B:398:LEU:HD21 | 1.68                     | 0.76              |
| 1:D:359:ASP:OD2  | 1:D:362:GLN:HG3  | 1.85                     | 0.76              |
| 1:B:401:PRO:O    | 1:B:405:ARG:HG3  | 1.86                     | 0.75              |
| 1:D:298:ILE:CG2  | 1:D:300:LYS:HB2  | 2.16                     | 0.75              |
| 1:A:154:HIS:O    | 1:A:197:ARG:HG3  | 1.87                     | 0.75              |
| 1:B:227:ARG:HH11 | 1:B:227:ARG:CG   | 1.98                     | 0.75              |
| 1:B:300:LYS:HB3  | 1:B:300:LYS:HZ2  | 1.52                     | 0.74              |
| 1:B:47:MSE:HE3   | 1:D:47:MSE:SE    | 2.38                     | 0.74              |
| 1:D:383:ILE:HG22 | 1:D:384:LEU:HD13 | 1.69                     | 0.74              |
| 1:B:177:MSE:O    | 1:B:180:PRO:HD2  | 1.87                     | 0.74              |
| 1:D:207:THR:O    | 1:D:224:LYS:HA   | 1.87                     | 0.74              |
| 1:A:405:ARG:HB2  | 1:A:405:ARG:NH1  | 2.02                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:33:ARG:HD3   | 1:D:196:ASP:HB3  | 1.71                     | 0.73              |
| 1:A:47:MSE:CE    | 1:A:566:LEU:HD22 | 2.19                     | 0.73              |
| 1:C:551:LYS:O    | 1:C:555:GLU:HB2  | 1.88                     | 0.73              |
| 1:A:371:GLU:CD   | 1:A:371:GLU:N    | 2.47                     | 0.72              |
| 1:D:400:THR:OG1  | 1:D:403:VAL:HG23 | 1.89                     | 0.72              |
| 1:A:227:ARG:HH11 | 1:A:227:ARG:CG   | 1.90                     | 0.72              |
| 1:B:105:GLU:HB2  | 5:B:4016:HOH:O   | 1.89                     | 0.72              |
| 1:D:548:ASP:OD1  | 1:D:551:LYS:HB2  | 1.90                     | 0.72              |
| 1:B:137:ILE:O    | 1:B:140:ARG:HG2  | 1.89                     | 0.72              |
| 1:B:332:LEU:HD21 | 1:B:340:LYS:HE3  | 1.71                     | 0.72              |
| 1:D:392:VAL:HG13 | 1:D:392:VAL:O    | 1.89                     | 0.72              |
| 1:B:385:LYS:HA   | 1:B:410:ILE:HD13 | 1.70                     | 0.72              |
| 1:B:75:MSE:HG2   | 1:B:80:GLU:CD    | 2.15                     | 0.71              |
| 1:A:123:TYR:HD2  | 1:A:219:MSE:HE1  | 1.53                     | 0.71              |
| 1:C:432:GLU:O    | 1:C:436:LEU:HB2  | 1.90                     | 0.71              |
| 1:D:240:LYS:HE3  | 1:D:273:TYR:OH   | 1.90                     | 0.71              |
| 1:D:468:VAL:HA   | 1:D:471:PHE:CE2  | 2.26                     | 0.71              |
| 1:C:75:MSE:HG2   | 1:C:80:GLU:CD    | 2.15                     | 0.71              |
| 1:B:22:LYS:NZ    | 1:D:27:PRO:HG2   | 2.05                     | 0.71              |
| 1:B:408:ALA:HB1  | 1:B:440:ARG:NH2  | 2.06                     | 0.71              |
| 1:B:324:VAL:O    | 1:B:328:VAL:HG13 | 1.91                     | 0.71              |
| 1:C:306:LYS:HG2  | 1:C:386:PRO:HA   | 1.72                     | 0.71              |
| 1:C:289:ALA:CB   | 1:C:498:LEU:HD23 | 2.21                     | 0.70              |
| 1:D:381:VAL:CG1  | 1:D:407:MSE:HE1  | 2.20                     | 0.70              |
| 1:C:355:LYS:HE2  | 1:C:355:LYS:CA   | 2.19                     | 0.70              |
| 1:D:194:ARG:HB2  | 1:D:197:ARG:HG3  | 1.72                     | 0.70              |
| 1:A:392:VAL:O    | 1:A:392:VAL:HG13 | 1.89                     | 0.70              |
| 1:A:81:LYS:O     | 1:A:85:ILE:HG23  | 1.91                     | 0.70              |
| 1:D:177:MSE:CE   | 1:D:180:PRO:HB2  | 2.22                     | 0.70              |
| 1:A:177:MSE:HE1  | 1:A:180:PRO:HB2  | 1.72                     | 0.70              |
| 1:B:90:GLU:OE1   | 1:B:131:LYS:HG3  | 1.92                     | 0.70              |
| 1:B:166:ILE:HG21 | 1:B:172:LEU:HD12 | 1.73                     | 0.70              |
| 1:B:354:ARG:HE   | 1:B:358:ILE:HD11 | 1.55                     | 0.70              |
| 1:D:253:GLN:HB2  | 1:D:276:PHE:CE2  | 2.26                     | 0.70              |
| 1:D:520:GLN:HE22 | 1:D:521:GLU:CG   | 1.99                     | 0.70              |
| 1:B:335:GLN:HG3  | 1:B:339:LYS:HE3  | 1.74                     | 0.70              |
| 1:D:194:ARG:HG2  | 1:D:194:ARG:HH11 | 1.55                     | 0.70              |
| 1:B:302:ILE:HA   | 1:B:305:HIS:ND1  | 2.07                     | 0.70              |
| 1:B:261:ASN:ND2  | 1:B:264:ARG:CZ   | 2.55                     | 0.70              |
| 1:D:300:LYS:NZ   | 1:D:300:LYS:HB3  | 2.04                     | 0.70              |
| 1:A:401:PRO:HB3  | 1:A:436:LEU:HD21 | 1.72                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:520:GLN:H    | 1:A:520:GLN:NE2  | 1.88                     | 0.69              |
| 1:B:433:ALA:O    | 1:B:437:THR:HG23 | 1.92                     | 0.69              |
| 1:C:197:ARG:HG3  | 1:C:197:ARG:NH1  | 1.98                     | 0.69              |
| 1:B:24:LYS:O     | 1:D:22:LYS:HE3   | 1.91                     | 0.69              |
| 1:C:520:GLN:H    | 1:C:520:GLN:HE21 | 1.40                     | 0.69              |
| 1:D:415:VAL:HG22 | 1:D:442:LEU:HD12 | 1.74                     | 0.69              |
| 1:C:434:TYR:CD1  | 1:C:452:VAL:HG11 | 2.28                     | 0.69              |
| 1:C:81:LYS:O     | 1:C:85:ILE:HG23  | 1.92                     | 0.69              |
| 1:A:405:ARG:HH11 | 1:A:405:ARG:CB   | 2.06                     | 0.69              |
| 1:B:537:ASN:N    | 1:B:537:ASN:HD22 | 1.91                     | 0.68              |
| 1:D:551:LYS:O    | 1:D:555:GLU:HB2  | 1.93                     | 0.68              |
| 1:B:305:HIS:HB2  | 1:B:340:LYS:HZ1  | 1.58                     | 0.68              |
| 1:A:91:ARG:NE    | 5:A:4055:HOH:O   | 2.26                     | 0.68              |
| 1:B:347:TYR:HB2  | 1:B:354:ARG:HH12 | 1.58                     | 0.68              |
| 1:C:133:LEU:HB2  | 1:C:199:LEU:HD11 | 1.75                     | 0.68              |
| 1:D:43:GLN:OE1   | 1:D:47:MSE:HE2   | 1.93                     | 0.68              |
| 1:D:211:ALA:HA   | 1:D:214:LYS:CE   | 2.22                     | 0.68              |
| 1:C:357:LYS:H    | 1:C:357:LYS:HD2  | 1.59                     | 0.68              |
| 1:B:328:VAL:HA   | 1:B:332:LEU:O    | 1.93                     | 0.68              |
| 1:B:60:THR:OG1   | 1:B:63:ILE:HG13  | 1.93                     | 0.68              |
| 1:B:528:ILE:O    | 1:B:532:GLU:HG3  | 1.94                     | 0.68              |
| 1:A:79:LEU:HB2   | 1:A:118:LEU:HD21 | 1.76                     | 0.67              |
| 1:B:205:VAL:HG11 | 1:B:231:TYR:HD1  | 1.59                     | 0.67              |
| 1:D:64:GLN:NE2   | 1:D:562:TYR:OH   | 2.25                     | 0.67              |
| 1:D:306:LYS:CG   | 1:D:386:PRO:HA   | 2.23                     | 0.67              |
| 1:A:398:LEU:HD23 | 1:A:398:LEU:N    | 2.09                     | 0.67              |
| 1:C:23:GLU:OE1   | 1:C:23:GLU:HA    | 1.93                     | 0.67              |
| 1:D:550:ALA:O    | 1:D:554:LYS:HG2  | 1.95                     | 0.67              |
| 1:A:45:ARG:HB3   | 1:A:51:GLN:HG2   | 1.76                     | 0.67              |
| 1:D:31:ASN:ND2   | 1:D:34:THR:HG23  | 2.09                     | 0.67              |
| 1:B:81:LYS:O     | 1:B:85:ILE:HG13  | 1.94                     | 0.67              |
| 1:B:291:LEU:HD13 | 1:B:417:PHE:CE2  | 2.29                     | 0.67              |
| 1:A:108:MSE:CE   | 1:A:516:LEU:HD11 | 2.24                     | 0.67              |
| 1:A:233:ASP:OD2  | 1:A:233:ASP:C    | 2.38                     | 0.67              |
| 1:A:137:ILE:HD12 | 1:A:234:LEU:HD22 | 1.77                     | 0.67              |
| 1:B:91:ARG:HG2   | 1:B:91:ARG:HH11  | 1.60                     | 0.67              |
| 1:B:253:GLN:HB2  | 1:B:276:PHE:CE2  | 2.30                     | 0.67              |
| 1:C:85:ILE:HD11  | 1:C:111:VAL:HG23 | 1.76                     | 0.67              |
| 1:A:140:ARG:HH22 | 1:A:233:ASP:HB3  | 1.57                     | 0.66              |
| 1:A:177:MSE:HE2  | 1:A:181:VAL:HG23 | 1.78                     | 0.66              |
| 1:A:453:LYS:CG   | 1:A:459:VAL:HG22 | 2.24                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:401:PRO:HB2  | 1:A:405:ARG:HH22 | 1.59                     | 0.66              |
| 1:B:422:PRO:HD2  | 1:B:425:GLN:HG2  | 1.77                     | 0.66              |
| 1:A:397:ARG:HG3  | 1:A:397:ARG:NH1  | 2.09                     | 0.66              |
| 1:C:298:ILE:HD13 | 1:C:413:ARG:HB2  | 1.76                     | 0.66              |
| 1:D:300:LYS:HB3  | 1:D:300:LYS:HZ2  | 1.59                     | 0.66              |
| 1:A:453:LYS:HG3  | 1:A:459:VAL:HG22 | 1.77                     | 0.66              |
| 1:B:240:LYS:HE3  | 1:B:244:ASP:OD2  | 1.94                     | 0.66              |
| 1:B:503:THR:HB   | 1:B:505:GLU:OE2  | 1.94                     | 0.66              |
| 1:B:51:GLN:NE2   | 5:B:4050:HOH:O   | 2.28                     | 0.66              |
| 1:D:51:GLN:HE21  | 1:D:51:GLN:HA    | 1.61                     | 0.66              |
| 1:D:327:MSE:CE   | 1:D:337:ALA:HB1  | 2.24                     | 0.66              |
| 1:C:79:LEU:HD22  | 1:C:118:LEU:HG   | 1.78                     | 0.66              |
| 1:B:60:THR:H     | 1:B:63:ILE:HD12  | 1.60                     | 0.66              |
| 1:D:137:ILE:O    | 1:D:140:ARG:HG2  | 1.95                     | 0.66              |
| 1:A:338:GLN:HB2  | 1:A:339:LYS:HZ2  | 1.61                     | 0.66              |
| 1:B:22:LYS:HZ3   | 1:D:27:PRO:HG2   | 1.59                     | 0.66              |
| 1:C:357:LYS:HD2  | 1:C:357:LYS:N    | 2.11                     | 0.66              |
| 1:A:156:LYS:HE3  | 1:A:479:ILE:HG23 | 1.77                     | 0.66              |
| 1:A:324:VAL:HA   | 1:A:327:MSE:CE   | 2.22                     | 0.66              |
| 1:B:395:ALA:HB3  | 1:B:398:LEU:CD2  | 2.26                     | 0.66              |
| 1:A:140:ARG:NH2  | 1:A:230:GLN:O    | 2.29                     | 0.65              |
| 1:D:437:THR:O    | 1:D:440:ARG:HG3  | 1.95                     | 0.65              |
| 1:D:505:GLU:O    | 1:D:508:ALA:HB3  | 1.96                     | 0.65              |
| 1:D:85:ILE:HD11  | 1:D:100:LEU:HD11 | 1.78                     | 0.65              |
| 1:B:22:LYS:O     | 1:D:24:LYS:HE3   | 1.97                     | 0.65              |
| 1:D:166:ILE:HD12 | 1:D:179:ILE:HG13 | 1.77                     | 0.65              |
| 1:A:392:VAL:O    | 1:A:392:VAL:CG1  | 2.44                     | 0.65              |
| 1:B:492:LEU:CD2  | 1:B:496:LYS:HE3  | 2.27                     | 0.65              |
| 1:C:314:GLU:HB2  | 3:C:2601:NAD:O1N | 1.96                     | 0.65              |
| 1:D:327:MSE:HE3  | 1:D:337:ALA:CB   | 2.25                     | 0.65              |
| 1:D:346:LYS:HE2  | 1:D:347:TYR:CZ   | 2.31                     | 0.65              |
| 1:D:350:LEU:N    | 1:D:350:LEU:HD23 | 2.11                     | 0.65              |
| 1:B:518:ASN:O    | 1:B:522:VAL:HG23 | 1.96                     | 0.65              |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:CD1  | 2.27                     | 0.65              |
| 1:B:81:LYS:HD2   | 5:B:4051:HOH:O   | 1.97                     | 0.65              |
| 1:B:309:PHE:HB2  | 1:B:343:MSE:HG3  | 1.79                     | 0.65              |
| 1:D:407:MSE:HE2  | 1:D:407:MSE:CA   | 2.27                     | 0.65              |
| 1:D:509:GLN:HG3  | 1:D:511:ARG:HG3  | 1.77                     | 0.65              |
| 1:D:520:GLN:NE2  | 1:D:521:GLU:N    | 2.43                     | 0.65              |
| 1:B:374:PRO:HG3  | 1:B:383:ILE:HD12 | 1.78                     | 0.64              |
| 1:A:310:LEU:HD21 | 1:A:398:LEU:HB2  | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:423:THR:HG23 | 1:B:447:SER:HB3  | 1.79                     | 0.64              |
| 1:A:358:ILE:HG23 | 1:A:362:GLN:HB2  | 1.79                     | 0.64              |
| 1:B:61:GLN:HG3   | 1:B:562:TYR:CE1  | 2.32                     | 0.64              |
| 1:A:328:VAL:HA   | 1:A:332:LEU:O    | 1.96                     | 0.64              |
| 1:D:385:LYS:HA   | 1:D:410:ILE:HD13 | 1.80                     | 0.64              |
| 1:A:467:ASN:H    | 1:A:467:ASN:ND2  | 1.94                     | 0.64              |
| 1:D:68:PHE:CE2   | 1:D:99:ILE:HG21  | 2.33                     | 0.64              |
| 1:D:286:VAL:HG11 | 1:D:466:ASN:O    | 1.98                     | 0.64              |
| 1:A:487:SER:HB3  | 1:A:539:MSE:CE   | 2.26                     | 0.64              |
| 1:A:177:MSE:HE3  | 1:A:180:PRO:HD2  | 1.80                     | 0.64              |
| 1:B:305:HIS:HB2  | 1:B:340:LYS:NZ   | 2.12                     | 0.64              |
| 1:B:492:LEU:HD21 | 1:B:496:LYS:HE3  | 1.80                     | 0.63              |
| 1:A:204:ASP:OD2  | 1:B:56:PRO:HG3   | 1.98                     | 0.63              |
| 1:B:273:TYR:O    | 1:B:485:HIS:HD2  | 1.81                     | 0.63              |
| 1:C:159:VAL:HG23 | 1:C:184:LEU:HD21 | 1.79                     | 0.63              |
| 1:D:210:ILE:HG12 | 1:D:211:ALA:N    | 2.14                     | 0.63              |
| 1:A:111:VAL:O    | 5:A:4046:HOH:O   | 2.15                     | 0.63              |
| 1:B:110:ILE:O    | 1:B:115:THR:HB   | 1.98                     | 0.63              |
| 1:A:504:ASP:OD2  | 1:A:504:ASP:N    | 2.31                     | 0.63              |
| 1:C:70:ARG:HH11  | 1:C:70:ARG:HG2   | 1.64                     | 0.63              |
| 1:A:61:GLN:HA    | 1:A:64:GLN:HE21  | 1.64                     | 0.63              |
| 1:A:88:ILE:HD13  | 1:A:91:ARG:HH21  | 1.64                     | 0.63              |
| 1:A:298:ILE:HG22 | 1:A:300:LYS:HB2  | 1.81                     | 0.63              |
| 1:B:261:ASN:ND2  | 1:B:264:ARG:NH1  | 2.47                     | 0.63              |
| 1:B:501:GLN:HE22 | 1:B:525:ASN:HB3  | 1.63                     | 0.63              |
| 1:D:153:ASN:H    | 1:D:153:ASN:ND2  | 1.97                     | 0.63              |
| 1:B:197:ARG:NH1  | 1:B:197:ARG:HG3  | 2.12                     | 0.63              |
| 1:C:90:GLU:OE1   | 1:C:131:LYS:HG3  | 1.98                     | 0.63              |
| 1:C:550:ALA:O    | 1:C:554:LYS:HG2  | 1.98                     | 0.63              |
| 1:B:346:LYS:NZ   | 1:B:346:LYS:HB2  | 2.14                     | 0.63              |
| 1:B:468:VAL:HA   | 1:B:471:PHE:CE2  | 2.34                     | 0.63              |
| 1:B:517:ALA:O    | 1:B:520:GLN:OE1  | 2.16                     | 0.63              |
| 1:A:310:LEU:HB3  | 1:A:391:GLY:HA2  | 1.81                     | 0.62              |
| 1:C:172:LEU:O    | 1:C:175:TYR:HB2  | 1.98                     | 0.62              |
| 1:B:197:ARG:HG3  | 1:B:197:ARG:HH11 | 1.64                     | 0.62              |
| 1:C:110:ILE:O    | 1:C:115:THR:HB   | 2.00                     | 0.62              |
| 1:D:306:LYS:HG2  | 1:D:386:PRO:HA   | 1.82                     | 0.62              |
| 1:D:481:CYS:HB3  | 1:D:540:ALA:HB1  | 1.79                     | 0.62              |
| 1:A:483:THR:OG1  | 1:A:534:LEU:HD13 | 1.99                     | 0.62              |
| 1:D:95:LEU:O     | 1:D:99:ILE:HG12  | 1.99                     | 0.62              |
| 1:A:177:MSE:CE   | 1:A:180:PRO:HB2  | 2.29                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:23:GLU:HA    | 1:B:23:GLU:OE1   | 1.99                     | 0.62              |
| 1:C:302:ILE:CD1  | 1:C:332:LEU:HD22 | 2.30                     | 0.62              |
| 1:B:515:PRO:HB2  | 1:B:518:ASN:HD22 | 1.65                     | 0.62              |
| 1:D:270:ARG:HG3  | 1:D:271:GLU:OE2  | 2.00                     | 0.62              |
| 1:A:29:MSE:HA    | 1:A:35:ASN:OD1   | 2.00                     | 0.62              |
| 1:D:286:VAL:HG21 | 1:D:467:ASN:CA   | 2.29                     | 0.62              |
| 1:B:295:GLN:HA   | 1:B:295:GLN:OE1  | 1.99                     | 0.61              |
| 1:D:108:MSE:HB3  | 1:D:109:PRO:HD3  | 1.80                     | 0.61              |
| 1:A:307:ILE:HG13 | 1:A:388:THR:HB   | 1.81                     | 0.61              |
| 1:C:112:TYR:CD2  | 1:C:113:THR:HG22 | 2.35                     | 0.61              |
| 1:D:33:ARG:NH1   | 1:D:93:GLU:OE1   | 2.33                     | 0.61              |
| 1:A:123:TYR:CD2  | 1:A:219:MSE:HE1  | 2.35                     | 0.61              |
| 1:A:132:GLY:HA2  | 1:A:200:PRO:HG2  | 1.81                     | 0.61              |
| 1:C:406:ALA:O    | 1:C:410:ILE:HG13 | 2.01                     | 0.61              |
| 1:C:437:THR:C    | 1:C:438:GLU:HG2  | 2.25                     | 0.61              |
| 1:D:286:VAL:CG2  | 1:D:467:ASN:HA   | 2.27                     | 0.61              |
| 1:C:221:LEU:HB3  | 1:C:223:GLN:HG2  | 1.82                     | 0.61              |
| 1:D:391:GLY:HA3  | 1:D:427:GLU:HG2  | 1.82                     | 0.61              |
| 1:A:475:ALA:O    | 1:A:479:ILE:HD12 | 2.00                     | 0.61              |
| 1:D:70:ARG:NH1   | 1:D:70:ARG:HG2   | 2.14                     | 0.61              |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:CD1  | 2.30                     | 0.61              |
| 1:A:55:PRO:HG3   | 1:B:219:MSE:HE3  | 1.83                     | 0.61              |
| 1:B:47:MSE:HE2   | 1:B:567:PRO:CG   | 2.29                     | 0.61              |
| 1:A:29:MSE:HE1   | 1:A:54:LEU:HD21  | 1.83                     | 0.61              |
| 1:C:21:ILE:HD12  | 1:C:22:LYS:N     | 2.16                     | 0.61              |
| 1:A:210:ILE:HD13 | 1:A:210:ILE:H    | 1.66                     | 0.61              |
| 1:C:61:GLN:HA    | 1:C:64:GLN:HE21  | 1.66                     | 0.61              |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:HB2  | 1.81                     | 0.61              |
| 1:C:434:TYR:HD1  | 1:C:452:VAL:HG11 | 1.64                     | 0.60              |
| 1:C:454:LEU:HD11 | 1:C:460:PHE:HE2  | 1.64                     | 0.60              |
| 1:D:70:ARG:CG    | 1:D:70:ARG:HH11  | 2.15                     | 0.60              |
| 1:D:179:ILE:HB   | 1:D:180:PRO:HD3  | 1.82                     | 0.60              |
| 1:B:177:MSE:O    | 1:B:181:VAL:HG23 | 2.00                     | 0.60              |
| 1:D:243:THR:HG21 | 1:D:273:TYR:CD2  | 2.36                     | 0.60              |
| 1:D:407:MSE:HE2  | 1:D:407:MSE:HA   | 1.82                     | 0.60              |
| 1:A:443:PHE:CZ   | 1:A:445:SER:HB3  | 2.37                     | 0.60              |
| 1:D:203:ILE:HD13 | 1:D:235:ILE:CD1  | 2.31                     | 0.60              |
| 1:C:70:ARG:HH11  | 1:C:70:ARG:CG    | 2.14                     | 0.60              |
| 1:D:306:LYS:HE2  | 1:D:342:TRP:NE1  | 2.17                     | 0.60              |
| 1:A:535:TYR:OH   | 1:A:542:ARG:HB3  | 2.01                     | 0.60              |
| 1:B:116:VAL:HG13 | 1:B:117:GLY:N    | 2.14                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:532:GLU:HG2  | 1:B:549:LYS:CG   | 2.31                     | 0.60              |
| 1:C:326:SER:O    | 1:C:329:GLU:HG2  | 2.02                     | 0.60              |
| 1:C:483:THR:OG1  | 1:C:534:LEU:HD13 | 2.01                     | 0.60              |
| 1:B:506:GLU:O    | 1:B:511:ARG:HB2  | 2.02                     | 0.59              |
| 1:C:165:ARG:NH2  | 1:C:256:ASP:OD1  | 2.34                     | 0.59              |
| 1:B:297:VAL:HG22 | 1:B:298:ILE:N    | 2.16                     | 0.59              |
| 1:C:68:PHE:CD2   | 1:C:99:ILE:HG13  | 2.37                     | 0.59              |
| 1:A:225:ARG:HH11 | 1:A:225:ARG:CG   | 2.16                     | 0.59              |
| 1:A:233:ASP:OD2  | 1:A:234:LEU:N    | 2.35                     | 0.59              |
| 1:B:24:LYS:NZ    | 1:D:22:LYS:HD3   | 2.17                     | 0.59              |
| 1:C:248:ARG:HH22 | 1:C:272:LYS:HZ2  | 1.49                     | 0.59              |
| 1:D:243:THR:HG21 | 1:D:273:TYR:CE2  | 2.37                     | 0.59              |
| 1:A:179:ILE:HB   | 1:A:180:PRO:HD3  | 1.83                     | 0.59              |
| 1:A:331:GLY:O    | 1:A:332:LEU:C    | 2.45                     | 0.59              |
| 1:C:21:ILE:HD12  | 1:C:22:LYS:H     | 1.67                     | 0.59              |
| 1:D:397:ARG:NH2  | 1:D:423:THR:O    | 2.35                     | 0.59              |
| 1:A:333:SER:OG   | 1:A:336:GLU:HG3  | 2.02                     | 0.59              |
| 1:B:397:ARG:NH2  | 1:B:426:ALA:HB3  | 2.17                     | 0.59              |
| 1:A:286:VAL:CG2  | 1:A:467:ASN:HA   | 2.32                     | 0.59              |
| 1:B:543:TYR:CZ   | 1:C:484:ARG:HG2  | 2.38                     | 0.59              |
| 1:A:57:LYS:HD3   | 1:B:218:TYR:O    | 2.02                     | 0.59              |
| 1:B:205:VAL:HG11 | 1:B:231:TYR:CD1  | 2.38                     | 0.59              |
| 1:C:307:ILE:N    | 1:C:307:ILE:HD12 | 2.18                     | 0.59              |
| 1:A:132:GLY:CA   | 1:A:200:PRO:HG2  | 2.33                     | 0.59              |
| 1:A:150:TRP:NE1  | 1:A:152:GLU:HB2  | 2.18                     | 0.59              |
| 1:A:221:LEU:HB3  | 1:A:223:GLN:HG2  | 1.84                     | 0.59              |
| 1:D:36:LYS:HE2   | 1:D:562:TYR:HB3  | 1.85                     | 0.58              |
| 1:D:140:ARG:NH2  | 1:D:230:GLN:HG2  | 2.17                     | 0.58              |
| 1:B:46:GLN:HG3   | 1:B:51:GLN:HG3   | 1.84                     | 0.58              |
| 1:B:346:LYS:HB2  | 1:B:346:LYS:HZ3  | 1.68                     | 0.58              |
| 1:C:552:TYR:O    | 1:C:556:ARG:HG2  | 2.02                     | 0.58              |
| 1:A:105:GLU:HG3  | 1:A:516:LEU:HB3  | 1.86                     | 0.58              |
| 1:C:453:LYS:HB2  | 1:C:459:VAL:HG22 | 1.85                     | 0.58              |
| 1:D:300:LYS:NZ   | 1:D:300:LYS:CB   | 2.65                     | 0.58              |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CZ   | 2.38                     | 0.58              |
| 1:A:350:LEU:HD11 | 1:A:362:GLN:NE2  | 2.17                     | 0.58              |
| 1:A:476:LEU:HD23 | 1:A:527:ALA:CB   | 2.34                     | 0.58              |
| 1:C:328:VAL:HA   | 1:C:332:LEU:O    | 2.02                     | 0.58              |
| 1:D:293:ALA:O    | 1:D:296:LYS:HB2  | 2.03                     | 0.58              |
| 1:A:207:THR:O    | 1:A:224:LYS:HA   | 2.04                     | 0.58              |
| 1:A:493:GLU:HG2  | 1:A:533:TYR:CD1  | 2.39                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:ARG:HD2   | 1:B:93:GLU:OE1   | 2.04                     | 0.58              |
| 1:B:301:PRO:HG2  | 1:B:304:GLU:OE2  | 2.03                     | 0.58              |
| 1:B:389:ILE:HG23 | 1:B:399:PHE:CZ   | 2.38                     | 0.58              |
| 1:D:518:ASN:HA   | 1:D:520:GLN:OE1  | 2.02                     | 0.58              |
| 1:A:177:MSE:HE1  | 1:A:200:PRO:HB2  | 1.86                     | 0.58              |
| 1:C:85:ILE:HD12  | 1:C:96:PHE:CE1   | 2.31                     | 0.58              |
| 1:D:38:MSE:SE    | 1:D:55:PRO:HG2   | 2.54                     | 0.58              |
| 1:A:397:ARG:HD2  | 1:A:426:ALA:O    | 2.03                     | 0.58              |
| 1:D:285:ALA:HB1  | 1:D:470:ILE:HD12 | 1.84                     | 0.58              |
| 1:A:57:LYS:HZ3   | 1:A:59:GLU:HG2   | 1.68                     | 0.57              |
| 1:A:152:GLU:OE1  | 1:A:152:GLU:N    | 2.36                     | 0.57              |
| 1:B:128:ARG:HG3  | 1:B:128:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:424:ALA:HB3  | 1:A:425:GLN:HE22 | 1.68                     | 0.57              |
| 1:B:515:PRO:HB2  | 1:B:518:ASN:ND2  | 2.19                     | 0.57              |
| 1:B:128:ARG:NE   | 5:B:4056:HOH:O   | 2.20                     | 0.57              |
| 1:C:420:SER:HA   | 3:C:2601:NAD:H1D | 1.86                     | 0.57              |
| 1:D:37:GLY:C     | 1:D:39:ALA:H     | 2.12                     | 0.57              |
| 1:A:55:PRO:CG    | 1:B:219:MSE:HE3  | 2.34                     | 0.57              |
| 1:A:350:LEU:HD13 | 1:A:358:ILE:CD1  | 2.34                     | 0.57              |
| 1:B:128:ARG:HG3  | 1:B:128:ARG:NH1  | 2.18                     | 0.57              |
| 1:B:354:ARG:HE   | 1:B:358:ILE:CD1  | 2.17                     | 0.57              |
| 1:C:231:TYR:CE2  | 1:C:265:PHE:HZ   | 2.23                     | 0.57              |
| 1:C:505:GLU:CD   | 1:C:505:GLU:H    | 2.11                     | 0.57              |
| 1:D:306:LYS:HG3  | 1:D:386:PRO:HA   | 1.85                     | 0.57              |
| 1:D:535:TYR:OH   | 1:D:542:ARG:HB3  | 2.05                     | 0.57              |
| 1:B:552:TYR:O    | 1:B:556:ARG:HG3  | 2.05                     | 0.57              |
| 1:D:43:GLN:HG2   | 1:D:566:LEU:CD1  | 2.32                     | 0.57              |
| 1:B:227:ARG:HG2  | 1:B:227:ARG:NH1  | 2.04                     | 0.57              |
| 1:D:86:MSE:HG3   | 1:D:131:LYS:HZ1  | 1.69                     | 0.57              |
| 1:D:481:CYS:HB3  | 1:D:540:ALA:CB   | 2.34                     | 0.57              |
| 1:B:29:MSE:CE    | 1:B:50:LEU:HD22  | 2.35                     | 0.57              |
| 1:B:343:MSE:HB3  | 1:B:350:LEU:HG   | 1.85                     | 0.57              |
| 1:D:456:ASP:OD2  | 1:D:458:ARG:NH1  | 2.37                     | 0.57              |
| 1:B:183:LYS:NZ   | 1:B:255:GLU:OE1  | 2.38                     | 0.57              |
| 1:B:456:ASP:OD2  | 1:B:458:ARG:NH1  | 2.37                     | 0.57              |
| 1:C:261:ASN:HD21 | 1:C:264:ARG:HH21 | 1.52                     | 0.57              |
| 1:C:446:GLY:N    | 5:C:4012:HOH:O   | 2.24                     | 0.57              |
| 1:D:526:ILE:O    | 1:D:530:VAL:HG23 | 2.05                     | 0.57              |
| 1:B:551:LYS:O    | 1:B:555:GLU:HB2  | 2.05                     | 0.57              |
| 1:C:412:GLU:O    | 1:C:440:ARG:NH1  | 2.37                     | 0.57              |
| 1:D:394:GLY:HA2  | 1:D:420:SER:HB3  | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:274:CYS:HB2  | 1:B:484:ARG:O    | 2.04                     | 0.57              |
| 1:C:41:THR:OG1   | 1:C:44:GLU:HG3   | 2.04                     | 0.57              |
| 1:A:503:THR:OG1  | 1:A:505:GLU:HG2  | 2.04                     | 0.56              |
| 1:D:381:VAL:CG2  | 1:D:389:ILE:HD11 | 2.35                     | 0.56              |
| 1:A:467:ASN:H    | 1:A:467:ASN:HD22 | 1.52                     | 0.56              |
| 1:B:227:ARG:CG   | 1:B:227:ARG:NH1  | 2.61                     | 0.56              |
| 1:C:40:PHE:HE2   | 1:C:565:LEU:CD1  | 2.17                     | 0.56              |
| 1:C:392:VAL:HG13 | 1:C:392:VAL:O    | 2.05                     | 0.56              |
| 1:A:61:GLN:OE1   | 1:A:98:ARG:HD3   | 2.05                     | 0.56              |
| 1:A:91:ARG:HD2   | 5:A:4055:HOH:O   | 2.04                     | 0.56              |
| 1:B:184:LEU:HD12 | 1:B:200:PRO:HB3  | 1.88                     | 0.56              |
| 1:B:396:GLY:O    | 1:B:427:GLU:HA   | 2.06                     | 0.56              |
| 1:B:552:TYR:CD1  | 1:B:556:ARG:NH1  | 2.73                     | 0.56              |
| 1:C:335:GLN:NE2  | 1:C:339:LYS:HZ1  | 2.04                     | 0.56              |
| 1:C:350:LEU:HD22 | 1:C:354:ARG:CZ   | 2.35                     | 0.56              |
| 1:D:81:LYS:O     | 1:D:85:ILE:HG22  | 2.06                     | 0.56              |
| 1:A:144:ARG:NE   | 1:A:148:ASP:OD1  | 2.38                     | 0.56              |
| 1:A:520:GLN:HE21 | 1:A:520:GLN:N    | 1.99                     | 0.56              |
| 1:A:527:ALA:O    | 1:A:531:THR:HG23 | 2.05                     | 0.56              |
| 1:B:478:VAL:HG13 | 1:B:483:THR:OG1  | 2.05                     | 0.56              |
| 1:C:221:LEU:HD23 | 1:C:223:GLN:CD   | 2.30                     | 0.56              |
| 1:D:86:MSE:HG3   | 1:D:131:LYS:NZ   | 2.20                     | 0.56              |
| 1:D:85:ILE:HG23  | 1:D:86:MSE:HE2   | 1.88                     | 0.56              |
| 1:D:432:GLU:OE2  | 5:D:4048:HOH:O   | 2.17                     | 0.56              |
| 1:A:306:LYS:HG2  | 1:A:386:PRO:HA   | 1.87                     | 0.56              |
| 1:A:398:LEU:N    | 1:A:398:LEU:CD2  | 2.68                     | 0.56              |
| 1:A:484:ARG:HG2  | 1:D:543:TYR:CE1  | 2.40                     | 0.56              |
| 1:C:61:GLN:OE1   | 1:C:98:ARG:HD3   | 2.06                     | 0.56              |
| 1:C:79:LEU:HB2   | 1:C:118:LEU:HD21 | 1.88                     | 0.56              |
| 1:D:72:LEU:HA    | 1:D:75:MSE:HG3   | 1.87                     | 0.56              |
| 1:B:286:VAL:HG21 | 1:B:467:ASN:HA   | 1.87                     | 0.56              |
| 1:C:248:ARG:NH1  | 1:C:273:TYR:CD2  | 2.74                     | 0.56              |
| 1:C:535:TYR:OH   | 1:C:542:ARG:HB3  | 2.06                     | 0.56              |
| 1:D:201:VAL:HG11 | 1:D:238:PHE:CE1  | 2.41                     | 0.56              |
| 1:D:441:CYS:O    | 1:D:442:LEU:HD23 | 2.06                     | 0.56              |
| 1:A:212:LEU:HD22 | 1:A:218:TYR:CD2  | 2.41                     | 0.56              |
| 1:B:297:VAL:CG2  | 1:B:298:ILE:N    | 2.68                     | 0.56              |
| 1:D:309:PHE:HB2  | 1:D:343:MSE:HG2  | 1.88                     | 0.56              |
| 1:A:91:ARG:CD    | 5:A:4055:HOH:O   | 2.53                     | 0.55              |
| 1:B:347:TYR:HB2  | 1:B:354:ARG:NH1  | 2.21                     | 0.55              |
| 1:C:371:GLU:HG2  | 1:C:372:SER:N    | 2.21                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:38:MSE:HE3   | 1:A:59:GLU:CG    | 2.36                     | 0.55              |
| 1:A:153:ASN:HD22 | 1:A:153:ASN:N    | 2.03                     | 0.55              |
| 1:A:177:MSE:O    | 1:A:177:MSE:HG3  | 2.06                     | 0.55              |
| 1:C:85:ILE:HG13  | 1:C:86:MSE:H     | 1.71                     | 0.55              |
| 1:A:225:ARG:O    | 1:A:227:ARG:HD2  | 2.06                     | 0.55              |
| 1:B:29:MSE:HE2   | 1:B:50:LEU:CD2   | 2.33                     | 0.55              |
| 1:C:42:LEU:O     | 1:C:46:GLN:HG3   | 2.05                     | 0.55              |
| 1:A:66:LEU:HD22  | 1:A:70:ARG:CD    | 2.37                     | 0.55              |
| 1:B:261:ASN:CG   | 1:B:264:ARG:NH1  | 2.64                     | 0.55              |
| 1:B:357:LYS:HD3  | 1:B:357:LYS:N    | 2.22                     | 0.55              |
| 1:D:36:LYS:HB3   | 1:D:39:ALA:HB3   | 1.88                     | 0.55              |
| 1:D:208:ASP:CG   | 1:D:227:ARG:HH22 | 2.14                     | 0.55              |
| 1:A:502:LEU:HD13 | 1:A:507:LEU:HD13 | 1.87                     | 0.55              |
| 1:B:556:ARG:HH11 | 1:B:556:ARG:CG   | 2.19                     | 0.55              |
| 1:C:302:ILE:HG23 | 1:C:303:SER:N    | 2.22                     | 0.55              |
| 1:D:261:ASN:HD21 | 1:D:264:ARG:HH21 | 1.53                     | 0.55              |
| 1:A:64:GLN:NE2   | 1:A:562:TYR:OH   | 2.37                     | 0.55              |
| 1:B:476:LEU:HD23 | 1:B:527:ALA:CB   | 2.37                     | 0.55              |
| 1:C:205:VAL:HG11 | 1:C:231:TYR:HD1  | 1.72                     | 0.55              |
| 1:C:242:ILE:CG2  | 1:C:243:THR:N    | 2.69                     | 0.55              |
| 1:B:75:MSE:HG2   | 1:B:80:GLU:OE1   | 2.07                     | 0.55              |
| 1:B:105:GLU:HG2  | 1:B:516:LEU:HB3  | 1.89                     | 0.55              |
| 1:B:154:HIS:O    | 1:B:197:ARG:HD2  | 2.07                     | 0.55              |
| 1:B:350:LEU:HD22 | 1:B:354:ARG:NH2  | 2.22                     | 0.55              |
| 1:C:45:ARG:HB3   | 1:C:51:GLN:HG2   | 1.89                     | 0.55              |
| 1:A:104:ILE:HG13 | 1:A:108:MSE:HE2  | 1.89                     | 0.55              |
| 1:A:305:HIS:O    | 1:A:340:LYS:HD3  | 2.07                     | 0.55              |
| 1:A:431:GLU:OE2  | 1:A:431:GLU:HA   | 2.07                     | 0.55              |
| 1:B:22:LYS:HZ3   | 1:D:27:PRO:CG    | 2.20                     | 0.55              |
| 1:B:446:GLY:O    | 1:B:466:ASN:ND2  | 2.38                     | 0.55              |
| 1:C:108:MSE:HB3  | 1:C:109:PRO:HD3  | 1.89                     | 0.55              |
| 1:A:59:GLU:CD    | 1:A:67:ARG:HH12  | 2.14                     | 0.54              |
| 1:A:146:ILE:O    | 1:A:149:ASN:HB2  | 2.08                     | 0.54              |
| 1:A:315:ALA:O    | 1:A:319:ILE:HG13 | 2.07                     | 0.54              |
| 1:B:179:ILE:HB   | 1:B:180:PRO:HD3  | 1.89                     | 0.54              |
| 1:B:432:GLU:O    | 1:B:436:LEU:HB2  | 2.07                     | 0.54              |
| 1:C:264:ARG:HG2  | 1:C:264:ARG:HH11 | 1.72                     | 0.54              |
| 1:C:389:ILE:HB   | 1:C:407:MSE:HE2  | 1.88                     | 0.54              |
| 1:D:25:GLY:C     | 1:D:27:PRO:HD2   | 2.32                     | 0.54              |
| 1:D:144:ARG:HA   | 1:D:147:VAL:HG22 | 1.89                     | 0.54              |
| 1:D:287:ALA:CB   | 1:D:319:ILE:HD13 | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:ARG:NH2  | 1:A:233:ASP:HB3  | 2.22                     | 0.54              |
| 1:C:325:MSE:HE1  | 1:C:489:SER:HA   | 1.88                     | 0.54              |
| 1:D:68:PHE:CE2   | 1:D:72:LEU:HD22  | 2.42                     | 0.54              |
| 1:A:153:ASN:N    | 1:A:153:ASN:ND2  | 2.55                     | 0.54              |
| 1:A:175:TYR:CE2  | 1:A:219:MSE:HE2  | 2.42                     | 0.54              |
| 1:A:298:ILE:CG2  | 1:A:300:LYS:HB2  | 2.37                     | 0.54              |
| 1:B:300:LYS:NZ   | 1:B:300:LYS:CB   | 2.62                     | 0.54              |
| 1:C:112:TYR:CD1  | 1:C:186:LEU:HD11 | 2.43                     | 0.54              |
| 1:D:194:ARG:HE   | 1:D:197:ARG:CZ   | 2.20                     | 0.54              |
| 1:A:261:ASN:ND2  | 1:A:264:ARG:HE   | 2.06                     | 0.54              |
| 1:D:379:ASP:O    | 1:D:383:ILE:HD13 | 2.07                     | 0.54              |
| 1:D:401:PRO:O    | 1:D:405:ARG:HG3  | 2.07                     | 0.54              |
| 1:A:137:ILE:HA   | 1:A:234:LEU:HD22 | 1.89                     | 0.54              |
| 1:A:177:MSE:CE   | 1:A:200:PRO:HB2  | 2.37                     | 0.54              |
| 1:C:46:GLN:HG2   | 1:C:51:GLN:HG3   | 1.90                     | 0.54              |
| 1:C:300:LYS:HG3  | 1:C:301:PRO:HD2  | 1.90                     | 0.54              |
| 1:D:475:ALA:O    | 1:D:479:ILE:HD12 | 2.08                     | 0.54              |
| 1:A:22:LYS:NZ    | 1:C:27:PRO:HG2   | 2.23                     | 0.54              |
| 1:A:24:LYS:HG3   | 1:C:22:LYS:HE2   | 1.89                     | 0.54              |
| 1:C:287:ALA:O    | 1:C:291:LEU:HD13 | 2.06                     | 0.54              |
| 1:D:242:ILE:HG22 | 1:D:243:THR:N    | 2.23                     | 0.54              |
| 1:D:307:ILE:HG13 | 1:D:388:THR:HB   | 1.90                     | 0.54              |
| 1:B:29:MSE:HE1   | 1:B:53:LEU:CB    | 2.34                     | 0.54              |
| 1:B:29:MSE:HE3   | 1:B:53:LEU:HD12  | 1.90                     | 0.54              |
| 1:C:552:TYR:CD1  | 1:C:556:ARG:NH1  | 2.75                     | 0.54              |
| 1:D:460:PHE:N    | 1:D:460:PHE:CD2  | 2.76                     | 0.54              |
| 1:D:486:ILE:N    | 1:D:486:ILE:HD12 | 2.22                     | 0.54              |
| 1:A:219:MSE:HG2  | 1:B:38:MSE:HE1   | 1.88                     | 0.54              |
| 1:A:282:GLY:O    | 1:A:286:VAL:HG23 | 2.07                     | 0.54              |
| 1:B:91:ARG:HG2   | 1:B:91:ARG:NH1   | 2.23                     | 0.54              |
| 1:B:331:GLY:O    | 1:B:332:LEU:O    | 2.26                     | 0.54              |
| 1:C:358:ILE:HG23 | 1:C:362:GLN:HB2  | 1.88                     | 0.54              |
| 1:C:354:ARG:HG2  | 1:C:358:ILE:HD11 | 1.90                     | 0.54              |
| 1:D:298:ILE:HG22 | 1:D:300:LYS:N    | 2.10                     | 0.54              |
| 1:A:68:PHE:HZ    | 1:A:85:ILE:HG22  | 1.71                     | 0.53              |
| 1:B:374:PRO:HB3  | 1:B:380:ALA:N    | 2.22                     | 0.53              |
| 1:B:431:GLU:OE2  | 1:B:452:VAL:HG13 | 2.07                     | 0.53              |
| 1:C:286:VAL:HG11 | 1:C:466:ASN:O    | 2.08                     | 0.53              |
| 1:C:335:GLN:NE2  | 1:C:339:LYS:NZ   | 2.56                     | 0.53              |
| 1:B:310:LEU:HB3  | 1:B:391:GLY:HA2  | 1.90                     | 0.53              |
| 1:D:21:ILE:N     | 1:D:21:ILE:HD12  | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:25:GLY:HA3   | 1:C:22:LYS:HE3   | 1.90                     | 0.53              |
| 1:A:37:GLY:C     | 1:A:39:ALA:H     | 2.17                     | 0.53              |
| 1:A:396:GLY:C    | 1:A:398:LEU:HD23 | 2.34                     | 0.53              |
| 1:A:397:ARG:HD3  | 1:A:397:ARG:N    | 2.24                     | 0.53              |
| 1:B:22:LYS:HD2   | 1:D:24:LYS:HE3   | 1.90                     | 0.53              |
| 1:B:58:ILE:HG22  | 1:B:58:ILE:O     | 2.07                     | 0.53              |
| 1:B:77:SER:OG    | 1:B:80:GLU:HB3   | 2.08                     | 0.53              |
| 1:B:401:PRO:HB3  | 1:B:436:LEU:HD21 | 1.90                     | 0.53              |
| 1:C:227:ARG:NH1  | 1:C:227:ARG:HG2  | 2.23                     | 0.53              |
| 1:C:527:ALA:O    | 1:C:531:THR:CG2  | 2.56                     | 0.53              |
| 1:D:70:ARG:NH1   | 1:D:70:ARG:CG    | 2.71                     | 0.53              |
| 1:D:414:PRO:HD2  | 1:D:441:CYS:HA   | 1.89                     | 0.53              |
| 1:A:210:ILE:H    | 1:A:210:ILE:CD1  | 2.22                     | 0.53              |
| 1:A:434:TYR:CZ   | 1:A:443:PHE:HB3  | 2.44                     | 0.53              |
| 1:A:505:GLU:O    | 1:A:508:ALA:HB3  | 2.08                     | 0.53              |
| 1:B:546:PRO:HG2  | 1:B:549:LYS:HD2  | 1.90                     | 0.53              |
| 1:B:133:LEU:HB2  | 1:B:199:LEU:HD11 | 1.90                     | 0.53              |
| 1:C:227:ARG:HG2  | 1:C:227:ARG:HH11 | 1.72                     | 0.53              |
| 1:D:245:ARG:HD3  | 1:D:246:TYR:CZ   | 2.44                     | 0.53              |
| 1:D:294:ALA:O    | 1:D:297:VAL:HG22 | 2.09                     | 0.53              |
| 1:D:556:ARG:NH1  | 1:D:556:ARG:HG2  | 2.24                     | 0.53              |
| 1:B:137:ILE:HA   | 1:B:234:LEU:HD22 | 1.90                     | 0.53              |
| 1:B:261:ASN:HA   | 1:B:264:ARG:HG2  | 1.91                     | 0.53              |
| 1:B:363:GLU:HB3  | 1:B:364:PRO:HD3  | 1.91                     | 0.53              |
| 1:B:453:LYS:CG   | 1:B:459:VAL:HG12 | 2.36                     | 0.53              |
| 1:C:331:GLY:O    | 1:C:332:LEU:O    | 2.27                     | 0.53              |
| 1:D:412:GLU:HG3  | 1:D:413:ARG:CD   | 2.38                     | 0.53              |
| 1:D:427:GLU:OE1  | 1:D:427:GLU:N    | 2.41                     | 0.53              |
| 1:C:194:ARG:CB   | 1:C:197:ARG:HG2  | 2.32                     | 0.53              |
| 1:D:274:CYS:SG   | 1:D:486:ILE:HD11 | 2.49                     | 0.53              |
| 1:A:300:LYS:HB3  | 1:A:300:LYS:HZ2  | 1.74                     | 0.53              |
| 1:A:411:ASN:HB2  | 1:A:414:PRO:HG3  | 1.90                     | 0.53              |
| 1:B:177:MSE:HG2  | 1:B:202:CYS:HB2  | 1.91                     | 0.53              |
| 1:B:30:LEU:O     | 1:B:32:PRO:HD3   | 2.09                     | 0.53              |
| 1:B:45:ARG:HB3   | 1:B:51:GLN:HG2   | 1.91                     | 0.53              |
| 1:B:402:ASP:OD2  | 1:B:402:ASP:N    | 2.42                     | 0.53              |
| 1:C:116:VAL:HG13 | 1:C:117:GLY:N    | 2.23                     | 0.53              |
| 1:A:300:LYS:NZ   | 1:A:305:HIS:HD2  | 2.07                     | 0.52              |
| 1:B:184:LEU:O    | 1:B:187:TYR:HB2  | 2.09                     | 0.52              |
| 1:B:239:MSE:CE   | 1:B:252:ILE:HD12 | 2.39                     | 0.52              |
| 1:C:527:ALA:O    | 1:C:531:THR:HG23 | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:400:THR:OG1  | 1:B:403:VAL:HG23 | 2.09                     | 0.52              |
| 1:D:70:ARG:HG2   | 1:D:70:ARG:HH11  | 1.74                     | 0.52              |
| 1:B:354:ARG:NH1  | 1:B:356:ALA:HB3  | 2.24                     | 0.52              |
| 1:B:484:ARG:HG2  | 1:C:543:TYR:CZ   | 2.44                     | 0.52              |
| 1:C:301:PRO:HG2  | 1:C:304:GLU:CD   | 2.34                     | 0.52              |
| 1:A:359:ASP:OD2  | 1:A:361:TYR:N    | 2.41                     | 0.52              |
| 1:A:382:ASN:O    | 1:A:385:LYS:HD2  | 2.09                     | 0.52              |
| 1:B:197:ARG:HH11 | 1:B:197:ARG:CG   | 2.22                     | 0.52              |
| 1:B:466:ASN:HB3  | 1:B:468:VAL:HG12 | 1.92                     | 0.52              |
| 1:C:89:GLN:NE2   | 1:C:185:CYS:SG   | 2.82                     | 0.52              |
| 1:B:88:ILE:HD13  | 1:B:99:ILE:HD13  | 1.91                     | 0.52              |
| 1:B:239:MSE:HE1  | 1:B:252:ILE:HD12 | 1.92                     | 0.52              |
| 1:B:261:ASN:HD21 | 1:B:264:ARG:CZ   | 2.21                     | 0.52              |
| 1:B:358:ILE:HG23 | 1:B:362:GLN:HB2  | 1.92                     | 0.52              |
| 1:B:293:ALA:O    | 1:B:296:LYS:HB2  | 2.10                     | 0.52              |
| 1:D:194:ARG:HE   | 1:D:197:ARG:HE   | 1.57                     | 0.52              |
| 1:D:295:GLN:HA   | 1:D:295:GLN:OE1  | 2.10                     | 0.52              |
| 1:C:454:LEU:CD1  | 1:C:460:PHE:HE2  | 2.22                     | 0.52              |
| 1:D:306:LYS:HB2  | 1:D:306:LYS:HZ2  | 1.75                     | 0.52              |
| 1:A:146:ILE:HG23 | 1:B:52:GLY:HA3   | 1.91                     | 0.52              |
| 1:B:215:ASP:OD2  | 1:B:218:TYR:N    | 2.42                     | 0.52              |
| 1:B:343:MSE:HE3  | 1:B:350:LEU:CD1  | 2.39                     | 0.52              |
| 1:C:248:ARG:HH22 | 1:C:272:LYS:NZ   | 2.08                     | 0.52              |
| 1:D:165:ARG:NH2  | 4:D:3603:TTN:O1  | 2.43                     | 0.52              |
| 1:D:350:LEU:N    | 1:D:350:LEU:CD2  | 2.72                     | 0.52              |
| 1:D:194:ARG:HG2  | 1:D:194:ARG:NH1  | 2.25                     | 0.52              |
| 1:A:96:PHE:O     | 1:A:100:LEU:HD22 | 2.10                     | 0.51              |
| 1:C:298:ILE:HD11 | 1:C:442:LEU:HD12 | 1.91                     | 0.51              |
| 1:D:174:VAL:C    | 1:D:176:GLY:H    | 2.18                     | 0.51              |
| 1:A:261:ASN:HA   | 1:A:264:ARG:HG2  | 1.92                     | 0.51              |
| 1:B:260:HIS:CD2  | 1:B:264:ARG:HH11 | 2.28                     | 0.51              |
| 1:B:528:ILE:O    | 1:B:531:THR:HG23 | 2.10                     | 0.51              |
| 1:D:184:LEU:HD12 | 1:D:200:PRO:HB3  | 1.91                     | 0.51              |
| 1:D:300:LYS:HE3  | 1:D:305:HIS:CE1  | 2.45                     | 0.51              |
| 1:C:429:THR:HG23 | 1:C:432:GLU:OE2  | 2.10                     | 0.51              |
| 1:D:520:GLN:CD   | 1:D:520:GLN:H    | 2.17                     | 0.51              |
| 1:D:191:ALA:HB3  | 1:D:193:ILE:HD12 | 1.93                     | 0.51              |
| 1:B:31:ASN:HB3   | 1:B:34:THR:OG1   | 2.10                     | 0.51              |
| 1:B:116:VAL:CG1  | 1:B:117:GLY:N    | 2.73                     | 0.51              |
| 1:B:452:VAL:O    | 1:B:459:VAL:HA   | 2.11                     | 0.51              |
| 1:C:150:TRP:CE2  | 1:C:199:LEU:HD13 | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:357:LYS:N    | 1:C:357:LYS:CD   | 2.73                     | 0.51              |
| 1:A:24:LYS:C     | 1:C:22:LYS:HE2   | 2.35                     | 0.51              |
| 1:B:228:THR:OG1  | 1:B:230:GLN:HB2  | 2.10                     | 0.51              |
| 1:C:132:GLY:HA3  | 1:C:177:MSE:HE3  | 1.92                     | 0.51              |
| 1:C:327:MSE:HE3  | 1:C:337:ALA:CB   | 2.29                     | 0.51              |
| 1:D:306:LYS:HE2  | 1:D:342:TRP:HE1  | 1.75                     | 0.51              |
| 1:A:175:TYR:CE2  | 1:A:218:TYR:HA   | 2.45                     | 0.51              |
| 1:A:307:ILE:HD12 | 1:A:307:ILE:N    | 2.25                     | 0.51              |
| 1:B:88:ILE:HG22  | 1:B:96:PHE:HB2   | 1.92                     | 0.51              |
| 1:A:61:GLN:HG3   | 1:A:562:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:306:LYS:C    | 1:A:307:ILE:HD12 | 2.36                     | 0.51              |
| 1:D:309:PHE:CE1  | 1:D:316:ALA:HA   | 2.46                     | 0.51              |
| 1:A:144:ARG:HE   | 1:A:148:ASP:CG   | 2.19                     | 0.51              |
| 1:C:137:ILE:HA   | 1:C:234:LEU:HD22 | 1.93                     | 0.51              |
| 1:D:331:GLY:O    | 1:D:332:LEU:C    | 2.53                     | 0.51              |
| 1:A:300:LYS:NZ   | 1:A:305:HIS:CD2  | 2.79                     | 0.50              |
| 1:B:150:TRP:CE2  | 1:B:199:LEU:HD13 | 2.45                     | 0.50              |
| 1:B:194:ARG:NH2  | 1:B:196:ASP:OD2  | 2.44                     | 0.50              |
| 1:B:374:PRO:HG3  | 1:B:383:ILE:CD1  | 2.40                     | 0.50              |
| 1:C:164:GLU:HG3  | 1:C:225:ARG:NE   | 2.26                     | 0.50              |
| 1:C:454:LEU:HD11 | 1:C:460:PHE:CE2  | 2.45                     | 0.50              |
| 1:C:520:GLN:H    | 1:C:520:GLN:NE2  | 2.05                     | 0.50              |
| 1:D:397:ARG:HA   | 1:D:427:GLU:O    | 2.11                     | 0.50              |
| 1:A:184:LEU:HD13 | 1:A:198:CYS:HB3  | 1.94                     | 0.50              |
| 1:A:267:ARG:O    | 1:A:267:ARG:HG3  | 2.11                     | 0.50              |
| 1:C:57:LYS:HG3   | 1:C:58:ILE:N     | 2.25                     | 0.50              |
| 1:C:207:THR:CG2  | 1:C:213:LEU:HD13 | 2.41                     | 0.50              |
| 1:C:401:PRO:HA   | 1:C:404:ILE:HG13 | 1.92                     | 0.50              |
| 1:A:346:LYS:HD3  | 1:A:347:TYR:CE1  | 2.47                     | 0.50              |
| 1:A:506:GLU:O    | 1:A:511:ARG:HG3  | 2.11                     | 0.50              |
| 1:D:68:PHE:CD2   | 1:D:99:ILE:HG21  | 2.47                     | 0.50              |
| 1:D:86:MSE:HE2   | 1:D:86:MSE:N     | 2.26                     | 0.50              |
| 1:D:291:LEU:HD13 | 1:D:417:PHE:CE2  | 2.45                     | 0.50              |
| 1:B:505:GLU:O    | 1:B:509:GLN:HG2  | 2.12                     | 0.50              |
| 1:B:534:LEU:CD2  | 1:B:539:MSE:HE2  | 2.42                     | 0.50              |
| 1:D:61:GLN:HG3   | 1:D:562:TYR:CE1  | 2.47                     | 0.50              |
| 1:D:144:ARG:HG2  | 1:D:144:ARG:HH11 | 1.76                     | 0.50              |
| 1:D:392:VAL:O    | 1:D:392:VAL:CG1  | 2.58                     | 0.50              |
| 1:A:319:ILE:O    | 1:A:323:ILE:HG13 | 2.12                     | 0.50              |
| 1:D:359:ASP:OD2  | 1:D:359:ASP:C    | 2.55                     | 0.50              |
| 1:D:482:ASN:HD21 | 3:D:3602:NAD:H4B | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:GLN:O     | 1:A:47:MSE:HB2   | 2.11                     | 0.50              |
| 1:B:24:LYS:HZ3   | 1:D:22:LYS:HD3   | 1.76                     | 0.50              |
| 1:B:327:MSE:HG2  | 1:B:332:LEU:HD22 | 1.94                     | 0.50              |
| 1:B:315:ALA:HB3  | 1:B:392:VAL:HG21 | 1.94                     | 0.50              |
| 1:A:57:LYS:NZ    | 1:A:59:GLU:HG2   | 2.26                     | 0.50              |
| 1:B:68:PHE:CD2   | 1:B:99:ILE:HG12  | 2.46                     | 0.50              |
| 1:B:177:MSE:C    | 1:B:180:PRO:HD2  | 2.36                     | 0.50              |
| 1:B:239:MSE:HE2  | 1:B:273:TYR:CD1  | 2.47                     | 0.50              |
| 1:A:407:MSE:HA   | 1:A:407:MSE:CE   | 2.38                     | 0.49              |
| 1:A:472:PRO:HD2  | 5:A:4029:HOH:O   | 2.10                     | 0.49              |
| 1:B:286:VAL:CG2  | 1:B:467:ASN:HA   | 2.42                     | 0.49              |
| 1:C:350:LEU:HD22 | 1:C:354:ARG:NH2  | 2.27                     | 0.49              |
| 1:D:210:ILE:O    | 1:D:214:LYS:HG3  | 2.12                     | 0.49              |
| 1:D:346:LYS:HE2  | 1:D:347:TYR:OH   | 2.12                     | 0.49              |
| 1:A:412:GLU:HG3  | 1:A:413:ARG:HG2  | 1.93                     | 0.49              |
| 1:B:297:VAL:HG21 | 1:B:442:LEU:HD21 | 1.94                     | 0.49              |
| 1:C:217:PHE:HZ   | 1:D:66:LEU:HD13  | 1.76                     | 0.49              |
| 1:C:286:VAL:HG13 | 1:C:470:ILE:HG12 | 1.93                     | 0.49              |
| 1:D:177:MSE:HE3  | 1:D:180:PRO:HD2  | 1.94                     | 0.49              |
| 1:D:527:ALA:O    | 1:D:531:THR:CG2  | 2.60                     | 0.49              |
| 1:A:38:MSE:HE3   | 1:A:59:GLU:HG3   | 1.94                     | 0.49              |
| 1:A:226:ASP:C    | 1:A:226:ASP:OD1  | 2.55                     | 0.49              |
| 1:A:273:TYR:HB2  | 1:A:275:THR:CG2  | 2.42                     | 0.49              |
| 1:A:376:THR:O    | 1:A:379:ASP:HB2  | 2.11                     | 0.49              |
| 1:B:93:GLU:OE1   | 1:B:195:PRO:HB2  | 2.12                     | 0.49              |
| 1:C:276:PHE:HB2  | 1:C:281:GLN:OE1  | 2.12                     | 0.49              |
| 1:B:248:ARG:HB3  | 1:C:543:TYR:CZ   | 2.48                     | 0.49              |
| 1:C:36:LYS:HE2   | 1:C:562:TYR:HB3  | 1.93                     | 0.49              |
| 1:C:146:ILE:O    | 1:C:149:ASN:HB2  | 2.13                     | 0.49              |
| 1:D:212:LEU:HD22 | 1:D:218:TYR:CD2  | 2.48                     | 0.49              |
| 1:A:140:ARG:NH2  | 1:A:230:GLN:HA   | 2.27                     | 0.49              |
| 1:C:408:ALA:HB1  | 1:C:440:ARG:NH2  | 2.28                     | 0.49              |
| 1:C:79:LEU:HD22  | 1:C:118:LEU:CG   | 2.41                     | 0.49              |
| 1:C:298:ILE:HD11 | 1:C:442:LEU:CD1  | 2.43                     | 0.49              |
| 1:A:24:LYS:O     | 1:C:22:LYS:HE2   | 2.12                     | 0.49              |
| 1:A:184:LEU:O    | 1:A:187:TYR:HB2  | 2.12                     | 0.49              |
| 1:B:140:ARG:CZ   | 1:B:230:GLN:HG3  | 2.43                     | 0.49              |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:HD12 | 1.95                     | 0.49              |
| 1:D:556:ARG:NE   | 3:D:3602:NAD:O2A | 2.46                     | 0.49              |
| 1:C:25:GLY:C     | 1:C:27:PRO:HD2   | 2.37                     | 0.49              |
| 1:C:418:ALA:O    | 5:C:4012:HOH:O   | 2.18                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:208:ASP:OD2  | 1:D:227:ARG:NH2  | 2.34                     | 0.49              |
| 1:D:239:MSE:O    | 1:D:243:THR:HG23 | 2.13                     | 0.49              |
| 1:D:405:ARG:HG3  | 1:D:405:ARG:HH11 | 1.78                     | 0.49              |
| 1:A:89:GLN:HB2   | 1:A:96:PHE:CD2   | 2.48                     | 0.49              |
| 1:A:310:LEU:HD22 | 1:A:399:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:397:ARG:NH1  | 1:A:397:ARG:CG   | 2.75                     | 0.49              |
| 1:A:467:ASN:O    | 1:A:471:PHE:HD2  | 1.95                     | 0.49              |
| 1:B:207:THR:O    | 1:B:224:LYS:HA   | 2.13                     | 0.49              |
| 1:B:521:GLU:HG2  | 1:B:525:ASN:ND2  | 2.28                     | 0.49              |
| 1:A:327:MSE:CE   | 1:A:337:ALA:HB1  | 2.30                     | 0.48              |
| 1:A:333:SER:H    | 1:A:336:GLU:CD   | 2.21                     | 0.48              |
| 1:B:451:PRO:HG3  | 1:B:461:THR:HG23 | 1.94                     | 0.48              |
| 1:B:518:ASN:HA   | 1:B:520:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:165:ARG:NH2  | 4:C:2603:TTN:O1  | 2.46                     | 0.48              |
| 1:C:197:ARG:HH11 | 1:C:197:ARG:CG   | 2.13                     | 0.48              |
| 1:D:226:ASP:C    | 1:D:226:ASP:OD1  | 2.55                     | 0.48              |
| 1:A:72:LEU:HA    | 1:A:75:MSE:HG3   | 1.94                     | 0.48              |
| 1:A:245:ARG:HD3  | 1:A:246:TYR:CE1  | 2.48                     | 0.48              |
| 1:A:385:LYS:HA   | 1:A:410:ILE:HD13 | 1.95                     | 0.48              |
| 1:B:266:LEU:O    | 1:B:270:ARG:HB3  | 2.12                     | 0.48              |
| 1:C:116:VAL:CG1  | 1:C:117:GLY:N    | 2.75                     | 0.48              |
| 1:D:144:ARG:HD2  | 1:D:147:VAL:HG21 | 1.91                     | 0.48              |
| 1:A:194:ARG:HG3  | 3:A:602:NAD:C6A  | 2.43                     | 0.48              |
| 1:A:300:LYS:HZ1  | 1:A:304:GLU:C    | 2.21                     | 0.48              |
| 1:B:29:MSE:CE    | 1:B:50:LEU:HB3   | 2.40                     | 0.48              |
| 1:D:314:GLU:HB2  | 3:D:3601:NAD:O1N | 2.12                     | 0.48              |
| 1:D:333:SER:H    | 1:D:336:GLU:CG   | 2.26                     | 0.48              |
| 1:A:29:MSE:HE1   | 1:A:54:LEU:CD2   | 2.43                     | 0.48              |
| 1:B:235:ILE:O    | 1:B:239:MSE:HG2  | 2.14                     | 0.48              |
| 1:B:453:LYS:HG2  | 1:B:459:VAL:CG1  | 2.34                     | 0.48              |
| 1:D:45:ARG:CZ    | 1:D:58:ILE:HD13  | 2.43                     | 0.48              |
| 1:D:156:LYS:HD3  | 1:D:479:ILE:HG23 | 1.94                     | 0.48              |
| 1:A:225:ARG:HH11 | 1:A:225:ARG:HG2  | 1.79                     | 0.48              |
| 1:A:248:ARG:HH11 | 1:A:248:ARG:HG2  | 1.79                     | 0.48              |
| 1:A:377:PHE:CZ   | 1:A:389:ILE:HD12 | 2.49                     | 0.48              |
| 1:B:339:LYS:HA   | 1:B:367:HIS:CE1  | 2.49                     | 0.48              |
| 1:C:309:PHE:HE2  | 1:C:341:ILE:HG23 | 1.79                     | 0.48              |
| 1:D:371:GLU:H    | 1:D:371:GLU:HG3  | 1.39                     | 0.48              |
| 1:A:300:LYS:HB3  | 1:A:300:LYS:NZ   | 2.29                     | 0.48              |
| 1:B:370:PRO:O    | 1:B:371:GLU:C    | 2.57                     | 0.48              |
| 1:D:381:VAL:CG1  | 1:D:407:MSE:CE   | 2.91                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:389:ILE:HG22 | 1:B:416:ILE:HA   | 1.95                     | 0.48              |
| 1:D:140:ARG:CZ   | 1:D:230:GLN:HG2  | 2.44                     | 0.48              |
| 1:D:506:GLU:O    | 1:D:509:GLN:HG2  | 2.12                     | 0.48              |
| 1:A:294:ALA:O    | 1:A:297:VAL:HG22 | 2.13                     | 0.48              |
| 1:A:394:GLY:HA2  | 1:A:420:SER:HB3  | 1.96                     | 0.48              |
| 1:A:502:LEU:CD1  | 1:A:507:LEU:HD13 | 2.44                     | 0.48              |
| 1:B:412:GLU:O    | 1:B:440:ARG:NH1  | 2.46                     | 0.48              |
| 1:B:501:GLN:NE2  | 1:B:525:ASN:HB3  | 2.28                     | 0.48              |
| 1:C:468:VAL:HA   | 1:C:471:PHE:CE2  | 2.49                     | 0.48              |
| 1:A:542:ARG:HH12 | 1:A:544:PRO:HD2  | 1.78                     | 0.48              |
| 1:A:559:ARG:HB3  | 1:A:561:GLU:HG2  | 1.95                     | 0.48              |
| 1:B:231:TYR:HE2  | 1:B:261:ASN:ND2  | 2.12                     | 0.48              |
| 1:B:255:GLU:OE2  | 1:B:278:ASP:CB   | 2.62                     | 0.48              |
| 1:B:520:GLN:O    | 1:B:524:ILE:HD12 | 2.13                     | 0.48              |
| 1:C:235:ILE:HG13 | 1:C:265:PHE:CZ   | 2.49                     | 0.48              |
| 1:A:26:LYS:N     | 1:A:27:PRO:CD    | 2.77                     | 0.48              |
| 1:A:397:ARG:HA   | 1:A:427:GLU:O    | 2.14                     | 0.48              |
| 1:C:166:ILE:HD12 | 1:C:179:ILE:HG13 | 1.95                     | 0.48              |
| 1:C:396:GLY:O    | 1:C:427:GLU:HA   | 2.14                     | 0.48              |
| 1:A:137:ILE:HG13 | 1:A:137:ILE:O    | 2.13                     | 0.47              |
| 1:A:194:ARG:HG3  | 3:A:602:NAD:N1A  | 2.29                     | 0.47              |
| 1:B:359:ASP:C    | 1:B:359:ASP:OD1  | 2.57                     | 0.47              |
| 1:B:537:ASN:N    | 1:B:537:ASN:ND2  | 2.59                     | 0.47              |
| 1:B:556:ARG:NH1  | 1:B:556:ARG:CG   | 2.74                     | 0.47              |
| 1:B:169:LEU:HD13 | 1:B:422:PRO:HD3  | 1.95                     | 0.47              |
| 3:C:2602:NAD:O3B | 5:C:4060:HOH:O   | 2.10                     | 0.47              |
| 1:D:24:LYS:HA    | 1:D:28:LEU:CD1   | 2.44                     | 0.47              |
| 1:D:177:MSE:CE   | 1:D:200:PRO:HB2  | 2.44                     | 0.47              |
| 1:D:415:VAL:CG2  | 1:D:442:LEU:HD12 | 2.44                     | 0.47              |
| 1:A:362:GLN:O    | 1:A:363:GLU:C    | 2.57                     | 0.47              |
| 1:A:150:TRP:CD1  | 1:A:152:GLU:HB2  | 2.49                     | 0.47              |
| 1:A:159:VAL:HG13 | 1:A:253:GLN:NE2  | 2.29                     | 0.47              |
| 1:A:468:VAL:HA   | 1:A:471:PHE:HE2  | 1.72                     | 0.47              |
| 1:B:92:ASN:HB2   | 5:B:4003:HOH:O   | 2.14                     | 0.47              |
| 1:B:163:GLY:HA2  | 1:B:166:ILE:HD11 | 1.96                     | 0.47              |
| 1:C:294:ALA:O    | 1:C:297:VAL:HG13 | 2.13                     | 0.47              |
| 1:D:239:MSE:HE3  | 1:D:252:ILE:HD13 | 1.96                     | 0.47              |
| 1:D:377:PHE:CE2  | 1:D:399:PHE:CE2  | 3.02                     | 0.47              |
| 1:A:25:GLY:HA3   | 1:C:22:LYS:CE    | 2.45                     | 0.47              |
| 1:A:150:TRP:HE1  | 1:A:152:GLU:HB2  | 1.78                     | 0.47              |
| 1:A:417:PHE:CD1  | 1:A:444:ALA:HB3  | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:165:ARG:NH2  | 4:B:1603:TTN:O1  | 2.48                     | 0.47              |
| 1:B:443:PHE:CZ   | 1:B:445:SER:HB3  | 2.50                     | 0.47              |
| 1:C:171:ASP:CG   | 1:C:225:ARG:HH21 | 2.23                     | 0.47              |
| 1:A:137:ILE:HA   | 1:A:234:LEU:CD2  | 2.45                     | 0.47              |
| 1:A:208:ASP:O    | 1:A:210:ILE:HD13 | 2.14                     | 0.47              |
| 1:A:363:GLU:HB3  | 1:A:364:PRO:CD   | 2.44                     | 0.47              |
| 1:A:484:ARG:HD2  | 1:A:541:PHE:CD1  | 2.48                     | 0.47              |
| 1:A:559:ARG:HG3  | 1:A:561:GLU:OE1  | 2.15                     | 0.47              |
| 1:B:140:ARG:NH2  | 1:B:230:GLN:HG3  | 2.30                     | 0.47              |
| 1:B:194:ARG:HB2  | 1:B:197:ARG:CG   | 2.44                     | 0.47              |
| 1:C:264:ARG:HG2  | 1:C:264:ARG:NH1  | 2.29                     | 0.47              |
| 1:D:23:GLU:O     | 1:D:28:LEU:HD11  | 2.15                     | 0.47              |
| 1:D:152:GLU:HG2  | 1:D:196:ASP:O    | 2.14                     | 0.47              |
| 1:D:389:ILE:HG23 | 1:D:399:PHE:CE1  | 2.50                     | 0.47              |
| 1:D:405:ARG:HG3  | 1:D:405:ARG:NH1  | 2.30                     | 0.47              |
| 1:D:527:ALA:O    | 1:D:531:THR:HG23 | 2.15                     | 0.47              |
| 1:A:85:ILE:CG1   | 1:A:86:MSE:N     | 2.77                     | 0.47              |
| 1:A:184:LEU:HD22 | 1:A:198:CYS:HB3  | 1.95                     | 0.47              |
| 1:A:225:ARG:CG   | 1:A:225:ARG:NH1  | 2.73                     | 0.47              |
| 1:C:210:ILE:O    | 1:C:214:LYS:HG3  | 2.15                     | 0.47              |
| 1:D:542:ARG:NH1  | 1:D:544:PRO:HD2  | 2.30                     | 0.47              |
| 1:A:221:LEU:HD13 | 1:B:56:PRO:HB2   | 1.97                     | 0.47              |
| 1:B:75:MSE:HG2   | 1:B:80:GLU:CG    | 2.45                     | 0.47              |
| 1:B:208:ASP:OD1  | 1:B:224:LYS:HD3  | 2.15                     | 0.47              |
| 1:B:434:TYR:HD1  | 1:B:452:VAL:HG21 | 1.78                     | 0.47              |
| 1:D:82:TYR:C     | 1:D:82:TYR:CD2   | 2.93                     | 0.47              |
| 1:A:174:VAL:HG21 | 1:A:220:GLY:CA   | 2.45                     | 0.46              |
| 1:A:381:VAL:CG1  | 1:A:407:MSE:HE3  | 2.41                     | 0.46              |
| 1:A:484:ARG:HD2  | 1:A:541:PHE:CE1  | 2.51                     | 0.46              |
| 1:B:57:LYS:HG3   | 1:B:58:ILE:N     | 2.30                     | 0.46              |
| 1:B:166:ILE:O    | 1:B:169:LEU:HB2  | 2.15                     | 0.46              |
| 1:C:61:GLN:HG3   | 1:C:562:TYR:CE1  | 2.50                     | 0.46              |
| 1:C:70:ARG:CG    | 1:C:70:ARG:NH1   | 2.76                     | 0.46              |
| 1:C:137:ILE:HG13 | 1:C:137:ILE:O    | 2.15                     | 0.46              |
| 1:C:382:ASN:O    | 1:C:385:LYS:NZ   | 2.48                     | 0.46              |
| 1:D:165:ARG:NH2  | 1:D:256:ASP:OD1  | 2.48                     | 0.46              |
| 1:A:561:GLU:CD   | 1:A:561:GLU:H    | 2.24                     | 0.46              |
| 1:C:277:ASN:C    | 1:C:277:ASN:HD22 | 2.24                     | 0.46              |
| 1:C:422:PRO:HD2  | 1:C:425:GLN:HE21 | 1.81                     | 0.46              |
| 1:D:298:ILE:HG21 | 1:D:300:LYS:HB2  | 1.94                     | 0.46              |
| 1:D:406:ALA:O    | 1:D:410:ILE:HG13 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:520:GLN:HE21 | 1:D:521:GLU:N    | 2.12                     | 0.46              |
| 1:A:487:SER:CB   | 1:A:539:MSE:HE1  | 2.41                     | 0.46              |
| 1:C:302:ILE:CG2  | 1:C:303:SER:N    | 2.78                     | 0.46              |
| 1:C:363:GLU:N    | 1:C:364:PRO:CD   | 2.77                     | 0.46              |
| 1:A:286:VAL:HG21 | 1:A:467:ASN:CA   | 2.39                     | 0.46              |
| 1:C:359:ASP:OD1  | 1:C:362:GLN:CD   | 2.59                     | 0.46              |
| 1:D:79:LEU:O     | 1:D:83:ILE:HG13  | 2.14                     | 0.46              |
| 1:D:385:LYS:HG3  | 1:D:410:ILE:HD13 | 1.98                     | 0.46              |
| 1:D:407:MSE:HG3  | 1:D:414:PRO:CB   | 2.45                     | 0.46              |
| 1:A:29:MSE:HE2   | 1:A:29:MSE:HB3   | 1.89                     | 0.46              |
| 1:A:484:ARG:HG2  | 1:D:543:TYR:CZ   | 2.51                     | 0.46              |
| 1:B:194:ARG:NH2  | 1:B:196:ASP:CG   | 2.74                     | 0.46              |
| 1:B:331:GLY:O    | 1:B:332:LEU:C    | 2.57                     | 0.46              |
| 1:B:549:LYS:O    | 1:B:553:VAL:HG23 | 2.16                     | 0.46              |
| 1:C:129:ARG:NH2  | 1:D:91:ARG:HB2   | 2.31                     | 0.46              |
| 1:D:112:TYR:OH   | 1:D:183:LYS:HE2  | 2.15                     | 0.46              |
| 1:D:289:ALA:CB   | 1:D:498:LEU:HD23 | 2.45                     | 0.46              |
| 1:A:46:GLN:CG    | 1:A:51:GLN:HG3   | 2.46                     | 0.46              |
| 1:A:424:ALA:HB3  | 1:A:425:GLN:NE2  | 2.30                     | 0.46              |
| 1:B:29:MSE:HE2   | 1:B:50:LEU:CB    | 2.40                     | 0.46              |
| 1:B:387:SER:HA   | 1:B:411:ASN:OD1  | 2.16                     | 0.46              |
| 1:C:61:GLN:HA    | 1:C:64:GLN:NE2   | 2.29                     | 0.46              |
| 1:D:100:LEU:HD23 | 1:D:189:ALA:HB2  | 1.98                     | 0.46              |
| 1:D:401:PRO:HA   | 1:D:436:LEU:HD13 | 1.98                     | 0.46              |
| 1:A:152:GLU:HG3  | 1:A:196:ASP:O    | 2.16                     | 0.46              |
| 1:A:363:GLU:N    | 1:A:364:PRO:HD2  | 2.31                     | 0.46              |
| 1:D:476:LEU:HD23 | 1:D:527:ALA:CB   | 2.46                     | 0.46              |
| 1:B:109:PRO:HA   | 1:B:113:THR:O    | 2.15                     | 0.46              |
| 1:B:335:GLN:O    | 1:B:339:LYS:CG   | 2.59                     | 0.46              |
| 1:D:78:PRO:HB3   | 1:D:110:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:389:ILE:HD13 | 1:A:389:ILE:HA   | 1.76                     | 0.46              |
| 1:D:398:LEU:N    | 1:D:398:LEU:HD12 | 2.29                     | 0.46              |
| 1:D:484:ARG:HG3  | 1:D:541:PHE:CE1  | 2.50                     | 0.46              |
| 1:D:533:TYR:CZ   | 1:D:537:ASN:ND2  | 2.84                     | 0.46              |
| 1:A:96:PHE:CZ    | 1:A:100:LEU:HD21 | 2.50                     | 0.46              |
| 1:B:298:ILE:HG22 | 1:B:300:LYS:H    | 1.80                     | 0.46              |
| 1:B:520:GLN:CD   | 1:B:520:GLN:H    | 2.23                     | 0.46              |
| 1:C:394:GLY:HA2  | 1:C:420:SER:HB3  | 1.98                     | 0.46              |
| 1:D:144:ARG:NH1  | 1:D:244:ASP:HB3  | 2.31                     | 0.46              |
| 1:D:204:ASP:OD2  | 1:D:221:LEU:N    | 2.44                     | 0.46              |
| 1:A:136:SER:HB2  | 1:A:221:LEU:CD2  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:ILE:HD13 | 1:A:210:ILE:N    | 2.30                     | 0.45              |
| 1:A:343:MSE:HB2  | 1:A:350:LEU:HG   | 1.98                     | 0.45              |
| 1:C:155:VAL:HB   | 1:C:246:TYR:CD1  | 2.51                     | 0.45              |
| 1:D:253:GLN:O    | 1:D:253:GLN:HG2  | 2.16                     | 0.45              |
| 1:A:21:ILE:N     | 1:A:21:ILE:CD1   | 2.68                     | 0.45              |
| 1:A:266:LEU:O    | 1:A:270:ARG:HB3  | 2.16                     | 0.45              |
| 1:A:397:ARG:N    | 1:A:397:ARG:CD   | 2.80                     | 0.45              |
| 1:A:403:VAL:O    | 1:A:406:ALA:HB3  | 2.16                     | 0.45              |
| 1:B:22:LYS:HA    | 1:D:24:LYS:CE    | 2.46                     | 0.45              |
| 1:B:85:ILE:CD1   | 1:B:110:ILE:HG21 | 2.46                     | 0.45              |
| 1:D:21:ILE:HG21  | 1:D:28:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:105:GLU:OE2  | 1:A:517:ALA:HB2  | 2.15                     | 0.45              |
| 1:A:492:LEU:HD22 | 1:A:496:LYS:HD2  | 1.97                     | 0.45              |
| 1:B:310:LEU:HD21 | 1:B:398:LEU:CB   | 2.46                     | 0.45              |
| 1:C:69:HIS:HE1   | 1:C:102:ASP:OD2  | 1.98                     | 0.45              |
| 1:B:24:LYS:NZ    | 1:D:22:LYS:CD    | 2.79                     | 0.45              |
| 1:B:371:GLU:CD   | 1:B:371:GLU:N    | 2.63                     | 0.45              |
| 1:D:175:TYR:CD1  | 1:D:212:LEU:HD21 | 2.52                     | 0.45              |
| 1:D:412:GLU:HG3  | 1:D:413:ARG:HD2  | 1.99                     | 0.45              |
| 1:D:496:LYS:HA   | 1:D:499:THR:HG22 | 1.99                     | 0.45              |
| 1:A:26:LYS:HA    | 1:A:29:MSE:HG3   | 1.98                     | 0.45              |
| 1:A:327:MSE:HG2  | 1:A:332:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:229:GLN:HG3  | 1:C:233:ASP:OD2  | 2.16                     | 0.45              |
| 1:C:289:ALA:HB2  | 1:C:498:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:297:VAL:HG22 | 1:C:298:ILE:HG12 | 1.97                     | 0.45              |
| 1:D:36:LYS:O     | 1:D:39:ALA:HB3   | 2.16                     | 0.45              |
| 1:A:327:MSE:HE3  | 1:A:337:ALA:CB   | 2.32                     | 0.45              |
| 1:A:335:GLN:CD   | 1:A:339:LYS:HZ3  | 2.24                     | 0.45              |
| 1:A:509:GLN:HG2  | 1:A:511:ARG:HG3  | 1.99                     | 0.45              |
| 1:B:171:ASP:CG   | 1:B:225:ARG:HE   | 2.23                     | 0.45              |
| 1:C:26:LYS:N     | 1:C:27:PRO:CD    | 2.80                     | 0.45              |
| 1:C:194:ARG:HB2  | 1:C:197:ARG:CG   | 2.36                     | 0.45              |
| 1:D:174:VAL:C    | 1:D:176:GLY:N    | 2.71                     | 0.45              |
| 1:D:441:CYS:C    | 1:D:442:LEU:HD23 | 2.42                     | 0.45              |
| 1:D:545:GLU:OE2  | 1:D:549:LYS:NZ   | 2.37                     | 0.45              |
| 1:A:156:LYS:HE3  | 1:A:156:LYS:HB3  | 1.73                     | 0.45              |
| 1:A:529:LYS:HE3  | 1:A:529:LYS:HA   | 1.99                     | 0.45              |
| 1:B:24:LYS:HZ2   | 1:D:22:LYS:CD    | 2.30                     | 0.45              |
| 1:C:78:PRO:HB3   | 1:C:110:ILE:CD1  | 2.47                     | 0.45              |
| 1:C:104:ILE:HG12 | 1:C:108:MSE:CE   | 2.46                     | 0.45              |
| 1:C:184:LEU:O    | 1:C:187:TYR:HB2  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:392:VAL:O    | 3:C:2601:NAD:H51N | 2.15                     | 0.45              |
| 1:D:61:GLN:OE1   | 1:D:98:ARG:HD3    | 2.17                     | 0.45              |
| 1:A:227:ARG:NH1  | 1:A:227:ARG:CG    | 2.56                     | 0.45              |
| 1:A:359:ASP:OD2  | 1:A:361:TYR:HD1   | 2.00                     | 0.45              |
| 1:B:343:MSE:HE1  | 1:B:365:PHE:HB2   | 1.99                     | 0.45              |
| 1:B:343:MSE:HE2  | 1:B:343:MSE:HB2   | 1.81                     | 0.45              |
| 1:D:517:ALA:O    | 1:D:520:GLN:OE1   | 2.35                     | 0.45              |
| 1:C:285:ALA:HB3  | 1:C:470:ILE:HG13  | 1.99                     | 0.45              |
| 1:C:373:ILE:O    | 1:C:373:ILE:CG2   | 2.65                     | 0.45              |
| 1:D:43:GLN:CD    | 1:D:47:MSE:HE2    | 2.42                     | 0.45              |
| 1:A:46:GLN:HG3   | 1:A:51:GLN:HG3    | 1.99                     | 0.45              |
| 1:B:535:TYR:CZ   | 1:B:546:PRO:HD2   | 2.52                     | 0.45              |
| 1:A:165:ARG:O    | 1:A:256:ASP:HB3   | 2.17                     | 0.44              |
| 1:A:194:ARG:HD3  | 1:A:197:ARG:NE    | 2.32                     | 0.44              |
| 1:B:172:LEU:O    | 1:B:175:TYR:HB2   | 2.17                     | 0.44              |
| 1:C:552:TYR:CE1  | 1:C:556:ARG:NH1   | 2.85                     | 0.44              |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:HD12  | 1.99                     | 0.44              |
| 1:A:297:VAL:CG2  | 1:A:442:LEU:HD11  | 2.47                     | 0.44              |
| 1:B:36:LYS:HB3   | 1:B:39:ALA:HB3    | 1.98                     | 0.44              |
| 1:B:342:TRP:CH2  | 1:B:370:PRO:HD3   | 2.52                     | 0.44              |
| 1:B:444:ALA:HB2  | 1:B:512:LEU:HD12  | 2.00                     | 0.44              |
| 1:D:150:TRP:CE2  | 1:D:199:LEU:HD13  | 2.52                     | 0.44              |
| 1:A:33:ARG:HD2   | 1:A:93:GLU:OE1    | 2.18                     | 0.44              |
| 1:A:340:LYS:C    | 1:A:341:ILE:HD13  | 2.42                     | 0.44              |
| 1:B:255:GLU:OE2  | 1:B:278:ASP:HB3   | 2.17                     | 0.44              |
| 1:B:261:ASN:ND2  | 1:B:265:PHE:CE1   | 2.86                     | 0.44              |
| 1:C:217:PHE:CZ   | 1:D:66:LEU:HD13   | 2.52                     | 0.44              |
| 1:A:156:LYS:CE   | 1:A:479:ILE:HG23  | 2.47                     | 0.44              |
| 1:A:166:ILE:HG21 | 1:A:172:LEU:HD12  | 2.00                     | 0.44              |
| 1:B:229:GLN:O    | 1:B:229:GLN:HG3   | 2.16                     | 0.44              |
| 1:B:395:ALA:CB   | 1:B:398:LEU:HD21  | 2.43                     | 0.44              |
| 1:B:408:ALA:HB1  | 1:B:440:ARG:HH22  | 1.78                     | 0.44              |
| 1:C:282:GLY:O    | 1:C:286:VAL:HG22  | 2.18                     | 0.44              |
| 1:D:212:LEU:HD13 | 1:D:218:TYR:CE2   | 2.52                     | 0.44              |
| 1:A:235:ILE:O    | 1:A:239:MSE:HG2   | 2.18                     | 0.44              |
| 1:A:412:GLU:O    | 1:A:440:ARG:HD2   | 2.18                     | 0.44              |
| 1:B:332:LEU:HD21 | 1:B:340:LYS:CE    | 2.46                     | 0.44              |
| 1:A:24:LYS:HE2   | 1:C:22:LYS:HA     | 1.99                     | 0.44              |
| 1:A:346:LYS:HD2  | 3:A:601:NAD:O2B   | 2.18                     | 0.44              |
| 1:A:429:THR:OG1  | 1:A:432:GLU:HG2   | 2.17                     | 0.44              |
| 1:A:552:TYR:O    | 1:A:556:ARG:NH1   | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:346:LYS:NZ   | 1:B:346:LYS:CB   | 2.74                     | 0.44              |
| 1:B:359:ASP:OD1  | 1:B:362:GLN:HG3  | 2.17                     | 0.44              |
| 1:C:92:ASN:HB2   | 5:C:4011:HOH:O   | 2.16                     | 0.44              |
| 1:C:205:VAL:HG11 | 1:C:231:TYR:CD1  | 2.53                     | 0.44              |
| 1:C:352:LYS:N    | 1:C:366:THR:HG22 | 2.32                     | 0.44              |
| 1:C:505:GLU:O    | 1:C:508:ALA:HB3  | 2.18                     | 0.44              |
| 1:B:481:CYS:HB3  | 1:B:483:THR:CG2  | 2.47                     | 0.44              |
| 1:C:231:TYR:HE2  | 1:C:265:PHE:HZ   | 1.65                     | 0.44              |
| 1:D:43:GLN:O     | 1:D:47:MSE:HG3   | 2.16                     | 0.44              |
| 1:D:306:LYS:HZ2  | 1:D:306:LYS:CB   | 2.31                     | 0.44              |
| 1:D:329:GLU:C    | 1:D:330:ASN:HD22 | 2.26                     | 0.44              |
| 1:A:261:ASN:HD22 | 1:A:264:ARG:HE   | 1.65                     | 0.44              |
| 1:A:317:LEU:HD21 | 1:A:343:MSE:HE1  | 2.00                     | 0.44              |
| 1:A:429:THR:HA   | 1:A:449:PHE:CE1  | 2.53                     | 0.44              |
| 1:A:453:LYS:HG2  | 1:A:459:VAL:HG22 | 1.97                     | 0.44              |
| 1:B:261:ASN:HD21 | 1:B:264:ARG:NH2  | 2.14                     | 0.44              |
| 1:B:343:MSE:CE   | 1:B:350:LEU:HD12 | 2.41                     | 0.44              |
| 1:C:57:LYS:HD3   | 1:D:218:TYR:O    | 2.17                     | 0.44              |
| 1:A:391:GLY:HA3  | 1:A:427:GLU:HG2  | 2.00                     | 0.44              |
| 1:A:401:PRO:HB2  | 1:A:405:ARG:NH2  | 2.31                     | 0.44              |
| 1:B:108:MSE:HB3  | 1:B:109:PRO:CD   | 2.48                     | 0.44              |
| 1:B:174:VAL:HG12 | 1:B:174:VAL:O    | 2.18                     | 0.44              |
| 1:B:317:LEU:HD21 | 1:B:362:GLN:HG2  | 2.00                     | 0.44              |
| 1:C:75:MSE:HG2   | 1:C:80:GLU:CG    | 2.48                     | 0.44              |
| 1:C:164:GLU:HG3  | 1:C:225:ARG:CZ   | 2.47                     | 0.44              |
| 1:C:174:VAL:O    | 1:C:174:VAL:CG1  | 2.65                     | 0.44              |
| 1:C:420:SER:OG   | 1:C:427:GLU:OE2  | 2.36                     | 0.44              |
| 1:D:310:LEU:HD21 | 1:D:398:LEU:HB2  | 2.00                     | 0.44              |
| 1:B:397:ARG:HA   | 1:B:427:GLU:O    | 2.18                     | 0.43              |
| 1:C:559:ARG:HG2  | 1:C:561:GLU:HG2  | 2.00                     | 0.43              |
| 1:D:85:ILE:HD11  | 1:D:100:LEU:CD1  | 2.46                     | 0.43              |
| 1:D:215:ASP:OD1  | 1:D:216:PRO:HD2  | 2.18                     | 0.43              |
| 1:B:97:TYR:CE2   | 1:B:188:THR:HB   | 2.53                     | 0.43              |
| 1:B:306:LYS:HD3  | 1:B:384:LEU:O    | 2.18                     | 0.43              |
| 1:C:73:LYS:HE2   | 1:C:73:LYS:HA    | 2.00                     | 0.43              |
| 1:C:335:GLN:HE21 | 1:C:335:GLN:HB3  | 1.57                     | 0.43              |
| 1:D:68:PHE:CD2   | 1:D:68:PHE:C     | 2.96                     | 0.43              |
| 1:D:253:GLN:HB2  | 1:D:276:PHE:HE2  | 1.81                     | 0.43              |
| 1:D:358:ILE:HG12 | 1:D:366:THR:OG1  | 2.18                     | 0.43              |
| 1:B:298:ILE:HG22 | 1:B:300:LYS:HB2  | 2.00                     | 0.43              |
| 1:B:423:THR:HG23 | 1:B:447:SER:CB   | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:556:ARG:HG2  | 1:D:556:ARG:HH11 | 1.82                     | 0.43              |
| 1:A:350:LEU:N    | 1:A:350:LEU:HD23 | 2.33                     | 0.43              |
| 1:A:468:VAL:HA   | 1:A:471:PHE:CD2  | 2.51                     | 0.43              |
| 1:C:164:GLU:HG3  | 1:C:225:ARG:CD   | 2.48                     | 0.43              |
| 1:C:174:VAL:CG2  | 1:C:204:ASP:HB2  | 2.49                     | 0.43              |
| 1:C:218:TYR:O    | 1:D:57:LYS:HE3   | 2.17                     | 0.43              |
| 1:C:382:ASN:OD1  | 1:C:382:ASN:N    | 2.51                     | 0.43              |
| 1:D:136:SER:HA   | 1:D:204:ASP:O    | 2.18                     | 0.43              |
| 1:D:554:LYS:HG2  | 1:D:554:LYS:H    | 1.50                     | 0.43              |
| 1:A:308:LEU:HB3  | 1:A:389:ILE:HD13 | 1.99                     | 0.43              |
| 1:A:419:LEU:O    | 3:A:601:NAD:H2N  | 2.18                     | 0.43              |
| 1:B:21:ILE:HD12  | 1:B:21:ILE:HA    | 1.77                     | 0.43              |
| 1:B:128:ARG:CD   | 5:B:4056:HOH:O   | 2.64                     | 0.43              |
| 1:B:525:ASN:HA   | 1:B:528:ILE:HD12 | 2.00                     | 0.43              |
| 1:D:60:THR:OG1   | 1:D:63:ILE:HG12  | 2.17                     | 0.43              |
| 1:D:298:ILE:HD11 | 1:D:442:LEU:HD11 | 1.99                     | 0.43              |
| 1:D:556:ARG:HH11 | 1:D:556:ARG:CG   | 2.32                     | 0.43              |
| 1:A:164:GLU:OE1  | 1:A:225:ARG:HD3  | 2.17                     | 0.43              |
| 1:A:284:ALA:CB   | 1:A:322:LEU:HD12 | 2.48                     | 0.43              |
| 1:C:248:ARG:NH2  | 1:C:272:LYS:NZ   | 2.66                     | 0.43              |
| 1:D:110:ILE:O    | 1:D:115:THR:HB   | 2.18                     | 0.43              |
| 1:A:82:TYR:CD2   | 1:A:82:TYR:C     | 2.95                     | 0.43              |
| 1:B:174:VAL:HG21 | 1:B:220:GLY:HA3  | 2.00                     | 0.43              |
| 1:B:429:THR:HG23 | 1:B:432:GLU:OE2  | 2.19                     | 0.43              |
| 1:C:75:MSE:HG2   | 1:C:80:GLU:HG2   | 2.01                     | 0.43              |
| 1:C:134:PHE:HB3  | 1:D:56:PRO:HD3   | 2.01                     | 0.43              |
| 1:D:306:LYS:HG3  | 1:D:306:LYS:O    | 2.18                     | 0.43              |
| 1:A:384:LEU:O    | 1:A:385:LYS:HB2  | 2.18                     | 0.43              |
| 1:A:401:PRO:HA   | 1:A:436:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:420:SER:HA   | 3:A:601:NAD:H1D  | 2.01                     | 0.43              |
| 1:B:120:CYS:C    | 1:B:122:GLN:N    | 2.77                     | 0.43              |
| 1:B:165:ARG:NH2  | 1:B:256:ASP:OD1  | 2.52                     | 0.43              |
| 1:D:146:ILE:O    | 1:D:149:ASN:HB2  | 2.19                     | 0.43              |
| 1:D:301:PRO:O    | 1:D:302:ILE:C    | 2.60                     | 0.43              |
| 1:B:243:THR:HG21 | 1:B:273:TYR:CD2  | 2.54                     | 0.43              |
| 1:B:343:MSE:CE   | 1:B:365:PHE:HB2  | 2.49                     | 0.43              |
| 1:B:392:VAL:O    | 1:B:392:VAL:HG13 | 2.18                     | 0.43              |
| 1:B:477:ALA:O    | 1:B:481:CYS:HB2  | 2.18                     | 0.43              |
| 1:C:55:PRO:CG    | 1:D:219:MSE:HE3  | 2.49                     | 0.43              |
| 1:C:133:LEU:HD23 | 1:D:53:LEU:HD23  | 2.01                     | 0.43              |
| 1:C:528:ILE:HA   | 1:C:531:THR:HG23 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:23:GLU:OE2   | 1:D:23:GLU:CA    | 2.61                     | 0.43              |
| 1:D:26:LYS:N     | 1:D:27:PRO:CD    | 2.82                     | 0.43              |
| 1:D:61:GLN:HG3   | 1:D:562:TYR:CZ   | 2.54                     | 0.43              |
| 1:A:153:ASN:HD22 | 1:A:153:ASN:H    | 1.66                     | 0.43              |
| 1:A:302:ILE:HG23 | 1:A:332:LEU:HD22 | 2.01                     | 0.43              |
| 1:B:40:PHE:HE2   | 1:B:565:LEU:CD1  | 2.31                     | 0.43              |
| 1:B:77:SER:HA    | 1:B:78:PRO:HD3   | 1.86                     | 0.43              |
| 1:C:38:MSE:HB3   | 1:C:59:GLU:HG3   | 2.01                     | 0.43              |
| 1:C:329:GLU:HG3  | 1:C:330:ASN:ND2  | 2.34                     | 0.43              |
| 1:D:269:TYR:O    | 1:D:270:ARG:C    | 2.62                     | 0.43              |
| 1:D:502:LEU:HD13 | 1:D:507:LEU:HD11 | 2.01                     | 0.43              |
| 1:A:37:GLY:C     | 1:A:39:ALA:N     | 2.77                     | 0.42              |
| 1:A:160:VAL:HG22 | 1:A:161:THR:N    | 2.34                     | 0.42              |
| 1:B:260:HIS:CD2  | 1:B:264:ARG:NH1  | 2.87                     | 0.42              |
| 1:B:358:ILE:CG2  | 1:B:359:ASP:N    | 2.81                     | 0.42              |
| 1:D:177:MSE:HE1  | 1:D:200:PRO:HB2  | 2.00                     | 0.42              |
| 1:D:305:HIS:HD2  | 1:D:307:ILE:HD11 | 1.84                     | 0.42              |
| 1:A:429:THR:HG22 | 1:A:449:PHE:CZ   | 2.54                     | 0.42              |
| 1:B:213:LEU:CD1  | 1:B:224:LYS:HZ2  | 2.32                     | 0.42              |
| 1:B:302:ILE:CG2  | 1:B:303:SER:N    | 2.82                     | 0.42              |
| 1:C:38:MSE:HG2   | 1:C:57:LYS:O     | 2.18                     | 0.42              |
| 1:C:99:ILE:HD13  | 1:C:99:ILE:HA    | 1.69                     | 0.42              |
| 1:C:108:MSE:HE3  | 1:C:108:MSE:HB2  | 1.77                     | 0.42              |
| 1:C:161:THR:HA   | 1:C:257:PHE:CE1  | 2.54                     | 0.42              |
| 1:C:164:GLU:HG3  | 1:C:225:ARG:HD3  | 2.01                     | 0.42              |
| 1:C:238:PHE:CE1  | 1:C:242:ILE:HD13 | 2.55                     | 0.42              |
| 1:C:242:ILE:HG22 | 1:C:243:THR:N    | 2.33                     | 0.42              |
| 1:C:295:GLN:OE1  | 1:C:295:GLN:HA   | 2.18                     | 0.42              |
| 1:C:373:ILE:HA   | 1:C:374:PRO:HD2  | 1.90                     | 0.42              |
| 1:C:402:ASP:N    | 1:C:402:ASP:OD1  | 2.52                     | 0.42              |
| 1:B:22:LYS:HA    | 1:D:24:LYS:HE2   | 2.01                     | 0.42              |
| 1:C:171:ASP:OD2  | 1:C:225:ARG:NE   | 2.36                     | 0.42              |
| 1:C:331:GLY:O    | 1:C:332:LEU:C    | 2.62                     | 0.42              |
| 1:D:377:PHE:CE2  | 1:D:399:PHE:HE2  | 2.37                     | 0.42              |
| 1:A:22:LYS:HZ1   | 1:C:27:PRO:HG2   | 1.84                     | 0.42              |
| 1:A:467:ASN:ND2  | 3:A:601:NAD:O7N  | 2.45                     | 0.42              |
| 1:A:529:LYS:HA   | 1:A:532:GLU:HG3  | 2.01                     | 0.42              |
| 1:B:297:VAL:HG22 | 1:B:298:ILE:H    | 1.83                     | 0.42              |
| 1:D:483:THR:OG1  | 1:D:534:LEU:HD13 | 2.19                     | 0.42              |
| 1:B:354:ARG:CZ   | 1:B:356:ALA:HB3  | 2.49                     | 0.42              |
| 1:B:419:LEU:O    | 3:B:1601:NAD:H2N | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:239:MSE:HE2  | 1:C:269:TYR:CD1  | 2.55                     | 0.42              |
| 1:C:452:VAL:O    | 1:C:452:VAL:HG22 | 2.18                     | 0.42              |
| 1:C:528:ILE:HG12 | 1:C:550:ALA:HA   | 2.01                     | 0.42              |
| 1:C:572:TRP:HA   | 1:C:573:PRO:HD3  | 1.90                     | 0.42              |
| 1:D:59:GLU:HB3   | 1:D:63:ILE:HG13  | 2.01                     | 0.42              |
| 1:A:68:PHE:CD2   | 1:A:68:PHE:C     | 2.97                     | 0.42              |
| 1:A:454:LEU:O    | 1:A:455:THR:C    | 2.63                     | 0.42              |
| 1:B:300:LYS:HE2  | 1:B:304:GLU:O    | 2.19                     | 0.42              |
| 1:C:104:ILE:HG12 | 1:C:108:MSE:HE1  | 2.02                     | 0.42              |
| 1:C:104:ILE:CG2  | 1:C:105:GLU:N    | 2.83                     | 0.42              |
| 1:C:158:VAL:HA   | 1:C:199:LEU:O    | 2.20                     | 0.42              |
| 1:C:475:ALA:O    | 1:C:479:ILE:HD12 | 2.20                     | 0.42              |
| 1:A:85:ILE:HG12  | 1:A:86:MSE:N     | 2.34                     | 0.42              |
| 1:A:165:ARG:NH2  | 1:A:256:ASP:OD1  | 2.52                     | 0.42              |
| 1:A:344:PHE:CZ   | 1:A:348:GLY:HA2  | 2.55                     | 0.42              |
| 1:A:509:GLN:HE21 | 1:A:509:GLN:HB3  | 1.64                     | 0.42              |
| 1:C:283:THR:O    | 1:C:286:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:297:VAL:HG12 | 1:D:507:LEU:HD23 | 2.00                     | 0.42              |
| 1:D:443:PHE:O    | 5:D:4062:HOH:O   | 2.22                     | 0.42              |
| 1:A:286:VAL:HG11 | 1:A:466:ASN:O    | 2.18                     | 0.42              |
| 1:A:453:LYS:NZ   | 1:A:457:GLY:HA2  | 2.34                     | 0.42              |
| 1:B:389:ILE:HB   | 1:B:407:MSE:HE2  | 2.02                     | 0.42              |
| 1:C:534:LEU:HD23 | 1:C:534:LEU:HA   | 1.80                     | 0.42              |
| 1:D:64:GLN:HB3   | 1:D:95:LEU:CD2   | 2.50                     | 0.42              |
| 1:D:94:LYS:NZ    | 1:D:561:GLU:O    | 2.53                     | 0.42              |
| 1:A:174:VAL:HG21 | 1:A:220:GLY:HA3  | 2.02                     | 0.42              |
| 1:A:349:LEU:HD23 | 1:A:351:VAL:CG1  | 2.50                     | 0.42              |
| 1:C:108:MSE:SE   | 1:C:516:LEU:HD21 | 2.69                     | 0.42              |
| 1:C:335:GLN:O    | 1:C:339:LYS:HE3  | 2.19                     | 0.42              |
| 1:C:453:LYS:CB   | 1:C:459:VAL:HG22 | 2.49                     | 0.42              |
| 1:A:218:TYR:O    | 1:B:57:LYS:HD3   | 2.20                     | 0.42              |
| 1:A:255:GLU:OE2  | 1:A:278:ASP:HB3  | 2.20                     | 0.42              |
| 1:A:432:GLU:O    | 1:A:436:LEU:HB2  | 2.19                     | 0.42              |
| 1:B:492:LEU:HD23 | 1:B:496:LYS:HE3  | 2.00                     | 0.42              |
| 1:C:213:LEU:HD12 | 1:C:213:LEU:HA   | 1.83                     | 0.42              |
| 1:D:197:ARG:NH1  | 3:D:3602:NAD:O2B | 2.53                     | 0.42              |
| 1:D:229:GLN:HA   | 1:D:229:GLN:NE2  | 2.34                     | 0.42              |
| 1:D:515:PRO:HG2  | 1:D:518:ASN:OD1  | 2.20                     | 0.42              |
| 1:A:291:LEU:HD12 | 1:A:291:LEU:HA   | 1.81                     | 0.41              |
| 1:A:344:PHE:CE2  | 1:A:348:GLY:HA2  | 2.55                     | 0.41              |
| 1:A:399:PHE:CG   | 1:A:427:GLU:HB3  | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:133:LEU:HD11 | 1:C:146:ILE:HG22 | 2.01                     | 0.41              |
| 1:D:85:ILE:HG12  | 1:D:96:PHE:HE1   | 1.85                     | 0.41              |
| 1:D:144:ARG:O    | 1:D:147:VAL:CG2  | 2.68                     | 0.41              |
| 1:D:263:PHE:CZ   | 1:D:314:GLU:HA   | 2.55                     | 0.41              |
| 1:A:161:THR:HA   | 1:A:257:PHE:CE1  | 2.56                     | 0.41              |
| 1:A:174:VAL:CG2  | 1:A:220:GLY:HA3  | 2.50                     | 0.41              |
| 1:B:144:ARG:HA   | 1:B:144:ARG:HD2  | 1.94                     | 0.41              |
| 1:B:210:ILE:O    | 1:B:214:LYS:HG2  | 2.20                     | 0.41              |
| 1:C:174:VAL:O    | 1:C:174:VAL:HG12 | 2.20                     | 0.41              |
| 1:D:26:LYS:HD3   | 1:D:26:LYS:O     | 2.20                     | 0.41              |
| 1:D:132:GLY:CA   | 1:D:200:PRO:HG2  | 2.50                     | 0.41              |
| 1:D:239:MSE:HE1  | 1:D:252:ILE:HG21 | 2.02                     | 0.41              |
| 1:D:269:TYR:O    | 1:D:271:GLU:N    | 2.53                     | 0.41              |
| 1:A:108:MSE:HB3  | 1:A:109:PRO:CD   | 2.40                     | 0.41              |
| 1:A:174:VAL:C    | 1:A:176:GLY:H    | 2.28                     | 0.41              |
| 1:B:103:ASP:OD2  | 1:B:106:SER:HB3  | 2.20                     | 0.41              |
| 1:D:381:VAL:HG22 | 1:D:389:ILE:HD11 | 2.02                     | 0.41              |
| 1:D:407:MSE:HG3  | 1:D:414:PRO:HB2  | 2.02                     | 0.41              |
| 1:D:478:VAL:HG13 | 1:D:483:THR:HB   | 2.01                     | 0.41              |
| 1:A:401:PRO:HB3  | 1:A:436:LEU:CD2  | 2.47                     | 0.41              |
| 1:B:105:GLU:HG3  | 1:B:517:ALA:N    | 2.36                     | 0.41              |
| 1:B:225:ARG:HG2  | 1:B:225:ARG:HH11 | 1.85                     | 0.41              |
| 1:B:521:GLU:HG2  | 1:B:525:ASN:HD22 | 1.84                     | 0.41              |
| 1:D:300:LYS:HE3  | 1:D:305:HIS:HD1  | 1.82                     | 0.41              |
| 1:D:389:ILE:HD12 | 1:D:407:MSE:SE   | 2.70                     | 0.41              |
| 1:B:68:PHE:CD1   | 1:B:88:ILE:HD11  | 2.55                     | 0.41              |
| 1:B:128:ARG:HD3  | 5:B:4056:HOH:O   | 2.20                     | 0.41              |
| 1:C:287:ALA:HB3  | 1:C:319:ILE:HG12 | 2.02                     | 0.41              |
| 1:C:389:ILE:HG23 | 1:C:399:PHE:CZ   | 2.55                     | 0.41              |
| 1:D:496:LYS:O    | 1:D:500:SER:HB3  | 2.20                     | 0.41              |
| 1:A:296:LYS:HE2  | 1:A:296:LYS:HB2  | 1.75                     | 0.41              |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:HA   | 1.77                     | 0.41              |
| 1:A:429:THR:H    | 1:A:432:GLU:CG   | 2.32                     | 0.41              |
| 1:B:82:TYR:HA    | 1:B:85:ILE:HD12  | 2.03                     | 0.41              |
| 1:B:94:LYS:HB3   | 1:B:562:TYR:CE2  | 2.56                     | 0.41              |
| 1:B:174:VAL:HG22 | 1:B:204:ASP:HB2  | 2.02                     | 0.41              |
| 1:B:454:LEU:CD1  | 1:B:460:PHE:HE2  | 2.34                     | 0.41              |
| 1:C:183:LYS:NZ   | 4:C:2603:TTN:C3  | 2.83                     | 0.41              |
| 1:D:261:ASN:HD22 | 1:D:264:ARG:HE   | 1.68                     | 0.41              |
| 1:D:456:ASP:C    | 1:D:456:ASP:OD1  | 2.63                     | 0.41              |
| 1:A:90:GLU:OE2   | 1:A:131:LYS:HD2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:219:MSE:HE3  | 1:A:219:MSE:HB2  | 1.86                     | 0.41              |
| 1:A:284:ALA:HB1  | 1:A:322:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:401:PRO:O    | 1:A:405:ARG:NH1  | 2.53                     | 0.41              |
| 1:B:235:ILE:HG22 | 1:B:269:TYR:OH   | 2.21                     | 0.41              |
| 1:C:215:ASP:HA   | 1:C:216:PRO:HD3  | 1.83                     | 0.41              |
| 1:C:274:CYS:HB2  | 1:C:484:ARG:O    | 2.20                     | 0.41              |
| 1:D:29:MSE:HE3   | 1:D:54:LEU:HG    | 2.02                     | 0.41              |
| 1:A:66:LEU:HD22  | 1:A:70:ARG:NE    | 2.36                     | 0.41              |
| 1:B:25:GLY:C     | 1:B:27:PRO:HD2   | 2.45                     | 0.41              |
| 1:C:260:HIS:CD2  | 1:C:264:ARG:HE   | 2.39                     | 0.41              |
| 1:D:104:ILE:HG21 | 1:D:519:ILE:HG22 | 2.03                     | 0.41              |
| 1:D:240:LYS:O    | 1:D:241:ALA:C    | 2.64                     | 0.41              |
| 1:A:23:GLU:OE1   | 1:A:23:GLU:CA    | 2.57                     | 0.41              |
| 1:A:26:LYS:HD3   | 1:A:29:MSE:HG3   | 2.03                     | 0.41              |
| 1:A:169:LEU:HD22 | 1:A:422:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:308:LEU:HB3  | 1:A:389:ILE:CD1  | 2.51                     | 0.41              |
| 1:A:372:SER:O    | 1:A:383:ILE:HD13 | 2.21                     | 0.41              |
| 1:A:396:GLY:O    | 1:A:398:LEU:HD23 | 2.21                     | 0.41              |
| 1:A:434:TYR:OH   | 1:A:443:PHE:HB3  | 2.21                     | 0.41              |
| 1:B:112:TYR:CD2  | 1:B:113:THR:HG22 | 2.56                     | 0.41              |
| 1:C:33:ARG:HD2   | 1:C:93:GLU:OE2   | 2.21                     | 0.41              |
| 1:C:418:ALA:O    | 1:C:445:SER:HA   | 2.21                     | 0.41              |
| 1:D:37:GLY:C     | 1:D:39:ALA:N     | 2.75                     | 0.41              |
| 1:D:77:SER:O     | 1:D:81:LYS:HG3   | 2.21                     | 0.41              |
| 1:D:456:ASP:OD1  | 1:D:458:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:22:LYS:HE3   | 1:C:24:LYS:O     | 2.20                     | 0.41              |
| 1:A:133:LEU:HB2  | 1:A:199:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:104:ILE:HG23 | 1:B:105:GLU:N    | 2.35                     | 0.41              |
| 1:B:194:ARG:NH2  | 1:B:196:ASP:OD1  | 2.54                     | 0.41              |
| 1:B:315:ALA:CB   | 1:B:392:VAL:HG21 | 2.51                     | 0.41              |
| 1:C:262:ALA:HB1  | 1:C:280:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:419:LEU:O    | 3:C:2601:NAD:H2N | 2.21                     | 0.41              |
| 1:D:380:ALA:O    | 1:D:384:LEU:HB2  | 2.21                     | 0.41              |
| 1:D:407:MSE:CA   | 1:D:407:MSE:CE   | 2.98                     | 0.41              |
| 1:D:408:ALA:HB2  | 1:D:437:THR:HG22 | 2.02                     | 0.41              |
| 1:B:194:ARG:HE   | 1:B:194:ARG:HB3  | 1.34                     | 0.40              |
| 1:B:355:LYS:HE2  | 1:B:355:LYS:HB2  | 1.97                     | 0.40              |
| 1:B:543:TYR:CE1  | 1:C:484:ARG:HG2  | 2.55                     | 0.40              |
| 1:C:79:LEU:HD12  | 1:C:79:LEU:O     | 2.21                     | 0.40              |
| 1:C:295:GLN:O    | 1:C:299:SER:N    | 2.43                     | 0.40              |
| 1:C:550:ALA:O    | 1:C:554:LYS:CG   | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:174:VAL:O    | 1:D:174:VAL:HG12 | 2.21                     | 0.40              |
| 1:D:218:TYR:OH   | 5:D:4067:HOH:O   | 2.18                     | 0.40              |
| 1:D:233:ASP:CG   | 1:D:234:LEU:N    | 2.79                     | 0.40              |
| 1:D:302:ILE:HG22 | 1:D:303:SER:N    | 2.37                     | 0.40              |
| 1:A:380:ALA:O    | 1:A:384:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:526:ILE:O    | 1:A:530:VAL:HG23 | 2.22                     | 0.40              |
| 1:B:60:THR:O     | 1:B:64:GLN:HG3   | 2.22                     | 0.40              |
| 1:B:66:LEU:O     | 1:B:70:ARG:HB2   | 2.21                     | 0.40              |
| 1:B:89:GLN:NE2   | 1:B:185:CYS:SG   | 2.95                     | 0.40              |
| 1:B:380:ALA:O    | 1:B:384:LEU:HB2  | 2.21                     | 0.40              |
| 1:C:193:ILE:HD11 | 1:C:476:LEU:HB2  | 2.03                     | 0.40              |
| 1:C:201:VAL:HG12 | 1:C:202:CYS:N    | 2.35                     | 0.40              |
| 1:C:235:ILE:O    | 1:C:239:MSE:HG2  | 2.21                     | 0.40              |
| 1:A:24:LYS:O     | 1:C:22:LYS:CE    | 2.69                     | 0.40              |
| 1:A:97:TYR:CE2   | 1:A:188:THR:HB   | 2.56                     | 0.40              |
| 1:A:123:TYR:HB3  | 1:A:219:MSE:HE1  | 2.02                     | 0.40              |
| 1:A:297:VAL:CG2  | 1:A:298:ILE:N    | 2.84                     | 0.40              |
| 1:A:332:LEU:HD12 | 1:A:332:LEU:HA   | 1.83                     | 0.40              |
| 1:A:559:ARG:HA   | 1:A:559:ARG:HD3  | 1.92                     | 0.40              |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:CG   | 2.29                     | 0.40              |
| 1:B:298:ILE:CG2  | 1:B:300:LYS:HB2  | 2.51                     | 0.40              |
| 1:D:177:MSE:O    | 1:D:180:PRO:HD2  | 2.21                     | 0.40              |
| 1:D:221:LEU:HB3  | 1:D:223:GLN:HG2  | 2.03                     | 0.40              |
| 1:A:352:LYS:HG3  | 1:A:367:HIS:C    | 2.47                     | 0.40              |
| 1:B:66:LEU:HD23  | 1:B:66:LEU:HA    | 1.89                     | 0.40              |
| 1:B:69:HIS:HE1   | 1:B:102:ASP:OD2  | 2.05                     | 0.40              |
| 1:B:174:VAL:CG2  | 1:B:220:GLY:HA3  | 2.50                     | 0.40              |
| 1:B:358:ILE:HG22 | 1:B:359:ASP:N    | 2.36                     | 0.40              |
| 1:B:552:TYR:CE1  | 1:B:556:ARG:CZ   | 3.05                     | 0.40              |
| 1:C:399:PHE:CG   | 1:C:427:GLU:HB3  | 2.56                     | 0.40              |
| 1:A:44:GLU:O     | 1:A:45:ARG:C     | 2.64                     | 0.40              |
| 1:A:177:MSE:CE   | 1:A:177:MSE:O    | 2.70                     | 0.40              |
| 1:B:228:THR:C    | 1:B:230:GLN:N    | 2.78                     | 0.40              |
| 1:B:248:ARG:HB3  | 1:C:543:TYR:OH   | 2.22                     | 0.40              |
| 5:B:4078:HOH:O   | 1:C:543:TYR:HD1  | 2.05                     | 0.40              |
| 1:C:75:MSE:HE1   | 1:C:84:TYR:CG    | 2.56                     | 0.40              |
| 1:D:33:ARG:NH1   | 1:D:33:ARG:HG3   | 2.36                     | 0.40              |
| 1:D:398:LEU:N    | 1:D:398:LEU:CD1  | 2.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 551/584 (94%)   | 516 (94%)  | 33 (6%)  | 2 (0%)   | 30          | 51 |
| 1   | B     | 551/584 (94%)   | 513 (93%)  | 35 (6%)  | 3 (0%)   | 24          | 46 |
| 1   | C     | 551/584 (94%)   | 525 (95%)  | 23 (4%)  | 3 (0%)   | 24          | 46 |
| 1   | D     | 551/584 (94%)   | 515 (94%)  | 32 (6%)  | 4 (1%)   | 18          | 38 |
| All | All   | 2204/2336 (94%) | 2069 (94%) | 123 (6%) | 12 (0%)  | 24          | 46 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 332 | LEU  |
| 1   | C     | 332 | LEU  |
| 1   | C     | 392 | VAL  |
| 1   | A     | 332 | LEU  |
| 1   | D     | 270 | ARG  |
| 1   | D     | 332 | LEU  |
| 1   | A     | 433 | ALA  |
| 1   | B     | 121 | SER  |
| 1   | C     | 441 | CYS  |
| 1   | D     | 392 | VAL  |
| 1   | B     | 392 | VAL  |
| 1   | D     | 472 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 469/483 (97%)   | 365 (78%)  | 104 (22%) | 1           | 2 |
| 1   | B     | 469/483 (97%)   | 355 (76%)  | 114 (24%) | 1           | 1 |
| 1   | C     | 469/483 (97%)   | 373 (80%)  | 96 (20%)  | 1           | 2 |
| 1   | D     | 469/483 (97%)   | 370 (79%)  | 99 (21%)  | 1           | 2 |
| All | All   | 1876/1932 (97%) | 1463 (78%) | 413 (22%) | 1           | 2 |

All (413) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 21  | ILE  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 23  | GLU  |
| 1   | A     | 26  | LYS  |
| 1   | A     | 29  | MSE  |
| 1   | A     | 43  | GLN  |
| 1   | A     | 45  | ARG  |
| 1   | A     | 47  | MSE  |
| 1   | A     | 57  | LYS  |
| 1   | A     | 60  | THR  |
| 1   | A     | 66  | LEU  |
| 1   | A     | 74  | LYS  |
| 1   | A     | 75  | MSE  |
| 1   | A     | 76  | THR  |
| 1   | A     | 81  | LYS  |
| 1   | A     | 85  | ILE  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 100 | LEU  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 110 | ILE  |
| 1   | A     | 118 | LEU  |
| 1   | A     | 121 | SER  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 138 | SER  |
| 1   | A     | 140 | ARG  |
| 1   | A     | 152 | GLU  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 165 | ARG  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 183 | LYS  |
| 1   | A     | 185 | CYS  |
| 1   | A     | 193 | ILE  |
| 1   | A     | 197 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 203 | ILE  |
| 1   | A     | 210 | ILE  |
| 1   | A     | 221 | LEU  |
| 1   | A     | 225 | ARG  |
| 1   | A     | 226 | ASP  |
| 1   | A     | 227 | ARG  |
| 1   | A     | 233 | ASP  |
| 1   | A     | 236 | ASP  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 267 | ARG  |
| 1   | A     | 275 | THR  |
| 1   | A     | 281 | GLN  |
| 1   | A     | 286 | VAL  |
| 1   | A     | 291 | LEU  |
| 1   | A     | 292 | LEU  |
| 1   | A     | 295 | GLN  |
| 1   | A     | 296 | LYS  |
| 1   | A     | 297 | VAL  |
| 1   | A     | 298 | ILE  |
| 1   | A     | 300 | LYS  |
| 1   | A     | 302 | ILE  |
| 1   | A     | 303 | SER  |
| 1   | A     | 306 | LYS  |
| 1   | A     | 327 | MSE  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 336 | GLU  |
| 1   | A     | 339 | LYS  |
| 1   | A     | 340 | LYS  |
| 1   | A     | 346 | LYS  |
| 1   | A     | 350 | LEU  |
| 1   | A     | 355 | LYS  |
| 1   | A     | 359 | ASP  |
| 1   | A     | 360 | SER  |
| 1   | A     | 363 | GLU  |
| 1   | A     | 371 | GLU  |
| 1   | A     | 375 | ASP  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 389 | ILE  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 397 | ARG  |
| 1   | A     | 398 | LEU  |
| 1   | A     | 405 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 409 | SER  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 431 | GLU  |
| 1   | A     | 432 | GLU  |
| 1   | A     | 436 | LEU  |
| 1   | A     | 454 | LEU  |
| 1   | A     | 467 | ASN  |
| 1   | A     | 478 | VAL  |
| 1   | A     | 484 | ARG  |
| 1   | A     | 487 | SER  |
| 1   | A     | 488 | ASP  |
| 1   | A     | 489 | SER  |
| 1   | A     | 492 | LEU  |
| 1   | A     | 493 | GLU  |
| 1   | A     | 499 | THR  |
| 1   | A     | 502 | LEU  |
| 1   | A     | 504 | ASP  |
| 1   | A     | 505 | GLU  |
| 1   | A     | 507 | LEU  |
| 1   | A     | 509 | GLN  |
| 1   | A     | 511 | ARG  |
| 1   | A     | 516 | LEU  |
| 1   | A     | 519 | ILE  |
| 1   | A     | 520 | GLN  |
| 1   | A     | 529 | LYS  |
| 1   | A     | 556 | ARG  |
| 1   | A     | 559 | ARG  |
| 1   | A     | 561 | GLU  |
| 1   | A     | 571 | GLU  |
| 1   | B     | 21  | ILE  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 23  | GLU  |
| 1   | B     | 24  | LYS  |
| 1   | B     | 26  | LYS  |
| 1   | B     | 33  | ARG  |
| 1   | B     | 43  | GLN  |
| 1   | B     | 47  | MSE  |
| 1   | B     | 57  | LYS  |
| 1   | B     | 66  | LEU  |
| 1   | B     | 70  | ARG  |
| 1   | B     | 73  | LYS  |
| 1   | B     | 74  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 80  | GLU  |
| 1   | B     | 94  | LYS  |
| 1   | B     | 99  | ILE  |
| 1   | B     | 100 | LEU  |
| 1   | B     | 104 | ILE  |
| 1   | B     | 105 | GLU  |
| 1   | B     | 111 | VAL  |
| 1   | B     | 118 | LEU  |
| 1   | B     | 121 | SER  |
| 1   | B     | 128 | ARG  |
| 1   | B     | 129 | ARG  |
| 1   | B     | 131 | LYS  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 136 | SER  |
| 1   | B     | 138 | SER  |
| 1   | B     | 140 | ARG  |
| 1   | B     | 156 | LYS  |
| 1   | B     | 164 | GLU  |
| 1   | B     | 165 | ARG  |
| 1   | B     | 177 | MSE  |
| 1   | B     | 183 | LYS  |
| 1   | B     | 194 | ARG  |
| 1   | B     | 197 | ARG  |
| 1   | B     | 203 | ILE  |
| 1   | B     | 210 | ILE  |
| 1   | B     | 214 | LYS  |
| 1   | B     | 223 | GLN  |
| 1   | B     | 224 | LYS  |
| 1   | B     | 225 | ARG  |
| 1   | B     | 227 | ARG  |
| 1   | B     | 230 | GLN  |
| 1   | B     | 232 | ASP  |
| 1   | B     | 233 | ASP  |
| 1   | B     | 236 | ASP  |
| 1   | B     | 242 | ILE  |
| 1   | B     | 248 | ARG  |
| 1   | B     | 251 | LEU  |
| 1   | B     | 252 | ILE  |
| 1   | B     | 264 | ARG  |
| 1   | B     | 271 | GLU  |
| 1   | B     | 272 | LYS  |
| 1   | B     | 283 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 286 | VAL  |
| 1   | B     | 291 | LEU  |
| 1   | B     | 292 | LEU  |
| 1   | B     | 296 | LYS  |
| 1   | B     | 297 | VAL  |
| 1   | B     | 300 | LYS  |
| 1   | B     | 302 | ILE  |
| 1   | B     | 303 | SER  |
| 1   | B     | 304 | GLU  |
| 1   | B     | 328 | VAL  |
| 1   | B     | 334 | GLU  |
| 1   | B     | 335 | GLN  |
| 1   | B     | 340 | LYS  |
| 1   | B     | 343 | MSE  |
| 1   | B     | 346 | LYS  |
| 1   | B     | 350 | LEU  |
| 1   | B     | 352 | LYS  |
| 1   | B     | 354 | ARG  |
| 1   | B     | 355 | LYS  |
| 1   | B     | 357 | LYS  |
| 1   | B     | 372 | SER  |
| 1   | B     | 384 | LEU  |
| 1   | B     | 385 | LYS  |
| 1   | B     | 389 | ILE  |
| 1   | B     | 397 | ARG  |
| 1   | B     | 398 | LEU  |
| 1   | B     | 402 | ASP  |
| 1   | B     | 405 | ARG  |
| 1   | B     | 409 | SER  |
| 1   | B     | 413 | ARG  |
| 1   | B     | 423 | THR  |
| 1   | B     | 429 | THR  |
| 1   | B     | 436 | LEU  |
| 1   | B     | 453 | LYS  |
| 1   | B     | 455 | THR  |
| 1   | B     | 458 | ARG  |
| 1   | B     | 459 | VAL  |
| 1   | B     | 480 | LEU  |
| 1   | B     | 481 | CYS  |
| 1   | B     | 486 | ILE  |
| 1   | B     | 499 | THR  |
| 1   | B     | 502 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 509 | GLN  |
| 1   | B     | 511 | ARG  |
| 1   | B     | 519 | ILE  |
| 1   | B     | 520 | GLN  |
| 1   | B     | 524 | ILE  |
| 1   | B     | 531 | THR  |
| 1   | B     | 537 | ASN  |
| 1   | B     | 547 | GLU  |
| 1   | B     | 549 | LYS  |
| 1   | B     | 551 | LYS  |
| 1   | B     | 554 | LYS  |
| 1   | B     | 556 | ARG  |
| 1   | B     | 557 | THR  |
| 1   | B     | 559 | ARG  |
| 1   | B     | 564 | SER  |
| 1   | B     | 569 | VAL  |
| 1   | B     | 571 | GLU  |
| 1   | C     | 21  | ILE  |
| 1   | C     | 22  | LYS  |
| 1   | C     | 23  | GLU  |
| 1   | C     | 24  | LYS  |
| 1   | C     | 33  | ARG  |
| 1   | C     | 38  | MSE  |
| 1   | C     | 43  | GLN  |
| 1   | C     | 57  | LYS  |
| 1   | C     | 58  | ILE  |
| 1   | C     | 66  | LEU  |
| 1   | C     | 70  | ARG  |
| 1   | C     | 73  | LYS  |
| 1   | C     | 74  | LYS  |
| 1   | C     | 79  | LEU  |
| 1   | C     | 85  | ILE  |
| 1   | C     | 99  | ILE  |
| 1   | C     | 100 | LEU  |
| 1   | C     | 104 | ILE  |
| 1   | C     | 108 | MSE  |
| 1   | C     | 118 | LEU  |
| 1   | C     | 122 | GLN  |
| 1   | C     | 129 | ARG  |
| 1   | C     | 131 | LYS  |
| 1   | C     | 133 | LEU  |
| 1   | C     | 137 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 140 | ARG  |
| 1   | C     | 156 | LYS  |
| 1   | C     | 164 | GLU  |
| 1   | C     | 169 | LEU  |
| 1   | C     | 193 | ILE  |
| 1   | C     | 197 | ARG  |
| 1   | C     | 210 | ILE  |
| 1   | C     | 213 | LEU  |
| 1   | C     | 214 | LYS  |
| 1   | C     | 219 | MSE  |
| 1   | C     | 224 | LYS  |
| 1   | C     | 230 | GLN  |
| 1   | C     | 236 | ASP  |
| 1   | C     | 240 | LYS  |
| 1   | C     | 242 | ILE  |
| 1   | C     | 245 | ARG  |
| 1   | C     | 248 | ARG  |
| 1   | C     | 267 | ARG  |
| 1   | C     | 272 | LYS  |
| 1   | C     | 277 | ASN  |
| 1   | C     | 286 | VAL  |
| 1   | C     | 292 | LEU  |
| 1   | C     | 297 | VAL  |
| 1   | C     | 298 | ILE  |
| 1   | C     | 299 | SER  |
| 1   | C     | 325 | MSE  |
| 1   | C     | 332 | LEU  |
| 1   | C     | 333 | SER  |
| 1   | C     | 335 | GLN  |
| 1   | C     | 346 | LYS  |
| 1   | C     | 350 | LEU  |
| 1   | C     | 355 | LYS  |
| 1   | C     | 357 | LYS  |
| 1   | C     | 360 | SER  |
| 1   | C     | 363 | GLU  |
| 1   | C     | 368 | SER  |
| 1   | C     | 372 | SER  |
| 1   | C     | 373 | ILE  |
| 1   | C     | 384 | LEU  |
| 1   | C     | 389 | ILE  |
| 1   | C     | 390 | ILE  |
| 1   | C     | 397 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 398 | LEU  |
| 1   | C     | 404 | ILE  |
| 1   | C     | 409 | SER  |
| 1   | C     | 412 | GLU  |
| 1   | C     | 420 | SER  |
| 1   | C     | 425 | GLN  |
| 1   | C     | 436 | LEU  |
| 1   | C     | 438 | GLU  |
| 1   | C     | 452 | VAL  |
| 1   | C     | 453 | LYS  |
| 1   | C     | 458 | ARG  |
| 1   | C     | 492 | LEU  |
| 1   | C     | 499 | THR  |
| 1   | C     | 502 | LEU  |
| 1   | C     | 504 | ASP  |
| 1   | C     | 505 | GLU  |
| 1   | C     | 507 | LEU  |
| 1   | C     | 509 | GLN  |
| 1   | C     | 519 | ILE  |
| 1   | C     | 520 | GLN  |
| 1   | C     | 521 | GLU  |
| 1   | C     | 529 | LYS  |
| 1   | C     | 531 | THR  |
| 1   | C     | 538 | LYS  |
| 1   | C     | 551 | LYS  |
| 1   | C     | 554 | LYS  |
| 1   | C     | 556 | ARG  |
| 1   | C     | 559 | ARG  |
| 1   | C     | 571 | GLU  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 23  | GLU  |
| 1   | D     | 24  | LYS  |
| 1   | D     | 47  | MSE  |
| 1   | D     | 51  | GLN  |
| 1   | D     | 57  | LYS  |
| 1   | D     | 62  | ASP  |
| 1   | D     | 63  | ILE  |
| 1   | D     | 66  | LEU  |
| 1   | D     | 70  | ARG  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 75  | MSE  |
| 1   | D     | 76  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 85  | ILE  |
| 1   | D     | 86  | MSE  |
| 1   | D     | 91  | ARG  |
| 1   | D     | 101 | GLN  |
| 1   | D     | 104 | ILE  |
| 1   | D     | 128 | ARG  |
| 1   | D     | 133 | LEU  |
| 1   | D     | 137 | ILE  |
| 1   | D     | 138 | SER  |
| 1   | D     | 146 | ILE  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 160 | VAL  |
| 1   | D     | 161 | THR  |
| 1   | D     | 169 | LEU  |
| 1   | D     | 183 | LYS  |
| 1   | D     | 193 | ILE  |
| 1   | D     | 210 | ILE  |
| 1   | D     | 214 | LYS  |
| 1   | D     | 221 | LEU  |
| 1   | D     | 224 | LYS  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 230 | GLN  |
| 1   | D     | 233 | ASP  |
| 1   | D     | 236 | ASP  |
| 1   | D     | 240 | LYS  |
| 1   | D     | 249 | ASN  |
| 1   | D     | 251 | LEU  |
| 1   | D     | 266 | LEU  |
| 1   | D     | 271 | GLU  |
| 1   | D     | 272 | LYS  |
| 1   | D     | 286 | VAL  |
| 1   | D     | 291 | LEU  |
| 1   | D     | 292 | LEU  |
| 1   | D     | 296 | LYS  |
| 1   | D     | 297 | VAL  |
| 1   | D     | 299 | SER  |
| 1   | D     | 300 | LYS  |
| 1   | D     | 302 | ILE  |
| 1   | D     | 303 | SER  |
| 1   | D     | 304 | GLU  |
| 1   | D     | 305 | HIS  |
| 1   | D     | 306 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 324 | VAL  |
| 1   | D     | 325 | MSE  |
| 1   | D     | 327 | MSE  |
| 1   | D     | 332 | LEU  |
| 1   | D     | 335 | GLN  |
| 1   | D     | 340 | LYS  |
| 1   | D     | 343 | MSE  |
| 1   | D     | 350 | LEU  |
| 1   | D     | 355 | LYS  |
| 1   | D     | 357 | LYS  |
| 1   | D     | 358 | ILE  |
| 1   | D     | 360 | SER  |
| 1   | D     | 371 | GLU  |
| 1   | D     | 373 | ILE  |
| 1   | D     | 378 | GLU  |
| 1   | D     | 384 | LEU  |
| 1   | D     | 389 | ILE  |
| 1   | D     | 392 | VAL  |
| 1   | D     | 397 | ARG  |
| 1   | D     | 407 | MSE  |
| 1   | D     | 409 | SER  |
| 1   | D     | 447 | SER  |
| 1   | D     | 455 | THR  |
| 1   | D     | 458 | ARG  |
| 1   | D     | 470 | ILE  |
| 1   | D     | 489 | SER  |
| 1   | D     | 492 | LEU  |
| 1   | D     | 500 | SER  |
| 1   | D     | 502 | LEU  |
| 1   | D     | 504 | ASP  |
| 1   | D     | 506 | GLU  |
| 1   | D     | 507 | LEU  |
| 1   | D     | 520 | GLN  |
| 1   | D     | 521 | GLU  |
| 1   | D     | 529 | LYS  |
| 1   | D     | 531 | THR  |
| 1   | D     | 543 | TYR  |
| 1   | D     | 551 | LYS  |
| 1   | D     | 554 | LYS  |
| 1   | D     | 555 | GLU  |
| 1   | D     | 556 | ARG  |
| 1   | D     | 559 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 561 | GLU  |
| 1   | D     | 564 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 64  | GLN  |
| 1   | A     | 89  | GLN  |
| 1   | A     | 101 | GLN  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 253 | GLN  |
| 1   | A     | 261 | ASN  |
| 1   | A     | 281 | GLN  |
| 1   | A     | 305 | HIS  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 482 | ASN  |
| 1   | A     | 520 | GLN  |
| 1   | B     | 43  | GLN  |
| 1   | B     | 64  | GLN  |
| 1   | B     | 101 | GLN  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 260 | HIS  |
| 1   | B     | 261 | ASN  |
| 1   | B     | 335 | GLN  |
| 1   | B     | 482 | ASN  |
| 1   | B     | 485 | HIS  |
| 1   | B     | 501 | GLN  |
| 1   | B     | 509 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 525 | ASN  |
| 1   | B     | 537 | ASN  |
| 1   | C     | 43  | GLN  |
| 1   | C     | 51  | GLN  |
| 1   | C     | 64  | GLN  |
| 1   | C     | 69  | HIS  |
| 1   | C     | 125 | HIS  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 261 | ASN  |
| 1   | C     | 277 | ASN  |
| 1   | C     | 321 | ASN  |
| 1   | C     | 335 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 425 | GLN  |
| 1   | C     | 482 | ASN  |
| 1   | C     | 509 | GLN  |
| 1   | C     | 520 | GLN  |
| 1   | D     | 51  | GLN  |
| 1   | D     | 64  | GLN  |
| 1   | D     | 153 | ASN  |
| 1   | D     | 154 | HIS  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 230 | GLN  |
| 1   | D     | 261 | ASN  |
| 1   | D     | 277 | ASN  |
| 1   | D     | 330 | ASN  |
| 1   | D     | 466 | ASN  |
| 1   | D     | 482 | ASN  |
| 1   | D     | 520 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 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 |
| 3   | NAD  | B     | 1602 | -    | 46,48,48     | 2.24 | 13 (28%) | 64,73,73    | 1.78 | 10 (15%) |
| 4   | TTN  | A     | 603  | 2    | 5,7,7        | 1.40 | 1 (20%)  | 3,9,9       | 1.69 | 1 (33%)  |
| 3   | NAD  | C     | 2601 | -    | 46,48,48     | 2.00 | 11 (23%) | 64,73,73    | 1.88 | 11 (17%) |
| 3   | NAD  | A     | 601  | -    | 46,48,48     | 1.93 | 13 (28%) | 64,73,73    | 1.89 | 11 (17%) |
| 3   | NAD  | B     | 1601 | -    | 46,48,48     | 1.99 | 13 (28%) | 64,73,73    | 1.89 | 13 (20%) |
| 3   | NAD  | D     | 3602 | -    | 46,48,48     | 2.36 | 14 (30%) | 64,73,73    | 1.82 | 12 (18%) |
| 3   | NAD  | A     | 602  | -    | 46,48,48     | 2.27 | 12 (26%) | 64,73,73    | 1.84 | 10 (15%) |
| 4   | TTN  | D     | 3603 | 2    | 5,7,7        | 1.39 | 1 (20%)  | 3,9,9       | 1.65 | 1 (33%)  |
| 3   | NAD  | D     | 3601 | -    | 46,48,48     | 2.04 | 12 (26%) | 64,73,73    | 1.91 | 11 (17%) |
| 4   | TTN  | C     | 2603 | 2    | 5,7,7        | 1.43 | 2 (40%)  | 3,9,9       | 1.78 | 1 (33%)  |
| 4   | TTN  | B     | 1603 | 2    | 5,7,7        | 1.40 | 1 (20%)  | 3,9,9       | 1.64 | 1 (33%)  |
| 3   | NAD  | C     | 2602 | -    | 46,48,48     | 2.58 | 14 (30%) | 64,73,73    | 1.79 | 10 (15%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 3   | NAD  | B     | 1602 | -    | -       | 11/30/62/62 | 0/5/5/5 |
| 4   | TTN  | A     | 603  | 2    | -       | 2/8/8/8     | -       |
| 3   | NAD  | C     | 2601 | -    | -       | 2/30/62/62  | 0/5/5/5 |
| 3   | NAD  | A     | 601  | -    | -       | 2/30/62/62  | 0/5/5/5 |
| 3   | NAD  | B     | 1601 | -    | -       | 3/30/62/62  | 0/5/5/5 |
| 3   | NAD  | D     | 3602 | -    | -       | 11/30/62/62 | 0/5/5/5 |
| 3   | NAD  | A     | 602  | -    | -       | 11/30/62/62 | 0/5/5/5 |
| 4   | TTN  | D     | 3603 | 2    | -       | 4/8/8/8     | -       |
| 3   | NAD  | D     | 3601 | -    | -       | 2/30/62/62  | 0/5/5/5 |
| 4   | TTN  | C     | 2603 | 2    | -       | 2/8/8/8     | -       |
| 4   | TTN  | B     | 1603 | 2    | -       | 2/8/8/8     | -       |
| 3   | NAD  | C     | 2602 | -    | -       | 9/30/62/62  | 0/5/5/5 |

All (107) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | D     | 3602 | NAD  | C2N-N1N | 8.38 | 1.44        | 1.35     |
| 3   | C     | 2602 | NAD  | C2N-N1N | 8.31 | 1.44        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 1602 | NAD  | C2N-N1N | 8.18  | 1.44        | 1.35     |
| 3   | A     | 602  | NAD  | C2N-N1N | 8.13  | 1.43        | 1.35     |
| 3   | C     | 2602 | NAD  | O4D-C1D | 7.37  | 1.50        | 1.40     |
| 3   | D     | 3602 | NAD  | O4D-C1D | 7.10  | 1.50        | 1.40     |
| 3   | A     | 601  | NAD  | C2N-N1N | 7.01  | 1.42        | 1.35     |
| 3   | C     | 2601 | NAD  | C2N-N1N | 6.67  | 1.42        | 1.35     |
| 3   | D     | 3601 | NAD  | C2N-N1N | 6.66  | 1.42        | 1.35     |
| 3   | C     | 2602 | NAD  | PA-O3   | -6.66 | 1.52        | 1.59     |
| 3   | B     | 1602 | NAD  | O4D-C1D | 6.40  | 1.49        | 1.40     |
| 3   | A     | 602  | NAD  | O4D-C1D | 6.23  | 1.49        | 1.40     |
| 3   | B     | 1601 | NAD  | C2N-N1N | 6.20  | 1.41        | 1.35     |
| 3   | B     | 1601 | NAD  | C5A-N7A | -4.54 | 1.30        | 1.39     |
| 3   | D     | 3601 | NAD  | C6N-N1N | 4.48  | 1.45        | 1.35     |
| 3   | D     | 3602 | NAD  | C5A-N7A | -4.33 | 1.31        | 1.39     |
| 3   | C     | 2601 | NAD  | C3N-C7N | 4.31  | 1.57        | 1.50     |
| 3   | A     | 602  | NAD  | C6N-N1N | 4.17  | 1.44        | 1.35     |
| 3   | C     | 2601 | NAD  | C6N-N1N | 4.17  | 1.44        | 1.35     |
| 3   | D     | 3602 | NAD  | C6N-N1N | 4.13  | 1.44        | 1.35     |
| 3   | C     | 2601 | NAD  | C5A-N7A | -4.10 | 1.31        | 1.39     |
| 3   | D     | 3601 | NAD  | C5A-N7A | -4.08 | 1.31        | 1.39     |
| 3   | A     | 601  | NAD  | C5A-N7A | -4.02 | 1.31        | 1.39     |
| 3   | C     | 2602 | NAD  | C6N-N1N | 4.02  | 1.44        | 1.35     |
| 3   | C     | 2602 | NAD  | C5A-N7A | -3.98 | 1.31        | 1.39     |
| 3   | D     | 3601 | NAD  | O4D-C1D | 3.96  | 1.46        | 1.40     |
| 3   | B     | 1601 | NAD  | O4D-C1D | 3.94  | 1.46        | 1.40     |
| 3   | A     | 602  | NAD  | C5A-N7A | -3.93 | 1.31        | 1.39     |
| 3   | B     | 1602 | NAD  | C6N-N1N | 3.92  | 1.44        | 1.35     |
| 3   | B     | 1601 | NAD  | C6N-N1N | 3.90  | 1.44        | 1.35     |
| 3   | B     | 1602 | NAD  | C5A-N7A | -3.88 | 1.32        | 1.39     |
| 3   | C     | 2601 | NAD  | C5A-C4A | -3.63 | 1.32        | 1.39     |
| 3   | D     | 3601 | NAD  | C3N-C7N | 3.62  | 1.56        | 1.50     |
| 3   | A     | 601  | NAD  | C6N-N1N | 3.57  | 1.43        | 1.35     |
| 3   | B     | 1601 | NAD  | C3N-C7N | 3.40  | 1.55        | 1.50     |
| 3   | A     | 601  | NAD  | C5A-C4A | -3.37 | 1.33        | 1.39     |
| 3   | D     | 3602 | NAD  | PN-O3   | 3.36  | 1.63        | 1.59     |
| 3   | B     | 1602 | NAD  | C3N-C7N | 3.32  | 1.55        | 1.50     |
| 3   | C     | 2602 | NAD  | O4D-C4D | 3.25  | 1.52        | 1.45     |
| 3   | C     | 2602 | NAD  | PN-O3   | -3.25 | 1.56        | 1.59     |
| 3   | B     | 1602 | NAD  | PA-O3   | -3.20 | 1.56        | 1.59     |
| 3   | C     | 2602 | NAD  | C3N-C7N | 3.18  | 1.55        | 1.50     |
| 3   | A     | 602  | NAD  | C3N-C7N | 3.17  | 1.55        | 1.50     |
| 3   | A     | 602  | NAD  | C5A-C4A | -3.13 | 1.33        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | A     | 601  | NAD  | C3N-C7N | 3.06  | 1.55        | 1.50     |
| 3   | B     | 1602 | NAD  | C5A-C4A | -3.04 | 1.33        | 1.39     |
| 3   | B     | 1601 | NAD  | C4A-N9A | -2.91 | 1.31        | 1.37     |
| 3   | B     | 1601 | NAD  | C5A-C4A | -2.89 | 1.33        | 1.39     |
| 3   | D     | 3602 | NAD  | C8A-N7A | 2.89  | 1.37        | 1.31     |
| 3   | A     | 602  | NAD  | PN-O3   | 2.88  | 1.62        | 1.59     |
| 3   | C     | 2602 | NAD  | C5A-C4A | -2.84 | 1.34        | 1.39     |
| 3   | D     | 3602 | NAD  | C3N-C7N | 2.84  | 1.54        | 1.50     |
| 3   | D     | 3601 | NAD  | C2A-N1A | 2.84  | 1.39        | 1.33     |
| 3   | D     | 3601 | NAD  | C4N-C3N | 2.80  | 1.43        | 1.39     |
| 3   | A     | 601  | NAD  | O4D-C1D | 2.76  | 1.44        | 1.40     |
| 3   | B     | 1601 | NAD  | C2A-N1A | 2.75  | 1.38        | 1.33     |
| 3   | D     | 3601 | NAD  | C5A-C4A | -2.74 | 1.34        | 1.39     |
| 3   | C     | 2601 | NAD  | C5N-C4N | 2.72  | 1.43        | 1.38     |
| 3   | A     | 602  | NAD  | C8A-N7A | 2.66  | 1.36        | 1.31     |
| 3   | C     | 2602 | NAD  | C8A-N7A | 2.64  | 1.36        | 1.31     |
| 3   | A     | 601  | NAD  | C4A-N9A | -2.61 | 1.32        | 1.37     |
| 3   | C     | 2601 | NAD  | O4D-C1D | 2.54  | 1.44        | 1.40     |
| 3   | C     | 2601 | NAD  | C4A-N9A | -2.53 | 1.32        | 1.37     |
| 3   | D     | 3602 | NAD  | C5A-C4A | -2.52 | 1.34        | 1.39     |
| 3   | B     | 1601 | NAD  | C2B-C1B | -2.46 | 1.45        | 1.53     |
| 3   | C     | 2602 | NAD  | PN-O5D  | 2.42  | 1.68        | 1.59     |
| 3   | D     | 3602 | NAD  | O4D-C4D | 2.42  | 1.50        | 1.45     |
| 3   | D     | 3601 | NAD  | C8A-N7A | 2.41  | 1.36        | 1.31     |
| 3   | A     | 601  | NAD  | O4B-C1B | 2.38  | 1.47        | 1.42     |
| 3   | D     | 3601 | NAD  | C2A-N3A | 2.36  | 1.38        | 1.33     |
| 3   | D     | 3602 | NAD  | C4N-C3N | 2.36  | 1.43        | 1.39     |
| 3   | A     | 601  | NAD  | C5N-C4N | 2.36  | 1.42        | 1.38     |
| 3   | B     | 1602 | NAD  | C4N-C3N | 2.35  | 1.43        | 1.39     |
| 3   | B     | 1601 | NAD  | C5N-C4N | 2.34  | 1.42        | 1.38     |
| 3   | D     | 3601 | NAD  | O4B-C1B | 2.33  | 1.47        | 1.42     |
| 3   | D     | 3602 | NAD  | C2A-N3A | 2.33  | 1.38        | 1.33     |
| 3   | B     | 1601 | NAD  | C8A-N7A | 2.33  | 1.36        | 1.31     |
| 3   | C     | 2601 | NAD  | C4N-C3N | 2.32  | 1.42        | 1.39     |
| 3   | A     | 602  | NAD  | C4N-C3N | 2.32  | 1.42        | 1.39     |
| 3   | C     | 2602 | NAD  | C4N-C3N | 2.30  | 1.42        | 1.39     |
| 3   | A     | 601  | NAD  | C2A-N1A | 2.30  | 1.38        | 1.33     |
| 3   | A     | 601  | NAD  | C8A-N7A | 2.28  | 1.36        | 1.31     |
| 3   | A     | 601  | NAD  | C2A-N3A | 2.28  | 1.38        | 1.33     |
| 3   | B     | 1601 | NAD  | C4N-C3N | 2.27  | 1.42        | 1.39     |
| 3   | D     | 3602 | NAD  | C4A-N9A | -2.23 | 1.33        | 1.37     |
| 3   | B     | 1602 | NAD  | C2A-N1A | 2.22  | 1.37        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 1602 | NAD  | C8A-N7A | 2.21  | 1.35        | 1.31     |
| 3   | A     | 602  | NAD  | O4D-C4D | 2.21  | 1.49        | 1.45     |
| 4   | C     | 2603 | TTN  | O2-C1   | -2.20 | 1.23        | 1.30     |
| 4   | C     | 2603 | TTN  | O5-C3   | -2.18 | 1.23        | 1.30     |
| 4   | B     | 1603 | TTN  | O2-C1   | -2.17 | 1.23        | 1.30     |
| 3   | D     | 3602 | NAD  | C2A-N1A | 2.17  | 1.37        | 1.33     |
| 3   | C     | 2601 | NAD  | C2A-N3A | 2.16  | 1.37        | 1.33     |
| 3   | B     | 1602 | NAD  | C2A-N3A | 2.14  | 1.37        | 1.33     |
| 3   | B     | 1601 | NAD  | O4B-C1B | 2.12  | 1.46        | 1.42     |
| 3   | C     | 2602 | NAD  | C2A-N1A | 2.11  | 1.37        | 1.33     |
| 3   | D     | 3601 | NAD  | C4A-N9A | -2.10 | 1.33        | 1.37     |
| 4   | A     | 603  | TTN  | O2-C1   | -2.10 | 1.24        | 1.30     |
| 3   | B     | 1602 | NAD  | O4D-C4D | 2.09  | 1.49        | 1.45     |
| 3   | A     | 602  | NAD  | O4B-C1B | 2.09  | 1.46        | 1.42     |
| 3   | A     | 602  | NAD  | C2A-N3A | 2.06  | 1.37        | 1.33     |
| 3   | D     | 3602 | NAD  | C1B-N9A | 2.05  | 1.52        | 1.46     |
| 3   | C     | 2602 | NAD  | O4B-C1B | 2.05  | 1.46        | 1.42     |
| 3   | A     | 601  | NAD  | C4N-C3N | 2.04  | 1.42        | 1.39     |
| 3   | C     | 2601 | NAD  | C2A-N1A | 2.03  | 1.37        | 1.33     |
| 4   | D     | 3603 | TTN  | O2-C1   | -2.02 | 1.24        | 1.30     |
| 3   | B     | 1602 | NAD  | C5N-C4N | 2.02  | 1.42        | 1.38     |

All (92) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | A     | 602  | NAD  | C5A-C4A-N3A | -6.20 | 118.18      | 126.72   |
| 3   | C     | 2602 | NAD  | C5A-C4A-N3A | -6.08 | 118.35      | 126.72   |
| 3   | D     | 3602 | NAD  | C5A-C4A-N3A | -6.03 | 118.42      | 126.72   |
| 3   | B     | 1602 | NAD  | C5A-C4A-N3A | -5.91 | 118.58      | 126.72   |
| 3   | D     | 3601 | NAD  | C5A-C4A-N3A | -5.84 | 118.68      | 126.72   |
| 3   | A     | 601  | NAD  | C5A-C4A-N3A | -5.79 | 118.75      | 126.72   |
| 3   | C     | 2601 | NAD  | C5A-C4A-N3A | -5.66 | 118.93      | 126.72   |
| 3   | B     | 1601 | NAD  | C5A-C4A-N3A | -5.63 | 118.96      | 126.72   |
| 3   | C     | 2601 | NAD  | N3A-C2A-N1A | -5.46 | 120.32      | 128.58   |
| 3   | D     | 3601 | NAD  | C6A-C5A-N7A | -5.31 | 121.85      | 132.09   |
| 3   | A     | 602  | NAD  | N3A-C2A-N1A | -5.29 | 120.57      | 128.58   |
| 3   | A     | 601  | NAD  | N3A-C2A-N1A | -5.25 | 120.64      | 128.58   |
| 3   | B     | 1601 | NAD  | C6A-C5A-N7A | -5.24 | 121.98      | 132.09   |
| 3   | D     | 3601 | NAD  | C6A-C5A-C4A | 5.24  | 124.33      | 117.18   |
| 3   | B     | 1601 | NAD  | N3A-C2A-N1A | -5.17 | 120.75      | 128.58   |
| 3   | D     | 3601 | NAD  | N3A-C2A-N1A | -5.16 | 120.78      | 128.58   |
| 3   | B     | 1601 | NAD  | C6A-C5A-C4A | 5.13  | 124.18      | 117.18   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 3602 | NAD  | N3A-C2A-N1A | -5.09 | 120.88      | 128.58   |
| 3   | C     | 2601 | NAD  | C6A-C5A-N7A | -5.08 | 122.29      | 132.09   |
| 3   | A     | 601  | NAD  | C6A-C5A-N7A | -5.05 | 122.35      | 132.09   |
| 3   | D     | 3601 | NAD  | N3A-C4A-N9A | 5.00  | 135.67      | 127.17   |
| 3   | B     | 1602 | NAD  | N3A-C2A-N1A | -4.98 | 121.04      | 128.58   |
| 3   | A     | 602  | NAD  | N3A-C4A-N9A | 4.93  | 135.55      | 127.17   |
| 3   | C     | 2601 | NAD  | N3A-C4A-N9A | 4.90  | 135.50      | 127.17   |
| 3   | C     | 2601 | NAD  | C6A-C5A-C4A | 4.90  | 123.87      | 117.18   |
| 3   | C     | 2602 | NAD  | N3A-C2A-N1A | -4.85 | 121.24      | 128.58   |
| 3   | D     | 3602 | NAD  | C6A-C5A-C4A | 4.85  | 123.80      | 117.18   |
| 3   | A     | 601  | NAD  | C6A-C5A-C4A | 4.84  | 123.78      | 117.18   |
| 3   | B     | 1602 | NAD  | N3A-C4A-N9A | 4.83  | 135.38      | 127.17   |
| 3   | B     | 1601 | NAD  | N3A-C4A-N9A | 4.77  | 135.28      | 127.17   |
| 3   | D     | 3602 | NAD  | C6A-C5A-N7A | -4.77 | 122.90      | 132.09   |
| 3   | A     | 602  | NAD  | C6A-C5A-N7A | -4.76 | 122.91      | 132.09   |
| 3   | A     | 601  | NAD  | N3A-C4A-N9A | 4.75  | 135.25      | 127.17   |
| 3   | C     | 2602 | NAD  | N3A-C4A-N9A | 4.73  | 135.21      | 127.17   |
| 3   | B     | 1602 | NAD  | C6A-C5A-C4A | 4.72  | 123.62      | 117.18   |
| 3   | C     | 2602 | NAD  | C6A-C5A-C4A | 4.63  | 123.50      | 117.18   |
| 3   | A     | 602  | NAD  | C6A-C5A-C4A | 4.59  | 123.45      | 117.18   |
| 3   | C     | 2602 | NAD  | C6A-C5A-N7A | -4.59 | 123.23      | 132.09   |
| 3   | D     | 3602 | NAD  | N3A-C4A-N9A | 4.57  | 134.94      | 127.17   |
| 3   | B     | 1602 | NAD  | C6A-C5A-N7A | -4.55 | 123.33      | 132.09   |
| 3   | A     | 601  | NAD  | N9A-C8A-N7A | -3.96 | 108.31      | 113.94   |
| 3   | C     | 2601 | NAD  | N9A-C8A-N7A | -3.85 | 108.47      | 113.94   |
| 3   | B     | 1602 | NAD  | N9A-C8A-N7A | -3.81 | 108.53      | 113.94   |
| 3   | D     | 3601 | NAD  | N9A-C8A-N7A | -3.78 | 108.57      | 113.94   |
| 3   | B     | 1601 | NAD  | N9A-C8A-N7A | -3.77 | 108.59      | 113.94   |
| 3   | C     | 2602 | NAD  | N9A-C8A-N7A | -3.60 | 108.83      | 113.94   |
| 3   | A     | 602  | NAD  | N9A-C8A-N7A | -3.56 | 108.89      | 113.94   |
| 3   | A     | 602  | NAD  | C2A-N3A-C4A | 3.53  | 120.46      | 111.83   |
| 3   | D     | 3602 | NAD  | N9A-C8A-N7A | -3.52 | 108.94      | 113.94   |
| 3   | C     | 2602 | NAD  | C2A-N3A-C4A | 3.40  | 120.13      | 111.83   |
| 3   | C     | 2601 | NAD  | C4D-O4D-C1D | -3.39 | 106.82      | 109.92   |
| 3   | D     | 3601 | NAD  | C4D-O4D-C1D | -3.39 | 106.82      | 109.92   |
| 3   | B     | 1602 | NAD  | C2A-N3A-C4A | 3.33  | 119.96      | 111.83   |
| 3   | D     | 3602 | NAD  | C2A-N3A-C4A | 3.28  | 119.85      | 111.83   |
| 3   | A     | 601  | NAD  | C2A-N3A-C4A | 3.21  | 119.66      | 111.83   |
| 3   | C     | 2601 | NAD  | C2A-N3A-C4A | 3.17  | 119.56      | 111.83   |
| 3   | A     | 601  | NAD  | C4D-O4D-C1D | -3.16 | 107.03      | 109.92   |
| 3   | B     | 1601 | NAD  | O4B-C1B-N9A | 3.13  | 114.10      | 108.09   |
| 3   | B     | 1601 | NAD  | C4D-O4D-C1D | -3.12 | 107.07      | 109.92   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | B     | 1601 | NAD  | C2A-N3A-C4A | 3.08  | 119.36      | 111.83   |
| 3   | D     | 3601 | NAD  | C2A-N3A-C4A | 3.08  | 119.35      | 111.83   |
| 3   | D     | 3602 | NAD  | C6N-N1N-C2N | -3.06 | 119.28      | 121.88   |
| 3   | A     | 602  | NAD  | C6N-N1N-C2N | -3.05 | 119.28      | 121.88   |
| 3   | A     | 601  | NAD  | C4A-C5A-N7A | 2.86  | 113.85      | 110.58   |
| 3   | B     | 1601 | NAD  | C4A-C5A-N7A | 2.85  | 113.84      | 110.58   |
| 3   | C     | 2601 | NAD  | C4A-C5A-N7A | 2.84  | 113.83      | 110.58   |
| 3   | D     | 3601 | NAD  | C4A-C5A-N7A | 2.83  | 113.82      | 110.58   |
| 3   | C     | 2602 | NAD  | C6N-N1N-C2N | -2.78 | 119.52      | 121.88   |
| 3   | A     | 602  | NAD  | C4A-C5A-N7A | 2.67  | 113.64      | 110.58   |
| 3   | A     | 601  | NAD  | O4B-C1B-N9A | 2.63  | 113.14      | 108.09   |
| 3   | B     | 1602 | NAD  | C6N-N1N-C2N | -2.62 | 119.65      | 121.88   |
| 3   | D     | 3601 | NAD  | O4B-C1B-N9A | 2.57  | 113.03      | 108.09   |
| 4   | C     | 2603 | TTN  | O2-C1-O1    | -2.40 | 118.63      | 124.08   |
| 3   | D     | 3602 | NAD  | C4A-C5A-N7A | 2.38  | 113.30      | 110.58   |
| 3   | C     | 2602 | NAD  | C4A-C5A-N7A | 2.34  | 113.26      | 110.58   |
| 4   | A     | 603  | TTN  | O2-C1-O1    | -2.32 | 118.82      | 124.08   |
| 3   | D     | 3602 | NAD  | C3B-C2B-C1B | 2.27  | 105.75      | 101.46   |
| 3   | D     | 3602 | NAD  | C2D-C3D-C4D | 2.26  | 106.97      | 102.61   |
| 4   | D     | 3603 | TTN  | O2-C1-O1    | -2.24 | 118.99      | 124.08   |
| 3   | B     | 1601 | NAD  | C3N-C7N-N7N | -2.24 | 114.98      | 117.74   |
| 3   | C     | 2601 | NAD  | O4B-C1B-N9A | 2.23  | 112.37      | 108.09   |
| 3   | A     | 602  | NAD  | C2D-C3D-C4D | 2.22  | 106.91      | 102.61   |
| 4   | B     | 1603 | TTN  | O2-C1-O1    | -2.21 | 119.07      | 124.08   |
| 3   | B     | 1601 | NAD  | C6N-N1N-C2N | -2.20 | 120.00      | 121.88   |
| 3   | C     | 2602 | NAD  | C2D-C3D-C4D | 2.17  | 106.81      | 102.61   |
| 3   | B     | 1602 | NAD  | C2D-C3D-C4D | 2.16  | 106.79      | 102.61   |
| 3   | B     | 1602 | NAD  | C4A-C5A-N7A | 2.16  | 113.05      | 110.58   |
| 3   | A     | 601  | NAD  | C6N-N1N-C2N | -2.13 | 120.07      | 121.88   |
| 3   | D     | 3602 | NAD  | O4B-C1B-N9A | 2.04  | 112.01      | 108.09   |
| 3   | C     | 2601 | NAD  | C4A-N9A-C8A | 2.03  | 107.86      | 105.74   |
| 3   | D     | 3601 | NAD  | C6N-N1N-C2N | -2.01 | 120.17      | 121.88   |
| 3   | B     | 1601 | NAD  | C4A-N9A-C8A | 2.01  | 107.85      | 105.74   |

There are no chirality outliers.

All (61) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 601 | NAD  | O4D-C1D-N1N-C6N |
| 3   | A     | 602 | NAD  | C5B-O5B-PA-O1A  |
| 3   | A     | 602 | NAD  | C5B-O5B-PA-O3   |
| 3   | A     | 602 | NAD  | PA-O3-PN-O5D    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 602  | NAD  | C5D-O5D-PN-O3   |
| 3   | A     | 602  | NAD  | C5D-O5D-PN-O2N  |
| 3   | A     | 602  | NAD  | C3D-C4D-C5D-O5D |
| 3   | B     | 1601 | NAD  | O4D-C1D-N1N-C6N |
| 3   | B     | 1602 | NAD  | C5B-O5B-PA-O1A  |
| 3   | B     | 1602 | NAD  | C5B-O5B-PA-O3   |
| 3   | B     | 1602 | NAD  | C5D-O5D-PN-O3   |
| 3   | B     | 1602 | NAD  | C5D-O5D-PN-O2N  |
| 3   | B     | 1602 | NAD  | C3D-C4D-C5D-O5D |
| 3   | C     | 2601 | NAD  | O4D-C1D-N1N-C6N |
| 3   | C     | 2602 | NAD  | C5B-O5B-PA-O1A  |
| 3   | C     | 2602 | NAD  | C5B-O5B-PA-O3   |
| 3   | C     | 2602 | NAD  | C5D-O5D-PN-O3   |
| 3   | C     | 2602 | NAD  | C5D-O5D-PN-O1N  |
| 3   | C     | 2602 | NAD  | C5D-O5D-PN-O2N  |
| 3   | C     | 2602 | NAD  | O4D-C4D-C5D-O5D |
| 3   | C     | 2602 | NAD  | C3D-C4D-C5D-O5D |
| 3   | D     | 3601 | NAD  | O4D-C1D-N1N-C6N |
| 3   | D     | 3602 | NAD  | C5B-O5B-PA-O1A  |
| 3   | D     | 3602 | NAD  | C5B-O5B-PA-O3   |
| 3   | D     | 3602 | NAD  | PA-O3-PN-O5D    |
| 3   | D     | 3602 | NAD  | C5D-O5D-PN-O3   |
| 3   | D     | 3602 | NAD  | C5D-O5D-PN-O1N  |
| 3   | D     | 3602 | NAD  | C5D-O5D-PN-O2N  |
| 3   | D     | 3602 | NAD  | C3D-C4D-C5D-O5D |
| 4   | B     | 1603 | TTN  | O3-C2-C3-O4     |
| 4   | B     | 1603 | TTN  | O3-C2-C3-O5     |
| 3   | A     | 602  | NAD  | O4D-C4D-C5D-O5D |
| 3   | B     | 1602 | NAD  | O4D-C4D-C5D-O5D |
| 3   | D     | 3602 | NAD  | O4D-C4D-C5D-O5D |
| 4   | C     | 2603 | TTN  | O3-C2-C3-O4     |
| 4   | C     | 2603 | TTN  | O3-C2-C3-O5     |
| 4   | A     | 603  | TTN  | O3-C2-C3-O4     |
| 4   | A     | 603  | TTN  | O3-C2-C3-O5     |
| 3   | A     | 602  | NAD  | O4B-C4B-C5B-O5B |
| 4   | D     | 3603 | TTN  | O3-C2-C3-O4     |
| 3   | B     | 1602 | NAD  | PA-O3-PN-O5D    |
| 3   | D     | 3602 | NAD  | O4B-C4B-C5B-O5B |
| 4   | D     | 3603 | TTN  | O3-C2-C3-O5     |
| 3   | A     | 602  | NAD  | C4D-C5D-O5D-PN  |
| 3   | D     | 3602 | NAD  | C4D-C5D-O5D-PN  |
| 3   | A     | 602  | NAD  | C5B-O5B-PA-O2A  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | B     | 1602 | NAD  | C5B-O5B-PA-O2A  |
| 3   | C     | 2602 | NAD  | C5B-O5B-PA-O2A  |
| 3   | D     | 3602 | NAD  | C5B-O5B-PA-O2A  |
| 3   | C     | 2602 | NAD  | C4D-C5D-O5D-PN  |
| 3   | A     | 601  | NAD  | O4D-C1D-N1N-C2N |
| 3   | B     | 1601 | NAD  | O4D-C1D-N1N-C2N |
| 3   | C     | 2601 | NAD  | O4D-C1D-N1N-C2N |
| 3   | D     | 3601 | NAD  | O4D-C1D-N1N-C2N |
| 4   | D     | 3603 | TTN  | O2-C1-C2-O3     |
| 3   | B     | 1602 | NAD  | C4D-C5D-O5D-PN  |
| 3   | B     | 1602 | NAD  | O4B-C4B-C5B-O5B |
| 3   | B     | 1602 | NAD  | C4B-C5B-O5B-PA  |
| 3   | B     | 1601 | NAD  | O4B-C4B-C5B-O5B |
| 4   | D     | 3603 | TTN  | O1-C1-C2-O3     |
| 3   | A     | 602  | NAD  | C3B-C4B-C5B-O5B |

There are no ring outliers.

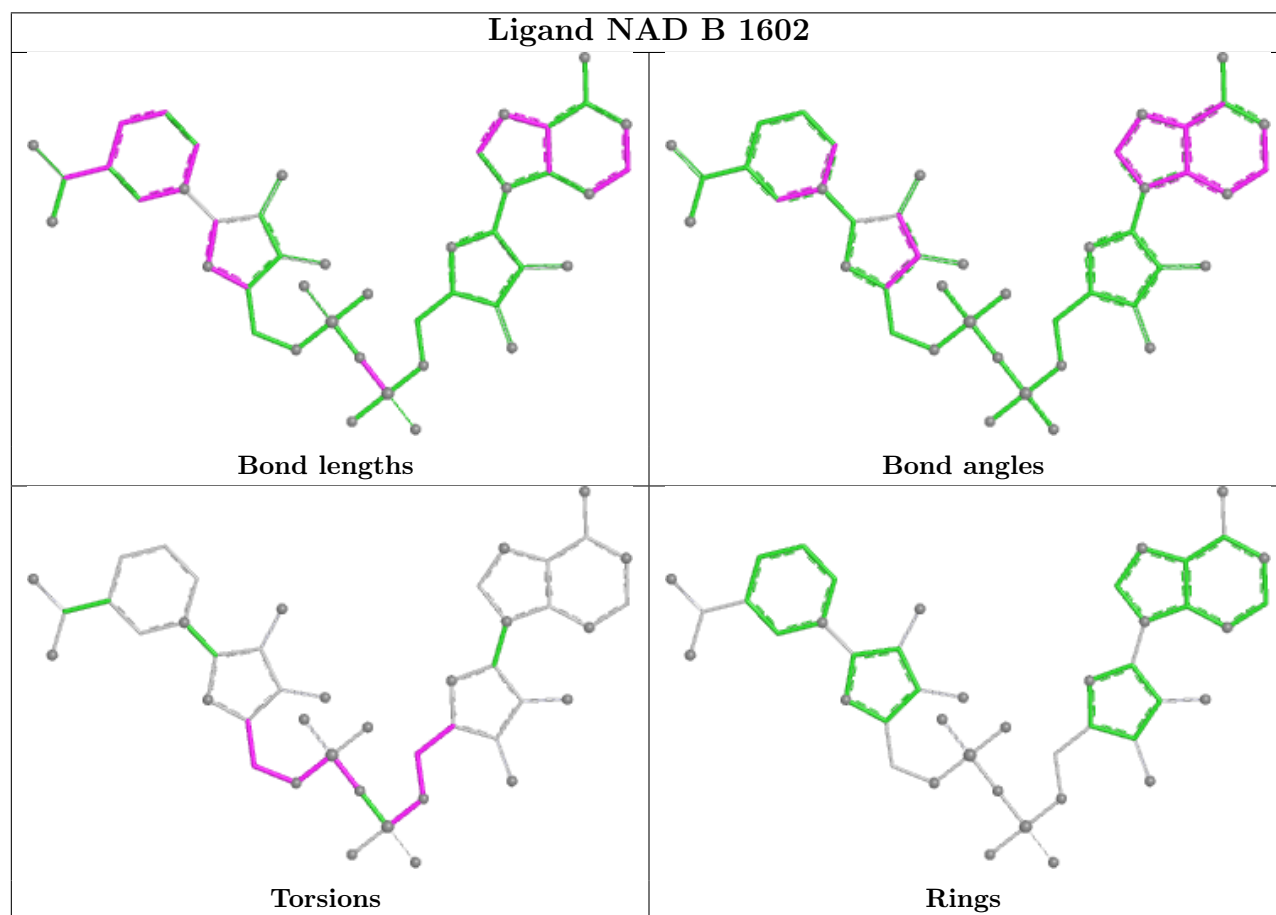
11 monomers are involved in 21 short contacts:

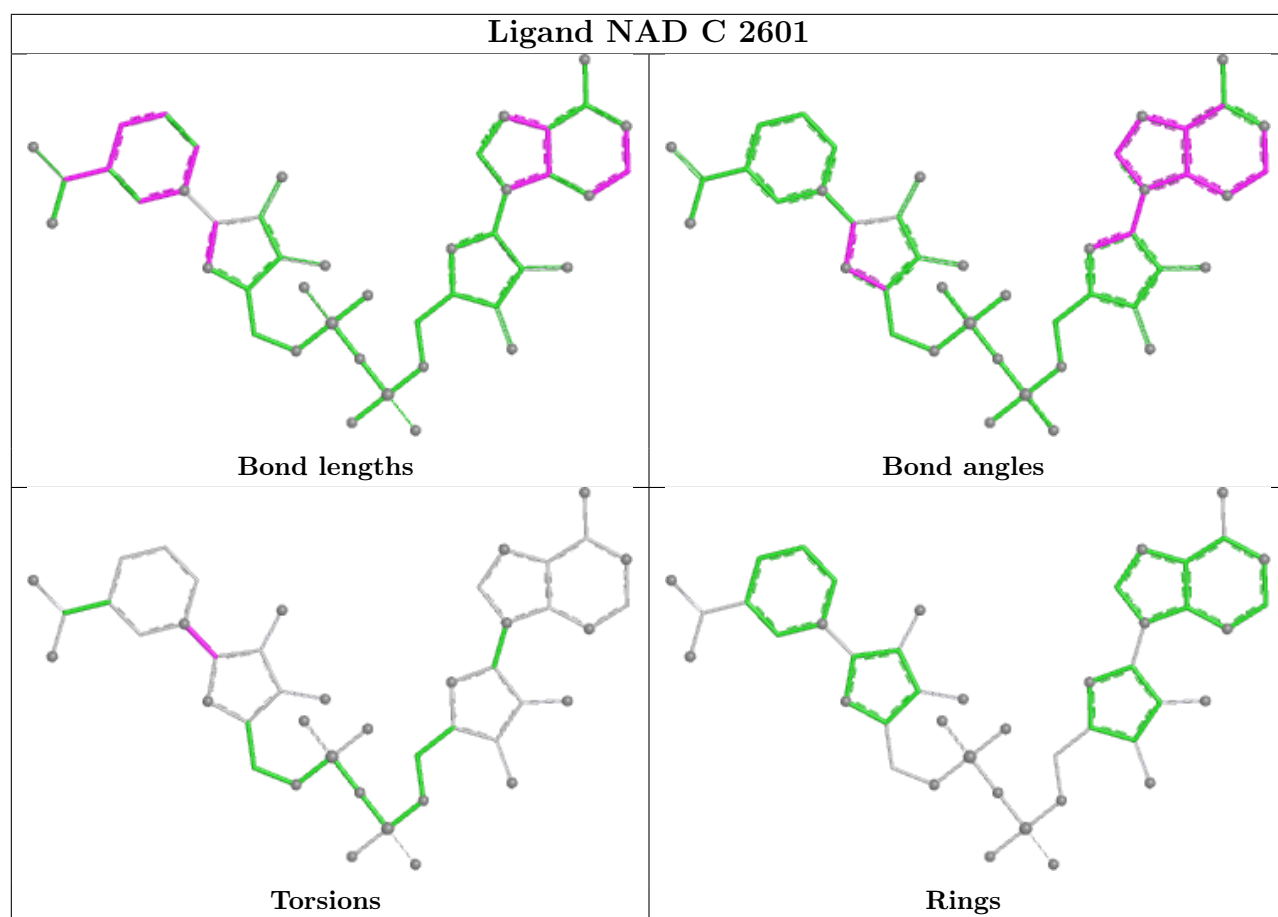
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 1602 | NAD  | 1       | 0            |
| 3   | C     | 2601 | NAD  | 4       | 0            |
| 3   | A     | 601  | NAD  | 4       | 0            |
| 3   | B     | 1601 | NAD  | 1       | 0            |
| 3   | D     | 3602 | NAD  | 3       | 0            |
| 3   | A     | 602  | NAD  | 2       | 0            |
| 4   | D     | 3603 | TTN  | 1       | 0            |
| 3   | D     | 3601 | NAD  | 1       | 0            |
| 4   | C     | 2603 | TTN  | 2       | 0            |
| 4   | B     | 1603 | TTN  | 1       | 0            |
| 3   | C     | 2602 | NAD  | 1       | 0            |

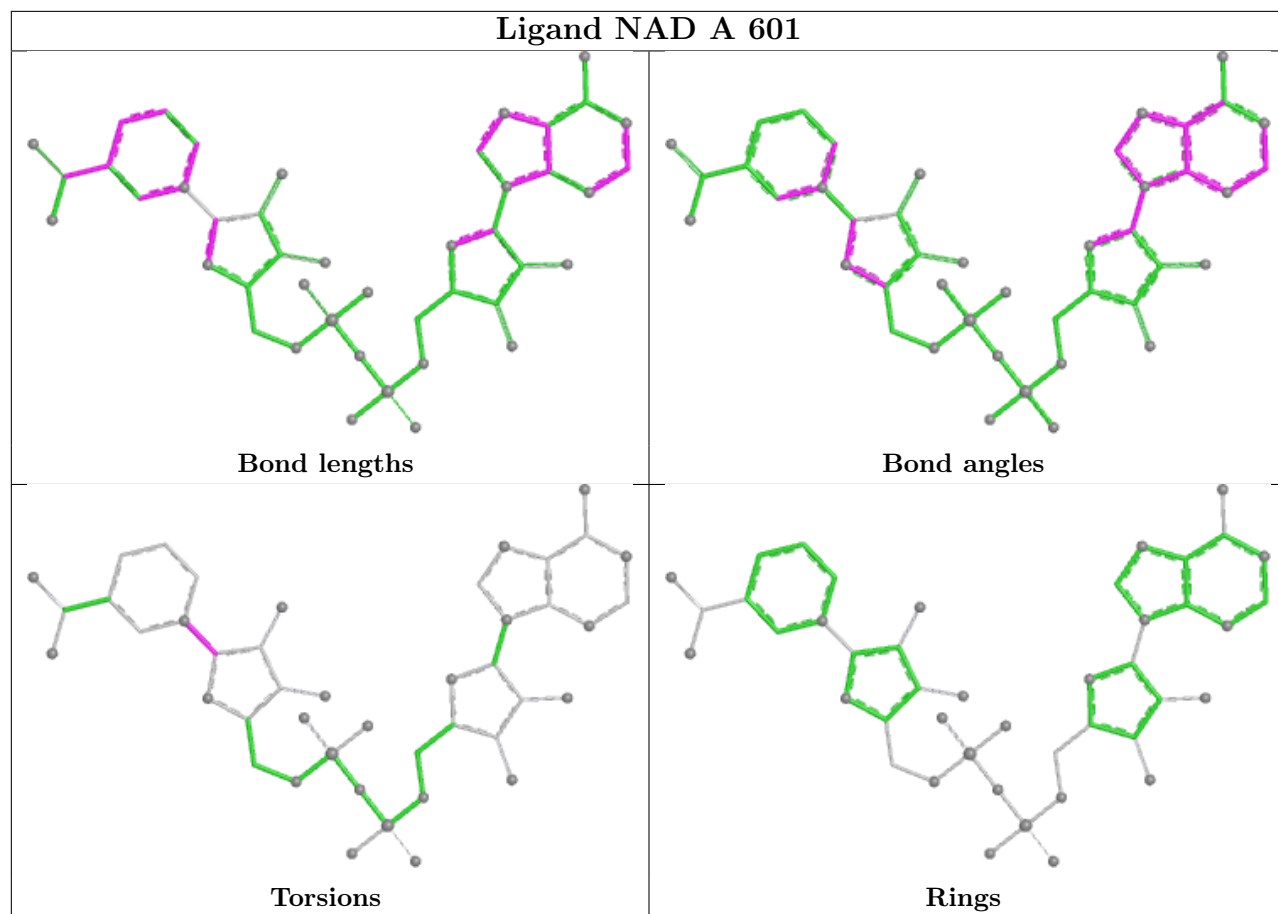
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

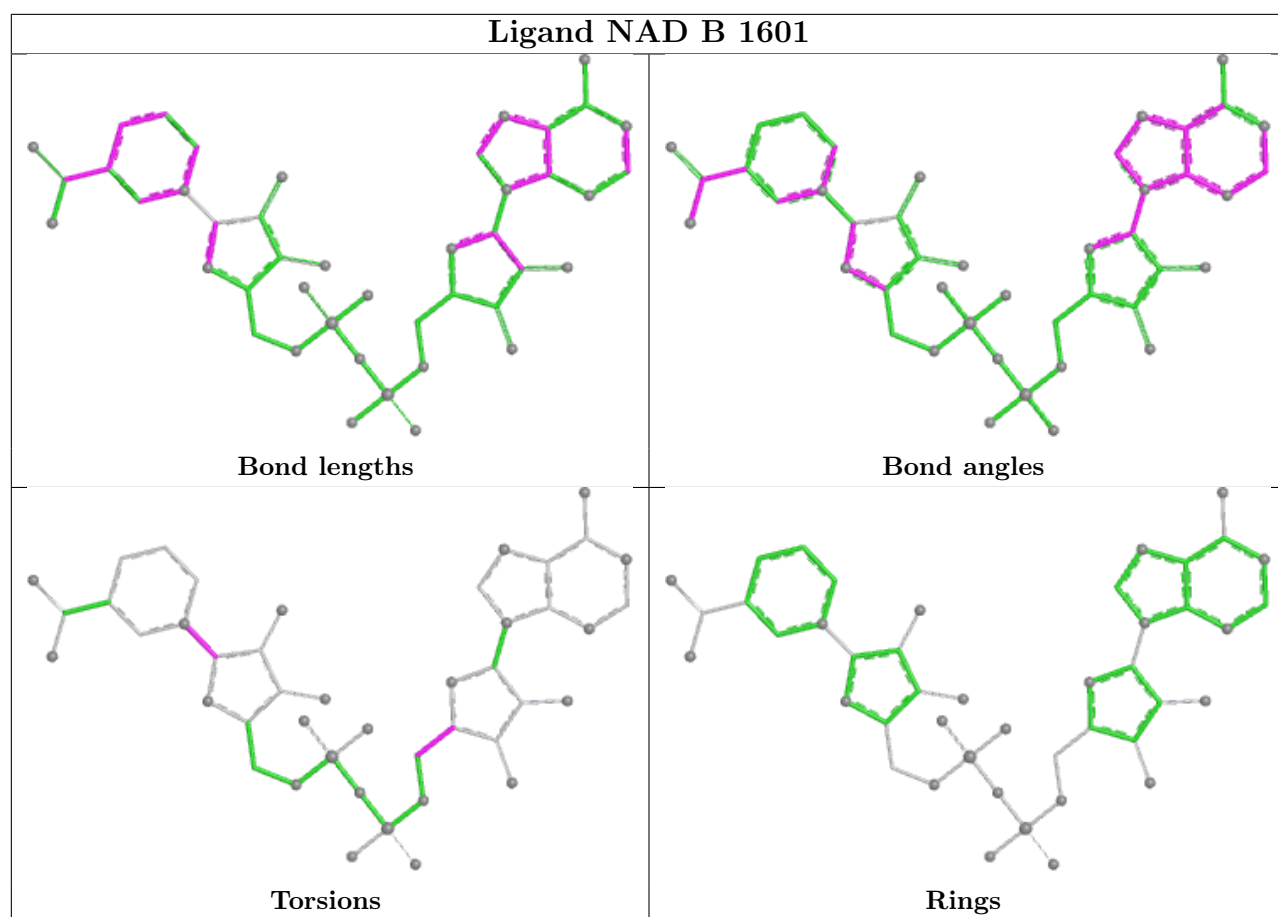


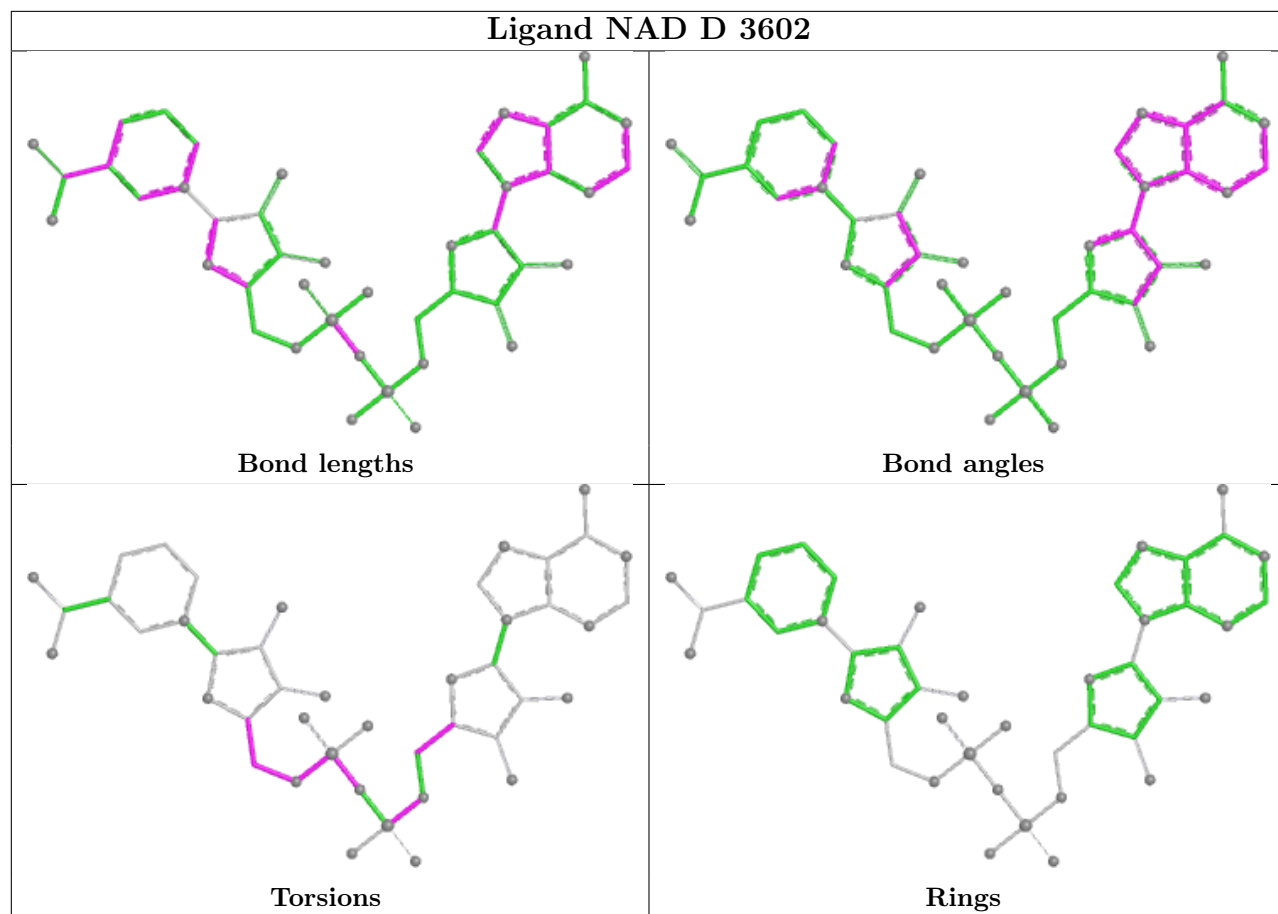
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

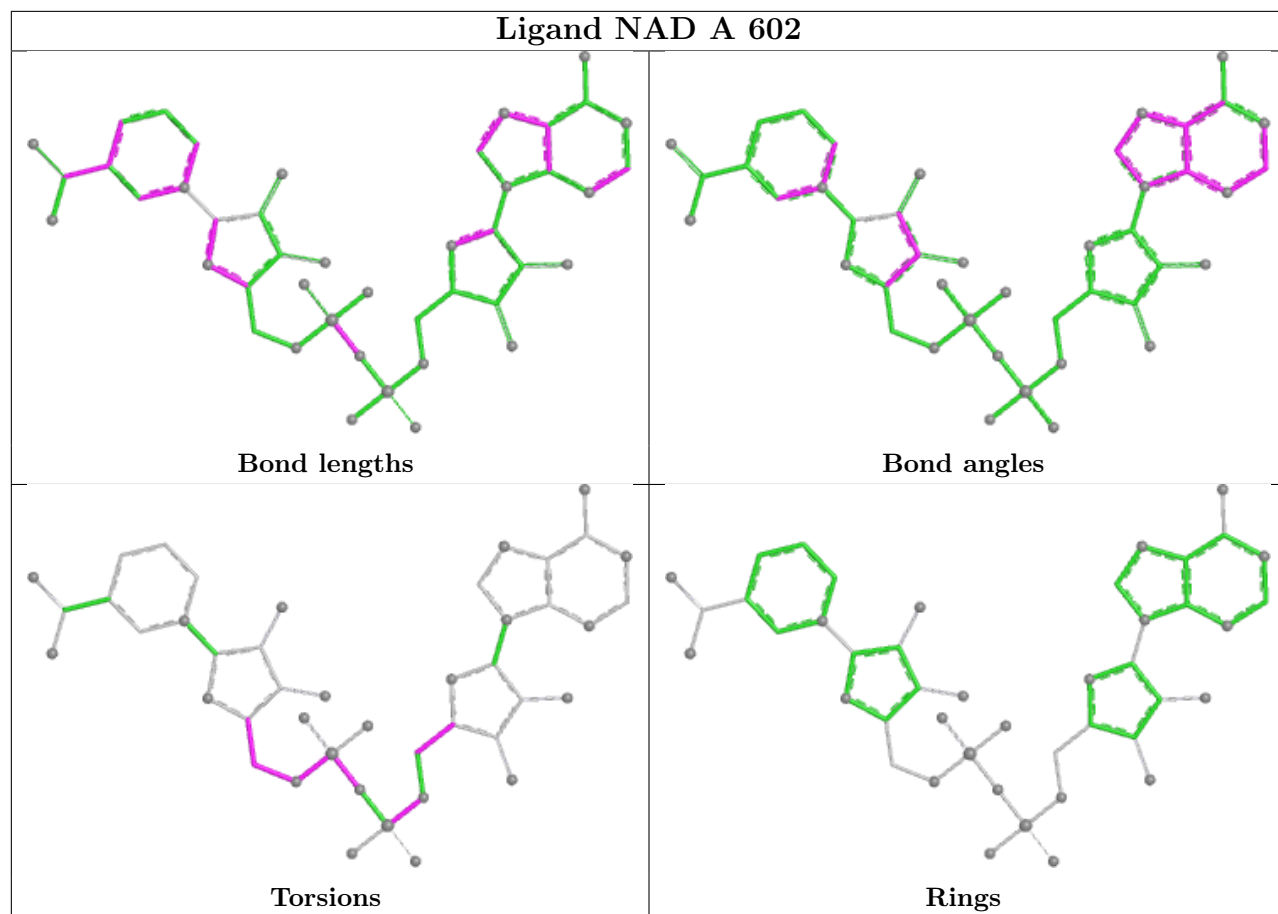


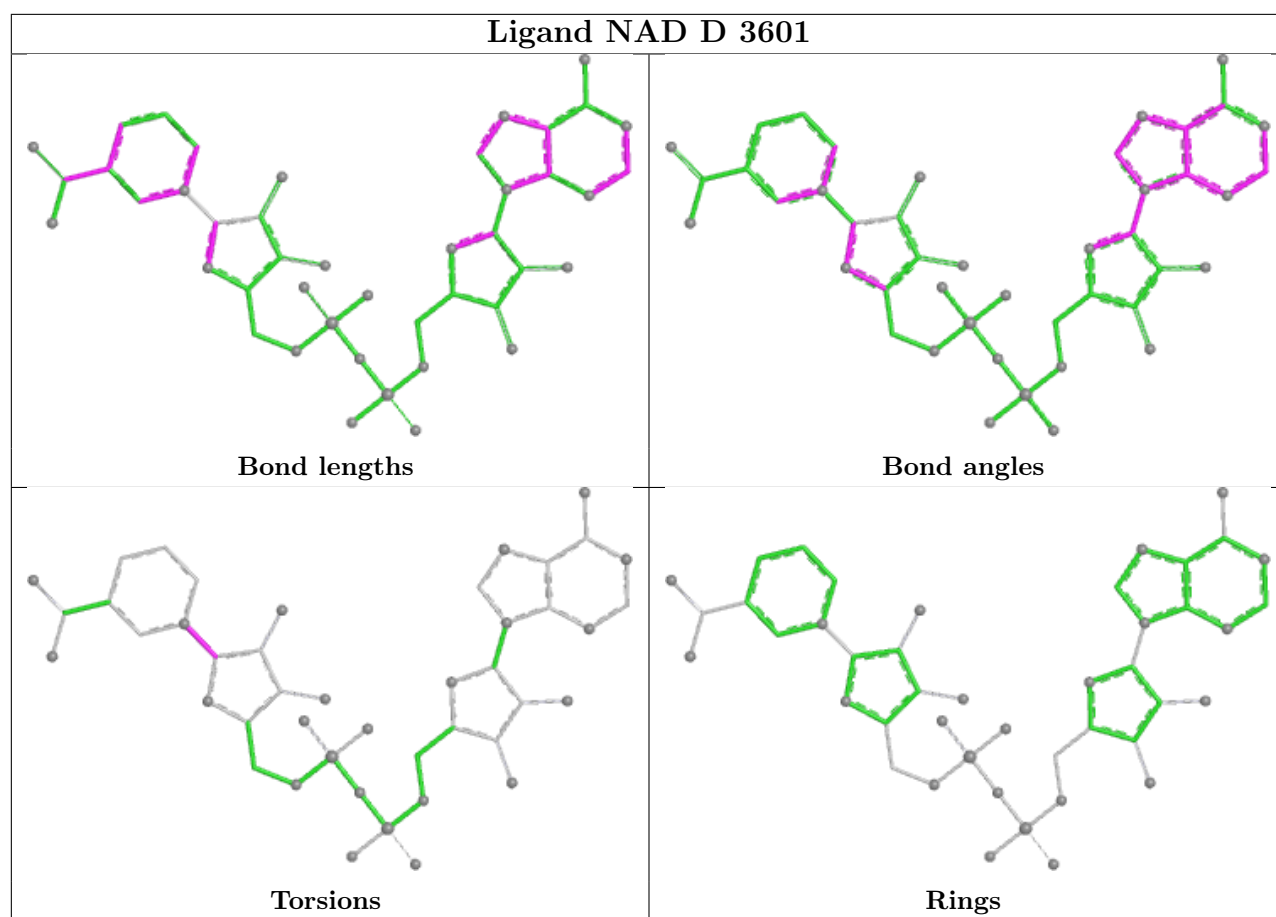


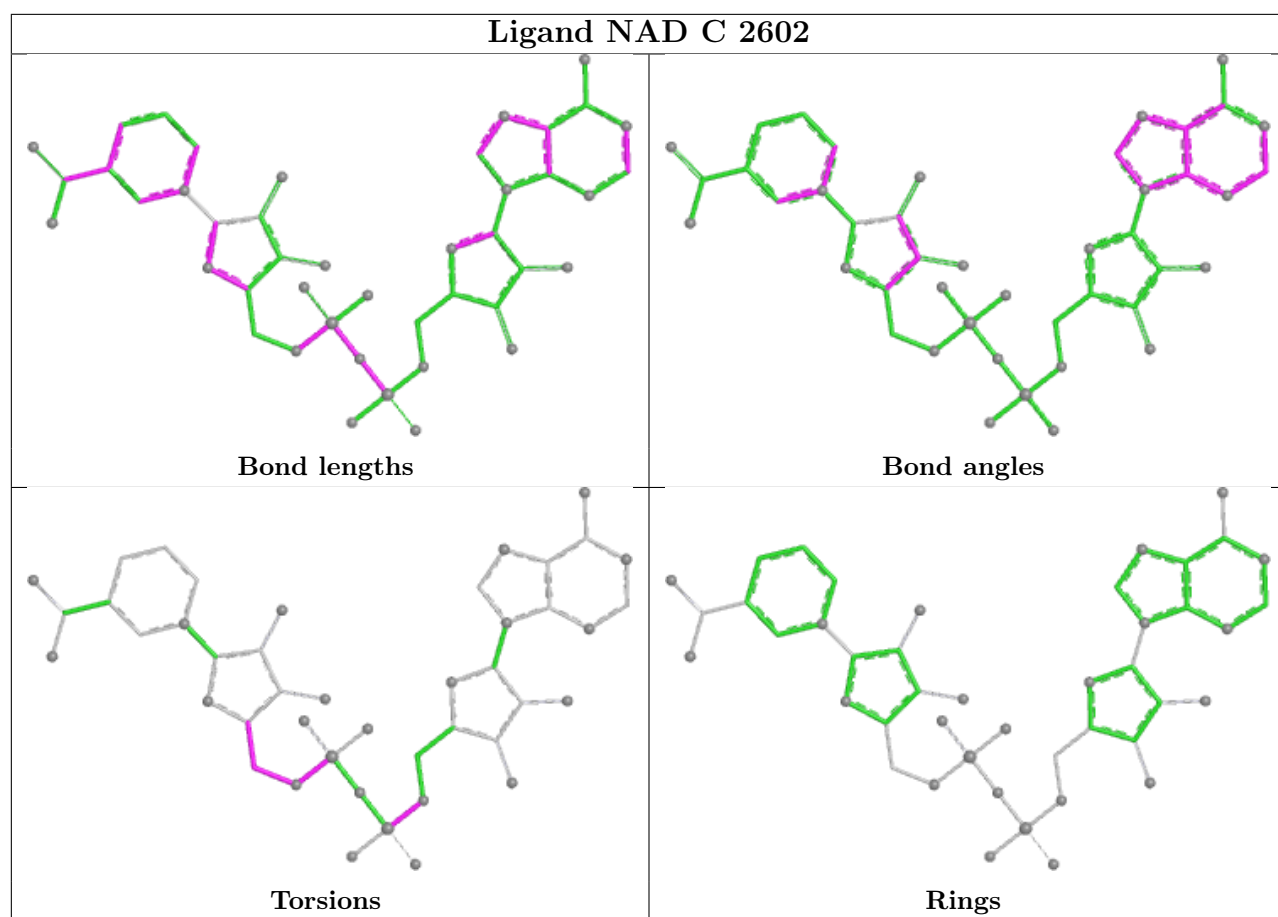












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.