



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:49 PM UTC

PDB ID : 1DDO / pdb\_00001ddo  
Title : REDUCED D-AMINO ACID OXIDASE FROM PIG KIDNEY IN COMPLEX  
WITH IMINO-TRP  
Authors : Todone, F.; Mattevi, A.  
Deposited on : 1997-01-16  
Resolution : 3.10 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>.

---

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

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

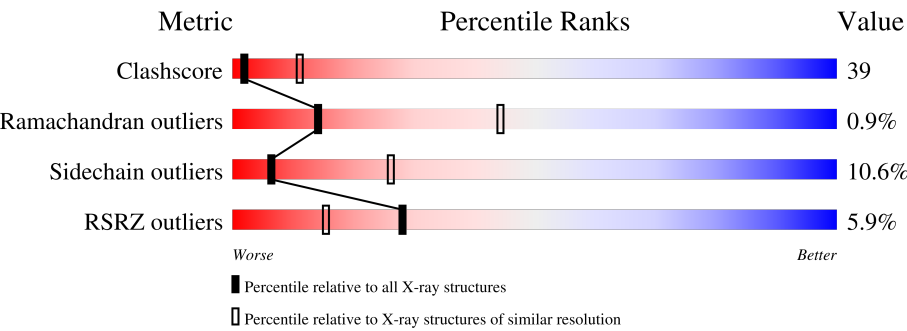
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                      |
|-----|-------|--------|-------------------------------------------------------------------------------------------------------|
| 1   | A     | 347    | <div><div>5%</div><div><div></div><div>40%</div><div>42%</div><div>14%</div><div>..</div></div></div> |
| 1   | B     | 347    | <div><div>6%</div><div><div></div><div>40%</div><div>44%</div><div>13%</div><div>..</div></div></div> |
| 1   | C     | 347    | <div><div>5%</div><div><div></div><div>40%</div><div>46%</div><div>11%</div><div>..</div></div></div> |
| 1   | D     | 347    | <div><div>7%</div><div><div></div><div>39%</div><div>44%</div><div>12%</div><div>..</div></div></div> |
| 1   | E     | 347    | <div><div>5%</div><div><div></div><div>43%</div><div>42%</div><div>11%</div><div>..</div></div></div> |
| 1   | F     | 347    | <div><div>4%</div><div><div></div><div>41%</div><div>42%</div><div>13%</div><div>..</div></div></div> |
| 1   | G     | 347    | <div><div>7%</div><div><div></div><div>41%</div><div>43%</div><div>12%</div><div>..</div></div></div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | H     | 347    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | DTR  | E     | 350 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22441 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 D-AMINO ACID OXIDASE.

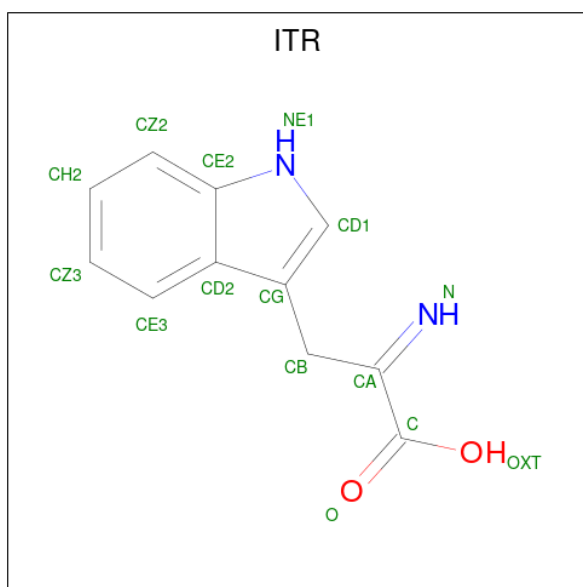
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 339      | Total | C    | N   | O   | S | 161     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | B     | 339      | Total | C    | N   | O   | S | 190     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | C     | 339      | Total | C    | N   | O   | S | 173     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | D     | 339      | Total | C    | N   | O   | S | 131     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | E     | 339      | Total | C    | N   | O   | S | 164     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | F     | 339      | Total | C    | N   | O   | S | 154     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | G     | 339      | Total | C    | N   | O   | S | 210     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |
| 1   | H     | 339      | Total | C    | N   | O   | S | 166     | 0       | 0     |
|     |       |          | 2720  | 1749 | 473 | 489 | 9 |         |         |       |

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



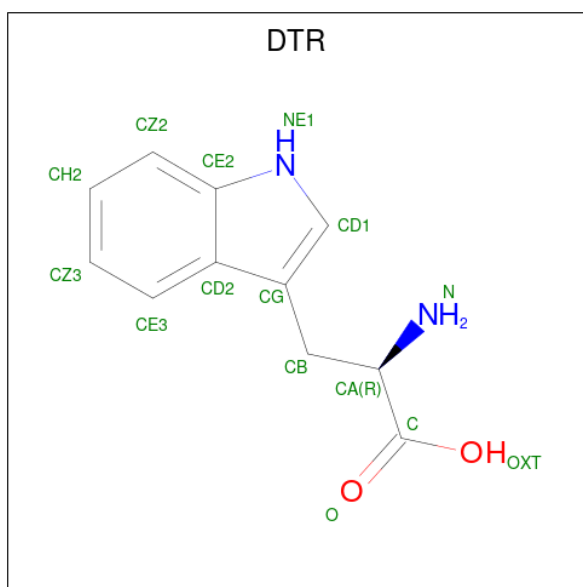
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 3 is IMINO-TRYPTOPHAN (CCD ID: ITR) (formula: C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |

- Molecule 4 is D-TRYPTOPHAN (CCD ID: DTR) (formula:  $C_{11}H_{12}N_2O_2$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |
| 4   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 15    | 11 | 2 | 2 |         |         |

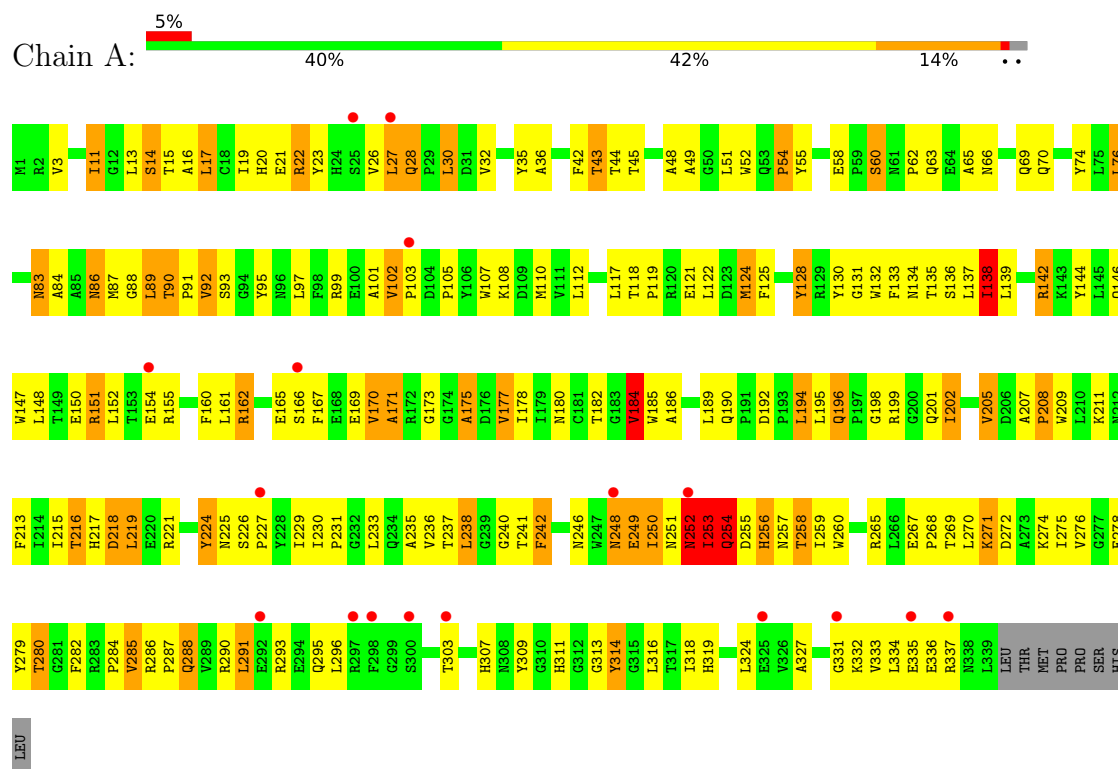
- Molecule 5 is water.

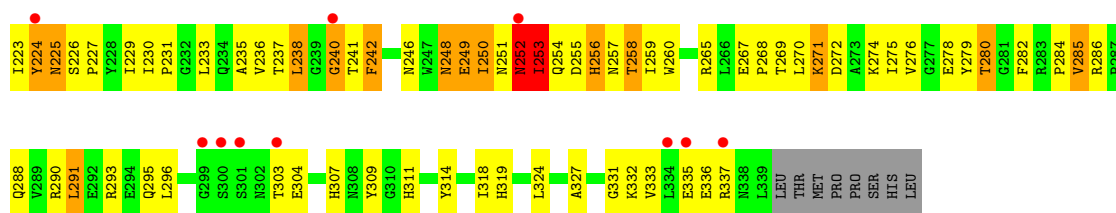
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 5   | B     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 5   | C     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 5   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 5   | E     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 5   | F     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 5   | G     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | H     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |

### 3 Residue-property plots [i](#)

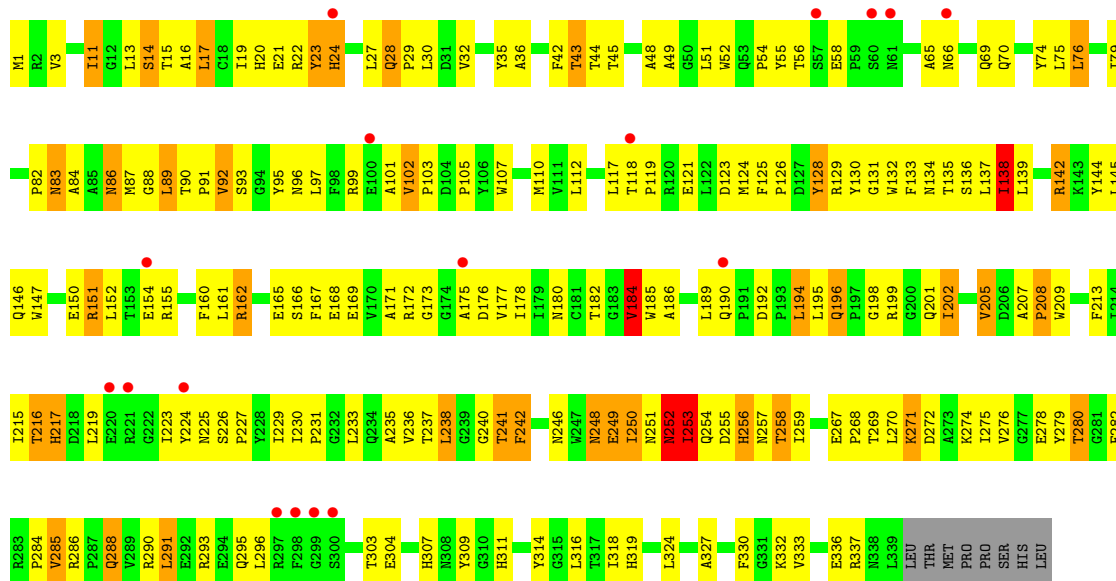
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: D-AMINO ACID OXIDASE

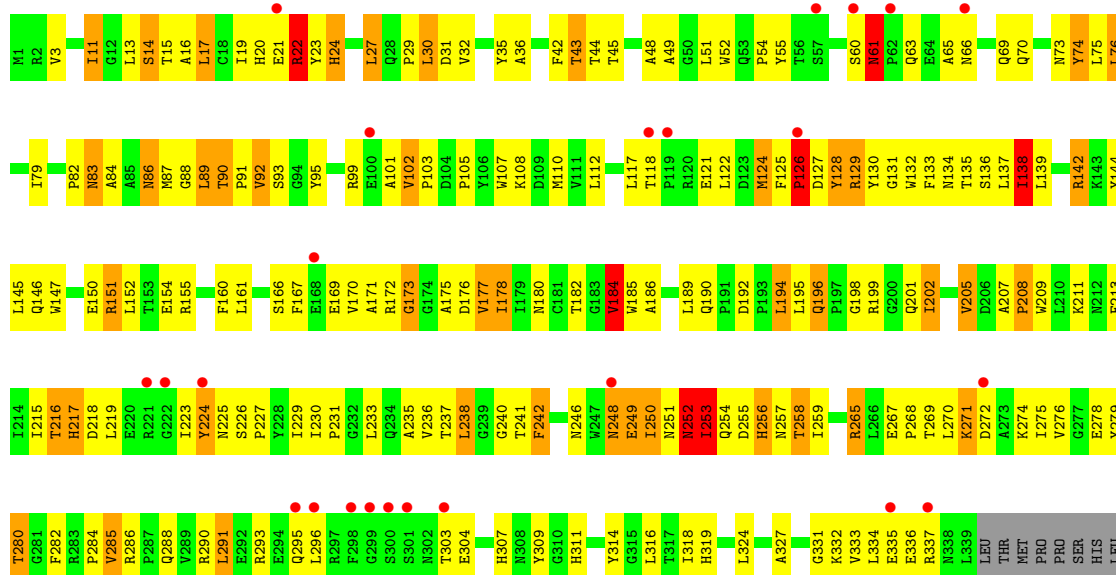




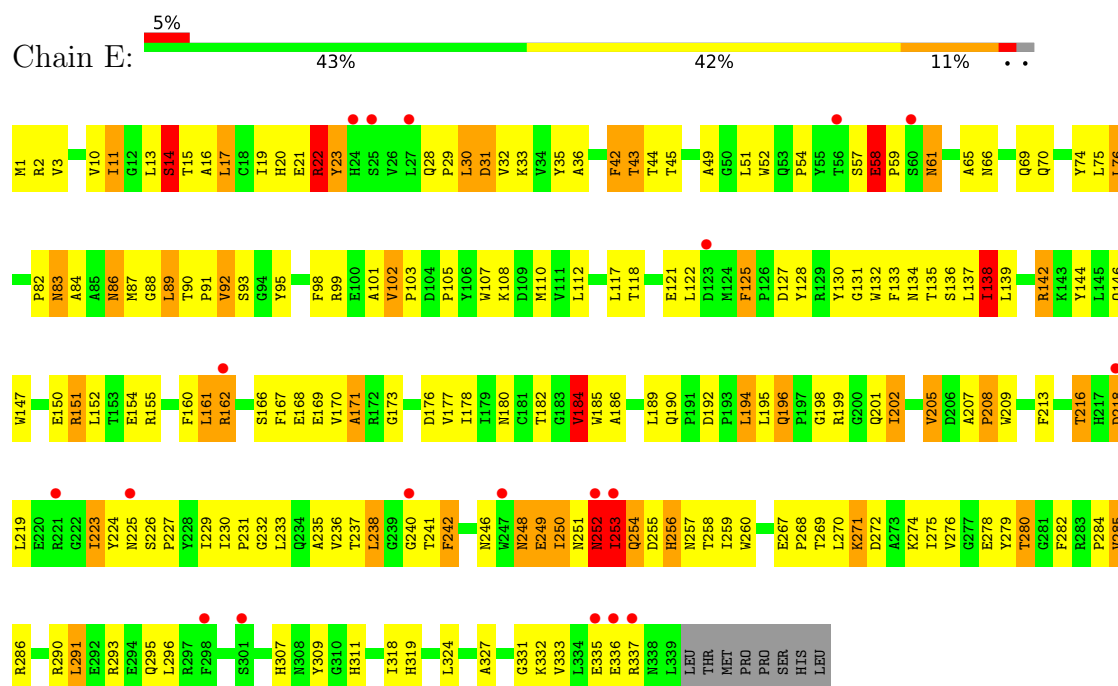
● Molecule 1: D-AMINO ACID OXIDASE



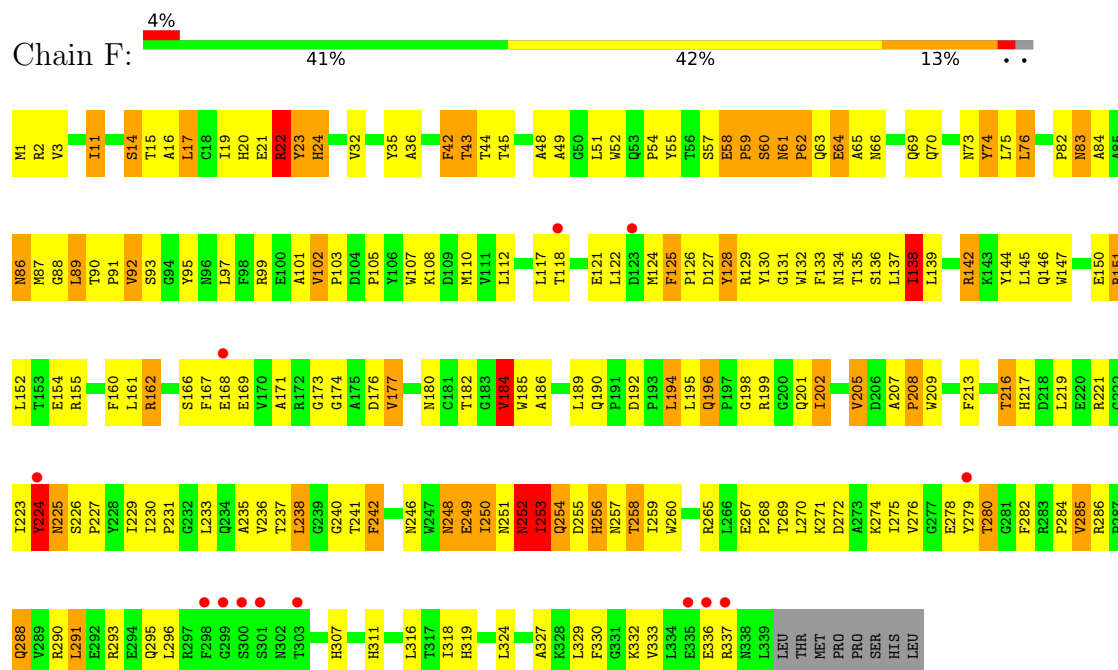
● Molecule 1: D-AMINO ACID OXIDASE



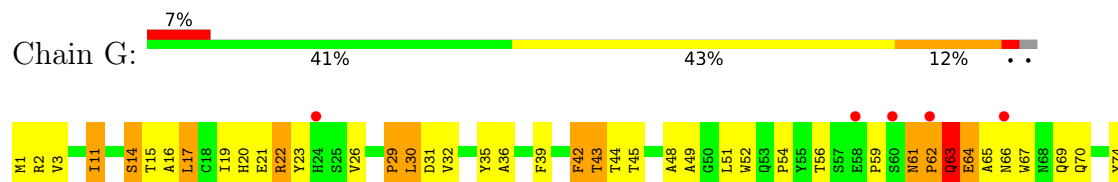
● Molecule 1: D-AMINO ACID OXIDASE

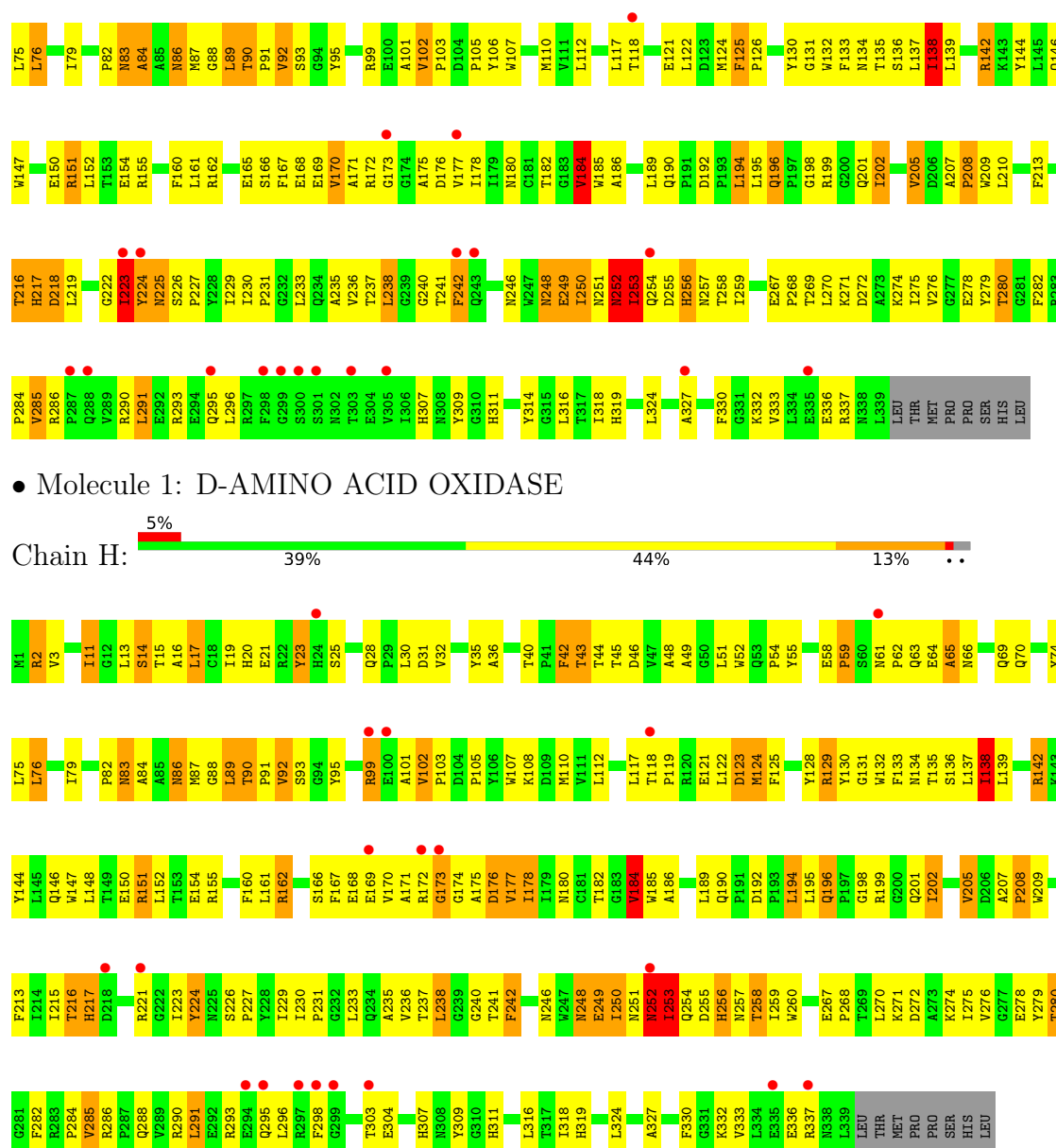


- Molecule 1: D-AMINO ACID OXIDASE



- Molecule 1: D-AMINO ACID OXIDASE





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 325.20Å 137.10Å 196.80Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.10<br>20.00 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (20.00-3.10)<br>97.8 (20.00-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 6.18 (at 3.13Å)                                             | Xtriage          |
| Refinement program                                                      | TNT 5E                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.236 , 0.250<br>0.235 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.345                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.53 , 172.2                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 22441                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTR, ITR, FAD

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     | 1.16         | 8/2796 (0.3%)   | 1.79        | 69/3808 (1.8%)   |
| 1   | B     | 1.12         | 4/2796 (0.1%)   | 1.75        | 59/3808 (1.5%)   |
| 1   | C     | 1.12         | 5/2796 (0.2%)   | 1.72        | 61/3808 (1.6%)   |
| 1   | D     | 1.21         | 14/2796 (0.5%)  | 1.78        | 64/3808 (1.7%)   |
| 1   | E     | 1.13         | 3/2796 (0.1%)   | 1.71        | 60/3808 (1.6%)   |
| 1   | F     | 1.15         | 4/2796 (0.1%)   | 1.76        | 68/3808 (1.8%)   |
| 1   | G     | 1.09         | 4/2796 (0.1%)   | 1.72        | 61/3808 (1.6%)   |
| 1   | H     | 1.13         | 4/2796 (0.1%)   | 1.74        | 61/3808 (1.6%)   |
| All | All   | 1.14         | 46/22368 (0.2%) | 1.75        | 503/30464 (1.7%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | D     | 1                   | 0                   |
| 1   | E     | 0                   | 2                   |
| 1   | F     | 0                   | 1                   |
| All | All   | 1                   | 4                   |

All (46) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 177 | VAL  | CA-CB | -6.38 | 1.45        | 1.54     |
| 1   | D     | 288 | GLN  | C-O   | 6.33  | 1.31        | 1.23     |
| 1   | D     | 178 | ILE  | CA-CB | -6.25 | 1.46        | 1.54     |
| 1   | A     | 225 | ASN  | C-O   | 6.08  | 1.31        | 1.24     |
| 1   | D     | 124 | MET  | SD-CE | -6.03 | 1.64        | 1.79     |
| 1   | D     | 271 | LYS  | CA-C  | -6.01 | 1.44        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 314 | TYR  | CA-C  | -5.90 | 1.46        | 1.52     |
| 1   | D     | 265 | ARG  | C-O   | -5.85 | 1.16        | 1.24     |
| 1   | B     | 225 | ASN  | C-O   | 5.84  | 1.31        | 1.24     |
| 1   | A     | 177 | VAL  | CA-CB | -5.81 | 1.46        | 1.54     |
| 1   | B     | 65  | ALA  | CA-CB | -5.74 | 1.44        | 1.53     |
| 1   | C     | 178 | ILE  | C-N   | 5.74  | 1.40        | 1.33     |
| 1   | H     | 65  | ALA  | CA-CB | -5.70 | 1.44        | 1.53     |
| 1   | C     | 65  | ALA  | CA-CB | -5.70 | 1.44        | 1.53     |
| 1   | A     | 60  | SER  | CB-OG | 5.69  | 1.53        | 1.42     |
| 1   | A     | 65  | ALA  | CA-CB | -5.66 | 1.44        | 1.53     |
| 1   | F     | 65  | ALA  | CA-CB | -5.65 | 1.44        | 1.53     |
| 1   | D     | 175 | ALA  | CA-CB | -5.61 | 1.46        | 1.53     |
| 1   | E     | 65  | ALA  | CA-CB | -5.60 | 1.44        | 1.53     |
| 1   | D     | 271 | LYS  | C-N   | -5.58 | 1.25        | 1.33     |
| 1   | B     | 235 | ALA  | CA-CB | -5.51 | 1.44        | 1.53     |
| 1   | F     | 235 | ALA  | CA-CB | -5.50 | 1.44        | 1.53     |
| 1   | D     | 65  | ALA  | CA-CB | -5.50 | 1.44        | 1.53     |
| 1   | G     | 235 | ALA  | CA-CB | -5.48 | 1.44        | 1.53     |
| 1   | D     | 235 | ALA  | CA-CB | -5.48 | 1.44        | 1.53     |
| 1   | H     | 235 | ALA  | CA-CB | -5.47 | 1.44        | 1.53     |
| 1   | A     | 235 | ALA  | CA-CB | -5.47 | 1.44        | 1.53     |
| 1   | E     | 235 | ALA  | CA-CB | -5.47 | 1.44        | 1.53     |
| 1   | C     | 235 | ALA  | CA-CB | -5.46 | 1.44        | 1.53     |
| 1   | G     | 65  | ALA  | CA-CB | -5.45 | 1.44        | 1.53     |
| 1   | D     | 61  | ASN  | C-O   | -5.37 | 1.18        | 1.24     |
| 1   | F     | 124 | MET  | SD-CE | 5.37  | 1.93        | 1.79     |
| 1   | G     | 225 | ASN  | C-O   | 5.37  | 1.30        | 1.23     |
| 1   | H     | 124 | MET  | SD-CE | -5.26 | 1.66        | 1.79     |
| 1   | G     | 138 | ILE  | CA-CB | -5.21 | 1.48        | 1.54     |
| 1   | C     | 138 | ILE  | CA-CB | -5.20 | 1.48        | 1.54     |
| 1   | A     | 138 | ILE  | CA-CB | -5.19 | 1.48        | 1.54     |
| 1   | F     | 138 | ILE  | CA-CB | -5.19 | 1.48        | 1.54     |
| 1   | H     | 138 | ILE  | CA-CB | -5.18 | 1.48        | 1.54     |
| 1   | D     | 138 | ILE  | CA-CB | -5.18 | 1.48        | 1.54     |
| 1   | E     | 138 | ILE  | CA-CB | -5.17 | 1.48        | 1.54     |
| 1   | A     | 63  | GLN  | C-O   | -5.15 | 1.17        | 1.24     |
| 1   | B     | 138 | ILE  | CA-CB | -5.14 | 1.48        | 1.54     |
| 1   | C     | 56  | THR  | CA-CB | 5.13  | 1.61        | 1.53     |
| 1   | D     | 217 | HIS  | CA-C  | 5.04  | 1.58        | 1.52     |
| 1   | D     | 126 | PRO  | N-CA  | -5.00 | 1.41        | 1.47     |

All (503) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 224 | TYR  | N-CA-C  | 16.25  | 133.38      | 113.23   |
| 1   | B     | 223 | ILE  | N-CA-C  | 14.72  | 127.19      | 111.58   |
| 1   | B     | 23  | TYR  | N-CA-C  | 13.61  | 130.69      | 113.55   |
| 1   | D     | 23  | TYR  | N-CA-C  | 11.40  | 127.40      | 113.38   |
| 1   | D     | 42  | PHE  | N-CA-C  | 11.37  | 127.26      | 113.16   |
| 1   | C     | 42  | PHE  | N-CA-C  | 11.36  | 127.25      | 113.16   |
| 1   | B     | 42  | PHE  | N-CA-C  | 11.36  | 127.24      | 113.16   |
| 1   | G     | 42  | PHE  | N-CA-C  | 11.35  | 127.23      | 113.16   |
| 1   | F     | 42  | PHE  | N-CA-C  | 11.34  | 127.22      | 113.16   |
| 1   | A     | 42  | PHE  | N-CA-C  | 11.34  | 127.22      | 113.16   |
| 1   | E     | 42  | PHE  | N-CA-C  | 11.33  | 127.21      | 113.16   |
| 1   | H     | 42  | PHE  | N-CA-C  | 11.33  | 127.21      | 113.16   |
| 1   | D     | 27  | LEU  | CB-CA-C | -10.88 | 96.81       | 111.82   |
| 1   | C     | 27  | LEU  | N-CA-C  | -10.21 | 96.10       | 110.50   |
| 1   | D     | 127 | ASP  | N-CA-C  | 9.55   | 121.69      | 111.28   |
| 1   | D     | 172 | ARG  | N-CA-C  | -9.51  | 101.84      | 113.15   |
| 1   | C     | 24  | HIS  | N-CA-C  | -9.49  | 97.84       | 113.50   |
| 1   | F     | 24  | HIS  | N-CA-C  | -9.47  | 101.49      | 113.23   |
| 1   | A     | 171 | ALA  | N-CA-C  | -9.28  | 101.12      | 111.14   |
| 1   | A     | 254 | GLN  | CB-CA-C | -9.27  | 95.40       | 110.79   |
| 1   | B     | 225 | ASN  | CA-C-N  | -9.19  | 106.33      | 121.03   |
| 1   | B     | 225 | ASN  | C-N-CA  | -9.19  | 106.33      | 121.03   |
| 1   | H     | 2   | ARG  | CA-C-N  | -8.94  | 110.52      | 122.94   |
| 1   | H     | 2   | ARG  | C-N-CA  | -8.94  | 110.52      | 122.94   |
| 1   | D     | 126 | PRO  | CA-C-N  | -8.93  | 108.31      | 120.28   |
| 1   | D     | 126 | PRO  | C-N-CA  | -8.93  | 108.31      | 120.28   |
| 1   | E     | 22  | ARG  | N-CA-C  | 8.79   | 123.30      | 112.23   |
| 1   | F     | 184 | VAL  | CB-CA-C | -8.68  | 99.38       | 112.05   |
| 1   | A     | 184 | VAL  | CB-CA-C | -8.67  | 99.39       | 112.05   |
| 1   | B     | 184 | VAL  | CB-CA-C | -8.67  | 99.39       | 112.05   |
| 1   | E     | 184 | VAL  | CB-CA-C | -8.66  | 99.40       | 112.05   |
| 1   | D     | 173 | GLY  | N-CA-C  | -8.66  | 100.54      | 115.61   |
| 1   | H     | 184 | VAL  | CB-CA-C | -8.66  | 99.41       | 112.05   |
| 1   | C     | 184 | VAL  | CB-CA-C | -8.65  | 99.42       | 112.05   |
| 1   | D     | 184 | VAL  | CB-CA-C | -8.64  | 99.43       | 112.05   |
| 1   | G     | 184 | VAL  | CB-CA-C | -8.64  | 99.44       | 112.05   |
| 1   | F     | 61  | ASN  | N-CA-C  | -8.57  | 98.46       | 110.29   |
| 1   | A     | 219 | LEU  | N-CA-C  | 8.52   | 123.45      | 112.89   |
| 1   | H     | 25  | SER  | N-CA-C  | -8.51  | 101.76      | 112.90   |
| 1   | D     | 288 | GLN  | N-CA-C  | -8.28  | 96.12       | 108.79   |
| 1   | G     | 61  | ASN  | N-CA-C  | -8.27  | 97.97       | 109.71   |
| 1   | F     | 11  | ILE  | N-CA-C  | 8.19   | 118.24      | 110.30   |
| 1   | F     | 225 | ASN  | CA-C-O  | 8.16   | 127.70      | 118.97   |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 11  | ILE  | N-CA-C  | 8.16  | 118.22      | 110.30   |
| 1   | A     | 11  | ILE  | N-CA-C  | 8.14  | 118.20      | 110.30   |
| 1   | C     | 11  | ILE  | N-CA-C  | 8.14  | 118.20      | 110.30   |
| 1   | G     | 11  | ILE  | N-CA-C  | 8.14  | 118.20      | 110.30   |
| 1   | E     | 11  | ILE  | N-CA-C  | 8.14  | 118.19      | 110.30   |
| 1   | B     | 11  | ILE  | N-CA-C  | 8.13  | 118.19      | 110.30   |
| 1   | D     | 11  | ILE  | N-CA-C  | 8.13  | 118.19      | 110.30   |
| 1   | H     | 288 | GLN  | N-CA-C  | -8.12 | 96.73       | 109.07   |
| 1   | A     | 22  | ARG  | N-CA-C  | 8.11  | 123.00      | 113.18   |
| 1   | D     | 253 | ILE  | CB-CA-C | -8.09 | 101.61      | 111.97   |
| 1   | B     | 253 | ILE  | CB-CA-C | -8.07 | 101.64      | 111.97   |
| 1   | C     | 253 | ILE  | CB-CA-C | -8.06 | 101.65      | 111.97   |
| 1   | E     | 253 | ILE  | CB-CA-C | -8.06 | 101.65      | 111.97   |
| 1   | G     | 62  | PRO  | N-CA-C  | 8.05  | 129.05      | 112.47   |
| 1   | H     | 253 | ILE  | CB-CA-C | -8.05 | 101.67      | 111.97   |
| 1   | A     | 253 | ILE  | CB-CA-C | -8.04 | 101.67      | 111.97   |
| 1   | F     | 253 | ILE  | CB-CA-C | -8.04 | 101.68      | 111.97   |
| 1   | A     | 60  | SER  | N-CA-C  | -7.92 | 102.64      | 111.28   |
| 1   | B     | 170 | VAL  | CA-C-N  | -7.88 | 108.33      | 120.31   |
| 1   | B     | 170 | VAL  | C-N-CA  | -7.88 | 108.33      | 120.31   |
| 1   | G     | 253 | ILE  | CB-CA-C | -7.79 | 101.63      | 112.14   |
| 1   | A     | 92  | VAL  | CB-CA-C | -7.75 | 96.97       | 111.30   |
| 1   | D     | 92  | VAL  | CB-CA-C | -7.74 | 96.99       | 111.30   |
| 1   | F     | 92  | VAL  | CB-CA-C | -7.73 | 96.99       | 111.30   |
| 1   | C     | 92  | VAL  | CB-CA-C | -7.73 | 97.00       | 111.30   |
| 1   | H     | 92  | VAL  | CB-CA-C | -7.73 | 97.00       | 111.30   |
| 1   | E     | 92  | VAL  | CB-CA-C | -7.72 | 97.01       | 111.30   |
| 1   | B     | 92  | VAL  | CB-CA-C | -7.71 | 97.03       | 111.30   |
| 1   | G     | 92  | VAL  | CB-CA-C | -7.71 | 97.03       | 111.30   |
| 1   | F     | 14  | SER  | CB-CA-C | -7.67 | 98.83       | 110.88   |
| 1   | B     | 14  | SER  | CB-CA-C | -7.67 | 98.84       | 110.88   |
| 1   | E     | 14  | SER  | CB-CA-C | -7.66 | 98.85       | 110.88   |
| 1   | A     | 14  | SER  | CB-CA-C | -7.66 | 98.85       | 110.88   |
| 1   | G     | 14  | SER  | CB-CA-C | -7.66 | 98.85       | 110.88   |
| 1   | D     | 14  | SER  | CB-CA-C | -7.65 | 98.87       | 110.88   |
| 1   | C     | 14  | SER  | CB-CA-C | -7.64 | 98.88       | 110.88   |
| 1   | H     | 14  | SER  | CB-CA-C | -7.64 | 98.88       | 110.88   |
| 1   | C     | 24  | HIS  | CA-C-O  | 7.58  | 126.75      | 118.65   |
| 1   | A     | 225 | ASN  | CA-C-N  | -7.50 | 106.17      | 121.48   |
| 1   | A     | 225 | ASN  | C-N-CA  | -7.50 | 106.17      | 121.48   |
| 1   | A     | 170 | VAL  | CB-CA-C | -7.49 | 101.89      | 112.22   |
| 1   | H     | 178 | ILE  | N-CA-C  | -7.46 | 96.73       | 107.77   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 128 | TYR  | CA-CB-CG   | -7.44 | 100.50      | 113.90   |
| 1   | B     | 250 | ILE  | CB-CA-C    | -7.42 | 100.10      | 111.31   |
| 1   | F     | 250 | ILE  | CB-CA-C    | -7.41 | 100.11      | 111.31   |
| 1   | C     | 250 | ILE  | CB-CA-C    | -7.41 | 100.12      | 111.31   |
| 1   | D     | 250 | ILE  | CB-CA-C    | -7.41 | 100.12      | 111.31   |
| 1   | H     | 250 | ILE  | CB-CA-C    | -7.41 | 100.12      | 111.31   |
| 1   | E     | 250 | ILE  | CB-CA-C    | -7.40 | 100.13      | 111.31   |
| 1   | H     | 162 | ARG  | CA-C-N     | -7.40 | 113.22      | 122.84   |
| 1   | H     | 162 | ARG  | C-N-CA     | -7.40 | 113.22      | 122.84   |
| 1   | A     | 250 | ILE  | CB-CA-C    | -7.40 | 100.14      | 111.31   |
| 1   | G     | 250 | ILE  | CB-CA-C    | -7.39 | 100.14      | 111.31   |
| 1   | A     | 170 | VAL  | O-C-N      | 7.39  | 129.44      | 121.83   |
| 1   | D     | 176 | ASP  | N-CA-C     | 7.31  | 119.25      | 111.28   |
| 1   | G     | 61  | ASN  | C-N-CD     | -7.26 | 95.24       | 125.00   |
| 1   | E     | 23  | TYR  | CG-CD1-CE1 | -7.21 | 110.38      | 121.20   |
| 1   | B     | 249 | GLU  | N-CA-C     | 7.13  | 120.85      | 112.72   |
| 1   | A     | 249 | GLU  | N-CA-C     | 7.13  | 120.85      | 112.72   |
| 1   | C     | 249 | GLU  | N-CA-C     | 7.13  | 120.85      | 112.72   |
| 1   | E     | 249 | GLU  | N-CA-C     | 7.13  | 120.85      | 112.72   |
| 1   | H     | 249 | GLU  | N-CA-C     | 7.13  | 120.85      | 112.72   |
| 1   | G     | 22  | ARG  | N-CA-C     | 7.12  | 120.45      | 111.69   |
| 1   | F     | 249 | GLU  | N-CA-C     | 7.12  | 120.83      | 112.72   |
| 1   | D     | 249 | GLU  | N-CA-C     | 7.12  | 120.83      | 112.72   |
| 1   | G     | 249 | GLU  | N-CA-C     | 7.09  | 120.80      | 112.72   |
| 1   | A     | 271 | LYS  | O-C-N      | 7.04  | 131.49      | 122.33   |
| 1   | D     | 90  | THR  | N-CA-CB    | 7.00  | 122.82      | 110.37   |
| 1   | C     | 90  | THR  | N-CA-CB    | 6.99  | 122.81      | 110.37   |
| 1   | E     | 90  | THR  | N-CA-CB    | 6.98  | 122.79      | 110.37   |
| 1   | A     | 90  | THR  | N-CA-CB    | 6.97  | 122.78      | 110.37   |
| 1   | F     | 90  | THR  | N-CA-CB    | 6.97  | 122.78      | 110.37   |
| 1   | G     | 90  | THR  | N-CA-CB    | 6.97  | 122.78      | 110.37   |
| 1   | B     | 90  | THR  | N-CA-CB    | 6.96  | 122.77      | 110.37   |
| 1   | H     | 90  | THR  | N-CA-CB    | 6.96  | 122.76      | 110.37   |
| 1   | B     | 221 | ARG  | N-CA-C     | 6.94  | 121.19      | 113.21   |
| 1   | F     | 57  | SER  | N-CA-C     | 6.93  | 120.74      | 110.48   |
| 1   | D     | 27  | LEU  | CA-CB-CG   | 6.93  | 140.55      | 116.30   |
| 1   | D     | 265 | ARG  | CG-CD-NE   | -6.90 | 96.82       | 112.00   |
| 1   | F     | 22  | ARG  | N-CA-C     | 6.72  | 121.31      | 113.18   |
| 1   | B     | 56  | THR  | N-CA-C     | 6.68  | 119.39      | 111.71   |
| 1   | G     | 61  | ASN  | CA-C-N     | 6.68  | 128.19      | 119.84   |
| 1   | G     | 61  | ASN  | C-N-CA     | 6.68  | 128.19      | 119.84   |
| 1   | H     | 162 | ARG  | N-CA-C     | 6.63  | 120.09      | 108.75   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 24  | HIS  | CB-CA-C | 6.61  | 124.32      | 110.45   |
| 1   | E     | 171 | ALA  | N-CA-C  | -6.61 | 104.08      | 111.28   |
| 1   | A     | 162 | ARG  | CA-C-N  | -6.54 | 114.34      | 122.84   |
| 1   | A     | 162 | ARG  | C-N-CA  | -6.54 | 114.34      | 122.84   |
| 1   | H     | 31  | ASP  | CA-C-N  | -6.46 | 114.77      | 123.10   |
| 1   | H     | 31  | ASP  | C-N-CA  | -6.46 | 114.77      | 123.10   |
| 1   | D     | 225 | ASN  | CA-C-O  | 6.45  | 126.53      | 119.24   |
| 1   | H     | 59  | PRO  | N-CA-C  | 6.40  | 120.88      | 111.03   |
| 1   | F     | 44  | THR  | N-CA-C  | -6.38 | 104.40      | 111.36   |
| 1   | D     | 44  | THR  | N-CA-C  | -6.38 | 104.41      | 111.36   |
| 1   | H     | 44  | THR  | N-CA-C  | -6.37 | 104.42      | 111.36   |
| 1   | B     | 44  | THR  | N-CA-C  | -6.36 | 104.43      | 111.36   |
| 1   | A     | 44  | THR  | N-CA-C  | -6.36 | 104.43      | 111.36   |
| 1   | E     | 44  | THR  | N-CA-C  | -6.35 | 104.44      | 111.36   |
| 1   | A     | 196 | GLN  | N-CA-C  | 6.35  | 116.30      | 108.11   |
| 1   | C     | 44  | THR  | N-CA-C  | -6.33 | 104.46      | 111.36   |
| 1   | C     | 196 | GLN  | N-CA-C  | 6.33  | 116.27      | 108.11   |
| 1   | H     | 196 | GLN  | N-CA-C  | 6.33  | 116.27      | 108.11   |
| 1   | F     | 196 | GLN  | N-CA-C  | 6.32  | 116.26      | 108.11   |
| 1   | G     | 44  | THR  | N-CA-C  | -6.32 | 104.47      | 111.36   |
| 1   | E     | 196 | GLN  | N-CA-C  | 6.32  | 116.26      | 108.11   |
| 1   | B     | 196 | GLN  | N-CA-C  | 6.31  | 116.25      | 108.11   |
| 1   | G     | 196 | GLN  | N-CA-C  | 6.31  | 116.25      | 108.11   |
| 1   | D     | 196 | GLN  | N-CA-C  | 6.30  | 116.23      | 108.11   |
| 1   | C     | 126 | PRO  | N-CA-C  | 6.29  | 122.02      | 113.84   |
| 1   | B     | 198 | GLY  | N-CA-C  | -6.23 | 98.41       | 113.18   |
| 1   | C     | 198 | GLY  | N-CA-C  | -6.23 | 98.42       | 113.18   |
| 1   | D     | 27  | LEU  | N-CA-C  | 6.22  | 120.25      | 107.37   |
| 1   | G     | 198 | GLY  | N-CA-C  | -6.22 | 98.43       | 113.18   |
| 1   | F     | 198 | GLY  | N-CA-C  | -6.22 | 98.44       | 113.18   |
| 1   | B     | 125 | PHE  | CB-CA-C | -6.22 | 99.36       | 111.29   |
| 1   | E     | 198 | GLY  | N-CA-C  | -6.21 | 98.45       | 113.18   |
| 1   | H     | 198 | GLY  | N-CA-C  | -6.21 | 98.45       | 113.18   |
| 1   | A     | 198 | GLY  | N-CA-C  | -6.21 | 98.47       | 113.18   |
| 1   | H     | 318 | ILE  | CB-CA-C | -6.21 | 104.56      | 110.70   |
| 1   | D     | 198 | GLY  | N-CA-C  | -6.20 | 98.48       | 113.18   |
| 1   | C     | 23  | TYR  | CB-CA-C | -6.20 | 103.22      | 112.09   |
| 1   | F     | 224 | TYR  | CB-CA-C | -6.19 | 102.77      | 111.80   |
| 1   | E     | 318 | ILE  | CB-CA-C | -6.18 | 104.58      | 110.70   |
| 1   | D     | 318 | ILE  | CB-CA-C | -6.18 | 104.59      | 110.70   |
| 1   | F     | 318 | ILE  | CB-CA-C | -6.17 | 104.60      | 110.70   |
| 1   | F     | 265 | ARG  | CA-C-O  | 6.17  | 127.08      | 120.24   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 318 | ILE  | CB-CA-C  | -6.16 | 104.60      | 110.70   |
| 1   | B     | 318 | ILE  | CB-CA-C  | -6.16 | 104.60      | 110.70   |
| 1   | C     | 194 | LEU  | CA-CB-CG | -6.16 | 94.75       | 116.30   |
| 1   | D     | 194 | LEU  | CA-CB-CG | -6.16 | 94.75       | 116.30   |
| 1   | A     | 194 | LEU  | CA-CB-CG | -6.15 | 94.77       | 116.30   |
| 1   | E     | 194 | LEU  | CA-CB-CG | -6.15 | 94.77       | 116.30   |
| 1   | B     | 194 | LEU  | CA-CB-CG | -6.15 | 94.77       | 116.30   |
| 1   | F     | 194 | LEU  | CA-CB-CG | -6.15 | 94.77       | 116.30   |
| 1   | H     | 194 | LEU  | CA-CB-CG | -6.15 | 94.79       | 116.30   |
| 1   | G     | 194 | LEU  | CA-CB-CG | -6.14 | 94.79       | 116.30   |
| 1   | G     | 274 | LYS  | N-CA-C   | -6.14 | 100.00      | 109.76   |
| 1   | C     | 318 | ILE  | CB-CA-C  | -6.14 | 104.62      | 110.70   |
| 1   | A     | 274 | LYS  | N-CA-C   | -6.14 | 100.00      | 109.76   |
| 1   | E     | 274 | LYS  | N-CA-C   | -6.14 | 100.00      | 109.76   |
| 1   | G     | 318 | ILE  | CB-CA-C  | -6.14 | 104.62      | 110.70   |
| 1   | B     | 274 | LYS  | N-CA-C   | -6.13 | 100.02      | 109.76   |
| 1   | A     | 288 | GLN  | N-CA-C   | -6.12 | 99.09       | 108.76   |
| 1   | C     | 274 | LYS  | N-CA-C   | -6.12 | 100.03      | 109.76   |
| 1   | A     | 253 | ILE  | O-C-N    | -6.10 | 115.93      | 121.91   |
| 1   | F     | 176 | ASP  | CA-C-N   | -6.10 | 112.51      | 122.57   |
| 1   | F     | 176 | ASP  | C-N-CA   | -6.10 | 112.51      | 122.57   |
| 1   | H     | 217 | HIS  | CB-CA-C  | -6.08 | 100.78      | 110.14   |
| 1   | G     | 29  | PRO  | N-CA-C   | 6.07  | 124.97      | 112.47   |
| 1   | F     | 23  | TYR  | CA-C-N   | -6.05 | 111.01      | 121.66   |
| 1   | F     | 23  | TYR  | C-N-CA   | -6.05 | 111.01      | 121.66   |
| 1   | B     | 288 | GLN  | N-CA-C   | -6.04 | 99.50       | 108.99   |
| 1   | E     | 218 | ASP  | N-CA-C   | -6.04 | 98.88       | 108.73   |
| 1   | H     | 162 | ARG  | CG-CD-NE | -6.02 | 98.75       | 112.00   |
| 1   | E     | 31  | ASP  | N-CA-CB  | -6.00 | 100.80      | 110.69   |
| 1   | G     | 86  | ASN  | N-CA-C   | -5.99 | 105.23      | 112.54   |
| 1   | C     | 86  | ASN  | N-CA-C   | -5.99 | 105.23      | 112.54   |
| 1   | B     | 162 | ARG  | N-CA-CB  | -5.99 | 100.75      | 110.81   |
| 1   | A     | 86  | ASN  | N-CA-C   | -5.98 | 105.24      | 112.54   |
| 1   | B     | 86  | ASN  | N-CA-C   | -5.98 | 105.25      | 112.54   |
| 1   | D     | 86  | ASN  | N-CA-C   | -5.98 | 105.25      | 112.54   |
| 1   | H     | 86  | ASN  | N-CA-C   | -5.97 | 105.25      | 112.54   |
| 1   | D     | 129 | ARG  | CB-CA-C  | -5.97 | 100.19      | 109.80   |
| 1   | E     | 86  | ASN  | N-CA-C   | -5.96 | 105.27      | 112.54   |
| 1   | F     | 86  | ASN  | N-CA-C   | -5.95 | 105.28      | 112.54   |
| 1   | D     | 24  | HIS  | N-CA-C   | 5.94  | 117.83      | 111.36   |
| 1   | H     | 202 | ILE  | CB-CA-C  | -5.93 | 99.81       | 110.48   |
| 1   | D     | 285 | VAL  | N-CA-C   | 5.92  | 117.26      | 109.21   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 225 | ASN  | N-CA-C   | -5.92 | 106.40      | 113.97   |
| 1   | A     | 202 | ILE  | CB-CA-C  | -5.91 | 99.84       | 110.48   |
| 1   | G     | 126 | PRO  | N-CA-C   | 5.91  | 122.40      | 114.18   |
| 1   | F     | 202 | ILE  | CB-CA-C  | -5.91 | 99.84       | 110.48   |
| 1   | B     | 285 | VAL  | N-CA-C   | 5.90  | 117.24      | 109.21   |
| 1   | G     | 202 | ILE  | CB-CA-C  | -5.90 | 99.86       | 110.48   |
| 1   | C     | 202 | ILE  | CB-CA-C  | -5.90 | 99.86       | 110.48   |
| 1   | F     | 285 | VAL  | N-CA-C   | 5.89  | 117.22      | 109.21   |
| 1   | H     | 285 | VAL  | N-CA-C   | 5.89  | 117.23      | 109.21   |
| 1   | D     | 202 | ILE  | CB-CA-C  | -5.89 | 99.88       | 110.48   |
| 1   | B     | 202 | ILE  | CB-CA-C  | -5.89 | 99.88       | 110.48   |
| 1   | C     | 285 | VAL  | N-CA-C   | 5.88  | 117.21      | 109.21   |
| 1   | E     | 285 | VAL  | N-CA-C   | 5.88  | 117.21      | 109.21   |
| 1   | E     | 202 | ILE  | CB-CA-C  | -5.88 | 99.89       | 110.48   |
| 1   | G     | 87  | MET  | N-CA-C   | -5.88 | 106.09      | 113.20   |
| 1   | G     | 285 | VAL  | N-CA-C   | 5.88  | 117.20      | 109.21   |
| 1   | A     | 285 | VAL  | N-CA-C   | 5.87  | 117.20      | 109.21   |
| 1   | C     | 128 | TYR  | CA-CB-CG | -5.87 | 103.33      | 113.90   |
| 1   | H     | 208 | PRO  | CB-CA-C  | -5.86 | 103.06      | 112.21   |
| 1   | C     | 208 | PRO  | CB-CA-C  | -5.85 | 103.08      | 112.21   |
| 1   | F     | 208 | PRO  | CB-CA-C  | -5.85 | 103.08      | 112.21   |
| 1   | G     | 208 | PRO  | CB-CA-C  | -5.85 | 103.09      | 112.21   |
| 1   | D     | 87  | MET  | N-CA-C   | -5.84 | 106.13      | 113.20   |
| 1   | A     | 87  | MET  | N-CA-C   | -5.84 | 106.13      | 113.20   |
| 1   | E     | 87  | MET  | N-CA-C   | -5.84 | 106.13      | 113.20   |
| 1   | H     | 87  | MET  | N-CA-C   | -5.84 | 106.14      | 113.20   |
| 1   | B     | 87  | MET  | N-CA-C   | -5.83 | 106.15      | 113.20   |
| 1   | A     | 208 | PRO  | CB-CA-C  | -5.83 | 103.12      | 112.21   |
| 1   | D     | 208 | PRO  | CB-CA-C  | -5.82 | 103.13      | 112.21   |
| 1   | F     | 87  | MET  | N-CA-C   | -5.82 | 106.16      | 113.20   |
| 1   | B     | 60  | SER  | N-CA-C   | -5.82 | 106.03      | 113.01   |
| 1   | B     | 208 | PRO  | CB-CA-C  | -5.81 | 103.14      | 112.21   |
| 1   | E     | 208 | PRO  | CB-CA-C  | -5.81 | 103.15      | 112.21   |
| 1   | A     | 224 | TYR  | CA-C-N   | -5.80 | 110.19      | 120.99   |
| 1   | A     | 224 | TYR  | C-N-CA   | -5.80 | 110.19      | 120.99   |
| 1   | D     | 126 | PRO  | N-CA-C   | 5.79  | 124.41      | 112.47   |
| 1   | C     | 87  | MET  | N-CA-C   | -5.79 | 106.19      | 113.20   |
| 1   | F     | 83  | ASN  | N-CA-C   | 5.78  | 120.61      | 113.50   |
| 1   | G     | 83  | ASN  | N-CA-C   | 5.77  | 120.60      | 113.50   |
| 1   | A     | 83  | ASN  | N-CA-C   | 5.77  | 120.59      | 113.50   |
| 1   | C     | 162 | ARG  | CG-CD-NE | -5.76 | 99.33       | 112.00   |
| 1   | D     | 83  | ASN  | N-CA-C   | 5.76  | 120.59      | 113.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 63  | GLN  | N-CA-C   | -5.76 | 105.14      | 111.82   |
| 1   | B     | 83  | ASN  | N-CA-C   | 5.76  | 120.58      | 113.50   |
| 1   | E     | 83  | ASN  | N-CA-C   | 5.75  | 120.57      | 113.50   |
| 1   | H     | 83  | ASN  | N-CA-C   | 5.74  | 120.56      | 113.50   |
| 1   | C     | 83  | ASN  | N-CA-C   | 5.74  | 120.56      | 113.50   |
| 1   | D     | 125 | PHE  | C-N-CD   | -5.73 | 101.52      | 125.00   |
| 1   | D     | 274 | LYS  | N-CA-C   | -5.72 | 99.97       | 109.46   |
| 1   | H     | 274 | LYS  | N-CA-C   | -5.71 | 99.97       | 109.46   |
| 1   | F     | 274 | LYS  | N-CA-C   | -5.69 | 100.01      | 109.46   |
| 1   | C     | 162 | ARG  | CA-C-N   | -5.69 | 115.44      | 122.84   |
| 1   | C     | 162 | ARG  | C-N-CA   | -5.69 | 115.44      | 122.84   |
| 1   | E     | 177 | VAL  | CB-CA-C  | -5.69 | 101.74      | 110.50   |
| 1   | F     | 129 | ARG  | CA-CB-CG | 5.68  | 125.47      | 114.10   |
| 1   | F     | 225 | ASN  | N-CA-C   | -5.65 | 106.74      | 113.97   |
| 1   | D     | 74  | TYR  | N-CA-C   | -5.60 | 104.56      | 111.33   |
| 1   | G     | 218 | ASP  | N-CA-C   | -5.59 | 100.07      | 108.96   |
| 1   | F     | 74  | TYR  | N-CA-C   | -5.57 | 104.59      | 111.33   |
| 1   | H     | 74  | TYR  | N-CA-C   | -5.57 | 104.59      | 111.33   |
| 1   | E     | 74  | TYR  | N-CA-C   | -5.57 | 104.60      | 111.33   |
| 1   | G     | 217 | HIS  | CB-CA-C  | -5.57 | 103.06      | 110.79   |
| 1   | B     | 74  | TYR  | N-CA-C   | -5.56 | 104.60      | 111.33   |
| 1   | F     | 64  | GLU  | N-CA-C   | 5.56  | 117.03      | 110.97   |
| 1   | A     | 175 | ALA  | CA-C-N   | -5.55 | 111.65      | 121.81   |
| 1   | A     | 175 | ALA  | C-N-CA   | -5.55 | 111.65      | 121.81   |
| 1   | E     | 254 | GLN  | CB-CA-C  | -5.55 | 101.93      | 110.81   |
| 1   | G     | 64  | GLU  | CA-C-N   | -5.55 | 111.09      | 120.58   |
| 1   | G     | 64  | GLU  | C-N-CA   | -5.55 | 111.09      | 120.58   |
| 1   | C     | 178 | ILE  | CA-C-O   | -5.54 | 114.67      | 120.27   |
| 1   | C     | 74  | TYR  | N-CA-C   | -5.54 | 104.62      | 111.33   |
| 1   | C     | 19  | ILE  | N-CA-C   | -5.54 | 105.32      | 110.53   |
| 1   | G     | 19  | ILE  | N-CA-C   | -5.54 | 105.32      | 110.53   |
| 1   | A     | 74  | TYR  | N-CA-C   | -5.54 | 104.63      | 111.33   |
| 1   | G     | 173 | GLY  | N-CA-C   | 5.53  | 120.86      | 114.16   |
| 1   | B     | 19  | ILE  | N-CA-C   | -5.53 | 105.33      | 110.53   |
| 1   | G     | 74  | TYR  | N-CA-C   | -5.53 | 104.64      | 111.33   |
| 1   | A     | 19  | ILE  | N-CA-C   | -5.52 | 105.34      | 110.53   |
| 1   | F     | 19  | ILE  | N-CA-C   | -5.52 | 105.34      | 110.53   |
| 1   | B     | 257 | ASN  | CA-C-N   | -5.52 | 111.29      | 120.68   |
| 1   | B     | 257 | ASN  | C-N-CA   | -5.52 | 111.29      | 120.68   |
| 1   | H     | 19  | ILE  | N-CA-C   | -5.51 | 105.35      | 110.53   |
| 1   | F     | 127 | ASP  | CB-CA-C  | 5.51  | 121.83      | 110.31   |
| 1   | F     | 128 | TYR  | N-CA-C   | 5.51  | 118.61      | 110.46   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 19  | ILE  | N-CA-C  | -5.51 | 105.36      | 110.53   |
| 1   | E     | 257 | ASN  | CA-C-N  | -5.50 | 111.33      | 120.68   |
| 1   | E     | 257 | ASN  | C-N-CA  | -5.50 | 111.33      | 120.68   |
| 1   | E     | 19  | ILE  | N-CA-C  | -5.50 | 105.36      | 110.53   |
| 1   | G     | 257 | ASN  | CA-C-N  | -5.50 | 111.33      | 120.68   |
| 1   | G     | 257 | ASN  | C-N-CA  | -5.50 | 111.33      | 120.68   |
| 1   | H     | 257 | ASN  | CA-C-N  | -5.50 | 111.33      | 120.68   |
| 1   | H     | 257 | ASN  | C-N-CA  | -5.50 | 111.33      | 120.68   |
| 1   | C     | 257 | ASN  | CA-C-N  | -5.50 | 111.33      | 120.68   |
| 1   | C     | 257 | ASN  | C-N-CA  | -5.50 | 111.33      | 120.68   |
| 1   | C     | 196 | GLN  | CB-CA-C | -5.49 | 102.45      | 109.92   |
| 1   | F     | 257 | ASN  | CA-C-N  | -5.49 | 111.35      | 120.68   |
| 1   | F     | 257 | ASN  | C-N-CA  | -5.49 | 111.35      | 120.68   |
| 1   | A     | 257 | ASN  | CA-C-N  | -5.49 | 111.35      | 120.68   |
| 1   | A     | 257 | ASN  | C-N-CA  | -5.49 | 111.35      | 120.68   |
| 1   | D     | 257 | ASN  | CA-C-N  | -5.48 | 111.36      | 120.68   |
| 1   | D     | 257 | ASN  | C-N-CA  | -5.48 | 111.36      | 120.68   |
| 1   | A     | 27  | LEU  | CB-CA-C | -5.48 | 103.17      | 110.79   |
| 1   | B     | 337 | ARG  | N-CA-C  | -5.48 | 106.37      | 113.16   |
| 1   | E     | 161 | LEU  | CA-C-N  | -5.46 | 112.31      | 121.75   |
| 1   | E     | 161 | LEU  | C-N-CA  | -5.46 | 112.31      | 121.75   |
| 1   | F     | 337 | ARG  | N-CA-C  | -5.46 | 106.39      | 113.16   |
| 1   | H     | 196 | GLN  | CB-CA-C | -5.46 | 102.50      | 109.92   |
| 1   | A     | 196 | GLN  | CB-CA-C | -5.45 | 102.50      | 109.92   |
| 1   | A     | 337 | ARG  | N-CA-C  | -5.45 | 106.40      | 113.16   |
| 1   | G     | 337 | ARG  | N-CA-C  | -5.45 | 106.40      | 113.16   |
| 1   | E     | 337 | ARG  | N-CA-C  | -5.45 | 106.41      | 113.16   |
| 1   | G     | 208 | PRO  | CA-C-N  | -5.45 | 110.39      | 121.18   |
| 1   | G     | 208 | PRO  | C-N-CA  | -5.45 | 110.39      | 121.18   |
| 1   | E     | 196 | GLN  | CB-CA-C | -5.45 | 102.51      | 109.92   |
| 1   | C     | 337 | ARG  | N-CA-C  | -5.45 | 106.41      | 113.16   |
| 1   | F     | 196 | GLN  | CB-CA-C | -5.45 | 102.52      | 109.92   |
| 1   | H     | 337 | ARG  | N-CA-C  | -5.45 | 106.41      | 113.16   |
| 1   | G     | 64  | GLU  | N-CA-C  | -5.44 | 104.74      | 111.33   |
| 1   | H     | 176 | ASP  | N-CA-C  | 5.44  | 119.09      | 112.23   |
| 1   | D     | 196 | GLN  | CB-CA-C | -5.44 | 102.52      | 109.92   |
| 1   | E     | 271 | LYS  | CA-C-N  | -5.44 | 113.99      | 122.37   |
| 1   | E     | 271 | LYS  | C-N-CA  | -5.44 | 113.99      | 122.37   |
| 1   | G     | 196 | GLN  | CB-CA-C | -5.44 | 102.52      | 109.92   |
| 1   | B     | 208 | PRO  | CA-C-N  | -5.44 | 110.41      | 121.18   |
| 1   | B     | 208 | PRO  | C-N-CA  | -5.44 | 110.41      | 121.18   |
| 1   | E     | 30  | LEU  | N-CA-C  | 5.44  | 117.17      | 108.41   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 162 | ARG  | CA-C-O  | -5.44 | 115.46      | 121.33   |
| 1   | D     | 337 | ARG  | N-CA-C  | -5.43 | 106.42      | 113.16   |
| 1   | B     | 196 | GLN  | CB-CA-C | -5.43 | 102.53      | 109.92   |
| 1   | C     | 225 | ASN  | CA-C-O  | 5.42  | 124.87      | 118.90   |
| 1   | F     | 208 | PRO  | CA-C-N  | -5.42 | 110.46      | 121.18   |
| 1   | F     | 208 | PRO  | C-N-CA  | -5.42 | 110.46      | 121.18   |
| 1   | E     | 208 | PRO  | CA-C-N  | -5.42 | 110.46      | 121.18   |
| 1   | E     | 208 | PRO  | C-N-CA  | -5.42 | 110.46      | 121.18   |
| 1   | A     | 208 | PRO  | CA-C-N  | -5.41 | 110.47      | 121.18   |
| 1   | A     | 208 | PRO  | C-N-CA  | -5.41 | 110.47      | 121.18   |
| 1   | H     | 208 | PRO  | CA-C-N  | -5.41 | 110.48      | 121.18   |
| 1   | H     | 208 | PRO  | C-N-CA  | -5.41 | 110.48      | 121.18   |
| 1   | D     | 208 | PRO  | CA-C-N  | -5.40 | 110.48      | 121.18   |
| 1   | D     | 208 | PRO  | C-N-CA  | -5.40 | 110.48      | 121.18   |
| 1   | E     | 125 | PHE  | N-CA-C  | -5.40 | 96.75       | 108.74   |
| 1   | C     | 208 | PRO  | CA-C-N  | -5.39 | 110.50      | 121.18   |
| 1   | C     | 208 | PRO  | C-N-CA  | -5.39 | 110.50      | 121.18   |
| 1   | C     | 178 | ILE  | N-CA-C  | -5.38 | 99.81       | 107.77   |
| 1   | C     | 288 | GLN  | N-CA-C  | -5.38 | 100.89      | 109.07   |
| 1   | A     | 217 | HIS  | CA-C-N  | -5.37 | 115.30      | 122.72   |
| 1   | A     | 217 | HIS  | C-N-CA  | -5.37 | 115.30      | 122.72   |
| 1   | F     | 43  | THR  | N-CA-C  | 5.36  | 117.75      | 110.35   |
| 1   | A     | 43  | THR  | N-CA-C  | 5.36  | 117.75      | 110.35   |
| 1   | H     | 23  | TYR  | CA-C-N  | -5.36 | 111.30      | 121.54   |
| 1   | H     | 23  | TYR  | C-N-CA  | -5.36 | 111.30      | 121.54   |
| 1   | G     | 223 | ILE  | CB-CA-C | -5.35 | 103.70      | 111.68   |
| 1   | C     | 43  | THR  | N-CA-C  | 5.35  | 117.74      | 110.35   |
| 1   | F     | 59  | PRO  | N-CA-C  | 5.35  | 119.27      | 111.03   |
| 1   | D     | 43  | THR  | N-CA-C  | 5.35  | 117.73      | 110.35   |
| 1   | F     | 126 | PRO  | CA-C-N  | -5.35 | 111.79      | 120.72   |
| 1   | F     | 126 | PRO  | C-N-CA  | -5.35 | 111.79      | 120.72   |
| 1   | E     | 43  | THR  | N-CA-C  | 5.33  | 117.71      | 110.35   |
| 1   | H     | 43  | THR  | N-CA-C  | 5.33  | 117.71      | 110.35   |
| 1   | B     | 43  | THR  | N-CA-C  | 5.32  | 117.69      | 110.35   |
| 1   | G     | 63  | GLN  | N-CA-CB | -5.32 | 101.56      | 110.39   |
| 1   | F     | 174 | GLY  | CA-C-O  | 5.32  | 123.77      | 118.77   |
| 1   | B     | 219 | LEU  | N-CA-C  | 5.31  | 118.55      | 111.75   |
| 1   | C     | 252 | ASN  | N-CA-CB | -5.30 | 101.78      | 110.52   |
| 1   | G     | 43  | THR  | N-CA-C  | 5.30  | 117.66      | 110.35   |
| 1   | H     | 252 | ASN  | N-CA-CB | -5.30 | 101.78      | 110.52   |
| 1   | G     | 252 | ASN  | N-CA-CB | -5.30 | 101.78      | 110.52   |
| 1   | D     | 252 | ASN  | N-CA-CB | -5.28 | 101.81      | 110.52   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 252 | ASN  | N-CA-CB   | -5.28 | 101.81      | 110.52   |
| 1   | C     | 74  | TYR  | CA-C-N    | -5.28 | 113.68      | 120.65   |
| 1   | C     | 74  | TYR  | C-N-CA    | -5.28 | 113.68      | 120.65   |
| 1   | F     | 252 | ASN  | N-CA-CB   | -5.28 | 101.81      | 110.52   |
| 1   | B     | 252 | ASN  | N-CA-CB   | -5.28 | 101.82      | 110.52   |
| 1   | D     | 22  | ARG  | CA-C-N    | -5.27 | 113.14      | 122.26   |
| 1   | D     | 22  | ARG  | C-N-CA    | -5.27 | 113.14      | 122.26   |
| 1   | D     | 205 | VAL  | N-CA-CB   | -5.27 | 103.58      | 112.44   |
| 1   | A     | 252 | ASN  | N-CA-CB   | -5.27 | 101.82      | 110.52   |
| 1   | C     | 219 | LEU  | N-CA-C    | 5.27  | 117.02      | 111.28   |
| 1   | H     | 205 | VAL  | N-CA-CB   | -5.25 | 103.62      | 112.44   |
| 1   | A     | 205 | VAL  | N-CA-CB   | -5.25 | 103.62      | 112.44   |
| 1   | B     | 162 | ARG  | CA-C-O    | -5.25 | 113.82      | 120.28   |
| 1   | G     | 205 | VAL  | N-CA-CB   | -5.25 | 103.62      | 112.44   |
| 1   | B     | 205 | VAL  | N-CA-CB   | -5.25 | 103.63      | 112.44   |
| 1   | E     | 205 | VAL  | N-CA-CB   | -5.25 | 103.63      | 112.44   |
| 1   | D     | 128 | TYR  | N-CA-C    | 5.24  | 117.30      | 110.43   |
| 1   | E     | 127 | ASP  | CA-C-N    | -5.24 | 113.36      | 122.64   |
| 1   | E     | 127 | ASP  | C-N-CA    | -5.24 | 113.36      | 122.64   |
| 1   | F     | 125 | PHE  | CB-CA-C   | -5.24 | 104.80      | 110.98   |
| 1   | E     | 223 | ILE  | CB-CA-C   | -5.24 | 103.90      | 111.34   |
| 1   | F     | 205 | VAL  | N-CA-CB   | -5.24 | 103.64      | 112.44   |
| 1   | C     | 205 | VAL  | N-CA-CB   | -5.23 | 103.66      | 112.44   |
| 1   | C     | 95  | TYR  | N-CA-C    | 5.21  | 118.31      | 109.76   |
| 1   | B     | 124 | MET  | N-CA-C    | -5.20 | 105.79      | 111.82   |
| 1   | G     | 286 | ARG  | NE-CZ-NH1 | -5.18 | 116.32      | 121.50   |
| 1   | H     | 221 | ARG  | NE-CZ-NH2 | 5.18  | 123.86      | 119.20   |
| 1   | B     | 95  | TYR  | N-CA-C    | 5.17  | 118.25      | 109.76   |
| 1   | D     | 95  | TYR  | N-CA-C    | 5.17  | 118.24      | 109.76   |
| 1   | G     | 172 | ARG  | N-CA-C    | 5.17  | 119.90      | 111.37   |
| 1   | E     | 95  | TYR  | N-CA-C    | 5.17  | 118.23      | 109.76   |
| 1   | G     | 95  | TYR  | N-CA-C    | 5.17  | 118.23      | 109.76   |
| 1   | A     | 218 | ASP  | N-CA-CB   | 5.16  | 118.84      | 110.43   |
| 1   | H     | 95  | TYR  | N-CA-C    | 5.16  | 118.22      | 109.76   |
| 1   | A     | 95  | TYR  | N-CA-C    | 5.16  | 118.21      | 109.76   |
| 1   | F     | 74  | TYR  | CA-C-N    | -5.15 | 113.62      | 120.63   |
| 1   | F     | 74  | TYR  | C-N-CA    | -5.15 | 113.62      | 120.63   |
| 1   | F     | 248 | ASN  | CA-C-N    | -5.15 | 114.44      | 122.73   |
| 1   | F     | 248 | ASN  | C-N-CA    | -5.15 | 114.44      | 122.73   |
| 1   | F     | 95  | TYR  | N-CA-C    | 5.15  | 118.20      | 109.76   |
| 1   | B     | 74  | TYR  | CA-C-N    | -5.14 | 113.63      | 120.63   |
| 1   | B     | 74  | TYR  | C-N-CA    | -5.14 | 113.63      | 120.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 62  | PRO  | CA-C-O    | 5.14  | 127.36      | 119.55   |
| 1   | G     | 248 | ASN  | CA-C-N    | -5.14 | 114.45      | 122.73   |
| 1   | G     | 248 | ASN  | C-N-CA    | -5.14 | 114.45      | 122.73   |
| 1   | A     | 124 | MET  | CB-CG-SD  | -5.14 | 97.28       | 112.70   |
| 1   | C     | 58  | GLU  | N-CA-C    | -5.14 | 102.56      | 110.01   |
| 1   | C     | 248 | ASN  | CA-C-N    | -5.14 | 114.46      | 122.73   |
| 1   | C     | 248 | ASN  | C-N-CA    | -5.14 | 114.46      | 122.73   |
| 1   | D     | 286 | ARG  | NE-CZ-NH1 | -5.14 | 116.36      | 121.50   |
| 1   | B     | 248 | ASN  | CA-C-N    | -5.13 | 114.46      | 122.73   |
| 1   | B     | 248 | ASN  | C-N-CA    | -5.13 | 114.46      | 122.73   |
| 1   | E     | 248 | ASN  | CA-C-N    | -5.13 | 114.47      | 122.73   |
| 1   | E     | 248 | ASN  | C-N-CA    | -5.13 | 114.47      | 122.73   |
| 1   | A     | 248 | ASN  | CA-C-N    | -5.13 | 114.47      | 122.73   |
| 1   | A     | 248 | ASN  | C-N-CA    | -5.13 | 114.47      | 122.73   |
| 1   | F     | 162 | ARG  | NE-CZ-NH2 | 5.13  | 123.82      | 119.20   |
| 1   | G     | 74  | TYR  | CA-C-N    | -5.13 | 113.66      | 120.63   |
| 1   | G     | 74  | TYR  | C-N-CA    | -5.13 | 113.66      | 120.63   |
| 1   | H     | 248 | ASN  | CA-C-N    | -5.13 | 114.47      | 122.73   |
| 1   | H     | 248 | ASN  | C-N-CA    | -5.13 | 114.47      | 122.73   |
| 1   | E     | 286 | ARG  | NE-CZ-NH1 | -5.12 | 116.38      | 121.50   |
| 1   | C     | 286 | ARG  | NE-CZ-NH1 | -5.12 | 116.38      | 121.50   |
| 1   | F     | 58  | GLU  | CA-C-N    | 5.12  | 125.36      | 119.83   |
| 1   | F     | 58  | GLU  | C-N-CA    | 5.12  | 125.36      | 119.83   |
| 1   | H     | 286 | ARG  | NE-CZ-NH1 | -5.11 | 116.39      | 121.50   |
| 1   | H     | 74  | TYR  | CA-C-N    | -5.11 | 113.68      | 120.63   |
| 1   | H     | 74  | TYR  | C-N-CA    | -5.11 | 113.68      | 120.63   |
| 1   | E     | 74  | TYR  | CA-C-N    | -5.10 | 113.69      | 120.63   |
| 1   | E     | 74  | TYR  | C-N-CA    | -5.10 | 113.69      | 120.63   |
| 1   | D     | 248 | ASN  | CA-C-N    | -5.09 | 114.53      | 122.73   |
| 1   | D     | 248 | ASN  | C-N-CA    | -5.09 | 114.53      | 122.73   |
| 1   | D     | 74  | TYR  | CA-C-N    | -5.09 | 113.71      | 120.63   |
| 1   | D     | 74  | TYR  | C-N-CA    | -5.09 | 113.71      | 120.63   |
| 1   | F     | 2   | ARG  | N-CA-C    | 5.09  | 116.56      | 108.67   |
| 1   | F     | 286 | ARG  | NE-CZ-NH1 | -5.08 | 116.42      | 121.50   |
| 1   | C     | 172 | ARG  | N-CA-C    | -5.08 | 105.74      | 112.34   |
| 1   | A     | 74  | TYR  | CA-C-N    | -5.08 | 113.72      | 120.63   |
| 1   | A     | 74  | TYR  | C-N-CA    | -5.08 | 113.72      | 120.63   |
| 1   | H     | 84  | ALA  | CA-C-N    | -5.08 | 112.25      | 121.14   |
| 1   | H     | 84  | ALA  | C-N-CA    | -5.08 | 112.25      | 121.14   |
| 1   | C     | 275 | ILE  | CB-CA-C   | -5.08 | 104.55      | 111.15   |
| 1   | E     | 275 | ILE  | CB-CA-C   | -5.08 | 104.55      | 111.15   |
| 1   | A     | 286 | ARG  | NE-CZ-NH1 | -5.08 | 116.42      | 121.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 84  | ALA  | CA-C-N    | -5.08 | 112.26      | 121.14   |
| 1   | B     | 84  | ALA  | C-N-CA    | -5.08 | 112.26      | 121.14   |
| 1   | G     | 207 | ALA  | CA-C-N    | 5.07  | 124.86      | 119.28   |
| 1   | G     | 207 | ALA  | C-N-CA    | 5.07  | 124.86      | 119.28   |
| 1   | G     | 275 | ILE  | CB-CA-C   | -5.07 | 104.56      | 111.15   |
| 1   | B     | 286 | ARG  | NE-CZ-NH1 | -5.07 | 116.43      | 121.50   |
| 1   | A     | 275 | ILE  | CB-CA-C   | -5.07 | 104.56      | 111.15   |
| 1   | D     | 84  | ALA  | CA-C-N    | -5.07 | 112.28      | 121.14   |
| 1   | D     | 84  | ALA  | C-N-CA    | -5.07 | 112.28      | 121.14   |
| 1   | E     | 84  | ALA  | CA-C-N    | -5.07 | 112.28      | 121.14   |
| 1   | E     | 84  | ALA  | C-N-CA    | -5.07 | 112.28      | 121.14   |
| 1   | C     | 207 | ALA  | CA-C-N    | 5.06  | 124.85      | 119.28   |
| 1   | C     | 207 | ALA  | C-N-CA    | 5.06  | 124.85      | 119.28   |
| 1   | F     | 275 | ILE  | CB-CA-C   | -5.06 | 104.57      | 111.15   |
| 1   | H     | 207 | ALA  | CA-C-N    | 5.06  | 124.85      | 119.28   |
| 1   | H     | 207 | ALA  | C-N-CA    | 5.06  | 124.85      | 119.28   |
| 1   | B     | 171 | ALA  | N-CA-C    | -5.06 | 105.95      | 111.82   |
| 1   | D     | 207 | ALA  | CA-C-N    | 5.06  | 124.85      | 119.28   |
| 1   | D     | 207 | ALA  | C-N-CA    | 5.06  | 124.85      | 119.28   |
| 1   | C     | 84  | ALA  | CA-C-N    | -5.06 | 112.29      | 121.14   |
| 1   | C     | 84  | ALA  | C-N-CA    | -5.06 | 112.29      | 121.14   |
| 1   | A     | 84  | ALA  | CA-C-N    | -5.06 | 112.29      | 121.14   |
| 1   | A     | 84  | ALA  | C-N-CA    | -5.06 | 112.29      | 121.14   |
| 1   | F     | 84  | ALA  | CA-C-N    | -5.06 | 112.29      | 121.14   |
| 1   | F     | 84  | ALA  | C-N-CA    | -5.06 | 112.29      | 121.14   |
| 1   | D     | 275 | ILE  | CB-CA-C   | -5.05 | 104.58      | 111.15   |
| 1   | G     | 84  | ALA  | CA-C-N    | -5.05 | 112.29      | 121.14   |
| 1   | G     | 84  | ALA  | C-N-CA    | -5.05 | 112.29      | 121.14   |
| 1   | H     | 275 | ILE  | CB-CA-C   | -5.05 | 104.58      | 111.15   |
| 1   | B     | 275 | ILE  | CB-CA-C   | -5.05 | 104.58      | 111.15   |
| 1   | C     | 217 | HIS  | N-CA-C    | 5.05  | 116.62      | 108.34   |
| 1   | D     | 217 | HIS  | N-CA-C    | 5.05  | 116.64      | 108.26   |
| 1   | E     | 207 | ALA  | CA-C-N    | 5.04  | 124.83      | 119.28   |
| 1   | E     | 207 | ALA  | C-N-CA    | 5.04  | 124.83      | 119.28   |
| 1   | B     | 207 | ALA  | CA-C-N    | 5.02  | 124.81      | 119.28   |
| 1   | B     | 207 | ALA  | C-N-CA    | 5.02  | 124.81      | 119.28   |
| 1   | F     | 207 | ALA  | CA-C-N    | 5.02  | 124.80      | 119.28   |
| 1   | F     | 207 | ALA  | C-N-CA    | 5.02  | 124.80      | 119.28   |
| 1   | A     | 207 | ALA  | CA-C-N    | 5.02  | 124.80      | 119.28   |
| 1   | A     | 207 | ALA  | C-N-CA    | 5.02  | 124.80      | 119.28   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | D     | 23  | TYR  | CA   |

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 54  | PRO  | Mainchain |
| 1   | E     | 23  | TYR  | Sidechain |
| 1   | E     | 58  | GLU  | Sidechain |
| 1   | F     | 23  | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2720  | 0        | 2675     | 193     | 1            |
| 1   | B     | 2720  | 0        | 2675     | 208     | 0            |
| 1   | C     | 2720  | 0        | 2675     | 188     | 3            |
| 1   | D     | 2720  | 0        | 2675     | 233     | 1            |
| 1   | E     | 2720  | 0        | 2675     | 202     | 0            |
| 1   | F     | 2720  | 0        | 2675     | 198     | 0            |
| 1   | G     | 2720  | 0        | 2675     | 215     | 0            |
| 1   | H     | 2720  | 0        | 2675     | 202     | 3            |
| 2   | A     | 53    | 0        | 31       | 5       | 0            |
| 2   | B     | 53    | 0        | 31       | 3       | 0            |
| 2   | C     | 53    | 0        | 31       | 4       | 0            |
| 2   | D     | 53    | 0        | 31       | 4       | 0            |
| 2   | E     | 53    | 0        | 31       | 2       | 0            |
| 2   | F     | 53    | 0        | 31       | 4       | 0            |
| 2   | G     | 53    | 0        | 31       | 5       | 0            |
| 2   | H     | 53    | 0        | 31       | 5       | 0            |
| 3   | A     | 15    | 0        | 8        | 0       | 0            |
| 3   | B     | 15    | 0        | 8        | 0       | 0            |
| 3   | C     | 15    | 0        | 8        | 0       | 0            |
| 3   | D     | 15    | 0        | 8        | 0       | 0            |
| 3   | E     | 15    | 0        | 8        | 0       | 0            |
| 3   | F     | 15    | 0        | 8        | 1       | 0            |
| 3   | G     | 15    | 0        | 8        | 0       | 0            |
| 3   | H     | 15    | 0        | 8        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | E     | 15    | 0        | 11       | 7       | 0            |
| 4   | F     | 15    | 0        | 11       | 3       | 0            |
| 5   | A     | 17    | 0        | 0        | 0       | 0            |
| 5   | B     | 7     | 0        | 0        | 3       | 0            |
| 5   | C     | 12    | 0        | 0        | 2       | 0            |
| 5   | D     | 21    | 0        | 0        | 5       | 0            |
| 5   | E     | 16    | 0        | 0        | 0       | 0            |
| 5   | F     | 21    | 0        | 0        | 3       | 0            |
| 5   | G     | 3     | 0        | 0        | 1       | 0            |
| 5   | H     | 10    | 0        | 0        | 0       | 0            |
| All | All   | 22441 | 0        | 21734    | 1590    | 4            |

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 39.

All (1590) 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:D:223:ILE:HG13 | 1:D:224:TYR:CE1  | 1.52                     | 1.42              |
| 1:D:223:ILE:HG13 | 1:D:224:TYR:CD1  | 1.69                     | 1.27              |
| 1:A:253:ILE:HG12 | 1:F:42:PHE:CD1   | 1.73                     | 1.23              |
| 1:E:22:ARG:HH11  | 1:E:22:ARG:HG3   | 1.09                     | 1.14              |
| 1:F:223:ILE:HG12 | 1:F:224:TYR:CD1  | 1.85                     | 1.11              |
| 1:D:216:THR:HG22 | 1:D:226:SER:HB3  | 1.33                     | 1.11              |
| 1:B:201:GLN:HG3  | 1:B:280:THR:HG22 | 1.32                     | 1.10              |
| 1:F:201:GLN:HG3  | 1:F:280:THR:HG22 | 1.32                     | 1.10              |
| 1:B:216:THR:HG22 | 1:B:226:SER:HB3  | 1.33                     | 1.10              |
| 1:A:201:GLN:HG3  | 1:A:280:THR:HG22 | 1.32                     | 1.10              |
| 1:C:201:GLN:HG3  | 1:C:280:THR:HG22 | 1.32                     | 1.09              |
| 1:E:216:THR:HG22 | 1:E:226:SER:HB3  | 1.33                     | 1.09              |
| 1:E:201:GLN:HG3  | 1:E:280:THR:HG22 | 1.32                     | 1.08              |
| 1:F:216:THR:HG22 | 1:F:226:SER:HB3  | 1.33                     | 1.08              |
| 1:C:216:THR:HG22 | 1:C:226:SER:HB3  | 1.33                     | 1.08              |
| 1:D:27:LEU:HD12  | 1:D:30:LEU:HB2   | 1.13                     | 1.08              |
| 1:H:216:THR:HG22 | 1:H:226:SER:HB3  | 1.33                     | 1.08              |
| 1:A:216:THR:HG22 | 1:A:226:SER:HB3  | 1.33                     | 1.08              |
| 1:D:201:GLN:HG3  | 1:D:280:THR:HG22 | 1.32                     | 1.08              |
| 1:D:171:ALA:HB1  | 1:D:303:THR:HG21 | 1.36                     | 1.08              |
| 1:G:201:GLN:HG3  | 1:G:280:THR:HG22 | 1.32                     | 1.07              |
| 1:G:216:THR:HG22 | 1:G:226:SER:HB3  | 1.33                     | 1.06              |
| 1:D:223:ILE:CG1  | 1:D:224:TYR:CE1  | 2.37                     | 1.06              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:201:GLN:HG3  | 1:H:280:THR:HG22 | 1.32                     | 1.05              |
| 1:D:216:THR:CG2  | 1:D:226:SER:HB3  | 1.88                     | 1.04              |
| 1:E:256:HIS:ND1  | 1:E:278:GLU:OE2  | 1.91                     | 1.04              |
| 1:G:216:THR:CG2  | 1:G:226:SER:HB3  | 1.88                     | 1.04              |
| 1:D:256:HIS:ND1  | 1:D:278:GLU:OE2  | 1.91                     | 1.03              |
| 1:G:256:HIS:ND1  | 1:G:278:GLU:OE2  | 1.91                     | 1.03              |
| 1:H:216:THR:CG2  | 1:H:226:SER:HB3  | 1.88                     | 1.03              |
| 1:A:256:HIS:ND1  | 1:A:278:GLU:OE2  | 1.91                     | 1.03              |
| 1:F:216:THR:CG2  | 1:F:226:SER:HB3  | 1.88                     | 1.03              |
| 1:E:216:THR:CG2  | 1:E:226:SER:HB3  | 1.88                     | 1.02              |
| 1:B:256:HIS:ND1  | 1:B:278:GLU:OE2  | 1.91                     | 1.02              |
| 1:F:256:HIS:ND1  | 1:F:278:GLU:OE2  | 1.91                     | 1.02              |
| 1:B:216:THR:CG2  | 1:B:226:SER:HB3  | 1.88                     | 1.02              |
| 1:H:256:HIS:ND1  | 1:H:278:GLU:OE2  | 1.91                     | 1.02              |
| 1:C:256:HIS:ND1  | 1:C:278:GLU:OE2  | 1.91                     | 1.02              |
| 1:A:216:THR:CG2  | 1:A:226:SER:HB3  | 1.88                     | 1.01              |
| 1:C:216:THR:CG2  | 1:C:226:SER:HB3  | 1.88                     | 1.01              |
| 1:D:253:ILE:HG12 | 1:G:42:PHE:CD1   | 1.95                     | 1.01              |
| 1:D:223:ILE:HG13 | 1:D:224:TYR:HE1  | 1.25                     | 0.97              |
| 1:B:253:ILE:HG12 | 1:E:42:PHE:CD1   | 2.00                     | 0.95              |
| 1:G:30:LEU:HD12  | 1:G:31:ASP:N     | 1.81                     | 0.94              |
| 1:D:61:ASN:HD22  | 1:D:63:GLN:HE21  | 1.12                     | 0.94              |
| 1:D:22:ARG:HD2   | 1:D:22:ARG:O     | 1.67                     | 0.94              |
| 1:D:223:ILE:CG1  | 1:D:224:TYR:HE1  | 1.78                     | 0.93              |
| 1:G:62:PRO:HG2   | 1:G:63:GLN:HG3   | 1.52                     | 0.92              |
| 1:B:171:ALA:HB1  | 1:B:303:THR:HG21 | 1.51                     | 0.92              |
| 1:H:121:GLU:HA   | 1:H:124:MET:HE2  | 1.52                     | 0.91              |
| 1:B:216:THR:HG22 | 1:B:226:SER:CB   | 2.01                     | 0.90              |
| 1:H:216:THR:HG22 | 1:H:226:SER:CB   | 2.02                     | 0.90              |
| 1:C:216:THR:HG22 | 1:C:226:SER:CB   | 2.01                     | 0.90              |
| 1:D:69:GLN:HB2   | 1:D:110:MET:CE   | 2.02                     | 0.90              |
| 1:A:253:ILE:HG12 | 1:F:42:PHE:CE1   | 2.07                     | 0.90              |
| 1:D:216:THR:HG22 | 1:D:226:SER:CB   | 2.02                     | 0.90              |
| 1:F:61:ASN:OD1   | 1:F:63:GLN:HG3   | 1.71                     | 0.90              |
| 1:G:69:GLN:HB2   | 1:G:110:MET:CE   | 2.02                     | 0.90              |
| 1:C:69:GLN:HB2   | 1:C:110:MET:CE   | 2.02                     | 0.89              |
| 1:F:69:GLN:HB2   | 1:F:110:MET:CE   | 2.02                     | 0.89              |
| 1:G:216:THR:HG22 | 1:G:226:SER:CB   | 2.02                     | 0.89              |
| 1:E:69:GLN:HB2   | 1:E:110:MET:CE   | 2.02                     | 0.89              |
| 1:H:69:GLN:HB2   | 1:H:110:MET:CE   | 2.02                     | 0.89              |
| 1:E:216:THR:HG22 | 1:E:226:SER:CB   | 2.02                     | 0.89              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:2:ARG:HD3    | 4:E:350:DTR:CD2  | 2.03                     | 0.89              |
| 1:A:69:GLN:HB2   | 1:A:110:MET:CE   | 2.02                     | 0.89              |
| 1:A:216:THR:HG22 | 1:A:226:SER:CB   | 2.02                     | 0.89              |
| 1:C:253:ILE:HG12 | 1:H:42:PHE:CD1   | 2.07                     | 0.88              |
| 1:B:69:GLN:HB2   | 1:B:110:MET:CE   | 2.02                     | 0.88              |
| 1:F:216:THR:HG22 | 1:F:226:SER:CB   | 2.02                     | 0.88              |
| 1:D:27:LEU:CD1   | 1:D:30:LEU:HB2   | 2.02                     | 0.88              |
| 1:G:171:ALA:HA   | 1:G:175:ALA:HB3  | 1.56                     | 0.87              |
| 1:G:59:PRO:HG3   | 1:G:106:TYR:CZ   | 2.09                     | 0.87              |
| 1:F:223:ILE:HG12 | 1:F:224:TYR:HD1  | 1.40                     | 0.87              |
| 1:D:61:ASN:HD22  | 1:D:63:GLN:NE2   | 1.73                     | 0.86              |
| 1:A:253:ILE:CG1  | 1:F:42:PHE:CD1   | 2.57                     | 0.86              |
| 1:B:2:ARG:O      | 1:B:176:ASP:HB2  | 1.76                     | 0.86              |
| 1:B:250:ILE:CD1  | 1:E:250:ILE:HD13 | 2.05                     | 0.85              |
| 1:E:2:ARG:O      | 1:E:176:ASP:HB2  | 1.77                     | 0.85              |
| 1:H:168:GLU:HA   | 1:H:171:ALA:HB3  | 1.60                     | 0.84              |
| 1:D:90:THR:HG22  | 5:D:369:HOH:O    | 1.78                     | 0.84              |
| 1:D:121:GLU:HA   | 1:D:124:MET:HE2  | 1.60                     | 0.83              |
| 1:A:27:LEU:HD11  | 1:A:334:LEU:HD11 | 1.60                     | 0.83              |
| 1:H:2:ARG:NH1    | 1:H:173:GLY:O    | 2.12                     | 0.83              |
| 1:H:168:GLU:O    | 1:H:172:ARG:N    | 2.11                     | 0.83              |
| 1:G:216:THR:HB   | 1:G:227:PRO:O    | 1.79                     | 0.83              |
| 1:F:216:THR:HB   | 1:F:227:PRO:O    | 1.79                     | 0.82              |
| 1:D:30:LEU:C     | 1:D:30:LEU:HD12  | 2.04                     | 0.82              |
| 1:A:216:THR:HB   | 1:A:227:PRO:O    | 1.79                     | 0.82              |
| 1:H:216:THR:HB   | 1:H:227:PRO:O    | 1.79                     | 0.82              |
| 1:F:293:ARG:HH22 | 1:F:336:GLU:CD   | 1.88                     | 0.82              |
| 1:D:216:THR:HB   | 1:D:227:PRO:O    | 1.79                     | 0.82              |
| 1:H:293:ARG:HH22 | 1:H:336:GLU:CD   | 1.88                     | 0.82              |
| 1:D:293:ARG:HH22 | 1:D:336:GLU:CD   | 1.88                     | 0.82              |
| 1:D:223:ILE:HG23 | 1:D:224:TYR:CD1  | 2.14                     | 0.82              |
| 1:E:293:ARG:HH22 | 1:E:336:GLU:CD   | 1.88                     | 0.82              |
| 1:G:293:ARG:HH22 | 1:G:336:GLU:CD   | 1.88                     | 0.81              |
| 1:A:287:PRO:HB2  | 1:A:288:GLN:NE2  | 1.96                     | 0.81              |
| 1:F:60:SER:HB3   | 1:F:288:GLN:HG2  | 1.63                     | 0.81              |
| 1:A:293:ARG:HH22 | 1:A:336:GLU:CD   | 1.88                     | 0.81              |
| 1:C:293:ARG:HH22 | 1:C:336:GLU:CD   | 1.88                     | 0.81              |
| 1:E:216:THR:HB   | 1:E:227:PRO:O    | 1.79                     | 0.81              |
| 1:C:216:THR:HB   | 1:C:227:PRO:O    | 1.79                     | 0.81              |
| 1:B:293:ARG:HH22 | 1:B:336:GLU:CD   | 1.88                     | 0.81              |
| 1:D:171:ALA:CB   | 1:D:303:THR:HG21 | 2.10                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:216:THR:HB   | 1:B:227:PRO:O    | 1.79                     | 0.80              |
| 1:F:69:GLN:HB2   | 1:F:110:MET:HE2  | 1.63                     | 0.80              |
| 1:G:69:GLN:HB2   | 1:G:110:MET:HE2  | 1.63                     | 0.80              |
| 1:G:201:GLN:HE22 | 1:G:252:ASN:H    | 1.29                     | 0.80              |
| 1:C:201:GLN:HE22 | 1:C:252:ASN:H    | 1.29                     | 0.80              |
| 1:H:201:GLN:HE22 | 1:H:252:ASN:H    | 1.29                     | 0.80              |
| 1:C:69:GLN:HB2   | 1:C:110:MET:HE2  | 1.63                     | 0.80              |
| 1:A:69:GLN:HB2   | 1:A:110:MET:HE2  | 1.63                     | 0.80              |
| 1:E:69:GLN:HB2   | 1:E:110:MET:HE2  | 1.63                     | 0.80              |
| 1:D:69:GLN:HB2   | 1:D:110:MET:HE2  | 1.63                     | 0.80              |
| 1:B:59:PRO:HB2   | 1:B:61:ASN:O     | 1.82                     | 0.80              |
| 1:A:201:GLN:HE22 | 1:A:252:ASN:H    | 1.29                     | 0.79              |
| 1:B:201:GLN:HE22 | 1:B:252:ASN:H    | 1.29                     | 0.79              |
| 1:C:268:PRO:O    | 1:C:271:LYS:HB3  | 1.83                     | 0.79              |
| 1:D:223:ILE:CG1  | 1:D:224:TYR:CD1  | 2.59                     | 0.79              |
| 1:E:201:GLN:HE22 | 1:E:252:ASN:H    | 1.29                     | 0.79              |
| 1:G:62:PRO:HG2   | 1:G:63:GLN:CG    | 2.12                     | 0.79              |
| 1:B:69:GLN:HB2   | 1:B:110:MET:HE2  | 1.63                     | 0.79              |
| 1:B:250:ILE:HD13 | 1:E:250:ILE:HD13 | 1.64                     | 0.79              |
| 1:B:218:ASP:OD1  | 1:B:220:GLU:HG2  | 1.83                     | 0.79              |
| 1:D:61:ASN:HB2   | 1:D:63:GLN:HG3   | 1.65                     | 0.79              |
| 1:H:167:PHE:O    | 1:H:171:ALA:N    | 2.15                     | 0.79              |
| 1:B:118:THR:HG23 | 1:B:121:GLU:OE1  | 1.83                     | 0.79              |
| 1:C:66:ASN:O     | 1:C:70:GLN:HG3   | 1.83                     | 0.79              |
| 1:D:30:LEU:HD12  | 1:D:31:ASP:N     | 1.98                     | 0.79              |
| 1:H:66:ASN:O     | 1:H:70:GLN:HG3   | 1.83                     | 0.79              |
| 1:D:201:GLN:HE22 | 1:D:252:ASN:H    | 1.29                     | 0.78              |
| 1:A:66:ASN:O     | 1:A:70:GLN:HG3   | 1.83                     | 0.78              |
| 1:C:1:MET:HB2    | 1:C:176:ASP:OD2  | 1.83                     | 0.78              |
| 1:E:66:ASN:O     | 1:E:70:GLN:HG3   | 1.83                     | 0.78              |
| 1:E:118:THR:HG23 | 1:E:121:GLU:OE1  | 1.83                     | 0.78              |
| 1:F:118:THR:HG23 | 1:F:121:GLU:OE1  | 1.83                     | 0.78              |
| 1:A:118:THR:HG23 | 1:A:121:GLU:OE1  | 1.83                     | 0.78              |
| 1:D:118:THR:HG23 | 1:D:121:GLU:OE1  | 1.83                     | 0.78              |
| 1:D:66:ASN:O     | 1:D:70:GLN:HG3   | 1.83                     | 0.78              |
| 1:H:69:GLN:HB2   | 1:H:110:MET:HE2  | 1.63                     | 0.78              |
| 1:F:201:GLN:HE22 | 1:F:252:ASN:H    | 1.29                     | 0.78              |
| 1:F:66:ASN:O     | 1:F:70:GLN:HG3   | 1.83                     | 0.78              |
| 1:H:118:THR:HG23 | 1:H:121:GLU:OE1  | 1.83                     | 0.78              |
| 1:A:250:ILE:CD1  | 1:F:250:ILE:HD13 | 2.14                     | 0.78              |
| 1:B:66:ASN:O     | 1:B:70:GLN:HG3   | 1.83                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:251:ASN:OD1  | 1:B:280:THR:HG23 | 1.84                     | 0.77              |
| 1:F:251:ASN:OD1  | 1:F:280:THR:HG23 | 1.84                     | 0.77              |
| 1:C:253:ILE:HG12 | 1:H:42:PHE:CE1   | 2.18                     | 0.77              |
| 1:G:66:ASN:O     | 1:G:70:GLN:HG3   | 1.83                     | 0.77              |
| 1:G:118:THR:HG23 | 1:G:121:GLU:OE1  | 1.83                     | 0.77              |
| 1:C:251:ASN:OD1  | 1:C:280:THR:HG23 | 1.84                     | 0.77              |
| 1:G:251:ASN:OD1  | 1:G:280:THR:HG23 | 1.84                     | 0.77              |
| 1:D:223:ILE:C    | 1:D:224:TYR:HD1  | 1.93                     | 0.77              |
| 1:A:251:ASN:OD1  | 1:A:280:THR:HG23 | 1.84                     | 0.77              |
| 1:D:251:ASN:OD1  | 1:D:280:THR:HG23 | 1.84                     | 0.77              |
| 1:H:251:ASN:OD1  | 1:H:280:THR:HG23 | 1.84                     | 0.77              |
| 1:C:23:TYR:CE2   | 1:C:330:PHE:HD2  | 2.03                     | 0.77              |
| 1:C:118:THR:HG23 | 1:C:121:GLU:OE1  | 1.83                     | 0.77              |
| 1:E:251:ASN:OD1  | 1:E:280:THR:HG23 | 1.84                     | 0.77              |
| 1:A:250:ILE:HD11 | 1:F:250:ILE:HD13 | 1.67                     | 0.76              |
| 1:C:105:PRO:HD3  | 1:C:132:TRP:CZ2  | 2.21                     | 0.76              |
| 1:D:105:PRO:HD3  | 1:D:132:TRP:CZ2  | 2.21                     | 0.76              |
| 1:F:20:HIS:ND1   | 1:F:155:ARG:NH1  | 2.34                     | 0.76              |
| 1:F:58:GLU:HB3   | 1:F:59:PRO:HD2   | 1.67                     | 0.76              |
| 1:H:121:GLU:HA   | 1:H:124:MET:CE   | 2.15                     | 0.76              |
| 1:B:20:HIS:ND1   | 1:B:155:ARG:NH1  | 2.34                     | 0.76              |
| 1:F:105:PRO:HD3  | 1:F:132:TRP:CZ2  | 2.21                     | 0.76              |
| 1:B:105:PRO:HD3  | 1:B:132:TRP:CZ2  | 2.21                     | 0.75              |
| 1:B:250:ILE:HD11 | 1:E:250:ILE:CD1  | 2.16                     | 0.75              |
| 1:G:20:HIS:ND1   | 1:G:155:ARG:NH1  | 2.34                     | 0.75              |
| 1:D:20:HIS:ND1   | 1:D:155:ARG:NH1  | 2.34                     | 0.75              |
| 1:E:22:ARG:HG3   | 1:E:22:ARG:NH1   | 1.87                     | 0.75              |
| 1:E:105:PRO:HD3  | 1:E:132:TRP:CZ2  | 2.21                     | 0.75              |
| 1:F:223:ILE:HG23 | 1:F:224:TYR:CD1  | 2.21                     | 0.75              |
| 1:B:250:ILE:CD1  | 1:E:250:ILE:CD1  | 2.64                     | 0.75              |
| 1:E:20:HIS:ND1   | 1:E:155:ARG:NH1  | 2.34                     | 0.75              |
| 1:G:105:PRO:HD3  | 1:G:132:TRP:CZ2  | 2.21                     | 0.75              |
| 1:H:105:PRO:HD3  | 1:H:132:TRP:CZ2  | 2.21                     | 0.75              |
| 1:A:27:LEU:HD11  | 1:A:334:LEU:CD1  | 2.17                     | 0.74              |
| 1:A:27:LEU:HD12  | 1:A:30:LEU:HD22  | 1.69                     | 0.74              |
| 1:A:20:HIS:ND1   | 1:A:155:ARG:NH1  | 2.34                     | 0.74              |
| 1:A:105:PRO:HD3  | 1:A:132:TRP:CZ2  | 2.21                     | 0.74              |
| 1:H:20:HIS:ND1   | 1:H:155:ARG:NH1  | 2.34                     | 0.74              |
| 1:C:55:TYR:HE1   | 1:C:314:TYR:CD1  | 2.06                     | 0.74              |
| 1:C:20:HIS:ND1   | 1:C:155:ARG:NH1  | 2.34                     | 0.74              |
| 1:H:58:GLU:CG    | 1:H:59:PRO:HD2   | 2.17                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:269:THR:C    | 1:D:271:LYS:H    | 1.96                     | 0.73              |
| 1:B:253:ILE:HG22 | 1:B:254:GLN:N    | 2.02                     | 0.73              |
| 1:G:223:ILE:HB   | 1:G:224:TYR:CD1  | 2.24                     | 0.73              |
| 1:D:256:HIS:HD1  | 1:D:278:GLU:CD   | 1.97                     | 0.73              |
| 4:F:350:DTR:CE3  | 4:F:350:DTR:H    | 2.01                     | 0.73              |
| 1:C:256:HIS:HD1  | 1:C:278:GLU:CD   | 1.97                     | 0.72              |
| 1:H:224:TYR:HB2  | 1:H:242:PHE:HD2  | 1.54                     | 0.72              |
| 1:C:69:GLN:CB    | 1:C:110:MET:HE2  | 2.20                     | 0.72              |
| 1:D:102:VAL:HG13 | 1:D:103:PRO:HD2  | 1.72                     | 0.72              |
| 1:D:121:GLU:OE2  | 5:D:357:HOH:O    | 2.06                     | 0.72              |
| 1:B:69:GLN:CB    | 1:B:110:MET:HE2  | 2.20                     | 0.72              |
| 1:E:218:ASP:HB2  | 1:E:226:SER:OG   | 1.90                     | 0.72              |
| 1:F:102:VAL:HG13 | 1:F:103:PRO:HD2  | 1.72                     | 0.72              |
| 1:C:255:ASP:O    | 1:C:259:ILE:HG13 | 1.90                     | 0.71              |
| 1:G:201:GLN:CG   | 1:G:280:THR:HG22 | 2.18                     | 0.71              |
| 1:B:128:TYR:N    | 1:B:128:TYR:CD1  | 2.55                     | 0.71              |
| 1:C:201:GLN:CG   | 1:C:280:THR:HG22 | 2.18                     | 0.71              |
| 1:A:69:GLN:CB    | 1:A:110:MET:HE2  | 2.20                     | 0.71              |
| 1:B:256:HIS:HD1  | 1:B:278:GLU:CD   | 1.97                     | 0.71              |
| 1:D:255:ASP:O    | 1:D:259:ILE:HG13 | 1.90                     | 0.71              |
| 1:D:291:LEU:HA   | 1:D:307:HIS:O    | 1.91                     | 0.71              |
| 1:G:69:GLN:CB    | 1:G:110:MET:HE2  | 2.20                     | 0.71              |
| 1:F:69:GLN:CB    | 1:F:110:MET:HE2  | 2.20                     | 0.71              |
| 1:H:69:GLN:CB    | 1:H:110:MET:HE2  | 2.20                     | 0.71              |
| 1:F:61:ASN:CG    | 1:F:63:GLN:HG3   | 2.15                     | 0.71              |
| 1:G:63:GLN:O     | 1:G:67:TRP:N     | 2.14                     | 0.71              |
| 1:G:291:LEU:HA   | 1:G:307:HIS:O    | 1.91                     | 0.71              |
| 1:F:61:ASN:HD21  | 1:F:63:GLN:CD    | 1.97                     | 0.71              |
| 1:F:223:ILE:HG12 | 1:F:224:TYR:CE1  | 2.26                     | 0.71              |
| 1:A:201:GLN:CG   | 1:A:280:THR:HG22 | 2.18                     | 0.71              |
| 1:F:256:HIS:HD1  | 1:F:278:GLU:CD   | 1.97                     | 0.71              |
| 1:D:69:GLN:CB    | 1:D:110:MET:HE2  | 2.20                     | 0.70              |
| 1:E:69:GLN:CB    | 1:E:110:MET:HE2  | 2.20                     | 0.70              |
| 1:A:255:ASP:O    | 1:A:259:ILE:HG13 | 1.90                     | 0.70              |
| 1:C:102:VAL:HG13 | 1:C:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:F:255:ASP:O    | 1:F:259:ILE:HG13 | 1.90                     | 0.70              |
| 1:H:255:ASP:O    | 1:H:259:ILE:HG13 | 1.90                     | 0.70              |
| 1:B:102:VAL:HG13 | 1:B:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:E:255:ASP:O    | 1:E:259:ILE:HG13 | 1.90                     | 0.70              |
| 1:F:201:GLN:CG   | 1:F:280:THR:HG22 | 2.18                     | 0.70              |
| 1:B:255:ASP:O    | 1:B:259:ILE:HG13 | 1.90                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:291:LEU:HA   | 1:B:307:HIS:O    | 1.91                     | 0.70              |
| 1:G:256:HIS:HD1  | 1:G:278:GLU:CD   | 1.97                     | 0.70              |
| 1:H:102:VAL:HG13 | 1:H:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:H:256:HIS:HD1  | 1:H:278:GLU:CD   | 1.97                     | 0.70              |
| 1:F:291:LEU:HA   | 1:F:307:HIS:O    | 1.91                     | 0.70              |
| 1:G:255:ASP:O    | 1:G:259:ILE:HG13 | 1.90                     | 0.70              |
| 1:H:291:LEU:HA   | 1:H:307:HIS:O    | 1.91                     | 0.70              |
| 1:E:102:VAL:HG13 | 1:E:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:C:55:TYR:HE1   | 1:C:314:TYR:CE1  | 2.09                     | 0.70              |
| 1:G:102:VAL:HG13 | 1:G:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:G:224:TYR:HB2  | 1:G:242:PHE:HB2  | 1.73                     | 0.70              |
| 1:A:102:VAL:HG13 | 1:A:103:PRO:HD2  | 1.72                     | 0.70              |
| 1:C:291:LEU:HA   | 1:C:307:HIS:O    | 1.91                     | 0.70              |
| 1:G:121:GLU:HA   | 1:G:124:MET:HE2  | 1.73                     | 0.70              |
| 1:A:268:PRO:HB2  | 1:E:82:PRO:HA    | 1.72                     | 0.70              |
| 1:H:93:SER:OG    | 1:H:135:THR:HG23 | 1.92                     | 0.70              |
| 1:E:291:LEU:HA   | 1:E:307:HIS:O    | 1.91                     | 0.69              |
| 1:F:223:ILE:HG23 | 1:F:224:TYR:HD1  | 1.55                     | 0.69              |
| 1:G:92:VAL:HG21  | 1:G:138:ILE:HG13 | 1.74                     | 0.69              |
| 1:A:92:VAL:HG21  | 1:A:138:ILE:HG13 | 1.74                     | 0.69              |
| 1:A:93:SER:OG    | 1:A:135:THR:HG23 | 1.92                     | 0.69              |
| 1:D:211:LYS:O    | 5:D:370:HOH:O    | 2.09                     | 0.69              |
| 1:A:291:LEU:HA   | 1:A:307:HIS:O    | 1.91                     | 0.69              |
| 1:C:92:VAL:HG21  | 1:C:138:ILE:HG13 | 1.74                     | 0.69              |
| 1:F:93:SER:OG    | 1:F:135:THR:HG23 | 1.92                     | 0.69              |
| 1:G:93:SER:OG    | 1:G:135:THR:HG23 | 1.92                     | 0.69              |
| 1:A:250:ILE:HD11 | 1:F:250:ILE:CD1  | 2.22                     | 0.69              |
| 1:E:92:VAL:HG21  | 1:E:138:ILE:HG13 | 1.74                     | 0.69              |
| 1:B:171:ALA:CB   | 1:B:303:THR:HG21 | 2.21                     | 0.69              |
| 1:G:224:TYR:CD1  | 1:G:224:TYR:N    | 2.59                     | 0.69              |
| 1:H:58:GLU:HG3   | 1:H:59:PRO:CD    | 2.23                     | 0.69              |
| 1:B:201:GLN:CG   | 1:B:280:THR:HG22 | 2.18                     | 0.69              |
| 1:G:69:GLN:CA    | 1:G:110:MET:HE2  | 2.23                     | 0.69              |
| 1:H:69:GLN:HB2   | 1:H:110:MET:HE3  | 1.75                     | 0.69              |
| 1:B:69:GLN:CA    | 1:B:110:MET:HE2  | 2.23                     | 0.69              |
| 1:D:93:SER:OG    | 1:D:135:THR:HG23 | 1.92                     | 0.69              |
| 1:C:69:GLN:HB2   | 1:C:110:MET:HE3  | 1.75                     | 0.68              |
| 1:F:92:VAL:HG21  | 1:F:138:ILE:HG13 | 1.74                     | 0.68              |
| 1:H:253:ILE:HG22 | 1:H:254:GLN:N    | 2.03                     | 0.68              |
| 1:B:93:SER:OG    | 1:B:135:THR:HG23 | 1.92                     | 0.68              |
| 1:D:223:ILE:HG23 | 1:D:224:TYR:HD1  | 1.56                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:69:GLN:CA    | 1:F:110:MET:HE2  | 2.23                     | 0.68              |
| 1:B:55:TYR:HE1   | 1:B:314:TYR:CD1  | 2.10                     | 0.68              |
| 1:D:69:GLN:CA    | 1:D:110:MET:HE2  | 2.23                     | 0.68              |
| 1:E:93:SER:OG    | 1:E:135:THR:HG23 | 1.92                     | 0.68              |
| 1:G:223:ILE:C    | 1:G:224:TYR:HD1  | 2.00                     | 0.68              |
| 1:B:92:VAL:HG21  | 1:B:138:ILE:HG13 | 1.74                     | 0.68              |
| 1:C:93:SER:OG    | 1:C:135:THR:HG23 | 1.92                     | 0.68              |
| 1:E:256:HIS:HD1  | 1:E:278:GLU:CD   | 1.97                     | 0.68              |
| 1:H:69:GLN:CA    | 1:H:110:MET:HE2  | 2.23                     | 0.68              |
| 1:A:256:HIS:HD1  | 1:A:278:GLU:CD   | 1.97                     | 0.68              |
| 1:A:69:GLN:CA    | 1:A:110:MET:HE2  | 2.23                     | 0.68              |
| 1:E:69:GLN:CA    | 1:E:110:MET:HE2  | 2.23                     | 0.68              |
| 1:B:69:GLN:HB2   | 1:B:110:MET:HE3  | 1.75                     | 0.68              |
| 1:C:216:THR:HG21 | 1:C:226:SER:HB3  | 1.76                     | 0.68              |
| 1:D:92:VAL:HG21  | 1:D:138:ILE:HG13 | 1.74                     | 0.68              |
| 1:H:92:VAL:HG21  | 1:H:138:ILE:HG13 | 1.74                     | 0.68              |
| 1:E:69:GLN:HB2   | 1:E:110:MET:HE3  | 1.75                     | 0.68              |
| 1:G:69:GLN:HB2   | 1:G:110:MET:HE3  | 1.75                     | 0.68              |
| 1:A:69:GLN:HB2   | 1:A:110:MET:HE3  | 1.75                     | 0.68              |
| 1:B:199:ARG:HH22 | 1:B:201:GLN:NE2  | 1.92                     | 0.68              |
| 1:B:216:THR:HG21 | 1:B:226:SER:HB3  | 1.76                     | 0.68              |
| 1:C:69:GLN:CA    | 1:C:110:MET:HE2  | 2.23                     | 0.68              |
| 1:C:199:ARG:HH22 | 1:C:201:GLN:NE2  | 1.92                     | 0.68              |
| 1:D:61:ASN:HB2   | 1:D:63:GLN:CG    | 2.24                     | 0.68              |
| 1:H:23:TYR:O     | 1:H:30:LEU:HD22  | 1.93                     | 0.68              |
| 1:E:216:THR:HG21 | 1:E:226:SER:HB3  | 1.76                     | 0.68              |
| 1:H:199:ARG:HH22 | 1:H:201:GLN:NE2  | 1.92                     | 0.67              |
| 1:B:224:TYR:HB2  | 1:B:242:PHE:HB2  | 1.75                     | 0.67              |
| 1:A:253:ILE:HG22 | 1:A:254:GLN:N    | 2.06                     | 0.67              |
| 1:E:295:GLN:O    | 1:E:296:LEU:HD23 | 1.95                     | 0.67              |
| 1:H:295:GLN:O    | 1:H:296:LEU:HD23 | 1.95                     | 0.67              |
| 1:C:82:PRO:HA    | 1:G:268:PRO:HB2  | 1.76                     | 0.67              |
| 1:G:223:ILE:CG2  | 1:G:224:TYR:CE1  | 2.77                     | 0.67              |
| 1:H:151:ARG:NH2  | 1:H:154:GLU:OE2  | 2.28                     | 0.67              |
| 1:H:199:ARG:HH22 | 1:H:201:GLN:HE21 | 1.43                     | 0.67              |
| 1:E:199:ARG:HH22 | 1:E:201:GLN:HE21 | 1.43                     | 0.67              |
| 1:F:69:GLN:HB2   | 1:F:110:MET:HE3  | 1.75                     | 0.67              |
| 1:F:184:VAL:HG13 | 1:F:284:PRO:HA   | 1.77                     | 0.67              |
| 1:G:224:TYR:N    | 1:G:224:TYR:HD1  | 1.93                     | 0.67              |
| 1:D:69:GLN:HB2   | 1:D:110:MET:HE3  | 1.75                     | 0.67              |
| 1:D:199:ARG:HH22 | 1:D:201:GLN:HE21 | 1.43                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:184:VAL:HG13 | 1:E:284:PRO:HA   | 1.77                     | 0.67              |
| 1:D:199:ARG:HH22 | 1:D:201:GLN:NE2  | 1.92                     | 0.67              |
| 1:E:201:GLN:CG   | 1:E:280:THR:HG22 | 2.18                     | 0.67              |
| 1:F:61:ASN:OD1   | 1:F:62:PRO:N     | 2.28                     | 0.67              |
| 1:H:121:GLU:O    | 1:H:124:MET:HB2  | 1.95                     | 0.67              |
| 1:C:201:GLN:NE2  | 1:C:252:ASN:H    | 1.93                     | 0.67              |
| 1:C:295:GLN:O    | 1:C:296:LEU:HD23 | 1.95                     | 0.67              |
| 1:F:293:ARG:NH2  | 1:F:336:GLU:OE1  | 2.28                     | 0.67              |
| 1:G:293:ARG:NH2  | 1:G:336:GLU:OE1  | 2.28                     | 0.67              |
| 1:A:36:ALA:O     | 1:A:161:LEU:HD12 | 1.95                     | 0.67              |
| 1:A:151:ARG:NH2  | 1:A:154:GLU:OE2  | 2.28                     | 0.67              |
| 1:B:184:VAL:HG13 | 1:B:284:PRO:HA   | 1.77                     | 0.67              |
| 1:B:201:GLN:NE2  | 1:B:252:ASN:H    | 1.93                     | 0.67              |
| 1:B:293:ARG:NH2  | 1:B:336:GLU:OE1  | 2.28                     | 0.67              |
| 1:G:199:ARG:HH22 | 1:G:201:GLN:HE21 | 1.43                     | 0.67              |
| 1:A:201:GLN:NE2  | 1:A:252:ASN:H    | 1.93                     | 0.66              |
| 1:C:199:ARG:HH22 | 1:C:201:GLN:HE21 | 1.43                     | 0.66              |
| 1:D:36:ALA:O     | 1:D:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:D:184:VAL:HG13 | 1:D:284:PRO:HA   | 1.77                     | 0.66              |
| 1:F:199:ARG:HH22 | 1:F:201:GLN:HE21 | 1.43                     | 0.66              |
| 1:B:36:ALA:O     | 1:B:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:C:36:ALA:O     | 1:C:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:E:293:ARG:NH2  | 1:E:336:GLU:OE1  | 2.28                     | 0.66              |
| 1:F:36:ALA:O     | 1:F:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:F:199:ARG:HH22 | 1:F:201:GLN:NE2  | 1.92                     | 0.66              |
| 1:G:170:VAL:HB   | 1:G:178:ILE:HD11 | 1.76                     | 0.66              |
| 1:A:199:ARG:HH22 | 1:A:201:GLN:NE2  | 1.92                     | 0.66              |
| 1:F:295:GLN:O    | 1:F:296:LEU:HD23 | 1.95                     | 0.66              |
| 1:G:199:ARG:HH22 | 1:G:201:GLN:NE2  | 1.92                     | 0.66              |
| 1:H:201:GLN:NE2  | 1:H:252:ASN:H    | 1.93                     | 0.66              |
| 1:H:201:GLN:CG   | 1:H:280:THR:HG22 | 2.18                     | 0.66              |
| 1:A:199:ARG:HH22 | 1:A:201:GLN:HE21 | 1.43                     | 0.66              |
| 1:B:199:ARG:HH22 | 1:B:201:GLN:HE21 | 1.43                     | 0.66              |
| 1:C:293:ARG:NH2  | 1:C:336:GLU:OE1  | 2.28                     | 0.66              |
| 1:E:151:ARG:NH2  | 1:E:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:B:177:VAL:HG22 | 1:B:304:GLU:HB2  | 1.77                     | 0.66              |
| 1:C:151:ARG:NH2  | 1:C:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:E:199:ARG:HH22 | 1:E:201:GLN:NE2  | 1.92                     | 0.66              |
| 1:F:254:GLN:O    | 1:F:258:THR:HG23 | 1.94                     | 0.66              |
| 1:H:293:ARG:NH2  | 1:H:336:GLU:OE1  | 2.28                     | 0.66              |
| 1:B:151:ARG:NH2  | 1:B:154:GLU:OE2  | 2.28                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:151:ARG:NH2  | 1:F:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:A:216:THR:HG21 | 1:A:226:SER:HB3  | 1.76                     | 0.66              |
| 1:D:201:GLN:NE2  | 1:D:252:ASN:H    | 1.93                     | 0.66              |
| 1:D:215:ILE:HG22 | 1:D:217:HIS:CE1  | 2.31                     | 0.66              |
| 1:D:252:ASN:CG   | 1:D:254:GLN:HG2  | 2.20                     | 0.66              |
| 1:G:151:ARG:NH2  | 1:G:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:A:293:ARG:NH2  | 1:A:336:GLU:OE1  | 2.28                     | 0.66              |
| 1:A:295:GLN:O    | 1:A:296:LEU:HD23 | 1.95                     | 0.66              |
| 1:B:121:GLU:HA   | 1:B:124:MET:HE2  | 1.77                     | 0.66              |
| 1:D:151:ARG:NH2  | 1:D:154:GLU:OE2  | 2.28                     | 0.66              |
| 1:D:171:ALA:C    | 1:D:173:GLY:H    | 2.02                     | 0.66              |
| 1:D:216:THR:HG21 | 1:D:226:SER:HB3  | 1.76                     | 0.66              |
| 1:D:293:ARG:NH2  | 1:D:336:GLU:OE1  | 2.28                     | 0.66              |
| 1:E:36:ALA:O     | 1:E:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:D:295:GLN:O    | 1:D:296:LEU:HD23 | 1.95                     | 0.66              |
| 1:H:36:ALA:O     | 1:H:161:LEU:HD12 | 1.95                     | 0.66              |
| 1:C:22:ARG:HD3   | 1:C:23:TYR:CE1   | 2.31                     | 0.65              |
| 1:G:295:GLN:O    | 1:G:296:LEU:HD23 | 1.95                     | 0.65              |
| 1:B:295:GLN:O    | 1:B:296:LEU:HD23 | 1.95                     | 0.65              |
| 1:G:223:ILE:CB   | 1:G:224:TYR:HD1  | 2.09                     | 0.65              |
| 1:C:55:TYR:CE1   | 1:C:314:TYR:CD1  | 2.84                     | 0.65              |
| 1:G:36:ALA:O     | 1:G:161:LEU:HD12 | 1.95                     | 0.65              |
| 1:F:201:GLN:NE2  | 1:F:252:ASN:H    | 1.93                     | 0.65              |
| 1:H:184:VAL:HG13 | 1:H:284:PRO:HA   | 1.77                     | 0.65              |
| 1:D:61:ASN:OD1   | 1:D:61:ASN:N     | 2.30                     | 0.65              |
| 1:G:201:GLN:NE2  | 1:G:252:ASN:H    | 1.93                     | 0.65              |
| 1:C:254:GLN:O    | 1:C:258:THR:HG23 | 1.97                     | 0.65              |
| 1:C:23:TYR:O     | 1:C:30:LEU:HD23  | 1.97                     | 0.65              |
| 1:E:161:LEU:O    | 1:E:162:ARG:HG2  | 1.96                     | 0.65              |
| 1:E:201:GLN:NE2  | 1:E:252:ASN:H    | 1.93                     | 0.65              |
| 1:A:184:VAL:HG13 | 1:A:284:PRO:HA   | 1.77                     | 0.65              |
| 1:C:184:VAL:HG13 | 1:C:284:PRO:HA   | 1.77                     | 0.65              |
| 1:F:253:ILE:HG22 | 1:F:254:GLN:N    | 2.09                     | 0.65              |
| 1:G:184:VAL:HG13 | 1:G:284:PRO:HA   | 1.77                     | 0.65              |
| 1:C:23:TYR:HE2   | 1:C:330:PHE:HD2  | 1.43                     | 0.65              |
| 1:D:201:GLN:CG   | 1:D:280:THR:HG22 | 2.18                     | 0.65              |
| 1:B:171:ALA:HB1  | 1:B:303:THR:CG2  | 2.27                     | 0.64              |
| 1:E:33:LYS:HE3   | 4:E:350:DTR:CZ2  | 2.27                     | 0.64              |
| 1:G:223:ILE:CB   | 1:G:224:TYR:CD1  | 2.81                     | 0.64              |
| 1:B:180:ASN:HD22 | 1:B:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:D:121:GLU:O    | 1:D:124:MET:HB2  | 1.98                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:ILE:HG12 | 1:F:42:PHE:CG    | 2.29                     | 0.64              |
| 1:B:250:ILE:HD11 | 1:E:250:ILE:HD13 | 1.75                     | 0.64              |
| 1:D:180:ASN:HD22 | 1:D:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:H:180:ASN:HD22 | 1:H:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:A:180:ASN:HD22 | 1:A:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:A:253:ILE:HA   | 1:F:42:PHE:CZ    | 2.33                     | 0.64              |
| 1:C:180:ASN:HD22 | 1:C:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:E:180:ASN:HD22 | 1:E:307:HIS:HD2  | 1.46                     | 0.64              |
| 1:G:223:ILE:HG22 | 1:G:224:TYR:CD1  | 2.33                     | 0.64              |
| 1:E:22:ARG:HH11  | 1:E:22:ARG:CG    | 1.99                     | 0.64              |
| 1:F:168:GLU:O    | 1:F:171:ALA:HB3  | 1.96                     | 0.64              |
| 1:A:128:TYR:CD2  | 1:A:128:TYR:N    | 2.66                     | 0.63              |
| 1:E:253:ILE:HG22 | 1:E:254:GLN:N    | 2.04                     | 0.63              |
| 1:B:253:ILE:HG12 | 1:E:42:PHE:CG    | 2.33                     | 0.63              |
| 1:G:180:ASN:HD22 | 1:G:307:HIS:HD2  | 1.46                     | 0.63              |
| 1:B:192:ASP:OD1  | 1:B:194:LEU:HB2  | 1.99                     | 0.63              |
| 1:E:2:ARG:HD3    | 4:E:350:DTR:CE2  | 2.28                     | 0.63              |
| 1:H:172:ARG:C    | 1:H:174:GLY:H    | 2.05                     | 0.63              |
| 1:D:192:ASP:OD1  | 1:D:194:LEU:HB2  | 1.99                     | 0.62              |
| 1:H:224:TYR:HB2  | 1:H:242:PHE:CD2  | 2.32                     | 0.62              |
| 1:D:27:LEU:HD12  | 1:D:30:LEU:CB    | 2.09                     | 0.62              |
| 1:E:192:ASP:OD1  | 1:E:194:LEU:HB2  | 1.99                     | 0.62              |
| 1:D:82:PRO:HA    | 1:H:268:PRO:HB2  | 1.79                     | 0.62              |
| 1:B:250:ILE:HD13 | 1:E:250:ILE:CD1  | 2.30                     | 0.62              |
| 1:F:180:ASN:HD22 | 1:F:307:HIS:HD2  | 1.46                     | 0.62              |
| 1:F:192:ASP:OD1  | 1:F:194:LEU:HB2  | 1.99                     | 0.62              |
| 1:F:216:THR:HG21 | 1:F:226:SER:HB3  | 1.76                     | 0.62              |
| 1:G:192:ASP:OD1  | 1:G:194:LEU:HB2  | 1.99                     | 0.62              |
| 1:H:58:GLU:HG3   | 1:H:59:PRO:HD2   | 1.78                     | 0.62              |
| 1:H:216:THR:HG21 | 1:H:226:SER:HB3  | 1.76                     | 0.62              |
| 1:A:254:GLN:O    | 1:A:258:THR:HG23 | 2.00                     | 0.62              |
| 1:G:223:ILE:CG2  | 1:G:224:TYR:CD1  | 2.83                     | 0.62              |
| 1:E:138:ILE:HD11 | 1:E:231:PRO:O    | 2.00                     | 0.62              |
| 1:F:138:ILE:HD11 | 1:F:231:PRO:O    | 2.00                     | 0.62              |
| 1:H:122:LEU:C    | 1:H:124:MET:H    | 2.08                     | 0.62              |
| 1:C:124:MET:HE3  | 1:C:125:PHE:CE1  | 2.35                     | 0.62              |
| 1:D:223:ILE:HG12 | 1:D:224:TYR:HE1  | 1.61                     | 0.62              |
| 1:F:58:GLU:HB3   | 1:F:59:PRO:CD    | 2.30                     | 0.62              |
| 1:B:59:PRO:HG2   | 1:B:61:ASN:O     | 1.99                     | 0.61              |
| 1:G:216:THR:HG21 | 1:G:226:SER:HB3  | 1.76                     | 0.61              |
| 1:H:170:VAL:HB   | 1:H:178:ILE:HD11 | 1.82                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:ASP:OD1  | 1:C:194:LEU:HB2  | 1.99                     | 0.61              |
| 1:A:20:HIS:CE1   | 1:A:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:A:192:ASP:OD1  | 1:A:194:LEU:HB2  | 1.99                     | 0.61              |
| 1:H:192:ASP:OD1  | 1:H:194:LEU:HB2  | 1.99                     | 0.61              |
| 1:B:20:HIS:CE1   | 1:B:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:D:252:ASN:OD1  | 1:D:254:GLN:HG2  | 2.01                     | 0.61              |
| 1:B:138:ILE:HD11 | 1:B:231:PRO:O    | 2.00                     | 0.61              |
| 1:D:223:ILE:C    | 1:D:224:TYR:CD1  | 2.76                     | 0.61              |
| 1:D:252:ASN:ND2  | 1:D:254:GLN:HG2  | 2.16                     | 0.61              |
| 1:H:20:HIS:CE1   | 1:H:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:A:170:VAL:HG12 | 1:A:170:VAL:O    | 1.99                     | 0.61              |
| 1:H:168:GLU:O    | 1:H:171:ALA:N    | 2.33                     | 0.61              |
| 1:C:20:HIS:CE1   | 1:C:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:C:23:TYR:CE2   | 1:C:330:PHE:CD2  | 2.88                     | 0.61              |
| 1:F:20:HIS:CE1   | 1:F:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:F:246:ASN:OD1  | 1:F:248:ASN:N    | 2.26                     | 0.61              |
| 1:F:278:GLU:HG3  | 5:F:355:HOH:O    | 2.00                     | 0.61              |
| 1:G:142:ARG:O    | 1:G:146:GLN:HG3  | 2.01                     | 0.61              |
| 1:D:138:ILE:HD11 | 1:D:231:PRO:O    | 2.00                     | 0.61              |
| 1:D:142:ARG:O    | 1:D:146:GLN:HG3  | 2.01                     | 0.61              |
| 1:D:253:ILE:HG12 | 1:G:42:PHE:CE1   | 2.36                     | 0.61              |
| 1:G:138:ILE:HD11 | 1:G:231:PRO:O    | 2.00                     | 0.61              |
| 1:A:142:ARG:O    | 1:A:146:GLN:HG3  | 2.01                     | 0.61              |
| 1:B:59:PRO:CB    | 1:B:61:ASN:O     | 2.48                     | 0.61              |
| 1:B:246:ASN:OD1  | 1:B:248:ASN:N    | 2.26                     | 0.61              |
| 1:B:254:GLN:O    | 1:B:258:THR:HG23 | 2.00                     | 0.61              |
| 1:D:253:ILE:HG22 | 1:D:254:GLN:N    | 2.11                     | 0.61              |
| 1:E:142:ARG:O    | 1:E:146:GLN:HG3  | 2.01                     | 0.61              |
| 1:G:20:HIS:CE1   | 1:G:155:ARG:HH11 | 2.19                     | 0.61              |
| 1:H:142:ARG:O    | 1:H:146:GLN:HG3  | 2.01                     | 0.61              |
| 1:F:142:ARG:O    | 1:F:146:GLN:HG3  | 2.01                     | 0.60              |
| 1:G:223:ILE:HG21 | 1:G:224:TYR:HE1  | 1.66                     | 0.60              |
| 1:H:138:ILE:HD11 | 1:H:231:PRO:O    | 2.00                     | 0.60              |
| 1:B:142:ARG:O    | 1:B:146:GLN:HG3  | 2.01                     | 0.60              |
| 1:D:20:HIS:CE1   | 1:D:155:ARG:HH11 | 2.19                     | 0.60              |
| 1:F:223:ILE:CG1  | 1:F:224:TYR:CD1  | 2.76                     | 0.60              |
| 1:A:138:ILE:HD11 | 1:A:231:PRO:O    | 2.00                     | 0.60              |
| 1:C:142:ARG:O    | 1:C:146:GLN:HG3  | 2.01                     | 0.60              |
| 1:C:138:ILE:HD11 | 1:C:231:PRO:O    | 2.00                     | 0.60              |
| 1:E:58:GLU:CG    | 1:E:59:PRO:HD2   | 2.32                     | 0.60              |
| 1:G:252:ASN:OD1  | 1:G:254:GLN:N    | 2.35                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:30:LEU:HD11  | 1:D:32:VAL:HG23  | 1.84                     | 0.59              |
| 1:D:224:TYR:CD1  | 1:D:224:TYR:N    | 2.70                     | 0.59              |
| 1:E:20:HIS:CE1   | 1:E:155:ARG:HH11 | 2.19                     | 0.59              |
| 1:D:128:TYR:CD1  | 1:D:128:TYR:N    | 2.71                     | 0.59              |
| 1:D:296:LEU:HD11 | 5:D:354:HOH:O    | 2.02                     | 0.59              |
| 1:F:128:TYR:CD1  | 1:F:128:TYR:N    | 2.71                     | 0.59              |
| 1:C:55:TYR:HD2   | 1:C:223:ILE:HD13 | 1.68                     | 0.59              |
| 1:D:223:ILE:CG2  | 1:D:224:TYR:CD1  | 2.85                     | 0.59              |
| 1:A:246:ASN:OD1  | 1:A:248:ASN:N    | 2.26                     | 0.58              |
| 1:E:20:HIS:CE1   | 1:E:155:ARG:NH1  | 2.72                     | 0.58              |
| 1:G:62:PRO:CG    | 1:G:63:GLN:HG3   | 2.31                     | 0.58              |
| 1:G:246:ASN:OD1  | 1:G:248:ASN:N    | 2.26                     | 0.58              |
| 1:B:20:HIS:CE1   | 1:B:155:ARG:NH1  | 2.72                     | 0.58              |
| 1:E:168:GLU:O    | 1:E:171:ALA:HB3  | 2.04                     | 0.58              |
| 1:G:20:HIS:CE1   | 1:G:155:ARG:NH1  | 2.71                     | 0.58              |
| 1:B:225:ASN:ND2  | 1:B:240:GLY:O    | 2.35                     | 0.58              |
| 1:C:20:HIS:CE1   | 1:C:155:ARG:NH1  | 2.72                     | 0.58              |
| 1:D:269:THR:C    | 1:D:271:LYS:N    | 2.57                     | 0.58              |
| 1:H:20:HIS:CE1   | 1:H:155:ARG:NH1  | 2.72                     | 0.58              |
| 1:B:59:PRO:CG    | 1:B:61:ASN:O     | 2.51                     | 0.58              |
| 1:F:195:LEU:HD12 | 1:F:285:VAL:O    | 2.04                     | 0.58              |
| 1:A:20:HIS:CE1   | 1:A:155:ARG:NH1  | 2.71                     | 0.58              |
| 1:C:136:SER:OG   | 1:C:137:LEU:N    | 2.37                     | 0.58              |
| 1:C:195:LEU:HD12 | 1:C:285:VAL:O    | 2.04                     | 0.58              |
| 1:D:195:LEU:HD12 | 1:D:285:VAL:O    | 2.04                     | 0.58              |
| 1:F:92:VAL:CG2   | 1:F:138:ILE:HG13 | 2.34                     | 0.58              |
| 1:H:92:VAL:CG2   | 1:H:138:ILE:HG13 | 2.34                     | 0.58              |
| 1:H:121:GLU:O    | 1:H:124:MET:HE3  | 2.04                     | 0.58              |
| 1:B:253:ILE:HG12 | 1:E:42:PHE:CE1   | 2.38                     | 0.58              |
| 1:B:293:ARG:NH2  | 1:B:336:GLU:CD   | 2.61                     | 0.58              |
| 1:G:195:LEU:HD12 | 1:G:285:VAL:O    | 2.04                     | 0.58              |
| 1:B:83:ASN:O     | 1:B:86:ASN:N     | 2.37                     | 0.57              |
| 1:B:253:ILE:CG1  | 1:E:42:PHE:CD1   | 2.84                     | 0.57              |
| 1:D:20:HIS:CE1   | 1:D:155:ARG:NH1  | 2.71                     | 0.57              |
| 1:D:92:VAL:CG2   | 1:D:138:ILE:HG13 | 2.34                     | 0.57              |
| 1:G:83:ASN:O     | 1:G:86:ASN:N     | 2.37                     | 0.57              |
| 1:A:83:ASN:O     | 1:A:86:ASN:N     | 2.37                     | 0.57              |
| 1:B:136:SER:OG   | 1:B:137:LEU:N    | 2.37                     | 0.57              |
| 1:C:269:THR:C    | 1:C:271:LYS:H    | 2.11                     | 0.57              |
| 1:D:171:ALA:C    | 1:D:173:GLY:N    | 2.61                     | 0.57              |
| 1:H:136:SER:OG   | 1:H:137:LEU:N    | 2.37                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:83:ASN:O     | 1:D:86:ASN:N     | 2.37                     | 0.57              |
| 1:C:92:VAL:CG2   | 1:C:138:ILE:HG13 | 2.34                     | 0.57              |
| 1:H:170:VAL:HB   | 1:H:178:ILE:CD1  | 2.34                     | 0.57              |
| 1:D:90:THR:CG2   | 5:D:369:HOH:O    | 2.46                     | 0.57              |
| 1:D:252:ASN:OD1  | 1:D:254:GLN:N    | 2.37                     | 0.57              |
| 1:H:195:LEU:HD12 | 1:H:285:VAL:O    | 2.04                     | 0.57              |
| 1:A:195:LEU:HD12 | 1:A:285:VAL:O    | 2.04                     | 0.57              |
| 1:G:92:VAL:CG2   | 1:G:138:ILE:HG13 | 2.34                     | 0.57              |
| 1:B:92:VAL:CG2   | 1:B:138:ILE:HG13 | 2.34                     | 0.57              |
| 1:C:83:ASN:O     | 1:C:86:ASN:N     | 2.37                     | 0.57              |
| 1:F:20:HIS:CE1   | 1:F:155:ARG:NH1  | 2.71                     | 0.57              |
| 1:C:253:ILE:HG22 | 1:C:254:GLN:N    | 2.11                     | 0.57              |
| 1:C:293:ARG:NH2  | 1:C:336:GLU:CD   | 2.62                     | 0.57              |
| 1:D:136:SER:OG   | 1:D:137:LEU:N    | 2.37                     | 0.57              |
| 1:D:223:ILE:HG13 | 1:D:224:TYR:HD1  | 1.57                     | 0.57              |
| 1:C:128:TYR:N    | 1:C:128:TYR:CD2  | 2.73                     | 0.57              |
| 1:C:89:LEU:HD23  | 1:C:138:ILE:O    | 2.05                     | 0.56              |
| 1:E:92:VAL:CG2   | 1:E:138:ILE:HG13 | 2.34                     | 0.56              |
| 1:H:83:ASN:O     | 1:H:86:ASN:N     | 2.37                     | 0.56              |
| 1:A:92:VAL:CG2   | 1:A:138:ILE:HG13 | 2.34                     | 0.56              |
| 1:B:105:PRO:HD3  | 1:B:132:TRP:CH2  | 2.41                     | 0.56              |
| 1:B:195:LEU:HD12 | 1:B:285:VAL:O    | 2.04                     | 0.56              |
| 1:D:139:LEU:HD21 | 1:D:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:D:246:ASN:OD1  | 1:D:248:ASN:N    | 2.26                     | 0.56              |
| 1:E:83:ASN:O     | 1:E:86:ASN:N     | 2.37                     | 0.56              |
| 1:F:83:ASN:O     | 1:F:86:ASN:N     | 2.37                     | 0.56              |
| 1:F:139:LEU:HD21 | 1:F:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:H:89:LEU:HD23  | 1:H:138:ILE:O    | 2.05                     | 0.56              |
| 1:D:89:LEU:HD23  | 1:D:138:ILE:O    | 2.05                     | 0.56              |
| 1:H:139:LEU:HD21 | 1:H:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:A:121:GLU:O    | 1:A:124:MET:HG3  | 2.05                     | 0.56              |
| 1:F:61:ASN:ND2   | 1:F:63:GLN:HG3   | 2.21                     | 0.56              |
| 1:F:223:ILE:CG2  | 1:F:224:TYR:HD1  | 2.19                     | 0.56              |
| 1:E:195:LEU:HD12 | 1:E:285:VAL:O    | 2.04                     | 0.56              |
| 1:G:89:LEU:HD23  | 1:G:138:ILE:O    | 2.05                     | 0.56              |
| 1:A:287:PRO:HB2  | 1:A:288:GLN:CD   | 2.31                     | 0.56              |
| 1:E:139:LEU:HD21 | 1:E:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:A:139:LEU:HD21 | 1:A:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:C:139:LEU:HD21 | 1:C:144:TYR:CE2  | 2.41                     | 0.56              |
| 1:E:252:ASN:C    | 1:E:252:ASN:OD1  | 2.49                     | 0.56              |
| 1:F:252:ASN:OD1  | 1:F:252:ASN:C    | 2.49                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:223:ILE:C    | 1:G:224:TYR:CD1  | 2.83                     | 0.56              |
| 1:G:252:ASN:OD1  | 1:G:252:ASN:C    | 2.49                     | 0.56              |
| 1:G:293:ARG:NH2  | 1:G:336:GLU:CD   | 2.61                     | 0.56              |
| 1:D:252:ASN:OD1  | 1:D:252:ASN:C    | 2.49                     | 0.56              |
| 1:H:252:ASN:OD1  | 1:H:252:ASN:C    | 2.49                     | 0.56              |
| 1:A:89:LEU:HD23  | 1:A:138:ILE:O    | 2.06                     | 0.56              |
| 1:C:105:PRO:HD3  | 1:C:132:TRP:CH2  | 2.41                     | 0.56              |
| 1:D:170:VAL:CG1  | 1:D:178:ILE:HD13 | 2.36                     | 0.56              |
| 1:F:89:LEU:HD23  | 1:F:138:ILE:O    | 2.06                     | 0.56              |
| 1:G:253:ILE:HG22 | 1:G:254:GLN:N    | 2.16                     | 0.56              |
| 1:H:105:PRO:HD3  | 1:H:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:E:89:LEU:HD23  | 1:E:138:ILE:O    | 2.06                     | 0.55              |
| 1:H:122:LEU:C    | 1:H:124:MET:N    | 2.57                     | 0.55              |
| 1:A:250:ILE:CD1  | 1:F:250:ILE:CD1  | 2.80                     | 0.55              |
| 1:A:250:ILE:HD13 | 1:F:250:ILE:HD13 | 1.87                     | 0.55              |
| 1:A:253:ILE:HA   | 1:F:42:PHE:CE1   | 2.41                     | 0.55              |
| 1:B:89:LEU:HD23  | 1:B:138:ILE:O    | 2.05                     | 0.55              |
| 1:C:252:ASN:OD1  | 1:C:254:GLN:N    | 2.40                     | 0.55              |
| 1:E:160:PHE:CD1  | 1:E:162:ARG:NH2  | 2.75                     | 0.55              |
| 1:A:293:ARG:NH2  | 1:A:336:GLU:CD   | 2.61                     | 0.55              |
| 1:F:61:ASN:HD21  | 1:F:63:GLN:CG    | 2.19                     | 0.55              |
| 1:G:139:LEU:HD21 | 1:G:144:TYR:CE2  | 2.41                     | 0.55              |
| 1:F:105:PRO:HD3  | 1:F:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:B:252:ASN:C    | 1:B:252:ASN:OD1  | 2.49                     | 0.55              |
| 1:F:97:LEU:HD11  | 1:F:125:PHE:CD2  | 2.42                     | 0.55              |
| 1:H:23:TYR:CE2   | 1:H:330:PHE:HD2  | 2.25                     | 0.55              |
| 1:H:254:GLN:O    | 1:H:258:THR:HG23 | 2.07                     | 0.55              |
| 1:A:105:PRO:HD3  | 1:A:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:A:252:ASN:OD1  | 1:A:252:ASN:C    | 2.49                     | 0.55              |
| 1:E:105:PRO:HD3  | 1:E:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:G:105:PRO:HD3  | 1:G:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:G:171:ALA:HA   | 1:G:175:ALA:CB   | 2.33                     | 0.55              |
| 1:G:249:GLU:HB3  | 1:G:282:PHE:CZ   | 2.42                     | 0.55              |
| 1:B:139:LEU:HD21 | 1:B:144:TYR:CE2  | 2.41                     | 0.55              |
| 1:D:249:GLU:HB3  | 1:D:282:PHE:CZ   | 2.42                     | 0.55              |
| 1:H:293:ARG:NH2  | 1:H:336:GLU:CD   | 2.61                     | 0.55              |
| 1:D:105:PRO:HD3  | 1:D:132:TRP:CH2  | 2.41                     | 0.55              |
| 1:F:249:GLU:HB3  | 1:F:282:PHE:CZ   | 2.42                     | 0.55              |
| 1:C:252:ASN:OD1  | 1:C:252:ASN:C    | 2.49                     | 0.55              |
| 1:C:252:ASN:ND2  | 5:C:361:HOH:O    | 2.40                     | 0.55              |
| 1:E:249:GLU:HB3  | 1:E:282:PHE:CZ   | 2.42                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:249:GLU:HB3  | 1:A:282:PHE:CZ   | 2.42                     | 0.54              |
| 1:C:246:ASN:OD1  | 1:C:248:ASN:N    | 2.26                     | 0.54              |
| 1:C:269:THR:C    | 1:C:271:LYS:N    | 2.63                     | 0.54              |
| 1:G:2:ARG:N      | 1:G:176:ASP:OD2  | 2.31                     | 0.54              |
| 1:H:58:GLU:HG2   | 1:H:59:PRO:HD2   | 1.87                     | 0.54              |
| 1:G:23:TYR:CE2   | 1:G:330:PHE:HD2  | 2.25                     | 0.54              |
| 1:B:167:PHE:O    | 1:B:171:ALA:N    | 2.40                     | 0.54              |
| 1:C:249:GLU:HB3  | 1:C:282:PHE:CZ   | 2.42                     | 0.54              |
| 1:D:254:GLN:O    | 1:D:258:THR:HG23 | 2.08                     | 0.54              |
| 1:B:249:GLU:HB3  | 1:B:282:PHE:CZ   | 2.42                     | 0.54              |
| 1:G:177:VAL:HG12 | 1:G:178:ILE:N    | 2.21                     | 0.54              |
| 1:H:249:GLU:HB3  | 1:H:282:PHE:CZ   | 2.42                     | 0.54              |
| 1:G:59:PRO:HG3   | 1:G:106:TYR:CE1  | 2.43                     | 0.54              |
| 1:G:178:ILE:HG22 | 1:G:178:ILE:O    | 2.07                     | 0.54              |
| 1:C:150:GLU:O    | 1:C:154:GLU:HG3  | 2.08                     | 0.54              |
| 1:E:30:LEU:HD12  | 1:E:31:ASP:N     | 2.23                     | 0.54              |
| 1:F:150:GLU:O    | 1:F:154:GLU:HG3  | 2.08                     | 0.54              |
| 1:H:99:ARG:O     | 1:H:129:ARG:HG3  | 2.07                     | 0.54              |
| 1:B:22:ARG:HD2   | 1:B:23:TYR:CE1   | 2.42                     | 0.54              |
| 1:B:268:PRO:O    | 1:B:271:LYS:HB2  | 2.07                     | 0.54              |
| 1:E:151:ARG:HH21 | 1:E:154:GLU:CD   | 2.16                     | 0.54              |
| 1:H:150:GLU:O    | 1:H:154:GLU:HG3  | 2.08                     | 0.54              |
| 1:F:1:MET:SD     | 1:F:177:VAL:HG23 | 2.48                     | 0.54              |
| 1:G:30:LEU:HD12  | 1:G:30:LEU:C     | 2.32                     | 0.54              |
| 1:B:168:GLU:O    | 1:B:171:ALA:N    | 2.41                     | 0.54              |
| 1:G:151:ARG:HH21 | 1:G:154:GLU:CD   | 2.16                     | 0.54              |
| 1:D:21:GLU:HG3   | 1:D:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:D:27:LEU:HD12  | 1:D:30:LEU:CD2   | 2.39                     | 0.53              |
| 1:F:136:SER:OG   | 1:F:137:LEU:N    | 2.37                     | 0.53              |
| 1:A:165:GLU:HB3  | 1:A:169:GLU:CD   | 2.34                     | 0.53              |
| 1:B:136:SER:O    | 1:B:137:LEU:HD23 | 2.09                     | 0.53              |
| 1:D:151:ARG:HH21 | 1:D:154:GLU:CD   | 2.16                     | 0.53              |
| 1:E:21:GLU:HG3   | 1:E:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:F:293:ARG:NH2  | 1:F:336:GLU:CD   | 2.61                     | 0.53              |
| 1:A:150:GLU:O    | 1:A:154:GLU:HG3  | 2.08                     | 0.53              |
| 1:A:151:ARG:HH21 | 1:A:154:GLU:CD   | 2.16                     | 0.53              |
| 1:B:150:GLU:O    | 1:B:154:GLU:HG3  | 2.08                     | 0.53              |
| 1:C:136:SER:O    | 1:C:137:LEU:HD23 | 2.09                     | 0.53              |
| 1:E:22:ARG:NH1   | 1:E:22:ARG:CG    | 2.66                     | 0.53              |
| 1:F:136:SER:O    | 1:F:137:LEU:HD23 | 2.09                     | 0.53              |
| 1:H:136:SER:O    | 1:H:137:LEU:HD23 | 2.09                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:165:GLU:OE1  | 1:C:165:GLU:HA   | 2.07                     | 0.53              |
| 1:D:136:SER:O    | 1:D:137:LEU:HD23 | 2.09                     | 0.53              |
| 1:F:21:GLU:HG3   | 1:F:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:H:58:GLU:HG3   | 1:H:59:PRO:HD3   | 1.91                     | 0.53              |
| 1:A:21:GLU:HG3   | 1:A:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:C:21:GLU:HG3   | 1:C:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:H:246:ASN:OD1  | 1:H:248:ASN:N    | 2.26                     | 0.53              |
| 1:F:151:ARG:HH21 | 1:F:154:GLU:CD   | 2.16                     | 0.53              |
| 1:A:23:TYR:CD2   | 1:A:334:LEU:HD12 | 2.43                     | 0.53              |
| 1:E:150:GLU:O    | 1:E:154:GLU:HG3  | 2.08                     | 0.53              |
| 1:G:21:GLU:HG3   | 1:G:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:A:242:PHE:CD1  | 1:A:242:PHE:C    | 2.87                     | 0.53              |
| 1:E:256:HIS:C    | 1:E:256:HIS:CD2  | 2.87                     | 0.53              |
| 1:G:136:SER:O    | 1:G:137:LEU:HD23 | 2.09                     | 0.53              |
| 1:G:150:GLU:O    | 1:G:154:GLU:HG3  | 2.08                     | 0.53              |
| 1:H:21:GLU:HG3   | 1:H:155:ARG:NH2  | 2.23                     | 0.53              |
| 1:A:89:LEU:HA    | 1:A:138:ILE:O    | 2.09                     | 0.53              |
| 1:B:256:HIS:C    | 1:B:256:HIS:CD2  | 2.87                     | 0.53              |
| 1:C:151:ARG:HH21 | 1:C:154:GLU:CD   | 2.16                     | 0.53              |
| 1:E:293:ARG:NE   | 1:E:333:VAL:HG23 | 2.24                     | 0.53              |
| 1:G:269:THR:C    | 1:G:271:LYS:N    | 2.66                     | 0.53              |
| 1:H:215:ILE:HG22 | 1:H:217:HIS:CE1  | 2.43                     | 0.53              |
| 1:H:293:ARG:NE   | 1:H:333:VAL:HG23 | 2.24                     | 0.53              |
| 1:B:151:ARG:HH21 | 1:B:154:GLU:CD   | 2.16                     | 0.53              |
| 1:C:89:LEU:HA    | 1:C:138:ILE:O    | 2.09                     | 0.53              |
| 1:E:242:PHE:CD1  | 1:E:242:PHE:C    | 2.87                     | 0.53              |
| 1:A:313:GLY:C    | 1:A:314:TYR:CD1  | 2.87                     | 0.52              |
| 1:C:293:ARG:NE   | 1:C:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:D:150:GLU:O    | 1:D:154:GLU:HG3  | 2.08                     | 0.52              |
| 1:D:223:ILE:CG2  | 1:D:224:TYR:HD1  | 2.20                     | 0.52              |
| 1:E:58:GLU:CB    | 1:E:59:PRO:HD2   | 2.38                     | 0.52              |
| 1:E:136:SER:O    | 1:E:137:LEU:HD23 | 2.09                     | 0.52              |
| 1:G:89:LEU:HA    | 1:G:138:ILE:O    | 2.09                     | 0.52              |
| 1:B:21:GLU:HG3   | 1:B:155:ARG:NH2  | 2.23                     | 0.52              |
| 1:D:256:HIS:C    | 1:D:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:G:278:GLU:C    | 1:G:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:C:22:ARG:HG2   | 1:C:23:TYR:CE1   | 2.45                     | 0.52              |
| 1:C:96:ASN:OD1   | 1:C:217:HIS:HE1  | 1.92                     | 0.52              |
| 1:C:242:PHE:CD1  | 1:C:242:PHE:C    | 2.87                     | 0.52              |
| 1:C:278:GLU:C    | 1:C:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:D:89:LEU:HA    | 1:D:138:ILE:O    | 2.09                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:278:GLU:C    | 1:F:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:G:256:HIS:C    | 1:G:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:A:278:GLU:C    | 1:A:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:A:293:ARG:NE   | 1:A:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:B:278:GLU:C    | 1:B:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:C:253:ILE:CG1  | 1:H:42:PHE:CD1   | 2.88                     | 0.52              |
| 1:C:256:HIS:C    | 1:C:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:D:27:LEU:HD12  | 1:D:30:LEU:HD22  | 1.90                     | 0.52              |
| 1:G:242:PHE:CD1  | 1:G:242:PHE:C    | 2.87                     | 0.52              |
| 1:G:293:ARG:NE   | 1:G:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:A:136:SER:O    | 1:A:137:LEU:HD23 | 2.09                     | 0.52              |
| 1:A:252:ASN:OD1  | 1:A:254:GLN:HG2  | 2.10                     | 0.52              |
| 1:D:293:ARG:NE   | 1:D:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:B:293:ARG:NE   | 1:B:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:E:2:ARG:HD3    | 4:E:350:DTR:CG   | 2.40                     | 0.52              |
| 1:G:210:LEU:HB3  | 5:G:352:HOH:O    | 2.10                     | 0.52              |
| 1:H:256:HIS:C    | 1:H:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:B:242:PHE:CD1  | 1:B:242:PHE:C    | 2.87                     | 0.52              |
| 1:D:278:GLU:C    | 1:D:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:E:136:SER:OG   | 1:E:137:LEU:N    | 2.37                     | 0.52              |
| 1:F:89:LEU:HA    | 1:F:138:ILE:O    | 2.09                     | 0.52              |
| 1:H:151:ARG:HH21 | 1:H:154:GLU:CD   | 2.16                     | 0.52              |
| 1:A:256:HIS:C    | 1:A:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:B:251:ASN:HA   | 1:B:280:THR:HG21 | 1.92                     | 0.52              |
| 1:F:242:PHE:CD1  | 1:F:242:PHE:C    | 2.87                     | 0.52              |
| 1:H:89:LEU:HA    | 1:H:138:ILE:O    | 2.09                     | 0.52              |
| 1:F:293:ARG:NE   | 1:F:333:VAL:HG23 | 2.24                     | 0.52              |
| 1:B:89:LEU:HA    | 1:B:138:ILE:O    | 2.09                     | 0.52              |
| 1:E:89:LEU:HA    | 1:E:138:ILE:O    | 2.09                     | 0.52              |
| 1:E:278:GLU:C    | 1:E:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:F:223:ILE:CG2  | 1:F:224:TYR:CD1  | 2.91                     | 0.52              |
| 1:F:256:HIS:C    | 1:F:256:HIS:CD2  | 2.87                     | 0.52              |
| 1:H:278:GLU:C    | 1:H:279:TYR:CD1  | 2.88                     | 0.52              |
| 1:A:136:SER:OG   | 1:A:137:LEU:N    | 2.37                     | 0.51              |
| 1:G:251:ASN:HA   | 1:G:280:THR:HG21 | 1.92                     | 0.51              |
| 1:G:23:TYR:CD2   | 1:G:330:PHE:CD2  | 2.98                     | 0.51              |
| 1:G:122:LEU:O    | 1:G:125:PHE:O    | 2.28                     | 0.51              |
| 1:B:160:PHE:C    | 1:B:162:ARG:HG3  | 2.36                     | 0.51              |
| 1:B:119:PRO:HD3  | 5:B:356:HOH:O    | 2.11                     | 0.51              |
| 1:C:251:ASN:HA   | 1:C:280:THR:HG21 | 1.92                     | 0.51              |
| 1:D:224:TYR:HB2  | 1:D:242:PHE:HB2  | 1.91                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:268:PRO:HB2  | 1:H:82:PRO:HA    | 1.92                     | 0.51              |
| 1:F:1:MET:SD     | 1:F:177:VAL:CG2  | 2.99                     | 0.51              |
| 1:F:223:ILE:CG1  | 1:F:224:TYR:HD1  | 2.17                     | 0.51              |
| 1:H:242:PHE:C    | 1:H:242:PHE:HD1  | 2.18                     | 0.51              |
| 1:B:242:PHE:C    | 1:B:242:PHE:HD1  | 2.18                     | 0.51              |
| 1:F:251:ASN:HA   | 1:F:280:THR:HG21 | 1.92                     | 0.51              |
| 1:G:59:PRO:HG3   | 1:G:106:TYR:CE2  | 2.44                     | 0.51              |
| 1:A:242:PHE:C    | 1:A:242:PHE:HD1  | 2.18                     | 0.51              |
| 1:C:242:PHE:C    | 1:C:242:PHE:HD1  | 2.18                     | 0.51              |
| 1:E:293:ARG:NH2  | 1:E:336:GLU:CD   | 2.61                     | 0.51              |
| 1:H:251:ASN:HA   | 1:H:280:THR:HG21 | 1.92                     | 0.51              |
| 1:E:242:PHE:C    | 1:E:242:PHE:HD1  | 2.18                     | 0.51              |
| 1:F:22:ARG:O     | 1:F:22:ARG:HG3   | 2.11                     | 0.51              |
| 1:A:55:TYR:HB2   | 1:A:314:TYR:OH   | 2.11                     | 0.51              |
| 1:A:251:ASN:HA   | 1:A:280:THR:HG21 | 1.92                     | 0.51              |
| 1:C:23:TYR:CD2   | 1:C:330:PHE:CD2  | 2.99                     | 0.51              |
| 1:D:249:GLU:HG3  | 1:G:250:ILE:HD12 | 1.92                     | 0.51              |
| 1:D:251:ASN:HA   | 1:D:280:THR:HG21 | 1.92                     | 0.51              |
| 1:B:311:HIS:O    | 1:B:314:TYR:CD1  | 2.64                     | 0.51              |
| 1:D:61:ASN:ND2   | 1:D:63:GLN:HE21  | 1.95                     | 0.51              |
| 1:A:11:ILE:HD12  | 1:A:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:A:171:ALA:HB1  | 1:A:303:THR:HG21 | 1.93                     | 0.50              |
| 1:B:250:ILE:HD11 | 1:E:250:ILE:HD11 | 1.92                     | 0.50              |
| 1:D:27:LEU:CD1   | 1:D:30:LEU:HD22  | 2.41                     | 0.50              |
| 1:H:242:PHE:C    | 1:H:242:PHE:CD1  | 2.87                     | 0.50              |
| 1:B:293:ARG:HE   | 1:B:333:VAL:CG2  | 2.25                     | 0.50              |
| 4:F:350:DTR:H    | 4:F:350:DTR:HE3  | 1.75                     | 0.50              |
| 1:B:120:ARG:HH22 | 1:F:110:MET:C    | 2.19                     | 0.50              |
| 1:D:242:PHE:HD1  | 1:D:242:PHE:C    | 2.18                     | 0.50              |
| 1:G:144:TYR:CE2  | 1:G:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:G:269:THR:C    | 1:G:271:LYS:H    | 2.17                     | 0.50              |
| 1:D:11:ILE:HD12  | 1:D:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:E:246:ASN:OD1  | 1:E:248:ASN:N    | 2.26                     | 0.50              |
| 1:F:11:ILE:HD12  | 1:F:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:F:242:PHE:C    | 1:F:242:PHE:HD1  | 2.18                     | 0.50              |
| 1:G:11:ILE:HD12  | 1:G:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:H:58:GLU:CG    | 1:H:59:PRO:CD    | 2.83                     | 0.50              |
| 1:A:144:TYR:CE2  | 1:A:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:C:22:ARG:HD3   | 1:C:23:TYR:CZ    | 2.47                     | 0.50              |
| 1:D:265:ARG:HG3  | 1:D:265:ARG:HH11 | 1.76                     | 0.50              |
| 1:G:165:GLU:HA   | 1:G:165:GLU:OE1  | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:293:ARG:HE   | 1:G:333:VAL:CG2  | 2.25                     | 0.50              |
| 1:H:144:TYR:CE2  | 1:H:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:B:144:TYR:CE2  | 1:B:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:C:293:ARG:HE   | 1:C:333:VAL:CG2  | 2.25                     | 0.50              |
| 1:D:265:ARG:HG3  | 1:D:265:ARG:NH1  | 2.26                     | 0.50              |
| 1:E:144:TYR:CE2  | 1:E:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:F:17:LEU:CA    | 1:F:152:LEU:HD21 | 2.42                     | 0.50              |
| 1:G:242:PHE:C    | 1:G:242:PHE:HD1  | 2.18                     | 0.50              |
| 1:A:17:LEU:CA    | 1:A:152:LEU:HD21 | 2.42                     | 0.50              |
| 1:B:128:TYR:N    | 1:B:128:TYR:HD1  | 2.07                     | 0.50              |
| 1:D:144:TYR:CE2  | 1:D:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:E:59:PRO:HB2   | 1:E:61:ASN:O     | 2.12                     | 0.50              |
| 1:E:251:ASN:HA   | 1:E:280:THR:HG21 | 1.92                     | 0.50              |
| 1:H:11:ILE:HD12  | 1:H:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:B:11:ILE:HD12  | 1:B:311:HIS:CE1  | 2.47                     | 0.50              |
| 1:F:144:TYR:CE2  | 1:F:319:HIS:NE2  | 2.80                     | 0.50              |
| 1:A:293:ARG:HE   | 1:A:333:VAL:CG2  | 2.25                     | 0.49              |
| 1:F:252:ASN:OD1  | 1:F:254:GLN:N    | 2.45                     | 0.49              |
| 1:G:17:LEU:CA    | 1:G:152:LEU:HD21 | 2.42                     | 0.49              |
| 1:A:22:ARG:HG2   | 1:A:23:TYR:CE1   | 2.47                     | 0.49              |
| 1:B:170:VAL:HG12 | 1:B:175:ALA:CB   | 2.42                     | 0.49              |
| 1:B:250:ILE:CD1  | 1:E:250:ILE:HD11 | 2.40                     | 0.49              |
| 1:C:112:LEU:HB2  | 1:C:135:THR:HB   | 1.95                     | 0.49              |
| 1:F:293:ARG:HE   | 1:F:333:VAL:CG2  | 2.25                     | 0.49              |
| 1:C:268:PRO:HB2  | 1:G:82:PRO:HA    | 1.94                     | 0.49              |
| 1:A:97:LEU:HB3   | 1:A:128:TYR:CG   | 2.47                     | 0.49              |
| 1:A:251:ASN:OD1  | 1:A:280:THR:CG2  | 2.59                     | 0.49              |
| 1:C:17:LEU:CA    | 1:C:152:LEU:HD21 | 2.42                     | 0.49              |
| 1:D:293:ARG:HE   | 1:D:333:VAL:CG2  | 2.24                     | 0.49              |
| 1:F:130:TYR:CD1  | 1:F:131:GLY:N    | 2.81                     | 0.49              |
| 1:G:22:ARG:CG    | 1:G:22:ARG:O     | 2.60                     | 0.49              |
| 1:H:162:ARG:O    | 2:H:348:FAD:H2A  | 2.12                     | 0.49              |
| 1:C:130:TYR:CD1  | 1:C:131:GLY:N    | 2.81                     | 0.49              |
| 1:G:166:SER:O    | 1:G:170:VAL:HG23 | 2.12                     | 0.49              |
| 1:H:112:LEU:HB2  | 1:H:135:THR:HB   | 1.95                     | 0.49              |
| 1:A:130:TYR:CD1  | 1:A:131:GLY:N    | 2.81                     | 0.49              |
| 1:B:17:LEU:CA    | 1:B:152:LEU:HD21 | 2.42                     | 0.49              |
| 1:C:144:TYR:CE2  | 1:C:319:HIS:NE2  | 2.80                     | 0.49              |
| 1:D:17:LEU:CA    | 1:D:152:LEU:HD21 | 2.42                     | 0.49              |
| 1:D:170:VAL:HG12 | 1:D:178:ILE:CD1  | 2.42                     | 0.49              |
| 1:D:199:ARG:NH2  | 1:D:201:GLN:HE21 | 2.10                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:11:ILE:HD12 | 1:C:311:HIS:CE1  | 2.47                     | 0.49              |
| 1:D:242:PHE:C   | 1:D:242:PHE:CD1  | 2.87                     | 0.49              |
| 1:E:11:ILE:HD12 | 1:E:311:HIS:CE1  | 2.47                     | 0.49              |
| 1:G:130:TYR:CD1 | 1:G:131:GLY:N    | 2.81                     | 0.49              |
| 1:G:170:VAL:HB  | 1:G:178:ILE:CD1  | 2.42                     | 0.49              |
| 1:H:17:LEU:CA   | 1:H:152:LEU:HD21 | 2.42                     | 0.49              |
| 1:C:166:SER:O   | 1:C:169:GLU:HB3  | 2.13                     | 0.49              |
| 1:A:324:LEU:O   | 1:A:327:ALA:HB3  | 2.13                     | 0.49              |
| 1:D:213:PHE:CD1 | 1:D:213:PHE:C    | 2.91                     | 0.49              |
| 1:D:223:ILE:CB  | 1:D:224:TYR:HD1  | 2.26                     | 0.49              |
| 1:D:251:ASN:OD1 | 1:D:280:THR:CG2  | 2.59                     | 0.49              |
| 1:E:293:ARG:HE  | 1:E:333:VAL:CG2  | 2.24                     | 0.49              |
| 1:C:22:ARG:CD   | 1:C:23:TYR:CE1   | 2.96                     | 0.49              |
| 1:C:24:HIS:HD2  | 1:C:30:LEU:H     | 1.60                     | 0.49              |
| 1:D:55:TYR:CD1  | 1:D:55:TYR:N     | 2.77                     | 0.49              |
| 1:E:166:SER:O   | 1:E:169:GLU:HB3  | 2.13                     | 0.49              |
| 1:E:213:PHE:C   | 1:E:213:PHE:CD1  | 2.91                     | 0.49              |
| 1:F:62:PRO:C    | 1:F:64:GLU:N     | 2.67                     | 0.49              |
| 1:F:213:PHE:CD1 | 1:F:213:PHE:C    | 2.91                     | 0.49              |
| 1:G:166:SER:O   | 1:G:169:GLU:HB3  | 2.13                     | 0.49              |
| 1:H:293:ARG:HE  | 1:H:333:VAL:CG2  | 2.24                     | 0.49              |
| 1:B:55:TYR:CE1  | 1:B:314:TYR:CD1  | 2.97                     | 0.48              |
| 1:B:246:ASN:OD1 | 1:B:246:ASN:C    | 2.57                     | 0.48              |
| 1:D:112:LEU:HB2 | 1:D:135:THR:HB   | 1.94                     | 0.48              |
| 1:D:130:TYR:CD1 | 1:D:131:GLY:N    | 2.81                     | 0.48              |
| 1:E:17:LEU:CA   | 1:E:152:LEU:HD21 | 2.42                     | 0.48              |
| 1:E:130:TYR:CD1 | 1:E:131:GLY:N    | 2.81                     | 0.48              |
| 1:E:256:HIS:CE1 | 1:E:278:GLU:OE2  | 2.64                     | 0.48              |
| 1:F:11:ILE:HG13 | 2:F:348:FAD:O2P  | 2.13                     | 0.48              |
| 1:B:256:HIS:CE1 | 1:B:278:GLU:OE2  | 2.64                     | 0.48              |
| 1:C:246:ASN:OD1 | 1:C:246:ASN:C    | 2.56                     | 0.48              |
| 1:D:166:SER:O   | 1:D:169:GLU:HB3  | 2.13                     | 0.48              |
| 1:D:324:LEU:O   | 1:D:327:ALA:HB3  | 2.13                     | 0.48              |
| 1:E:173:GLY:O   | 4:E:350:DTR:HB3  | 2.13                     | 0.48              |
| 1:A:166:SER:O   | 1:A:169:GLU:HB3  | 2.13                     | 0.48              |
| 1:B:130:TYR:CD1 | 1:B:131:GLY:N    | 2.81                     | 0.48              |
| 1:B:324:LEU:O   | 1:B:327:ALA:HB3  | 2.13                     | 0.48              |
| 1:C:213:PHE:CD1 | 1:C:213:PHE:C    | 2.91                     | 0.48              |
| 1:D:249:GLU:HG3 | 1:G:250:ILE:CD1  | 2.44                     | 0.48              |
| 1:E:246:ASN:OD1 | 1:E:246:ASN:C    | 2.57                     | 0.48              |
| 1:G:324:LEU:O   | 1:G:327:ALA:HB3  | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:166:SER:O   | 1:H:169:GLU:HB3  | 2.13                     | 0.48              |
| 1:H:213:PHE:CD1 | 1:H:213:PHE:C    | 2.91                     | 0.48              |
| 1:B:268:PRO:HB2 | 1:F:82:PRO:HA    | 1.94                     | 0.48              |
| 1:B:269:THR:C   | 1:B:271:LYS:N    | 2.71                     | 0.48              |
| 1:D:55:TYR:N    | 1:D:55:TYR:HD1   | 2.12                     | 0.48              |
| 1:F:61:ASN:ND2  | 1:F:63:GLN:CG    | 2.77                     | 0.48              |
| 1:G:246:ASN:OD1 | 1:G:246:ASN:C    | 2.57                     | 0.48              |
| 1:H:246:ASN:OD1 | 1:H:246:ASN:C    | 2.57                     | 0.48              |
| 1:H:252:ASN:OD1 | 1:H:254:GLN:N    | 2.46                     | 0.48              |
| 1:B:11:ILE:HG13 | 2:B:348:FAD:O2P  | 2.13                     | 0.48              |
| 1:B:199:ARG:NH2 | 1:B:201:GLN:HE21 | 2.10                     | 0.48              |
| 1:E:112:LEU:HB2 | 1:E:135:THR:HB   | 1.95                     | 0.48              |
| 1:F:161:LEU:O   | 1:F:162:ARG:HD2  | 2.12                     | 0.48              |
| 1:F:166:SER:O   | 1:F:169:GLU:HB3  | 2.13                     | 0.48              |
| 1:H:130:TYR:CD1 | 1:H:131:GLY:N    | 2.81                     | 0.48              |
| 1:H:324:LEU:O   | 1:H:327:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:246:ASN:OD1 | 1:A:246:ASN:C    | 2.56                     | 0.48              |
| 1:E:251:ASN:OD1 | 1:E:280:THR:CG2  | 2.59                     | 0.48              |
| 1:G:23:TYR:CD2  | 1:G:330:PHE:HD2  | 2.32                     | 0.48              |
| 1:D:332:LYS:O   | 1:D:336:GLU:HG3  | 2.14                     | 0.48              |
| 1:E:11:ILE:HG13 | 2:E:348:FAD:O2P  | 2.14                     | 0.48              |
| 1:F:324:LEU:O   | 1:F:327:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:11:ILE:HG13 | 2:A:348:FAD:O2P  | 2.13                     | 0.48              |
| 1:B:213:PHE:CD1 | 1:B:213:PHE:C    | 2.91                     | 0.48              |
| 1:D:11:ILE:HG13 | 2:D:348:FAD:O2P  | 2.14                     | 0.48              |
| 1:F:112:LEU:HB2 | 1:F:135:THR:HB   | 1.95                     | 0.48              |
| 1:A:213:PHE:CD1 | 1:A:213:PHE:C    | 2.91                     | 0.48              |
| 1:A:332:LYS:O   | 1:A:336:GLU:HG3  | 2.14                     | 0.48              |
| 1:E:332:LYS:O   | 1:E:336:GLU:HG3  | 2.14                     | 0.48              |
| 1:G:11:ILE:HG13 | 2:G:348:FAD:O2P  | 2.14                     | 0.48              |
| 1:G:332:LYS:O   | 1:G:336:GLU:HG3  | 2.14                     | 0.48              |
| 1:B:22:ARG:CD   | 1:B:22:ARG:O     | 2.61                     | 0.48              |
| 1:B:55:TYR:N    | 1:B:55:TYR:CD1   | 2.82                     | 0.48              |
| 1:B:166:SER:O   | 1:B:169:GLU:HB3  | 2.13                     | 0.48              |
| 1:F:62:PRO:O    | 1:F:63:GLN:C     | 2.55                     | 0.48              |
| 1:G:168:GLU:O   | 1:G:171:ALA:HB3  | 2.13                     | 0.48              |
| 1:A:105:PRO:HB2 | 1:A:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:B:105:PRO:HB2 | 1:B:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:C:51:LEU:HD12 | 1:C:52:TRP:N     | 2.29                     | 0.47              |
| 1:C:230:ILE:HA  | 1:C:231:PRO:HD2  | 1.75                     | 0.47              |
| 1:C:332:LYS:O   | 1:C:336:GLU:HG3  | 2.14                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:105:PRO:HB2  | 1:D:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:D:170:VAL:HG11 | 1:D:178:ILE:HD13 | 1.96                     | 0.47              |
| 1:E:105:PRO:HB2  | 1:E:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:F:251:ASN:OD1  | 1:F:280:THR:CG2  | 2.59                     | 0.47              |
| 1:G:105:PRO:HB2  | 1:G:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:G:223:ILE:HG22 | 1:G:224:TYR:CE1  | 2.49                     | 0.47              |
| 1:H:229:ILE:C    | 1:H:230:ILE:HG13 | 2.39                     | 0.47              |
| 1:B:332:LYS:O    | 1:B:336:GLU:HG3  | 2.14                     | 0.47              |
| 1:H:35:TYR:CZ    | 1:H:162:ARG:NH1  | 2.83                     | 0.47              |
| 1:H:251:ASN:OD1  | 1:H:280:THR:CG2  | 2.59                     | 0.47              |
| 1:A:112:LEU:HB2  | 1:A:135:THR:HB   | 1.95                     | 0.47              |
| 1:B:112:LEU:HB2  | 1:B:135:THR:HB   | 1.95                     | 0.47              |
| 1:E:58:GLU:CB    | 1:E:59:PRO:CD    | 2.92                     | 0.47              |
| 1:E:252:ASN:OD1  | 1:E:254:GLN:N    | 2.47                     | 0.47              |
| 1:E:324:LEU:O    | 1:E:327:ALA:HB3  | 2.13                     | 0.47              |
| 1:A:229:ILE:C    | 1:A:230:ILE:HG13 | 2.40                     | 0.47              |
| 1:D:195:LEU:HA   | 1:D:285:VAL:O    | 2.14                     | 0.47              |
| 1:E:88:GLY:HA2   | 1:E:233:LEU:HD11 | 1.97                     | 0.47              |
| 1:F:3:VAL:HB     | 1:F:32:VAL:HG22  | 1.97                     | 0.47              |
| 1:F:246:ASN:OD1  | 1:F:246:ASN:C    | 2.57                     | 0.47              |
| 1:H:195:LEU:HA   | 1:H:285:VAL:O    | 2.14                     | 0.47              |
| 1:A:3:VAL:HB     | 1:A:32:VAL:HG22  | 1.97                     | 0.47              |
| 1:A:51:LEU:HD12  | 1:A:52:TRP:N     | 2.29                     | 0.47              |
| 1:B:88:GLY:HA2   | 1:B:233:LEU:HD11 | 1.97                     | 0.47              |
| 1:D:253:ILE:CG1  | 1:G:42:PHE:CD1   | 2.84                     | 0.47              |
| 1:E:51:LEU:HD12  | 1:E:52:TRP:N     | 2.29                     | 0.47              |
| 1:E:128:TYR:N    | 1:E:128:TYR:CD1  | 2.82                     | 0.47              |
| 1:G:112:LEU:HB2  | 1:G:135:THR:HB   | 1.95                     | 0.47              |
| 1:G:195:LEU:HA   | 1:G:285:VAL:O    | 2.14                     | 0.47              |
| 1:C:105:PRO:HB2  | 1:C:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:C:171:ALA:C    | 1:C:173:GLY:N    | 2.70                     | 0.47              |
| 1:D:3:VAL:HB     | 1:D:32:VAL:HG22  | 1.97                     | 0.47              |
| 1:D:88:GLY:HA2   | 1:D:233:LEU:HD11 | 1.97                     | 0.47              |
| 1:G:22:ARG:O     | 1:G:22:ARG:HG2   | 2.13                     | 0.47              |
| 1:H:11:ILE:HG13  | 2:H:348:FAD:O2P  | 2.14                     | 0.47              |
| 1:H:224:TYR:HB2  | 1:H:242:PHE:HB2  | 1.96                     | 0.47              |
| 1:H:332:LYS:O    | 1:H:336:GLU:HG3  | 2.14                     | 0.47              |
| 1:A:88:GLY:HA2   | 1:A:233:LEU:HD11 | 1.97                     | 0.47              |
| 1:A:195:LEU:HA   | 1:A:285:VAL:O    | 2.14                     | 0.47              |
| 1:A:208:PRO:HB2  | 1:E:233:LEU:O    | 2.15                     | 0.47              |
| 1:B:201:GLN:HA   | 1:B:279:TYR:O    | 2.15                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:3:VAL:HB     | 1:C:32:VAL:HG22  | 1.97                     | 0.47              |
| 1:C:11:ILE:HG13  | 2:C:348:FAD:O2P  | 2.13                     | 0.47              |
| 1:C:195:LEU:HA   | 1:C:285:VAL:O    | 2.14                     | 0.47              |
| 1:C:229:ILE:C    | 1:C:230:ILE:HG13 | 2.40                     | 0.47              |
| 1:D:51:LEU:HD12  | 1:D:52:TRP:N     | 2.29                     | 0.47              |
| 1:D:144:TYR:HE2  | 1:D:319:HIS:NE2  | 2.13                     | 0.47              |
| 1:D:246:ASN:OD1  | 1:D:246:ASN:C    | 2.57                     | 0.47              |
| 1:F:51:LEU:HD12  | 1:F:52:TRP:N     | 2.29                     | 0.47              |
| 1:G:144:TYR:HE2  | 1:G:319:HIS:NE2  | 2.13                     | 0.47              |
| 1:H:105:PRO:HB2  | 1:H:107:TRP:CE2  | 2.49                     | 0.47              |
| 1:H:201:GLN:HA   | 1:H:279:TYR:O    | 2.15                     | 0.47              |
| 1:A:144:TYR:HE2  | 1:A:319:HIS:NE2  | 2.13                     | 0.47              |
| 1:B:51:LEU:HD12  | 1:B:52:TRP:N     | 2.29                     | 0.47              |
| 1:B:139:LEU:HD21 | 1:B:144:TYR:CD2  | 2.50                     | 0.47              |
| 1:C:270:LEU:HD23 | 1:C:270:LEU:HA   | 1.71                     | 0.47              |
| 1:C:324:LEU:O    | 1:C:327:ALA:HB3  | 2.13                     | 0.47              |
| 1:F:229:ILE:C    | 1:F:230:ILE:HG13 | 2.40                     | 0.47              |
| 1:G:51:LEU:HD12  | 1:G:52:TRP:N     | 2.29                     | 0.47              |
| 1:G:213:PHE:CD1  | 1:G:213:PHE:C    | 2.91                     | 0.47              |
| 1:H:51:LEU:HD12  | 1:H:52:TRP:N     | 2.29                     | 0.47              |
| 1:H:129:ARG:O    | 1:H:130:TYR:HB2  | 2.14                     | 0.47              |
| 1:H:144:TYR:HE2  | 1:H:319:HIS:NE2  | 2.13                     | 0.47              |
| 1:B:127:ASP:HB2  | 1:B:128:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:293:ARG:NE   | 1:C:333:VAL:CG2  | 2.78                     | 0.47              |
| 1:D:293:ARG:NE   | 1:D:333:VAL:CG2  | 2.78                     | 0.47              |
| 1:E:195:LEU:HA   | 1:E:285:VAL:O    | 2.14                     | 0.47              |
| 1:B:229:ILE:C    | 1:B:230:ILE:HG13 | 2.40                     | 0.47              |
| 1:E:144:TYR:HE2  | 1:E:319:HIS:NE2  | 2.13                     | 0.47              |
| 1:F:88:GLY:HA2   | 1:F:233:LEU:HD11 | 1.97                     | 0.47              |
| 1:F:195:LEU:HA   | 1:F:285:VAL:O    | 2.14                     | 0.47              |
| 1:G:3:VAL:HB     | 1:G:32:VAL:HG22  | 1.97                     | 0.47              |
| 1:G:216:THR:CG2  | 1:G:217:HIS:N    | 2.75                     | 0.47              |
| 1:H:293:ARG:NE   | 1:H:333:VAL:CG2  | 2.78                     | 0.47              |
| 1:A:293:ARG:NE   | 1:A:333:VAL:CG2  | 2.78                     | 0.46              |
| 1:B:256:HIS:HB2  | 1:E:42:PHE:HZ    | 1.80                     | 0.46              |
| 1:D:60:SER:HB2   | 1:D:61:ASN:OD1   | 2.15                     | 0.46              |
| 1:E:122:LEU:HD23 | 1:E:122:LEU:HA   | 1.70                     | 0.46              |
| 1:F:105:PRO:HB2  | 1:F:107:TRP:CE2  | 2.49                     | 0.46              |
| 1:G:250:ILE:HD12 | 1:G:250:ILE:HG23 | 1.44                     | 0.46              |
| 1:H:61:ASN:O     | 1:H:64:GLU:HB2   | 2.15                     | 0.46              |
| 1:H:88:GLY:HA2   | 1:H:233:LEU:HD11 | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:133:PHE:CD1  | 1:A:133:PHE:C    | 2.93                     | 0.46              |
| 1:C:195:LEU:HD12 | 1:C:195:LEU:HA   | 1.63                     | 0.46              |
| 1:D:128:TYR:H    | 1:D:128:TYR:HD1  | 1.63                     | 0.46              |
| 1:D:229:ILE:C    | 1:D:230:ILE:HG13 | 2.40                     | 0.46              |
| 1:E:1:MET:HB2    | 1:E:176:ASP:OD2  | 2.15                     | 0.46              |
| 1:E:201:GLN:HA   | 1:E:279:TYR:O    | 2.15                     | 0.46              |
| 1:F:133:PHE:CD1  | 1:F:133:PHE:C    | 2.94                     | 0.46              |
| 1:F:139:LEU:HD21 | 1:F:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:F:144:TYR:HE2  | 1:F:319:HIS:NE2  | 2.13                     | 0.46              |
| 1:F:256:HIS:CE1  | 1:F:278:GLU:OE2  | 2.64                     | 0.46              |
| 1:G:30:LEU:HD12  | 1:G:31:ASP:H     | 1.74                     | 0.46              |
| 1:G:88:GLY:HA2   | 1:G:233:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:22:ARG:HD2   | 1:B:22:ARG:O     | 2.14                     | 0.46              |
| 1:B:251:ASN:OD1  | 1:B:280:THR:CG2  | 2.59                     | 0.46              |
| 1:C:201:GLN:HA   | 1:C:279:TYR:O    | 2.15                     | 0.46              |
| 1:D:139:LEU:HD21 | 1:D:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:F:332:LYS:O    | 1:F:336:GLU:HG3  | 2.14                     | 0.46              |
| 1:G:199:ARG:NH2  | 1:G:201:GLN:HE21 | 2.10                     | 0.46              |
| 1:H:3:VAL:HB     | 1:H:32:VAL:HG22  | 1.97                     | 0.46              |
| 1:H:139:LEU:HD21 | 1:H:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:H:176:ASP:C    | 1:H:177:VAL:HG23 | 2.39                     | 0.46              |
| 1:H:199:ARG:NH2  | 1:H:201:GLN:HE21 | 2.10                     | 0.46              |
| 1:C:133:PHE:C    | 1:C:133:PHE:CD1  | 2.93                     | 0.46              |
| 1:D:122:LEU:HA   | 1:D:122:LEU:HD23 | 1.70                     | 0.46              |
| 1:D:133:PHE:CD1  | 1:D:133:PHE:C    | 2.93                     | 0.46              |
| 1:D:253:ILE:HA   | 1:G:42:PHE:CE1   | 2.51                     | 0.46              |
| 1:E:139:LEU:HD21 | 1:E:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:E:199:ARG:NH2  | 1:E:201:GLN:HE21 | 2.10                     | 0.46              |
| 1:E:293:ARG:NE   | 1:E:333:VAL:CG2  | 2.78                     | 0.46              |
| 1:H:76:LEU:HD23  | 1:H:76:LEU:HA    | 1.62                     | 0.46              |
| 1:B:117:LEU:HD21 | 1:B:133:PHE:HB2  | 1.98                     | 0.46              |
| 1:E:117:LEU:HD21 | 1:E:133:PHE:HB2  | 1.98                     | 0.46              |
| 1:E:133:PHE:CD1  | 1:E:133:PHE:C    | 2.93                     | 0.46              |
| 1:F:293:ARG:NE   | 1:F:333:VAL:CG2  | 2.78                     | 0.46              |
| 1:H:13:LEU:HD23  | 1:H:13:LEU:HA    | 1.61                     | 0.46              |
| 1:H:208:PRO:HD2  | 1:H:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:A:117:LEU:HD21 | 1:A:133:PHE:HB2  | 1.98                     | 0.46              |
| 1:F:201:GLN:HA   | 1:F:279:TYR:O    | 2.15                     | 0.46              |
| 1:F:238:LEU:HD12 | 1:F:238:LEU:HA   | 1.56                     | 0.46              |
| 1:G:201:GLN:HA   | 1:G:279:TYR:O    | 2.15                     | 0.46              |
| 1:G:229:ILE:C    | 1:G:230:ILE:HG13 | 2.40                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:LEU:HD21 | 1:A:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:A:162:ARG:O    | 2:A:348:FAD:H2A  | 2.16                     | 0.46              |
| 1:A:201:GLN:HA   | 1:A:279:TYR:O    | 2.15                     | 0.46              |
| 1:B:3:VAL:HB     | 1:B:32:VAL:HG22  | 1.97                     | 0.46              |
| 1:B:195:LEU:HA   | 1:B:285:VAL:O    | 2.14                     | 0.46              |
| 1:C:139:LEU:HD21 | 1:C:144:TYR:CD2  | 2.50                     | 0.46              |
| 1:C:208:PRO:HD2  | 1:C:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:F:230:ILE:HA   | 1:F:231:PRO:HD2  | 1.75                     | 0.46              |
| 1:H:224:TYR:CB   | 1:H:242:PHE:HD2  | 2.23                     | 0.46              |
| 1:B:133:PHE:CD1  | 1:B:133:PHE:C    | 2.93                     | 0.46              |
| 1:B:144:TYR:HE2  | 1:B:319:HIS:NE2  | 2.13                     | 0.46              |
| 1:B:208:PRO:HD2  | 1:B:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:D:201:GLN:HA   | 1:D:279:TYR:O    | 2.15                     | 0.46              |
| 1:D:269:THR:O    | 1:D:271:LYS:N    | 2.49                     | 0.46              |
| 1:E:201:GLN:HG3  | 1:E:280:THR:CG2  | 2.24                     | 0.46              |
| 1:F:55:TYR:HE1   | 1:F:224:TYR:HH   | 1.53                     | 0.46              |
| 1:F:224:TYR:HE2  | 3:F:349:ITR:O    | 1.99                     | 0.46              |
| 1:F:270:LEU:HA   | 1:F:270:LEU:HD23 | 1.71                     | 0.46              |
| 1:H:128:TYR:CD1  | 1:H:128:TYR:N    | 2.84                     | 0.46              |
| 1:H:238:LEU:HD12 | 1:H:238:LEU:HA   | 1.56                     | 0.46              |
| 1:B:121:GLU:O    | 1:B:124:MET:HB2  | 2.16                     | 0.46              |
| 1:C:97:LEU:HB3   | 1:C:128:TYR:CB   | 2.46                     | 0.46              |
| 1:E:2:ARG:HB3    | 4:E:350:DTR:CH2  | 2.45                     | 0.46              |
| 1:E:30:LEU:HD12  | 1:E:30:LEU:C     | 2.41                     | 0.46              |
| 1:F:208:PRO:HD2  | 1:F:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:G:1:MET:O      | 1:G:30:LEU:HD13  | 2.15                     | 0.46              |
| 1:G:117:LEU:HD21 | 1:G:133:PHE:HB2  | 1.98                     | 0.46              |
| 1:H:168:GLU:CA   | 1:H:171:ALA:HB3  | 2.40                     | 0.46              |
| 1:A:90:THR:HG21  | 1:E:209:TRP:HD1  | 1.81                     | 0.46              |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:HA   | 1.63                     | 0.46              |
| 1:B:76:LEU:HA    | 1:B:76:LEU:HD23  | 1.62                     | 0.46              |
| 1:E:208:PRO:HD2  | 1:E:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:A:76:LEU:HA    | 1:A:76:LEU:HD23  | 1.62                     | 0.45              |
| 1:C:43:THR:OG1   | 1:C:45:THR:HB    | 2.16                     | 0.45              |
| 1:C:88:GLY:HA2   | 1:C:233:LEU:HD11 | 1.97                     | 0.45              |
| 1:C:236:VAL:HG12 | 1:C:237:THR:N    | 2.31                     | 0.45              |
| 1:D:250:ILE:CD1  | 1:G:249:GLU:HG3  | 2.45                     | 0.45              |
| 1:D:293:ARG:NH2  | 1:D:336:GLU:CD   | 2.61                     | 0.45              |
| 1:E:3:VAL:HB     | 1:E:32:VAL:HG22  | 1.97                     | 0.45              |
| 1:E:229:ILE:C    | 1:E:230:ILE:HG13 | 2.40                     | 0.45              |
| 1:G:139:LEU:HD21 | 1:G:144:TYR:CD2  | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:133:PHE:C    | 1:H:133:PHE:CD1  | 2.94                     | 0.45              |
| 1:A:43:THR:OG1   | 1:A:45:THR:HB    | 2.16                     | 0.45              |
| 1:A:199:ARG:NH2  | 1:A:201:GLN:HE21 | 2.10                     | 0.45              |
| 1:A:208:PRO:HD2  | 1:A:209:TRP:CE3  | 2.51                     | 0.45              |
| 1:B:236:VAL:HG12 | 1:B:237:THR:N    | 2.31                     | 0.45              |
| 1:B:293:ARG:NE   | 1:B:333:VAL:CG2  | 2.78                     | 0.45              |
| 1:B:311:HIS:O    | 1:B:314:TYR:CE1  | 2.68                     | 0.45              |
| 1:D:208:PRO:HD2  | 1:D:209:TRP:CE3  | 2.51                     | 0.45              |
| 1:E:218:ASP:HB2  | 1:E:226:SER:HG   | 1.78                     | 0.45              |
| 1:G:201:GLN:HG3  | 1:G:280:THR:CG2  | 2.24                     | 0.45              |
| 1:H:55:TYR:CD1   | 1:H:223:ILE:HD11 | 2.51                     | 0.45              |
| 1:H:117:LEU:HD21 | 1:H:133:PHE:HB2  | 1.98                     | 0.45              |
| 1:A:238:LEU:HD12 | 1:A:238:LEU:HA   | 1.56                     | 0.45              |
| 1:B:170:VAL:HB   | 1:B:178:ILE:HD11 | 1.99                     | 0.45              |
| 1:B:252:ASN:OD1  | 1:B:254:GLN:N    | 2.49                     | 0.45              |
| 1:D:43:THR:OG1   | 1:D:45:THR:HB    | 2.16                     | 0.45              |
| 1:E:17:LEU:HA    | 1:E:152:LEU:HD21 | 1.99                     | 0.45              |
| 1:F:117:LEU:HD21 | 1:F:133:PHE:HB2  | 1.98                     | 0.45              |
| 1:G:293:ARG:NE   | 1:G:333:VAL:CG2  | 2.78                     | 0.45              |
| 1:A:270:LEU:C    | 1:A:272:ASP:N    | 2.74                     | 0.45              |
| 1:C:79:ILE:CG2   | 1:G:124:MET:HG2  | 2.46                     | 0.45              |
| 1:F:17:LEU:HA    | 1:F:152:LEU:HD21 | 1.99                     | 0.45              |
| 1:G:63:GLN:HB2   | 1:G:67:TRP:CE2   | 2.51                     | 0.45              |
| 1:A:211:LYS:NZ   | 1:E:232:GLY:O    | 2.40                     | 0.45              |
| 1:B:290:ARG:NH2  | 1:B:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:C:290:ARG:NH2  | 1:C:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:D:76:LEU:HD23  | 1:D:76:LEU:HA    | 1.62                     | 0.45              |
| 1:F:316:LEU:HD23 | 1:F:316:LEU:HA   | 1.85                     | 0.45              |
| 1:G:133:PHE:CD1  | 1:G:133:PHE:C    | 2.93                     | 0.45              |
| 1:G:208:PRO:HD2  | 1:G:209:TRP:CE3  | 2.51                     | 0.45              |
| 1:G:251:ASN:OD1  | 1:G:280:THR:CG2  | 2.59                     | 0.45              |
| 1:H:177:VAL:HA   | 1:H:304:GLU:O    | 2.16                     | 0.45              |
| 1:H:236:VAL:HG12 | 1:H:237:THR:N    | 2.31                     | 0.45              |
| 1:C:144:TYR:HE2  | 1:C:319:HIS:NE2  | 2.13                     | 0.45              |
| 1:D:17:LEU:HA    | 1:D:152:LEU:HD21 | 1.99                     | 0.45              |
| 1:E:290:ARG:NH2  | 1:E:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:F:199:ARG:NH2  | 1:F:201:GLN:HE21 | 2.10                     | 0.45              |
| 1:G:223:ILE:HB   | 1:G:224:TYR:HD1  | 1.67                     | 0.45              |
| 1:H:270:LEU:C    | 1:H:272:ASP:N    | 2.74                     | 0.45              |
| 1:B:117:LEU:CD2  | 1:B:133:PHE:HB2  | 2.47                     | 0.45              |
| 1:G:290:ARG:NH2  | 1:G:307:HIS:CE1  | 2.85                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:290:ARG:NH2  | 1:H:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:A:290:ARG:NH2  | 1:A:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:B:17:LEU:HA    | 1:B:152:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:79:ILE:HD13  | 1:B:79:ILE:HA    | 1.78                     | 0.45              |
| 1:C:97:LEU:HD11  | 1:C:125:PHE:CD2  | 2.52                     | 0.45              |
| 1:D:270:LEU:HA   | 1:D:270:LEU:HD23 | 1.71                     | 0.45              |
| 1:E:270:LEU:HA   | 1:E:270:LEU:HD23 | 1.71                     | 0.45              |
| 1:F:102:VAL:HG13 | 1:F:103:PRO:CD   | 2.46                     | 0.45              |
| 1:F:117:LEU:CD2  | 1:F:133:PHE:HB2  | 2.47                     | 0.45              |
| 1:F:236:VAL:HG12 | 1:F:237:THR:N    | 2.31                     | 0.45              |
| 1:H:43:THR:OG1   | 1:H:45:THR:HB    | 2.17                     | 0.45              |
| 1:A:256:HIS:CE1  | 1:A:278:GLU:OE2  | 2.64                     | 0.45              |
| 1:C:23:TYR:CD2   | 1:C:330:PHE:CE2  | 3.05                     | 0.45              |
| 1:C:24:HIS:CD2   | 1:C:30:LEU:H     | 2.33                     | 0.45              |
| 1:C:117:LEU:HD21 | 1:C:133:PHE:HB2  | 1.98                     | 0.45              |
| 1:C:162:ARG:O    | 2:C:348:FAD:H2A  | 2.17                     | 0.45              |
| 1:D:30:LEU:HD11  | 1:D:32:VAL:CG2   | 2.45                     | 0.45              |
| 1:D:269:THR:H    | 1:D:269:THR:HG23 | 1.60                     | 0.45              |
| 1:E:43:THR:OG1   | 1:E:45:THR:HB    | 2.17                     | 0.45              |
| 1:A:122:LEU:HA   | 1:A:122:LEU:HD23 | 1.70                     | 0.45              |
| 1:A:270:LEU:HD23 | 1:A:270:LEU:HA   | 1.71                     | 0.45              |
| 1:C:117:LEU:CD2  | 1:C:133:PHE:HB2  | 2.47                     | 0.45              |
| 1:C:199:ARG:NH2  | 1:C:201:GLN:HE21 | 2.10                     | 0.45              |
| 1:D:30:LEU:C     | 1:D:30:LEU:CD1   | 2.72                     | 0.45              |
| 1:D:117:LEU:HD21 | 1:D:133:PHE:HB2  | 1.98                     | 0.45              |
| 1:D:290:ARG:NH2  | 1:D:307:HIS:CE1  | 2.85                     | 0.45              |
| 1:E:161:LEU:C    | 1:E:162:ARG:CG   | 2.90                     | 0.45              |
| 1:E:236:VAL:HG12 | 1:E:237:THR:N    | 2.31                     | 0.45              |
| 1:G:117:LEU:CD2  | 1:G:133:PHE:HB2  | 2.47                     | 0.45              |
| 1:G:324:LEU:HA   | 1:G:324:LEU:HD23 | 1.72                     | 0.45              |
| 1:A:97:LEU:HD11  | 1:A:125:PHE:CD1  | 2.52                     | 0.44              |
| 1:A:233:LEU:O    | 1:E:208:PRO:HB2  | 2.16                     | 0.44              |
| 1:B:43:THR:OG1   | 1:B:45:THR:HB    | 2.17                     | 0.44              |
| 1:B:169:GLU:O    | 1:B:172:ARG:HB2  | 2.16                     | 0.44              |
| 1:D:195:LEU:HD12 | 1:D:195:LEU:HA   | 1.63                     | 0.44              |
| 1:E:58:GLU:CD    | 1:E:59:PRO:HD2   | 2.43                     | 0.44              |
| 1:F:290:ARG:NH2  | 1:F:307:HIS:CE1  | 2.85                     | 0.44              |
| 1:G:182:THR:OG1  | 1:G:186:ALA:HA   | 2.17                     | 0.44              |
| 1:G:236:VAL:HG12 | 1:G:237:THR:N    | 2.31                     | 0.44              |
| 1:H:17:LEU:HA    | 1:H:152:LEU:HD21 | 1.99                     | 0.44              |
| 1:H:61:ASN:HA    | 1:H:62:PRO:HD2   | 1.73                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:316:LEU:HD23 | 1:H:316:LEU:HA   | 1.85                     | 0.44              |
| 1:A:182:THR:OG1  | 1:A:186:ALA:HA   | 2.17                     | 0.44              |
| 1:A:236:VAL:HG12 | 1:A:237:THR:N    | 2.31                     | 0.44              |
| 1:B:58:GLU:HG2   | 1:B:106:TYR:HB3  | 1.99                     | 0.44              |
| 1:B:133:PHE:CD1  | 1:B:134:ASN:N    | 2.86                     | 0.44              |
| 1:C:133:PHE:CD1  | 1:C:134:ASN:N    | 2.86                     | 0.44              |
| 1:C:184:VAL:HG23 | 1:C:185:TRP:CD2  | 2.53                     | 0.44              |
| 1:E:184:VAL:HG23 | 1:E:185:TRP:CD2  | 2.53                     | 0.44              |
| 1:G:30:LEU:CD1   | 1:G:31:ASP:N     | 2.67                     | 0.44              |
| 1:G:43:THR:OG1   | 1:G:45:THR:HB    | 2.16                     | 0.44              |
| 1:H:171:ALA:CB   | 1:H:298:PHE:CE2  | 3.00                     | 0.44              |
| 1:A:133:PHE:CD1  | 1:A:134:ASN:N    | 2.86                     | 0.44              |
| 1:C:17:LEU:HA    | 1:C:152:LEU:HD21 | 1.99                     | 0.44              |
| 1:C:256:HIS:CE1  | 1:C:278:GLU:OE2  | 2.64                     | 0.44              |
| 1:D:117:LEU:CD2  | 1:D:133:PHE:HB2  | 2.47                     | 0.44              |
| 1:D:236:VAL:HG12 | 1:D:237:THR:N    | 2.31                     | 0.44              |
| 1:D:270:LEU:C    | 1:D:272:ASP:N    | 2.74                     | 0.44              |
| 1:F:182:THR:OG1  | 1:F:186:ALA:HA   | 2.18                     | 0.44              |
| 1:G:270:LEU:C    | 1:G:272:ASP:N    | 2.74                     | 0.44              |
| 1:A:218:ASP:OD1  | 1:A:219:LEU:N    | 2.50                     | 0.44              |
| 1:D:182:THR:OG1  | 1:D:186:ALA:HA   | 2.17                     | 0.44              |
| 1:F:184:VAL:HG23 | 1:F:185:TRP:CD2  | 2.53                     | 0.44              |
| 1:G:59:PRO:HD3   | 1:G:106:TYR:CD1  | 2.52                     | 0.44              |
| 1:G:122:LEU:HA   | 1:G:122:LEU:HD23 | 1.70                     | 0.44              |
| 1:G:125:PHE:CD1  | 1:G:125:PHE:N    | 2.84                     | 0.44              |
| 1:H:117:LEU:CD2  | 1:H:133:PHE:HB2  | 2.47                     | 0.44              |
| 1:H:256:HIS:CE1  | 1:H:278:GLU:OE2  | 2.64                     | 0.44              |
| 1:A:201:GLN:HG3  | 1:A:280:THR:CG2  | 2.24                     | 0.44              |
| 1:B:184:VAL:HG23 | 1:B:185:TRP:CD2  | 2.53                     | 0.44              |
| 1:D:133:PHE:CD1  | 1:D:134:ASN:N    | 2.85                     | 0.44              |
| 1:E:117:LEU:CD2  | 1:E:133:PHE:HB2  | 2.47                     | 0.44              |
| 1:F:43:THR:OG1   | 1:F:45:THR:HB    | 2.16                     | 0.44              |
| 4:F:350:DTR:H    | 4:F:350:DTR:CD2  | 2.31                     | 0.44              |
| 1:G:196:GLN:O    | 1:G:285:VAL:HB   | 2.18                     | 0.44              |
| 1:H:230:ILE:HA   | 1:H:231:PRO:HD2  | 1.75                     | 0.44              |
| 1:A:117:LEU:CD2  | 1:A:133:PHE:HB2  | 2.47                     | 0.44              |
| 1:B:196:GLN:O    | 1:B:285:VAL:HB   | 2.18                     | 0.44              |
| 1:B:256:HIS:CB   | 1:E:42:PHE:HZ    | 2.30                     | 0.44              |
| 1:E:133:PHE:CD1  | 1:E:134:ASN:N    | 2.85                     | 0.44              |
| 1:E:279:TYR:CD1  | 1:E:279:TYR:N    | 2.86                     | 0.44              |
| 1:G:162:ARG:O    | 2:G:348:FAD:H2A  | 2.18                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:148:LEU:HD23 | 1:B:148:LEU:HA   | 1.86                     | 0.44              |
| 1:B:167:PHE:CZ   | 1:B:189:LEU:HB3  | 2.53                     | 0.44              |
| 1:C:270:LEU:C    | 1:C:272:ASP:H    | 2.26                     | 0.44              |
| 1:D:55:TYR:CD1   | 1:D:224:TYR:OH   | 2.66                     | 0.44              |
| 1:E:219:LEU:HD23 | 1:E:219:LEU:HA   | 1.73                     | 0.44              |
| 1:E:270:LEU:C    | 1:E:272:ASP:N    | 2.74                     | 0.44              |
| 1:H:2:ARG:HB2    | 1:H:176:ASP:OD2  | 2.18                     | 0.44              |
| 1:H:279:TYR:CD1  | 1:H:279:TYR:N    | 2.86                     | 0.44              |
| 1:A:265:ARG:O    | 1:A:265:ARG:HG2  | 2.17                     | 0.44              |
| 1:D:15:THR:O     | 1:D:16:ALA:C     | 2.61                     | 0.44              |
| 1:D:177:VAL:HG12 | 1:D:178:ILE:N    | 2.24                     | 0.44              |
| 1:D:223:ILE:HG23 | 1:D:223:ILE:O    | 2.18                     | 0.44              |
| 1:F:167:PHE:CZ   | 1:F:189:LEU:HB3  | 2.53                     | 0.44              |
| 1:G:238:LEU:HA   | 1:G:238:LEU:HD12 | 1.56                     | 0.44              |
| 1:A:267:GLU:N    | 1:A:268:PRO:HD3  | 2.33                     | 0.44              |
| 1:D:279:TYR:CD1  | 1:D:279:TYR:N    | 2.86                     | 0.44              |
| 1:G:79:ILE:HD13  | 1:G:79:ILE:HA    | 1.78                     | 0.44              |
| 1:G:133:PHE:CD1  | 1:G:134:ASN:N    | 2.86                     | 0.44              |
| 1:H:167:PHE:CZ   | 1:H:189:LEU:HB3  | 2.53                     | 0.44              |
| 1:B:55:TYR:CE2   | 1:B:224:TYR:OH   | 2.58                     | 0.43              |
| 1:C:251:ASN:OD1  | 1:C:280:THR:CG2  | 2.59                     | 0.43              |
| 1:D:184:VAL:HG23 | 1:D:185:TRP:CD2  | 2.53                     | 0.43              |
| 1:E:76:LEU:HD23  | 1:E:76:LEU:HA    | 1.62                     | 0.43              |
| 1:E:167:PHE:CZ   | 1:E:189:LEU:HB3  | 2.53                     | 0.43              |
| 1:E:196:GLN:O    | 1:E:285:VAL:HB   | 2.18                     | 0.43              |
| 1:F:270:LEU:C    | 1:F:272:ASP:N    | 2.74                     | 0.43              |
| 1:G:17:LEU:HA    | 1:G:152:LEU:HD21 | 1.99                     | 0.43              |
| 1:G:216:THR:HG23 | 1:G:217:HIS:N    | 2.32                     | 0.43              |
| 1:H:133:PHE:CD1  | 1:H:134:ASN:N    | 2.86                     | 0.43              |
| 1:C:23:TYR:O     | 1:C:30:LEU:CD2   | 2.66                     | 0.43              |
| 1:C:279:TYR:CD1  | 1:C:279:TYR:N    | 2.86                     | 0.43              |
| 1:D:145:LEU:HD23 | 1:D:145:LEU:HA   | 1.80                     | 0.43              |
| 1:D:196:GLN:O    | 1:D:285:VAL:HB   | 2.18                     | 0.43              |
| 1:F:279:TYR:CD1  | 1:F:279:TYR:N    | 2.86                     | 0.43              |
| 1:G:184:VAL:HG23 | 1:G:185:TRP:CD2  | 2.53                     | 0.43              |
| 1:H:176:ASP:C    | 1:H:177:VAL:CG2  | 2.91                     | 0.43              |
| 1:H:184:VAL:HG23 | 1:H:185:TRP:CD2  | 2.53                     | 0.43              |
| 1:H:324:LEU:HA   | 1:H:324:LEU:HD23 | 1.72                     | 0.43              |
| 1:A:22:ARG:O     | 1:A:22:ARG:CG    | 2.66                     | 0.43              |
| 1:D:167:PHE:CZ   | 1:D:189:LEU:HB3  | 2.53                     | 0.43              |
| 1:E:13:LEU:HD23  | 1:E:13:LEU:HA    | 1.62                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:15:THR:O     | 1:F:16:ALA:C     | 2.61                     | 0.43              |
| 1:F:196:GLN:O    | 1:F:285:VAL:HB   | 2.18                     | 0.43              |
| 1:G:256:HIS:CE1  | 1:G:278:GLU:OE2  | 2.64                     | 0.43              |
| 1:H:182:THR:OG1  | 1:H:186:ALA:HA   | 2.17                     | 0.43              |
| 1:H:251:ASN:HA   | 1:H:280:THR:CG2  | 2.49                     | 0.43              |
| 1:A:194:LEU:HA   | 1:A:194:LEU:HD23 | 1.08                     | 0.43              |
| 1:C:167:PHE:CZ   | 1:C:189:LEU:HB3  | 2.53                     | 0.43              |
| 1:C:182:THR:OG1  | 1:C:186:ALA:HA   | 2.17                     | 0.43              |
| 1:D:267:GLU:N    | 1:D:268:PRO:HD3  | 2.33                     | 0.43              |
| 1:G:152:LEU:HD23 | 1:G:152:LEU:HA   | 1.84                     | 0.43              |
| 1:G:167:PHE:CZ   | 1:G:189:LEU:HB3  | 2.53                     | 0.43              |
| 1:G:267:GLU:N    | 1:G:268:PRO:HD3  | 2.33                     | 0.43              |
| 1:H:196:GLN:O    | 1:H:285:VAL:HB   | 2.18                     | 0.43              |
| 1:A:196:GLN:O    | 1:A:285:VAL:HB   | 2.18                     | 0.43              |
| 1:A:251:ASN:HA   | 1:A:280:THR:CG2  | 2.49                     | 0.43              |
| 1:A:252:ASN:OD1  | 1:A:254:GLN:N    | 2.51                     | 0.43              |
| 1:B:91:PRO:HA    | 1:B:137:LEU:HD23 | 2.01                     | 0.43              |
| 1:B:182:THR:OG1  | 1:B:186:ALA:HA   | 2.18                     | 0.43              |
| 1:B:218:ASP:OD1  | 1:B:218:ASP:C    | 2.61                     | 0.43              |
| 1:B:270:LEU:C    | 1:B:272:ASP:N    | 2.74                     | 0.43              |
| 1:C:251:ASN:HA   | 1:C:280:THR:CG2  | 2.49                     | 0.43              |
| 1:D:251:ASN:HA   | 1:D:280:THR:CG2  | 2.49                     | 0.43              |
| 1:D:256:HIS:CE1  | 1:D:278:GLU:OE2  | 2.64                     | 0.43              |
| 1:E:58:GLU:CG    | 1:E:59:PRO:CD    | 2.96                     | 0.43              |
| 1:E:170:VAL:CG1  | 1:E:178:ILE:HD13 | 2.48                     | 0.43              |
| 1:F:133:PHE:CD1  | 1:F:134:ASN:N    | 2.86                     | 0.43              |
| 1:H:250:ILE:HG23 | 1:H:250:ILE:HD12 | 1.44                     | 0.43              |
| 1:A:17:LEU:HA    | 1:A:152:LEU:HD21 | 1.99                     | 0.43              |
| 1:B:238:LEU:HA   | 1:B:238:LEU:HD12 | 1.56                     | 0.43              |
| 1:B:249:GLU:HB3  | 1:B:282:PHE:CE2  | 2.54                     | 0.43              |
| 1:C:17:LEU:C     | 1:C:17:LEU:CD2   | 2.92                     | 0.43              |
| 1:C:233:LEU:HD23 | 1:C:233:LEU:HA   | 1.74                     | 0.43              |
| 1:D:250:ILE:HG23 | 1:D:250:ILE:HD12 | 1.44                     | 0.43              |
| 1:E:152:LEU:HD23 | 1:E:152:LEU:HA   | 1.83                     | 0.43              |
| 1:E:296:LEU:HD23 | 1:E:296:LEU:HA   | 1.50                     | 0.43              |
| 1:G:271:LYS:HG3  | 1:G:272:ASP:CG   | 2.44                     | 0.43              |
| 1:H:148:LEU:HD23 | 1:H:148:LEU:HA   | 1.86                     | 0.43              |
| 1:B:224:TYR:CG   | 1:B:242:PHE:HD2  | 2.36                     | 0.43              |
| 1:C:76:LEU:HD23  | 1:C:76:LEU:HA    | 1.62                     | 0.43              |
| 1:D:61:ASN:CB    | 1:D:63:GLN:HG3   | 2.43                     | 0.43              |
| 1:D:90:THR:HG21  | 1:H:209:TRP:HD1  | 1.83                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:2:ARG:NH1    | 4:E:350:DTR:CD1  | 2.82                     | 0.43              |
| 1:E:91:PRO:HA    | 1:E:137:LEU:HD23 | 2.01                     | 0.43              |
| 1:G:249:GLU:HB3  | 1:G:282:PHE:CE2  | 2.54                     | 0.43              |
| 1:H:175:ALA:O    | 1:H:303:THR:CG2  | 2.67                     | 0.43              |
| 1:A:177:VAL:HG12 | 1:A:178:ILE:N    | 2.34                     | 0.43              |
| 1:B:105:PRO:HD3  | 1:B:132:TRP:CE2  | 2.54                     | 0.43              |
| 1:D:293:ARG:HH11 | 1:D:293:ARG:HD3  | 1.65                     | 0.43              |
| 1:E:17:LEU:C     | 1:E:17:LEU:CD2   | 2.92                     | 0.43              |
| 1:E:182:THR:OG1  | 1:E:186:ALA:HA   | 2.17                     | 0.43              |
| 1:E:194:LEU:HA   | 1:E:194:LEU:HD23 | 1.08                     | 0.43              |
| 1:E:252:ASN:OD1  | 1:E:255:ASP:N    | 2.43                     | 0.43              |
| 1:F:105:PRO:HD3  | 1:F:132:TRP:CE2  | 2.54                     | 0.43              |
| 1:H:91:PRO:HA    | 1:H:137:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:17:LEU:C     | 1:A:17:LEU:CD2   | 2.92                     | 0.43              |
| 1:B:279:TYR:CD1  | 1:B:279:TYR:N    | 2.86                     | 0.43              |
| 1:C:91:PRO:HA    | 1:C:137:LEU:HD23 | 2.01                     | 0.43              |
| 1:C:215:ILE:HG22 | 1:C:217:HIS:CE1  | 2.54                     | 0.43              |
| 1:D:27:LEU:HD21  | 1:D:334:LEU:HD13 | 1.99                     | 0.43              |
| 1:D:79:ILE:HD13  | 1:D:79:ILE:HA    | 1.78                     | 0.43              |
| 1:H:35:TYR:HE1   | 1:H:160:PHE:CD2  | 2.37                     | 0.43              |
| 1:A:167:PHE:CZ   | 1:A:189:LEU:HB3  | 2.53                     | 0.43              |
| 1:B:267:GLU:N    | 1:B:268:PRO:HD3  | 2.33                     | 0.43              |
| 1:B:269:THR:H    | 1:B:269:THR:HG23 | 1.60                     | 0.43              |
| 1:D:35:TYR:HE1   | 1:D:160:PHE:CD2  | 2.37                     | 0.43              |
| 1:D:91:PRO:HA    | 1:D:137:LEU:HD23 | 2.01                     | 0.43              |
| 1:D:177:VAL:CG1  | 1:D:178:ILE:N    | 2.75                     | 0.43              |
| 1:D:324:LEU:HA   | 1:D:324:LEU:HD23 | 1.72                     | 0.43              |
| 1:E:293:ARG:HH11 | 1:E:293:ARG:HD3  | 1.65                     | 0.43              |
| 1:F:17:LEU:C     | 1:F:17:LEU:CD2   | 2.92                     | 0.43              |
| 1:F:249:GLU:HB3  | 1:F:282:PHE:CE2  | 2.54                     | 0.43              |
| 1:G:230:ILE:HA   | 1:G:231:PRO:HD2  | 1.75                     | 0.43              |
| 1:A:253:ILE:CG1  | 1:F:42:PHE:CG    | 2.95                     | 0.42              |
| 1:B:35:TYR:HE1   | 1:B:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:C:97:LEU:HB3   | 1:C:128:TYR:CG   | 2.54                     | 0.42              |
| 1:D:13:LEU:HA    | 1:D:13:LEU:HD23  | 1.62                     | 0.42              |
| 1:F:49:ALA:HB3   | 2:F:348:FAD:O4   | 2.20                     | 0.42              |
| 1:H:170:VAL:HG12 | 1:H:175:ALA:HB2  | 2.01                     | 0.42              |
| 1:H:249:GLU:HB3  | 1:H:282:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:91:PRO:HA    | 1:A:137:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:152:LEU:HD23 | 1:A:152:LEU:HA   | 1.84                     | 0.42              |
| 1:A:184:VAL:HG23 | 1:A:185:TRP:CD2  | 2.53                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:196:GLN:O    | 1:C:285:VAL:HB   | 2.18                     | 0.42              |
| 1:C:249:GLU:HB3  | 1:C:282:PHE:CE2  | 2.54                     | 0.42              |
| 1:D:233:LEU:HA   | 1:D:233:LEU:HD23 | 1.74                     | 0.42              |
| 1:E:35:TYR:HE1   | 1:E:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:G:251:ASN:HA   | 1:G:280:THR:CG2  | 2.49                     | 0.42              |
| 1:H:267:GLU:N    | 1:H:268:PRO:HD3  | 2.33                     | 0.42              |
| 1:A:331:GLY:O    | 1:A:335:GLU:N    | 2.50                     | 0.42              |
| 1:B:52:TRP:HE3   | 1:B:52:TRP:O     | 2.03                     | 0.42              |
| 1:C:105:PRO:HD3  | 1:C:132:TRP:CE2  | 2.54                     | 0.42              |
| 1:C:270:LEU:C    | 1:C:272:ASP:N    | 2.74                     | 0.42              |
| 1:D:295:GLN:C    | 1:D:296:LEU:HD23 | 2.45                     | 0.42              |
| 1:E:238:LEU:HA   | 1:E:238:LEU:HD12 | 1.56                     | 0.42              |
| 1:E:249:GLU:HB3  | 1:E:282:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:331:GLY:O    | 1:E:335:GLU:N    | 2.50                     | 0.42              |
| 1:G:17:LEU:C     | 1:G:17:LEU:CD2   | 2.92                     | 0.42              |
| 1:H:17:LEU:C     | 1:H:17:LEU:CD2   | 2.92                     | 0.42              |
| 1:H:102:VAL:HG13 | 1:H:103:PRO:CD   | 2.46                     | 0.42              |
| 1:A:279:TYR:CD1  | 1:A:279:TYR:N    | 2.86                     | 0.42              |
| 1:B:52:TRP:CZ3   | 1:B:54:PRO:HD3   | 2.55                     | 0.42              |
| 1:C:35:TYR:HE1   | 1:C:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:D:52:TRP:HE3   | 1:D:52:TRP:O     | 2.03                     | 0.42              |
| 1:D:170:VAL:HG12 | 1:D:178:ILE:HD11 | 2.00                     | 0.42              |
| 1:D:249:GLU:HB3  | 1:D:282:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:102:VAL:HG13 | 1:E:103:PRO:CD   | 2.46                     | 0.42              |
| 1:E:105:PRO:HD3  | 1:E:132:TRP:CE2  | 2.54                     | 0.42              |
| 1:E:251:ASN:HA   | 1:E:280:THR:CG2  | 2.49                     | 0.42              |
| 1:H:233:LEU:HA   | 1:H:233:LEU:HD23 | 1.74                     | 0.42              |
| 1:A:49:ALA:HB3   | 2:A:348:FAD:O4   | 2.20                     | 0.42              |
| 1:C:15:THR:O     | 1:C:16:ALA:C     | 2.61                     | 0.42              |
| 1:C:52:TRP:O     | 1:C:52:TRP:HE3   | 2.03                     | 0.42              |
| 1:C:267:GLU:N    | 1:C:268:PRO:HD3  | 2.33                     | 0.42              |
| 1:E:52:TRP:CZ3   | 1:E:54:PRO:HD3   | 2.55                     | 0.42              |
| 1:E:230:ILE:HA   | 1:E:231:PRO:HD2  | 1.75                     | 0.42              |
| 1:E:267:GLU:N    | 1:E:268:PRO:HD3  | 2.33                     | 0.42              |
| 1:F:52:TRP:CZ3   | 1:F:54:PRO:HD3   | 2.55                     | 0.42              |
| 1:F:138:ILE:HD13 | 1:F:138:ILE:HG21 | 1.72                     | 0.42              |
| 1:F:251:ASN:HA   | 1:F:280:THR:CG2  | 2.49                     | 0.42              |
| 1:F:267:GLU:N    | 1:F:268:PRO:HD3  | 2.33                     | 0.42              |
| 1:G:177:VAL:CG1  | 1:G:178:ILE:N    | 2.82                     | 0.42              |
| 1:G:279:TYR:CD1  | 1:G:279:TYR:N    | 2.86                     | 0.42              |
| 1:B:13:LEU:HA    | 1:B:13:LEU:HD23  | 1.61                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:219:LEU:HA   | 1:D:219:LEU:HD23 | 1.63                     | 0.42              |
| 1:D:219:LEU:HD23 | 1:D:219:LEU:N    | 2.27                     | 0.42              |
| 1:E:17:LEU:C     | 1:E:17:LEU:HD22  | 2.45                     | 0.42              |
| 1:G:63:GLN:O     | 1:G:64:GLU:C     | 2.62                     | 0.42              |
| 1:H:52:TRP:HE3   | 1:H:52:TRP:O     | 2.03                     | 0.42              |
| 1:H:105:PRO:HD3  | 1:H:132:TRP:CE2  | 2.54                     | 0.42              |
| 1:H:295:GLN:C    | 1:H:296:LEU:HD23 | 2.45                     | 0.42              |
| 1:A:35:TYR:HE1   | 1:A:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:A:295:GLN:C    | 1:A:296:LEU:HD23 | 2.45                     | 0.42              |
| 1:B:17:LEU:HD22  | 1:B:17:LEU:C     | 2.45                     | 0.42              |
| 1:B:101:ALA:HA   | 1:B:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:C:52:TRP:CZ3   | 1:C:54:PRO:HD3   | 2.55                     | 0.42              |
| 1:E:254:GLN:O    | 1:E:255:ASP:C    | 2.60                     | 0.42              |
| 1:G:39:PHE:O     | 1:G:42:PHE:N     | 2.42                     | 0.42              |
| 1:H:52:TRP:CZ3   | 1:H:54:PRO:HD3   | 2.55                     | 0.42              |
| 1:H:79:ILE:HD13  | 1:H:79:ILE:HA    | 1.78                     | 0.42              |
| 1:A:17:LEU:C     | 1:A:17:LEU:HD22  | 2.45                     | 0.42              |
| 1:A:118:THR:HG23 | 1:A:118:THR:H    | 1.56                     | 0.42              |
| 1:C:168:GLU:HA   | 1:C:171:ALA:HB3  | 2.01                     | 0.42              |
| 1:D:17:LEU:C     | 1:D:17:LEU:HD22  | 2.45                     | 0.42              |
| 1:D:238:LEU:HA   | 1:D:238:LEU:HD12 | 1.56                     | 0.42              |
| 1:D:265:ARG:NH1  | 1:D:265:ARG:CG   | 2.80                     | 0.42              |
| 1:E:101:ALA:HA   | 1:E:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:E:250:ILE:HD12 | 1:E:250:ILE:HG23 | 1.44                     | 0.42              |
| 1:F:171:ALA:C    | 1:F:173:GLY:N    | 2.77                     | 0.42              |
| 1:G:293:ARG:HH11 | 1:G:293:ARG:HD3  | 1.65                     | 0.42              |
| 1:H:101:ALA:HA   | 1:H:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:H:170:VAL:HG12 | 1:H:175:ALA:CB   | 2.50                     | 0.42              |
| 1:A:101:ALA:HA   | 1:A:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:A:170:VAL:HG12 | 1:A:175:ALA:HB2  | 2.02                     | 0.42              |
| 1:A:249:GLU:HB3  | 1:A:282:PHE:CE2  | 2.54                     | 0.42              |
| 1:A:265:ARG:O    | 1:A:265:ARG:CG   | 2.64                     | 0.42              |
| 1:D:102:VAL:HG13 | 1:D:103:PRO:CD   | 2.46                     | 0.42              |
| 1:D:177:VAL:HG22 | 1:D:304:GLU:HB2  | 2.02                     | 0.42              |
| 1:E:15:THR:O     | 1:E:16:ALA:C     | 2.61                     | 0.42              |
| 1:F:52:TRP:HE3   | 1:F:52:TRP:O     | 2.02                     | 0.42              |
| 1:G:91:PRO:HA    | 1:G:137:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:52:TRP:HE3   | 1:A:52:TRP:O     | 2.03                     | 0.42              |
| 1:A:314:TYR:CD1  | 1:A:314:TYR:N    | 2.87                     | 0.42              |
| 1:B:251:ASN:HA   | 1:B:280:THR:CG2  | 2.49                     | 0.42              |
| 1:C:101:ALA:HA   | 1:C:130:TYR:CD2  | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:49:ALA:HB3   | 2:D:348:FAD:O4   | 2.20                     | 0.42              |
| 1:D:101:ALA:HA   | 1:D:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:D:105:PRO:HD3  | 1:D:132:TRP:CE2  | 2.54                     | 0.42              |
| 1:D:128:TYR:C    | 1:D:129:ARG:HG2  | 2.45                     | 0.42              |
| 1:D:218:ASP:HB2  | 1:D:226:SER:OG   | 2.20                     | 0.42              |
| 1:E:49:ALA:HB3   | 2:E:348:FAD:O4   | 2.20                     | 0.42              |
| 1:F:35:TYR:HE1   | 1:F:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:F:101:ALA:HA   | 1:F:130:TYR:CD2  | 2.55                     | 0.42              |
| 1:F:217:HIS:CD2  | 5:F:363:HOH:O    | 2.73                     | 0.42              |
| 1:G:17:LEU:C     | 1:G:17:LEU:HD22  | 2.45                     | 0.42              |
| 1:G:35:TYR:HE1   | 1:G:160:PHE:CD2  | 2.37                     | 0.42              |
| 1:G:136:SER:OG   | 1:G:137:LEU:N    | 2.37                     | 0.42              |
| 1:H:59:PRO:HG3   | 1:H:65:ALA:HB2   | 2.02                     | 0.42              |
| 1:H:260:TRP:CD1  | 1:H:260:TRP:C    | 2.98                     | 0.42              |
| 1:A:13:LEU:HD23  | 1:A:13:LEU:HA    | 1.61                     | 0.41              |
| 1:B:119:PRO:CD   | 5:B:356:HOH:O    | 2.68                     | 0.41              |
| 1:F:17:LEU:C     | 1:F:17:LEU:HD22  | 2.45                     | 0.41              |
| 1:F:324:LEU:HD23 | 1:F:324:LEU:HA   | 1.72                     | 0.41              |
| 1:H:122:LEU:O    | 1:H:124:MET:N    | 2.53                     | 0.41              |
| 1:H:172:ARG:O    | 1:H:174:GLY:N    | 2.45                     | 0.41              |
| 1:A:313:GLY:C    | 1:A:314:TYR:CG   | 2.97                     | 0.41              |
| 1:C:49:ALA:HB3   | 2:C:348:FAD:O4   | 2.20                     | 0.41              |
| 1:C:75:LEU:O     | 1:C:76:LEU:C     | 2.63                     | 0.41              |
| 1:C:295:GLN:C    | 1:C:296:LEU:HD23 | 2.45                     | 0.41              |
| 1:D:147:TRP:CE2  | 1:D:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:F:269:THR:C    | 1:F:271:LYS:N    | 2.75                     | 0.41              |
| 1:G:43:THR:H     | 1:G:43:THR:HG23  | 1.66                     | 0.41              |
| 1:G:101:ALA:HA   | 1:G:130:TYR:CD2  | 2.55                     | 0.41              |
| 1:G:102:VAL:HG21 | 1:G:219:LEU:HD21 | 2.02                     | 0.41              |
| 1:H:49:ALA:HB3   | 2:H:348:FAD:O4   | 2.20                     | 0.41              |
| 1:H:172:ARG:C    | 1:H:174:GLY:N    | 2.74                     | 0.41              |
| 1:A:230:ILE:HA   | 1:A:231:PRO:HD2  | 1.75                     | 0.41              |
| 1:C:13:LEU:HD23  | 1:C:13:LEU:HA    | 1.62                     | 0.41              |
| 1:F:76:LEU:HA    | 1:F:76:LEU:HD23  | 1.62                     | 0.41              |
| 1:G:52:TRP:HE3   | 1:G:52:TRP:O     | 2.03                     | 0.41              |
| 1:H:122:LEU:O    | 1:H:125:PHE:N    | 2.41                     | 0.41              |
| 1:A:148:LEU:HD23 | 1:A:148:LEU:HA   | 1.86                     | 0.41              |
| 1:A:171:ALA:C    | 1:A:173:GLY:N    | 2.77                     | 0.41              |
| 1:C:69:GLN:N     | 1:C:110:MET:HE2  | 2.36                     | 0.41              |
| 1:C:324:LEU:HA   | 1:C:324:LEU:HD23 | 1.72                     | 0.41              |
| 1:D:130:TYR:CD1  | 1:D:130:TYR:C    | 2.99                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:295:GLN:C    | 1:E:296:LEU:HD23 | 2.45                     | 0.41              |
| 1:F:91:PRO:HA    | 1:F:137:LEU:HD23 | 2.01                     | 0.41              |
| 1:F:145:LEU:HD23 | 1:F:145:LEU:HA   | 1.80                     | 0.41              |
| 1:F:216:THR:CG2  | 1:F:217:HIS:N    | 2.80                     | 0.41              |
| 1:G:75:LEU:O     | 1:G:76:LEU:C     | 2.63                     | 0.41              |
| 1:G:105:PRO:HD3  | 1:G:132:TRP:CE2  | 2.54                     | 0.41              |
| 1:G:147:TRP:CE2  | 1:G:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:G:270:LEU:HD23 | 1:G:270:LEU:HA   | 1.71                     | 0.41              |
| 1:H:2:ARG:NH2    | 1:H:174:GLY:HA3  | 2.35                     | 0.41              |
| 1:H:75:LEU:O     | 1:H:76:LEU:C     | 2.63                     | 0.41              |
| 1:B:260:TRP:CD1  | 1:B:260:TRP:C    | 2.98                     | 0.41              |
| 1:D:52:TRP:CZ3   | 1:D:54:PRO:HD3   | 2.55                     | 0.41              |
| 1:D:223:ILE:CB   | 1:D:224:TYR:CD1  | 3.01                     | 0.41              |
| 1:E:52:TRP:HE3   | 1:E:52:TRP:O     | 2.03                     | 0.41              |
| 1:E:233:LEU:HA   | 1:E:233:LEU:HD23 | 1.74                     | 0.41              |
| 1:F:43:THR:H     | 1:F:43:THR:HG23  | 1.66                     | 0.41              |
| 1:F:69:GLN:N     | 1:F:110:MET:HE2  | 2.36                     | 0.41              |
| 1:G:295:GLN:C    | 1:G:296:LEU:HD23 | 2.45                     | 0.41              |
| 1:H:17:LEU:C     | 1:H:17:LEU:HD22  | 2.45                     | 0.41              |
| 1:A:15:THR:O     | 1:A:16:ALA:C     | 2.61                     | 0.41              |
| 1:A:170:VAL:C    | 1:A:173:GLY:H    | 2.29                     | 0.41              |
| 1:B:145:LEU:HA   | 1:B:145:LEU:HD23 | 1.80                     | 0.41              |
| 1:B:201:GLN:HG3  | 1:B:280:THR:CG2  | 2.24                     | 0.41              |
| 1:D:69:GLN:N     | 1:D:110:MET:HE2  | 2.36                     | 0.41              |
| 1:F:147:TRP:CE2  | 1:F:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:G:49:ALA:HB3   | 2:G:348:FAD:O4   | 2.19                     | 0.41              |
| 1:G:52:TRP:CZ3   | 1:G:54:PRO:HD3   | 2.55                     | 0.41              |
| 1:G:69:GLN:N     | 1:G:110:MET:HE2  | 2.36                     | 0.41              |
| 1:H:252:ASN:OD1  | 1:H:255:ASP:N    | 2.43                     | 0.41              |
| 1:A:52:TRP:CZ3   | 1:A:54:PRO:HD3   | 2.55                     | 0.41              |
| 1:A:147:TRP:CE2  | 1:A:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:A:269:THR:C    | 1:A:271:LYS:N    | 2.79                     | 0.41              |
| 1:A:316:LEU:HB2  | 2:A:348:FAD:O2   | 2.21                     | 0.41              |
| 1:B:17:LEU:C     | 1:B:17:LEU:CD2   | 2.92                     | 0.41              |
| 1:B:331:GLY:O    | 1:B:335:GLU:N    | 2.49                     | 0.41              |
| 1:C:17:LEU:C     | 1:C:17:LEU:HD22  | 2.45                     | 0.41              |
| 1:C:102:VAL:HG13 | 1:C:103:PRO:CD   | 2.46                     | 0.41              |
| 1:C:250:ILE:HD12 | 1:C:250:ILE:HG23 | 1.44                     | 0.41              |
| 1:D:17:LEU:C     | 1:D:17:LEU:CD2   | 2.92                     | 0.41              |
| 1:D:316:LEU:HB2  | 2:D:348:FAD:O2   | 2.21                     | 0.41              |
| 1:E:195:LEU:HD12 | 1:E:195:LEU:HA   | 1.63                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:48:ALA:HB1   | 2:F:348:FAD:C4X  | 2.51                     | 0.41              |
| 1:F:195:LEU:HD12 | 1:F:195:LEU:HA   | 1.63                     | 0.41              |
| 1:F:295:GLN:C    | 1:F:296:LEU:HD23 | 2.45                     | 0.41              |
| 1:G:316:LEU:HB2  | 2:G:348:FAD:O2   | 2.21                     | 0.41              |
| 1:H:40:THR:OG1   | 1:H:46:ASP:OD1   | 2.38                     | 0.41              |
| 1:H:69:GLN:N     | 1:H:110:MET:HE2  | 2.36                     | 0.41              |
| 1:A:69:GLN:N     | 1:A:110:MET:HE2  | 2.36                     | 0.41              |
| 1:B:49:ALA:HB3   | 2:B:348:FAD:O4   | 2.19                     | 0.41              |
| 1:B:75:LEU:O     | 1:B:76:LEU:C     | 2.63                     | 0.41              |
| 1:B:128:TYR:HD1  | 1:B:128:TYR:H    | 1.69                     | 0.41              |
| 1:B:147:TRP:CE2  | 1:B:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:B:160:PHE:CB   | 1:B:162:ARG:HG3  | 2.51                     | 0.41              |
| 1:B:253:ILE:HA   | 1:E:42:PHE:CZ    | 2.54                     | 0.41              |
| 1:E:118:THR:HG23 | 1:E:118:THR:H    | 1.56                     | 0.41              |
| 1:E:130:TYR:CD1  | 1:E:130:TYR:C    | 2.99                     | 0.41              |
| 1:E:260:TRP:CD1  | 1:E:260:TRP:C    | 2.98                     | 0.41              |
| 1:F:130:TYR:CD1  | 1:F:130:TYR:C    | 2.99                     | 0.41              |
| 1:G:48:ALA:HB1   | 2:G:348:FAD:C4X  | 2.51                     | 0.41              |
| 1:H:40:THR:OG1   | 1:H:142:ARG:NH1  | 2.53                     | 0.41              |
| 1:A:26:VAL:O     | 1:A:26:VAL:HG12  | 2.21                     | 0.41              |
| 1:A:48:ALA:HB1   | 2:A:348:FAD:C4X  | 2.51                     | 0.41              |
| 1:A:260:TRP:CD1  | 1:A:260:TRP:C    | 2.98                     | 0.41              |
| 1:A:268:PRO:HB2  | 1:E:82:PRO:CA    | 2.45                     | 0.41              |
| 1:B:55:TYR:HD1   | 1:B:55:TYR:H     | 1.68                     | 0.41              |
| 1:B:126:PRO:HD2  | 5:B:351:HOH:O    | 2.19                     | 0.41              |
| 1:B:152:LEU:HD23 | 1:B:152:LEU:HA   | 1.84                     | 0.41              |
| 1:B:195:LEU:HD12 | 1:B:195:LEU:HA   | 1.63                     | 0.41              |
| 1:B:295:GLN:C    | 1:B:296:LEU:HD23 | 2.45                     | 0.41              |
| 1:C:145:LEU:HD23 | 1:C:145:LEU:HA   | 1.80                     | 0.41              |
| 1:C:147:TRP:CE2  | 1:C:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:C:152:LEU:HA   | 1:C:152:LEU:HD23 | 1.84                     | 0.41              |
| 1:C:175:ALA:O    | 1:C:303:THR:HG22 | 2.21                     | 0.41              |
| 1:C:255:ASP:O    | 1:C:256:HIS:C    | 2.63                     | 0.41              |
| 1:C:316:LEU:HD23 | 1:C:316:LEU:HA   | 1.85                     | 0.41              |
| 1:D:107:TRP:O    | 1:D:108:LYS:C    | 2.64                     | 0.41              |
| 1:D:152:LEU:HD23 | 1:D:152:LEU:HA   | 1.83                     | 0.41              |
| 1:F:24:HIS:HB3   | 5:F:368:HOH:O    | 2.21                     | 0.41              |
| 1:G:102:VAL:HG13 | 1:G:103:PRO:CD   | 2.45                     | 0.41              |
| 1:G:124:MET:HE3  | 1:G:124:MET:HB2  | 1.87                     | 0.41              |
| 1:G:130:TYR:CD1  | 1:G:130:TYR:C    | 2.99                     | 0.41              |
| 1:G:224:TYR:CG   | 1:G:242:PHE:HD2  | 2.38                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:147:TRP:CE2  | 1:H:151:ARG:HD3  | 2.56                     | 0.41              |
| 1:H:316:LEU:HB2  | 2:H:348:FAD:O2   | 2.21                     | 0.41              |
| 1:A:51:LEU:HD23  | 1:A:215:ILE:HD11 | 2.03                     | 0.41              |
| 1:A:269:THR:H    | 1:A:269:THR:HG23 | 1.60                     | 0.41              |
| 1:B:130:TYR:CD1  | 1:B:130:TYR:C    | 2.99                     | 0.41              |
| 1:B:233:LEU:HD23 | 1:B:233:LEU:HA   | 1.74                     | 0.41              |
| 1:C:48:ALA:HB1   | 2:C:348:FAD:C4X  | 2.51                     | 0.41              |
| 1:C:195:LEU:HD22 | 1:C:309:TYR:CE1  | 2.56                     | 0.41              |
| 1:D:75:LEU:O     | 1:D:76:LEU:C     | 2.63                     | 0.41              |
| 1:E:98:PHE:O     | 1:E:128:TYR:HB3  | 2.21                     | 0.41              |
| 1:F:107:TRP:O    | 1:F:108:LYS:C    | 2.64                     | 0.41              |
| 1:F:122:LEU:HA   | 1:F:122:LEU:HD23 | 1.70                     | 0.41              |
| 1:G:291:LEU:HD12 | 1:G:291:LEU:C    | 2.46                     | 0.41              |
| 1:H:48:ALA:HB1   | 2:H:348:FAD:C4X  | 2.51                     | 0.41              |
| 1:A:195:LEU:HD22 | 1:A:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:B:15:THR:O     | 1:B:16:ALA:C     | 2.61                     | 0.40              |
| 1:B:69:GLN:N     | 1:B:110:MET:HE2  | 2.36                     | 0.40              |
| 1:B:73:ASN:O     | 1:B:74:TYR:C     | 2.64                     | 0.40              |
| 1:B:122:LEU:HD23 | 1:B:122:LEU:HA   | 1.70                     | 0.40              |
| 1:B:250:ILE:HG23 | 1:B:250:ILE:HD12 | 1.44                     | 0.40              |
| 1:B:291:LEU:C    | 1:B:291:LEU:HD12 | 2.46                     | 0.40              |
| 1:C:130:TYR:CD1  | 1:C:130:TYR:C    | 2.99                     | 0.40              |
| 1:C:291:LEU:HD12 | 1:C:291:LEU:C    | 2.46                     | 0.40              |
| 1:D:48:ALA:HB1   | 2:D:348:FAD:C4X  | 2.51                     | 0.40              |
| 1:D:73:ASN:O     | 1:D:74:TYR:C     | 2.64                     | 0.40              |
| 1:D:291:LEU:C    | 1:D:291:LEU:HD12 | 2.46                     | 0.40              |
| 1:E:107:TRP:O    | 1:E:108:LYS:C    | 2.64                     | 0.40              |
| 1:E:147:TRP:CE2  | 1:E:151:ARG:HD3  | 2.56                     | 0.40              |
| 1:E:195:LEU:HD22 | 1:E:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:F:233:LEU:HD23 | 1:F:233:LEU:HA   | 1.74                     | 0.40              |
| 1:F:291:LEU:HD12 | 1:F:291:LEU:C    | 2.46                     | 0.40              |
| 1:H:89:LEU:O     | 1:H:90:THR:HG23  | 2.22                     | 0.40              |
| 1:H:130:TYR:CD1  | 1:H:130:TYR:C    | 2.99                     | 0.40              |
| 1:A:105:PRO:HD3  | 1:A:132:TRP:CE2  | 2.54                     | 0.40              |
| 1:B:102:VAL:HG13 | 1:B:103:PRO:CD   | 2.46                     | 0.40              |
| 1:B:253:ILE:HD12 | 1:B:253:ILE:HG21 | 1.87                     | 0.40              |
| 1:D:55:TYR:CE1   | 1:D:314:TYR:HD1  | 2.39                     | 0.40              |
| 1:E:10:VAL:O     | 1:E:14:SER:OG    | 2.39                     | 0.40              |
| 1:E:269:THR:H    | 1:E:269:THR:HG23 | 1.60                     | 0.40              |
| 1:F:62:PRO:O     | 1:F:64:GLU:N     | 2.54                     | 0.40              |
| 1:F:63:GLN:HG3   | 1:F:63:GLN:H     | 1.63                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:75:LEU:O     | 1:F:76:LEU:C     | 2.63                     | 0.40              |
| 1:F:223:ILE:CG1  | 1:F:224:TYR:CE1  | 3.00                     | 0.40              |
| 1:G:76:LEU:HD23  | 1:G:76:LEU:HA    | 1.61                     | 0.40              |
| 1:G:118:THR:HG23 | 1:G:118:THR:H    | 1.56                     | 0.40              |
| 1:G:311:HIS:O    | 1:G:314:TYR:CD1  | 2.74                     | 0.40              |
| 1:H:291:LEU:C    | 1:H:291:LEU:HD12 | 2.46                     | 0.40              |
| 1:B:195:LEU:HD22 | 1:B:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:22:ARG:CG    | 1:C:23:TYR:CE1   | 3.04                     | 0.40              |
| 1:C:118:THR:CB   | 1:C:119:PRO:CD   | 3.00                     | 0.40              |
| 1:C:165:GLU:HB2  | 1:C:169:GLU:OE2  | 2.21                     | 0.40              |
| 1:D:195:LEU:HD22 | 1:D:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:D:331:GLY:O    | 1:D:335:GLU:N    | 2.49                     | 0.40              |
| 1:E:291:LEU:HD12 | 1:E:291:LEU:C    | 2.46                     | 0.40              |
| 1:F:73:ASN:O     | 1:F:74:TYR:C     | 2.64                     | 0.40              |
| 1:F:278:GLU:C    | 1:F:279:TYR:CG   | 3.00                     | 0.40              |
| 1:F:316:LEU:HB2  | 2:F:348:FAD:O2   | 2.21                     | 0.40              |
| 1:G:15:THR:O     | 1:G:16:ALA:C     | 2.61                     | 0.40              |
| 1:G:165:GLU:HB2  | 1:G:169:GLU:OE2  | 2.20                     | 0.40              |
| 1:G:195:LEU:HD22 | 1:G:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:H:15:THR:O     | 1:H:16:ALA:C     | 2.61                     | 0.40              |
| 1:H:107:TRP:O    | 1:H:108:LYS:C    | 2.64                     | 0.40              |
| 1:A:22:ARG:HG2   | 1:A:23:TYR:CD1   | 2.56                     | 0.40              |
| 1:A:118:THR:CB   | 1:A:119:PRO:CD   | 3.00                     | 0.40              |
| 1:B:48:ALA:HB1   | 2:B:348:FAD:C4X  | 2.51                     | 0.40              |
| 1:B:83:ASN:O     | 1:B:84:ALA:C     | 2.65                     | 0.40              |
| 1:B:89:LEU:O     | 1:B:90:THR:HG23  | 2.21                     | 0.40              |
| 1:B:256:HIS:CB   | 1:E:42:PHE:CZ    | 3.05                     | 0.40              |
| 1:C:165:GLU:HB2  | 1:C:169:GLU:CD   | 2.46                     | 0.40              |
| 1:C:238:LEU:HD12 | 1:C:238:LEU:HA   | 1.56                     | 0.40              |
| 1:E:69:GLN:N     | 1:E:110:MET:HE2  | 2.36                     | 0.40              |
| 1:E:75:LEU:O     | 1:E:76:LEU:C     | 2.63                     | 0.40              |
| 1:F:260:TRP:CD1  | 1:F:260:TRP:C    | 2.98                     | 0.40              |
| 1:G:89:LEU:O     | 1:G:90:THR:HG23  | 2.22                     | 0.40              |
| 1:G:195:LEU:HD12 | 1:G:195:LEU:HA   | 1.63                     | 0.40              |
| 1:H:118:THR:CB   | 1:H:119:PRO:CD   | 3.00                     | 0.40              |
| 1:H:195:LEU:HD22 | 1:H:309:TYR:CE1  | 2.56                     | 0.40              |
| 1:A:107:TRP:O    | 1:A:108:LYS:C    | 2.64                     | 0.40              |
| 1:A:130:TYR:CD1  | 1:A:130:TYR:C    | 2.99                     | 0.40              |
| 1:A:291:LEU:HD12 | 1:A:291:LEU:C    | 2.46                     | 0.40              |
| 1:B:255:ASP:O    | 1:B:256:HIS:C    | 2.63                     | 0.40              |
| 1:C:51:LEU:HD23  | 1:C:215:ILE:HD11 | 2.03                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:177:VAL:HA   | 1:C:304:GLU:O   | 2.21                     | 0.40              |
| 1:C:241:THR:N    | 5:C:357:HOH:O   | 2.20                     | 0.40              |
| 1:E:269:THR:C    | 1:E:271:LYS:N   | 2.79                     | 0.40              |
| 1:E:278:GLU:C    | 1:E:279:TYR:CG  | 3.00                     | 0.40              |
| 1:F:288:GLN:HE21 | 1:F:288:GLN:HB2 | 1.26                     | 0.40              |
| 1:F:329:LEU:O    | 1:F:330:PHE:C   | 2.65                     | 0.40              |
| 1:G:83:ASN:O     | 1:G:84:ALA:C    | 2.65                     | 0.40              |
| 1:G:194:LEU:HD23 | 1:G:194:LEU:HA  | 1.08                     | 0.40              |
| 1:H:278:GLU:C    | 1:H:279:TYR:CG  | 3.00                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:123:ASP:OD1 | 1:H:162:ARG:NH2[4_565] | 2.01                     | 0.19              |
| 1:A:332:LYS:NZ  | 1:D:126:PRO:CG[7_545]  | 2.11                     | 0.09              |
| 1:C:123:ASP:OD2 | 1:H:35:TYR:OH[4_565]   | 2.15                     | 0.05              |
| 1:C:162:ARG:NH2 | 1:H:123:ASP:OD1[3_655] | 2.17                     | 0.03              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 337/347 (97%) | 310 (92%) | 25 (7%) | 2 (1%)   | 21          | 52 |
| 1   | B     | 337/347 (97%) | 309 (92%) | 25 (7%) | 3 (1%)   | 14          | 44 |
| 1   | C     | 337/347 (97%) | 312 (93%) | 23 (7%) | 2 (1%)   | 21          | 52 |
| 1   | D     | 337/347 (97%) | 309 (92%) | 25 (7%) | 3 (1%)   | 14          | 44 |
| 1   | E     | 337/347 (97%) | 309 (92%) | 25 (7%) | 3 (1%)   | 14          | 44 |
| 1   | F     | 337/347 (97%) | 311 (92%) | 24 (7%) | 2 (1%)   | 21          | 52 |
| 1   | G     | 337/347 (97%) | 306 (91%) | 27 (8%) | 4 (1%)   | 10          | 37 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | H     | 337/347 (97%)   | 310 (92%)  | 23 (7%)  | 4 (1%)   | 10          | 37 |
| All | All   | 2696/2776 (97%) | 2476 (92%) | 197 (7%) | 23 (1%)  | 14          | 44 |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 28  | GLN  |
| 1   | E     | 28  | GLN  |
| 1   | A     | 28  | GLN  |
| 1   | B     | 24  | HIS  |
| 1   | G     | 222 | GLY  |
| 1   | A     | 240 | GLY  |
| 1   | B     | 240 | GLY  |
| 1   | C     | 240 | GLY  |
| 1   | D     | 240 | GLY  |
| 1   | E     | 29  | PRO  |
| 1   | E     | 240 | GLY  |
| 1   | F     | 221 | ARG  |
| 1   | F     | 240 | GLY  |
| 1   | G     | 240 | GLY  |
| 1   | H     | 123 | ASP  |
| 1   | H     | 240 | GLY  |
| 1   | H     | 271 | LYS  |
| 1   | B     | 271 | LYS  |
| 1   | D     | 29  | PRO  |
| 1   | D     | 126 | PRO  |
| 1   | G     | 26  | VAL  |
| 1   | H     | 173 | GLY  |
| 1   | G     | 29  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 290/298 (97%) | 259 (89%) | 31 (11%) | 6           | 25 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | B     | 290/298 (97%)   | 260 (90%)  | 30 (10%)  | 7           | 27 |
| 1   | C     | 290/298 (97%)   | 260 (90%)  | 30 (10%)  | 7           | 27 |
| 1   | D     | 290/298 (97%)   | 261 (90%)  | 29 (10%)  | 7           | 29 |
| 1   | E     | 290/298 (97%)   | 258 (89%)  | 32 (11%)  | 6           | 24 |
| 1   | F     | 290/298 (97%)   | 257 (89%)  | 33 (11%)  | 5           | 23 |
| 1   | G     | 290/298 (97%)   | 256 (88%)  | 34 (12%)  | 5           | 22 |
| 1   | H     | 290/298 (97%)   | 262 (90%)  | 28 (10%)  | 8           | 30 |
| All | All   | 2320/2384 (97%) | 2073 (89%) | 247 (11%) | 6           | 26 |

All (247) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | SER  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 28  | GLN  |
| 1   | A     | 30  | LEU  |
| 1   | A     | 58  | GLU  |
| 1   | A     | 60  | SER  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 89  | LEU  |
| 1   | A     | 99  | ARG  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 138 | ILE  |
| 1   | A     | 142 | ARG  |
| 1   | A     | 151 | ARG  |
| 1   | A     | 184 | VAL  |
| 1   | A     | 190 | GLN  |
| 1   | A     | 202 | ILE  |
| 1   | A     | 205 | VAL  |
| 1   | A     | 216 | THR  |
| 1   | A     | 221 | ARG  |
| 1   | A     | 224 | TYR  |
| 1   | A     | 238 | LEU  |
| 1   | A     | 241 | THR  |
| 1   | A     | 242 | PHE  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 253 | ILE  |
| 1   | A     | 254 | GLN  |
| 1   | A     | 256 | HIS  |
| 1   | A     | 258 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 276 | VAL  |
| 1   | A     | 280 | THR  |
| 1   | A     | 291 | LEU  |
| 1   | B     | 14  | SER  |
| 1   | B     | 17  | LEU  |
| 1   | B     | 55  | TYR  |
| 1   | B     | 56  | THR  |
| 1   | B     | 76  | LEU  |
| 1   | B     | 89  | LEU  |
| 1   | B     | 99  | ARG  |
| 1   | B     | 102 | VAL  |
| 1   | B     | 128 | TYR  |
| 1   | B     | 138 | ILE  |
| 1   | B     | 142 | ARG  |
| 1   | B     | 151 | ARG  |
| 1   | B     | 177 | VAL  |
| 1   | B     | 184 | VAL  |
| 1   | B     | 190 | GLN  |
| 1   | B     | 202 | ILE  |
| 1   | B     | 205 | VAL  |
| 1   | B     | 216 | THR  |
| 1   | B     | 224 | TYR  |
| 1   | B     | 238 | LEU  |
| 1   | B     | 241 | THR  |
| 1   | B     | 242 | PHE  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 253 | ILE  |
| 1   | B     | 256 | HIS  |
| 1   | B     | 258 | THR  |
| 1   | B     | 265 | ARG  |
| 1   | B     | 276 | VAL  |
| 1   | B     | 280 | THR  |
| 1   | B     | 291 | LEU  |
| 1   | C     | 14  | SER  |
| 1   | C     | 17  | LEU  |
| 1   | C     | 28  | GLN  |
| 1   | C     | 29  | PRO  |
| 1   | C     | 76  | LEU  |
| 1   | C     | 89  | LEU  |
| 1   | C     | 99  | ARG  |
| 1   | C     | 102 | VAL  |
| 1   | C     | 129 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 138 | ILE  |
| 1   | C     | 142 | ARG  |
| 1   | C     | 151 | ARG  |
| 1   | C     | 184 | VAL  |
| 1   | C     | 190 | GLN  |
| 1   | C     | 202 | ILE  |
| 1   | C     | 205 | VAL  |
| 1   | C     | 216 | THR  |
| 1   | C     | 224 | TYR  |
| 1   | C     | 238 | LEU  |
| 1   | C     | 241 | THR  |
| 1   | C     | 242 | PHE  |
| 1   | C     | 252 | ASN  |
| 1   | C     | 253 | ILE  |
| 1   | C     | 256 | HIS  |
| 1   | C     | 258 | THR  |
| 1   | C     | 271 | LYS  |
| 1   | C     | 276 | VAL  |
| 1   | C     | 280 | THR  |
| 1   | C     | 288 | GLN  |
| 1   | C     | 291 | LEU  |
| 1   | D     | 14  | SER  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 22  | ARG  |
| 1   | D     | 24  | HIS  |
| 1   | D     | 30  | LEU  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 76  | LEU  |
| 1   | D     | 89  | LEU  |
| 1   | D     | 99  | ARG  |
| 1   | D     | 102 | VAL  |
| 1   | D     | 138 | ILE  |
| 1   | D     | 142 | ARG  |
| 1   | D     | 151 | ARG  |
| 1   | D     | 184 | VAL  |
| 1   | D     | 190 | GLN  |
| 1   | D     | 202 | ILE  |
| 1   | D     | 205 | VAL  |
| 1   | D     | 216 | THR  |
| 1   | D     | 224 | TYR  |
| 1   | D     | 238 | LEU  |
| 1   | D     | 241 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 242 | PHE  |
| 1   | D     | 252 | ASN  |
| 1   | D     | 253 | ILE  |
| 1   | D     | 256 | HIS  |
| 1   | D     | 258 | THR  |
| 1   | D     | 276 | VAL  |
| 1   | D     | 280 | THR  |
| 1   | D     | 291 | LEU  |
| 1   | E     | 14  | SER  |
| 1   | E     | 17  | LEU  |
| 1   | E     | 22  | ARG  |
| 1   | E     | 57  | SER  |
| 1   | E     | 58  | GLU  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 76  | LEU  |
| 1   | E     | 89  | LEU  |
| 1   | E     | 99  | ARG  |
| 1   | E     | 102 | VAL  |
| 1   | E     | 125 | PHE  |
| 1   | E     | 138 | ILE  |
| 1   | E     | 142 | ARG  |
| 1   | E     | 151 | ARG  |
| 1   | E     | 184 | VAL  |
| 1   | E     | 190 | GLN  |
| 1   | E     | 202 | ILE  |
| 1   | E     | 205 | VAL  |
| 1   | E     | 216 | THR  |
| 1   | E     | 223 | ILE  |
| 1   | E     | 224 | TYR  |
| 1   | E     | 225 | ASN  |
| 1   | E     | 238 | LEU  |
| 1   | E     | 241 | THR  |
| 1   | E     | 242 | PHE  |
| 1   | E     | 252 | ASN  |
| 1   | E     | 253 | ILE  |
| 1   | E     | 256 | HIS  |
| 1   | E     | 258 | THR  |
| 1   | E     | 276 | VAL  |
| 1   | E     | 280 | THR  |
| 1   | E     | 291 | LEU  |
| 1   | F     | 14  | SER  |
| 1   | F     | 17  | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 22  | ARG  |
| 1   | F     | 60  | SER  |
| 1   | F     | 62  | PRO  |
| 1   | F     | 76  | LEU  |
| 1   | F     | 89  | LEU  |
| 1   | F     | 99  | ARG  |
| 1   | F     | 102 | VAL  |
| 1   | F     | 138 | ILE  |
| 1   | F     | 142 | ARG  |
| 1   | F     | 151 | ARG  |
| 1   | F     | 177 | VAL  |
| 1   | F     | 184 | VAL  |
| 1   | F     | 190 | GLN  |
| 1   | F     | 202 | ILE  |
| 1   | F     | 205 | VAL  |
| 1   | F     | 216 | THR  |
| 1   | F     | 219 | LEU  |
| 1   | F     | 224 | TYR  |
| 1   | F     | 225 | ASN  |
| 1   | F     | 238 | LEU  |
| 1   | F     | 241 | THR  |
| 1   | F     | 242 | PHE  |
| 1   | F     | 252 | ASN  |
| 1   | F     | 253 | ILE  |
| 1   | F     | 254 | GLN  |
| 1   | F     | 256 | HIS  |
| 1   | F     | 258 | THR  |
| 1   | F     | 276 | VAL  |
| 1   | F     | 280 | THR  |
| 1   | F     | 288 | GLN  |
| 1   | F     | 291 | LEU  |
| 1   | G     | 14  | SER  |
| 1   | G     | 17  | LEU  |
| 1   | G     | 30  | LEU  |
| 1   | G     | 56  | THR  |
| 1   | G     | 61  | ASN  |
| 1   | G     | 63  | GLN  |
| 1   | G     | 76  | LEU  |
| 1   | G     | 89  | LEU  |
| 1   | G     | 99  | ARG  |
| 1   | G     | 102 | VAL  |
| 1   | G     | 125 | PHE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 138 | ILE  |
| 1   | G     | 142 | ARG  |
| 1   | G     | 151 | ARG  |
| 1   | G     | 170 | VAL  |
| 1   | G     | 184 | VAL  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 202 | ILE  |
| 1   | G     | 205 | VAL  |
| 1   | G     | 216 | THR  |
| 1   | G     | 218 | ASP  |
| 1   | G     | 223 | ILE  |
| 1   | G     | 224 | TYR  |
| 1   | G     | 225 | ASN  |
| 1   | G     | 238 | LEU  |
| 1   | G     | 241 | THR  |
| 1   | G     | 242 | PHE  |
| 1   | G     | 252 | ASN  |
| 1   | G     | 253 | ILE  |
| 1   | G     | 256 | HIS  |
| 1   | G     | 258 | THR  |
| 1   | G     | 276 | VAL  |
| 1   | G     | 280 | THR  |
| 1   | G     | 291 | LEU  |
| 1   | H     | 14  | SER  |
| 1   | H     | 17  | LEU  |
| 1   | H     | 28  | GLN  |
| 1   | H     | 76  | LEU  |
| 1   | H     | 89  | LEU  |
| 1   | H     | 99  | ARG  |
| 1   | H     | 102 | VAL  |
| 1   | H     | 129 | ARG  |
| 1   | H     | 138 | ILE  |
| 1   | H     | 142 | ARG  |
| 1   | H     | 151 | ARG  |
| 1   | H     | 177 | VAL  |
| 1   | H     | 184 | VAL  |
| 1   | H     | 190 | GLN  |
| 1   | H     | 202 | ILE  |
| 1   | H     | 205 | VAL  |
| 1   | H     | 216 | THR  |
| 1   | H     | 224 | TYR  |
| 1   | H     | 238 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 241 | THR  |
| 1   | H     | 242 | PHE  |
| 1   | H     | 252 | ASN  |
| 1   | H     | 253 | ILE  |
| 1   | H     | 256 | HIS  |
| 1   | H     | 258 | THR  |
| 1   | H     | 276 | VAL  |
| 1   | H     | 280 | THR  |
| 1   | H     | 291 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | ASN  |
| 1   | A     | 63  | GLN  |
| 1   | A     | 134 | ASN  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 201 | GLN  |
| 1   | A     | 217 | HIS  |
| 1   | A     | 307 | HIS  |
| 1   | B     | 134 | ASN  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 201 | GLN  |
| 1   | B     | 217 | HIS  |
| 1   | B     | 288 | GLN  |
| 1   | B     | 307 | HIS  |
| 1   | C     | 24  | HIS  |
| 1   | C     | 134 | ASN  |
| 1   | C     | 146 | GLN  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 217 | HIS  |
| 1   | C     | 288 | GLN  |
| 1   | C     | 307 | HIS  |
| 1   | D     | 24  | HIS  |
| 1   | D     | 63  | GLN  |
| 1   | D     | 70  | GLN  |
| 1   | D     | 134 | ASN  |
| 1   | D     | 146 | GLN  |
| 1   | D     | 201 | GLN  |
| 1   | D     | 217 | HIS  |
| 1   | D     | 225 | ASN  |
| 1   | D     | 288 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 307 | HIS  |
| 1   | E     | 134 | ASN  |
| 1   | E     | 146 | GLN  |
| 1   | E     | 201 | GLN  |
| 1   | E     | 217 | HIS  |
| 1   | E     | 307 | HIS  |
| 1   | F     | 63  | GLN  |
| 1   | F     | 146 | GLN  |
| 1   | F     | 201 | GLN  |
| 1   | F     | 217 | HIS  |
| 1   | F     | 254 | GLN  |
| 1   | F     | 288 | GLN  |
| 1   | F     | 307 | HIS  |
| 1   | G     | 70  | GLN  |
| 1   | G     | 134 | ASN  |
| 1   | G     | 146 | GLN  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 217 | HIS  |
| 1   | G     | 225 | ASN  |
| 1   | G     | 307 | HIS  |
| 1   | H     | 70  | GLN  |
| 1   | H     | 134 | ASN  |
| 1   | H     | 146 | GLN  |
| 1   | H     | 201 | GLN  |
| 1   | H     | 217 | HIS  |
| 1   | H     | 307 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

18 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ITR  | G     | 349 | -    | 15,16,16     | 1.02 | 1 (6%)   | 17,22,22    | 0.67 | 0        |
| 2   | FAD  | C     | 348 | -    | 58,58,58     | 1.06 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 3   | ITR  | D     | 349 | -    | 15,16,16     | 1.02 | 2 (13%)  | 17,22,22    | 0.67 | 0        |
| 2   | FAD  | E     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.36 | 11 (12%) |
| 2   | FAD  | F     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 2   | FAD  | D     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 2   | FAD  | G     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 2   | FAD  | H     | 348 | -    | 58,58,58     | 1.08 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 3   | ITR  | F     | 349 | -    | 15,16,16     | 1.02 | 1 (6%)   | 17,22,22    | 0.66 | 0        |
| 3   | ITR  | C     | 349 | -    | 15,16,16     | 1.01 | 1 (6%)   | 17,22,22    | 0.66 | 0        |
| 3   | ITR  | E     | 349 | -    | 15,16,16     | 1.01 | 1 (6%)   | 17,22,22    | 0.67 | 0        |
| 2   | FAD  | A     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 3   | ITR  | B     | 349 | -    | 15,16,16     | 1.01 | 1 (6%)   | 17,22,22    | 0.67 | 0        |
| 2   | FAD  | B     | 348 | -    | 58,58,58     | 1.07 | 5 (8%)   | 85,89,89    | 1.35 | 11 (12%) |
| 4   | DTR  | E     | 350 | -    | 15,16,16     | 1.13 | 1 (6%)   | 18,22,22    | 0.79 | 1 (5%)   |
| 3   | ITR  | A     | 349 | -    | 15,16,16     | 1.01 | 2 (13%)  | 17,22,22    | 0.67 | 0        |
| 3   | ITR  | H     | 349 | -    | 15,16,16     | 1.01 | 2 (13%)  | 17,22,22    | 0.67 | 0        |
| 4   | DTR  | F     | 350 | -    | 15,16,16     | 1.34 | 2 (13%)  | 18,22,22    | 1.15 | 1 (5%)   |

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   | ITR  | G     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 2   | FAD  | C     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | ITR  | D     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 2   | FAD  | E     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 2   | FAD  | F     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 2   | FAD  | D     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 2   | FAD  | G     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 2   | FAD  | H     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 3   | ITR  | F     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 3   | ITR  | C     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 3   | ITR  | E     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 2   | FAD  | A     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 3   | ITR  | B     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 2   | FAD  | B     | 348 | -    | -       | 5/34/50/50 | 0/6/6/6 |
| 4   | DTR  | E     | 350 | -    | -       | 1/8/8/8    | 0/2/2/2 |
| 3   | ITR  | A     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 3   | ITR  | H     | 349 | -    | -       | 0/5/8/8    | 0/2/2/2 |
| 4   | DTR  | F     | 350 | -    | -       | 2/8/8/8    | 0/2/2/2 |

All (54) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 348 | FAD  | C5X-N5  | -3.44 | 1.33        | 1.39     |
| 2   | B     | 348 | FAD  | C5X-N5  | -3.43 | 1.33        | 1.39     |
| 2   | A     | 348 | FAD  | C5X-N5  | -3.41 | 1.33        | 1.39     |
| 2   | E     | 348 | FAD  | C5X-N5  | -3.41 | 1.33        | 1.39     |
| 2   | H     | 348 | FAD  | C5X-N5  | -3.40 | 1.33        | 1.39     |
| 2   | F     | 348 | FAD  | C5X-N5  | -3.40 | 1.33        | 1.39     |
| 2   | D     | 348 | FAD  | C5X-N5  | -3.39 | 1.33        | 1.39     |
| 2   | C     | 348 | FAD  | C5X-N5  | -3.37 | 1.33        | 1.39     |
| 2   | F     | 348 | FAD  | P-O3P   | 3.17  | 1.62        | 1.59     |
| 2   | H     | 348 | FAD  | P-O3P   | 3.16  | 1.62        | 1.59     |
| 2   | E     | 348 | FAD  | P-O3P   | 3.12  | 1.62        | 1.59     |
| 2   | D     | 348 | FAD  | P-O3P   | 3.09  | 1.62        | 1.59     |
| 2   | G     | 348 | FAD  | P-O3P   | 3.09  | 1.62        | 1.59     |
| 2   | B     | 348 | FAD  | P-O3P   | 3.08  | 1.62        | 1.59     |
| 2   | C     | 348 | FAD  | P-O3P   | 3.08  | 1.62        | 1.59     |
| 2   | A     | 348 | FAD  | P-O3P   | 3.07  | 1.62        | 1.59     |
| 4   | F     | 350 | DTR  | CB-CG   | -2.97 | 1.44        | 1.50     |
| 2   | H     | 348 | FAD  | C9A-N10 | -2.94 | 1.36        | 1.41     |
| 2   | D     | 348 | FAD  | C9A-N10 | -2.93 | 1.36        | 1.41     |
| 2   | G     | 348 | FAD  | C9A-N10 | -2.92 | 1.36        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 348 | FAD  | C9A-N10 | -2.92 | 1.36        | 1.41     |
| 2   | A     | 348 | FAD  | C9A-N10 | -2.91 | 1.36        | 1.41     |
| 2   | E     | 348 | FAD  | C9A-N10 | -2.89 | 1.36        | 1.41     |
| 2   | C     | 348 | FAD  | C9A-N10 | -2.86 | 1.36        | 1.41     |
| 2   | F     | 348 | FAD  | C9A-N10 | -2.85 | 1.36        | 1.41     |
| 2   | B     | 348 | FAD  | PA-O3P  | 2.49  | 1.62        | 1.59     |
| 2   | A     | 348 | FAD  | PA-O3P  | 2.47  | 1.62        | 1.59     |
| 2   | D     | 348 | FAD  | PA-O3P  | 2.47  | 1.62        | 1.59     |
| 2   | G     | 348 | FAD  | PA-O3P  | 2.45  | 1.62        | 1.59     |
| 2   | H     | 348 | FAD  | PA-O3P  | 2.40  | 1.62        | 1.59     |
| 2   | E     | 348 | FAD  | PA-O3P  | 2.39  | 1.62        | 1.59     |
| 2   | F     | 348 | FAD  | PA-O3P  | 2.39  | 1.62        | 1.59     |
| 2   | C     | 348 | FAD  | PA-O3P  | 2.37  | 1.62        | 1.59     |
| 3   | E     | 349 | ITR  | CA-N    | 2.31  | 1.32        | 1.27     |
| 3   | G     | 349 | ITR  | CA-N    | 2.29  | 1.32        | 1.27     |
| 3   | C     | 349 | ITR  | CA-N    | 2.26  | 1.32        | 1.27     |
| 3   | D     | 349 | ITR  | CA-N    | 2.26  | 1.32        | 1.27     |
| 3   | F     | 349 | ITR  | CA-N    | 2.26  | 1.32        | 1.27     |
| 3   | B     | 349 | ITR  | CA-N    | 2.26  | 1.32        | 1.27     |
| 3   | A     | 349 | ITR  | CA-N    | 2.25  | 1.32        | 1.27     |
| 3   | H     | 349 | ITR  | CA-N    | 2.25  | 1.32        | 1.27     |
| 4   | E     | 350 | DTR  | CB-CG   | -2.19 | 1.46        | 1.50     |
| 4   | F     | 350 | DTR  | CD2-CG  | -2.13 | 1.40        | 1.44     |
| 2   | E     | 348 | FAD  | C4X-N5  | 2.09  | 1.35        | 1.30     |
| 2   | H     | 348 | FAD  | C4X-N5  | 2.07  | 1.35        | 1.30     |
| 2   | A     | 348 | FAD  | C4X-N5  | 2.05  | 1.35        | 1.30     |
| 2   | G     | 348 | FAD  | C4X-N5  | 2.04  | 1.35        | 1.30     |
| 2   | F     | 348 | FAD  | C4X-N5  | 2.03  | 1.35        | 1.30     |
| 2   | B     | 348 | FAD  | C4X-N5  | 2.03  | 1.35        | 1.30     |
| 2   | C     | 348 | FAD  | C4X-N5  | 2.03  | 1.35        | 1.30     |
| 2   | D     | 348 | FAD  | C4X-N5  | 2.03  | 1.35        | 1.30     |
| 3   | D     | 349 | ITR  | OXT-C   | -2.01 | 1.25        | 1.30     |
| 3   | H     | 349 | ITR  | OXT-C   | -2.01 | 1.25        | 1.30     |
| 3   | A     | 349 | ITR  | OXT-C   | -2.00 | 1.25        | 1.30     |

All (90) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | H     | 348 | FAD  | C2B-C1B-N9A | 4.32 | 124.03      | 113.30   |
| 2   | C     | 348 | FAD  | C2B-C1B-N9A | 4.31 | 124.02      | 113.30   |
| 2   | G     | 348 | FAD  | C2B-C1B-N9A | 4.31 | 124.02      | 113.30   |
| 2   | E     | 348 | FAD  | C2B-C1B-N9A | 4.31 | 124.01      | 113.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 348 | FAD  | C2B-C1B-N9A | 4.31  | 124.01      | 113.30   |
| 2   | F     | 348 | FAD  | C2B-C1B-N9A | 4.31  | 124.01      | 113.30   |
| 2   | A     | 348 | FAD  | C2B-C1B-N9A | 4.30  | 123.99      | 113.30   |
| 2   | D     | 348 | FAD  | C2B-C1B-N9A | 4.30  | 123.99      | 113.30   |
| 2   | E     | 348 | FAD  | C5X-C9A-N10 | 3.79  | 121.40      | 117.97   |
| 2   | A     | 348 | FAD  | C5X-C9A-N10 | 3.77  | 121.37      | 117.97   |
| 2   | H     | 348 | FAD  | C5X-C9A-N10 | 3.75  | 121.36      | 117.97   |
| 2   | G     | 348 | FAD  | C5X-C9A-N10 | 3.74  | 121.35      | 117.97   |
| 2   | D     | 348 | FAD  | C5X-C9A-N10 | 3.74  | 121.35      | 117.97   |
| 2   | B     | 348 | FAD  | C5X-C9A-N10 | 3.73  | 121.34      | 117.97   |
| 2   | F     | 348 | FAD  | C5X-C9A-N10 | 3.73  | 121.34      | 117.97   |
| 2   | C     | 348 | FAD  | C5X-C9A-N10 | 3.72  | 121.33      | 117.97   |
| 2   | A     | 348 | FAD  | O2B-C2B-C3B | -3.13 | 101.78      | 111.82   |
| 2   | B     | 348 | FAD  | O2B-C2B-C3B | -3.13 | 101.78      | 111.82   |
| 2   | D     | 348 | FAD  | O2B-C2B-C3B | -3.13 | 101.78      | 111.82   |
| 2   | G     | 348 | FAD  | O2B-C2B-C3B | -3.13 | 101.79      | 111.82   |
| 2   | E     | 348 | FAD  | O2B-C2B-C3B | -3.13 | 101.79      | 111.82   |
| 2   | F     | 348 | FAD  | O2B-C2B-C3B | -3.12 | 101.81      | 111.82   |
| 2   | H     | 348 | FAD  | O2B-C2B-C3B | -3.12 | 101.83      | 111.82   |
| 2   | C     | 348 | FAD  | O2B-C2B-C3B | -3.12 | 101.83      | 111.82   |
| 2   | B     | 348 | FAD  | C4'-C3'-C2' | -3.03 | 108.53      | 113.57   |
| 2   | G     | 348 | FAD  | C4'-C3'-C2' | -3.00 | 108.57      | 113.57   |
| 2   | D     | 348 | FAD  | C4'-C3'-C2' | -2.99 | 108.59      | 113.57   |
| 2   | A     | 348 | FAD  | C4'-C3'-C2' | -2.99 | 108.59      | 113.57   |
| 2   | E     | 348 | FAD  | C4'-C3'-C2' | -2.99 | 108.59      | 113.57   |
| 2   | H     | 348 | FAD  | C4'-C3'-C2' | -2.99 | 108.60      | 113.57   |
| 2   | C     | 348 | FAD  | C4'-C3'-C2' | -2.97 | 108.63      | 113.57   |
| 2   | F     | 348 | FAD  | C4'-C3'-C2' | -2.97 | 108.63      | 113.57   |
| 2   | D     | 348 | FAD  | C3B-C2B-C1B | -2.91 | 95.96       | 101.46   |
| 2   | A     | 348 | FAD  | C3B-C2B-C1B | -2.90 | 95.99       | 101.46   |
| 2   | G     | 348 | FAD  | C3B-C2B-C1B | -2.89 | 95.99       | 101.46   |
| 2   | H     | 348 | FAD  | C3B-C2B-C1B | -2.89 | 95.99       | 101.46   |
| 2   | F     | 348 | FAD  | C3B-C2B-C1B | -2.89 | 95.99       | 101.46   |
| 2   | E     | 348 | FAD  | C3B-C2B-C1B | -2.89 | 95.99       | 101.46   |
| 2   | B     | 348 | FAD  | C3B-C2B-C1B | -2.89 | 96.00       | 101.46   |
| 2   | C     | 348 | FAD  | C3B-C2B-C1B | -2.88 | 96.01       | 101.46   |
| 2   | G     | 348 | FAD  | O4-C4-C4X   | -2.83 | 119.05      | 126.53   |
| 2   | B     | 348 | FAD  | O4-C4-C4X   | -2.82 | 119.09      | 126.53   |
| 2   | F     | 348 | FAD  | O4-C4-C4X   | -2.82 | 119.10      | 126.53   |
| 2   | E     | 348 | FAD  | O4-C4-C4X   | -2.81 | 119.12      | 126.53   |
| 2   | A     | 348 | FAD  | O4-C4-C4X   | -2.80 | 119.13      | 126.53   |
| 2   | H     | 348 | FAD  | O4-C4-C4X   | -2.80 | 119.13      | 126.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | D     | 348 | FAD  | O4-C4-C4X  | -2.80 | 119.14      | 126.53   |
| 2   | C     | 348 | FAD  | O4-C4-C4X  | -2.79 | 119.17      | 126.53   |
| 4   | F     | 350 | DTR  | CG-CD1-NE1 | -2.73 | 107.31      | 110.31   |
| 2   | C     | 348 | FAD  | O2P-P-O3P  | 2.69  | 114.55      | 107.27   |
| 2   | D     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.53      | 107.27   |
| 2   | E     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.52      | 107.27   |
| 2   | G     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.52      | 107.27   |
| 2   | H     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.52      | 107.27   |
| 2   | A     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.52      | 107.27   |
| 2   | F     | 348 | FAD  | O2P-P-O3P  | 2.68  | 114.52      | 107.27   |
| 2   | B     | 348 | FAD  | O2P-P-O3P  | 2.67  | 114.49      | 107.27   |
| 2   | E     | 348 | FAD  | C7M-C7-C6  | 2.54  | 124.05      | 119.57   |
| 2   | D     | 348 | FAD  | C7M-C7-C6  | 2.54  | 124.04      | 119.57   |
| 2   | H     | 348 | FAD  | C7M-C7-C6  | 2.53  | 124.02      | 119.57   |
| 2   | G     | 348 | FAD  | C7M-C7-C6  | 2.52  | 124.02      | 119.57   |
| 2   | C     | 348 | FAD  | C7M-C7-C6  | 2.52  | 124.02      | 119.57   |
| 2   | F     | 348 | FAD  | C7M-C7-C6  | 2.52  | 124.02      | 119.57   |
| 2   | A     | 348 | FAD  | C7M-C7-C6  | 2.52  | 124.02      | 119.57   |
| 2   | B     | 348 | FAD  | C7M-C7-C6  | 2.52  | 124.01      | 119.57   |
| 2   | H     | 348 | FAD  | C7M-C7-C8  | -2.36 | 115.94      | 120.76   |
| 2   | D     | 348 | FAD  | O4-C4-N3   | 2.36  | 124.55      | 120.11   |
| 2   | G     | 348 | FAD  | O4-C4-N3   | 2.36  | 124.55      | 120.11   |
| 2   | B     | 348 | FAD  | O4-C4-N3   | 2.36  | 124.55      | 120.11   |
| 2   | H     | 348 | FAD  | C10-N1-C2  | 2.35  | 121.94      | 116.85   |
| 2   | E     | 348 | FAD  | O4-C4-N3   | 2.35  | 124.53      | 120.11   |
| 2   | E     | 348 | FAD  | C7M-C7-C8  | -2.35 | 115.96      | 120.76   |
| 2   | F     | 348 | FAD  | O4-C4-N3   | 2.35  | 124.53      | 120.11   |
| 2   | A     | 348 | FAD  | C7M-C7-C8  | -2.35 | 115.97      | 120.76   |
| 2   | G     | 348 | FAD  | C10-N1-C2  | 2.35  | 121.93      | 116.85   |
| 2   | A     | 348 | FAD  | O4-C4-N3   | 2.35  | 124.52      | 120.11   |
| 2   | B     | 348 | FAD  | C7M-C7-C8  | -2.34 | 115.97      | 120.76   |
| 2   | F     | 348 | FAD  | C7M-C7-C8  | -2.34 | 115.98      | 120.76   |
| 2   | H     | 348 | FAD  | O4-C4-N3   | 2.34  | 124.52      | 120.11   |
| 2   | D     | 348 | FAD  | C7M-C7-C8  | -2.34 | 115.98      | 120.76   |
| 2   | C     | 348 | FAD  | O4-C4-N3   | 2.34  | 124.51      | 120.11   |
| 2   | C     | 348 | FAD  | C7M-C7-C8  | -2.34 | 115.98      | 120.76   |
| 2   | E     | 348 | FAD  | C10-N1-C2  | 2.34  | 121.91      | 116.85   |
| 2   | D     | 348 | FAD  | C10-N1-C2  | 2.33  | 121.89      | 116.85   |
| 2   | A     | 348 | FAD  | C10-N1-C2  | 2.32  | 121.88      | 116.85   |
| 2   | C     | 348 | FAD  | C10-N1-C2  | 2.32  | 121.87      | 116.85   |
| 2   | F     | 348 | FAD  | C10-N1-C2  | 2.32  | 121.87      | 116.85   |
| 2   | G     | 348 | FAD  | C7M-C7-C8  | -2.31 | 116.03      | 120.76   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 348 | FAD  | C10-N1-C2 | 2.31  | 121.84      | 116.85   |
| 4   | E     | 350 | DTR  | CA-CB-CG  | -2.04 | 109.62      | 113.49   |

There are no chirality outliers.

All (43) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | A     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | B     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | B     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | C     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | C     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | D     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | D     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | E     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | E     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | F     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | F     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | G     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | G     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | H     | 348 | FAD  | C5B-O5B-PA-O2A  |
| 2   | H     | 348 | FAD  | C5B-O5B-PA-O3P  |
| 2   | A     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | B     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | C     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | D     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | E     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | F     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | G     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | H     | 348 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | B     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | C     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | D     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | E     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | F     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | G     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | H     | 348 | FAD  | C3B-C4B-C5B-O5B |
| 2   | A     | 348 | FAD  | C5B-O5B-PA-O1A  |
| 2   | B     | 348 | FAD  | C5B-O5B-PA-O1A  |
| 2   | C     | 348 | FAD  | C5B-O5B-PA-O1A  |

*Continued on next page...*

*Continued from previous page...*

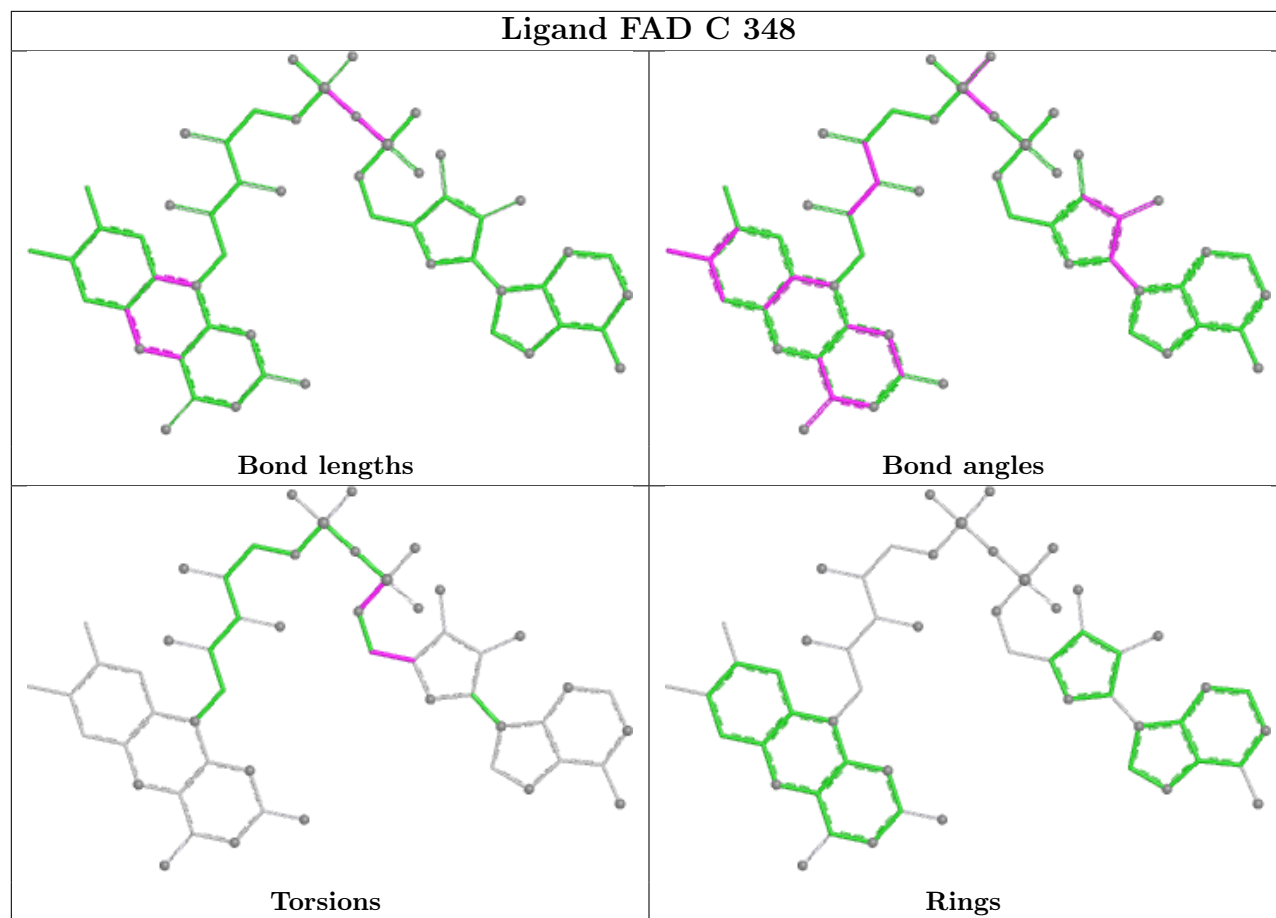
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | D     | 348 | FAD  | C5B-O5B-PA-O1A |
| 2   | E     | 348 | FAD  | C5B-O5B-PA-O1A |
| 2   | F     | 348 | FAD  | C5B-O5B-PA-O1A |
| 2   | G     | 348 | FAD  | C5B-O5B-PA-O1A |
| 2   | H     | 348 | FAD  | C5B-O5B-PA-O1A |
| 4   | F     | 350 | DTR  | OXT-C-CA-CB    |
| 4   | F     | 350 | DTR  | O-C-CA-CB      |
| 4   | E     | 350 | DTR  | OXT-C-CA-N     |

There are no ring outliers.

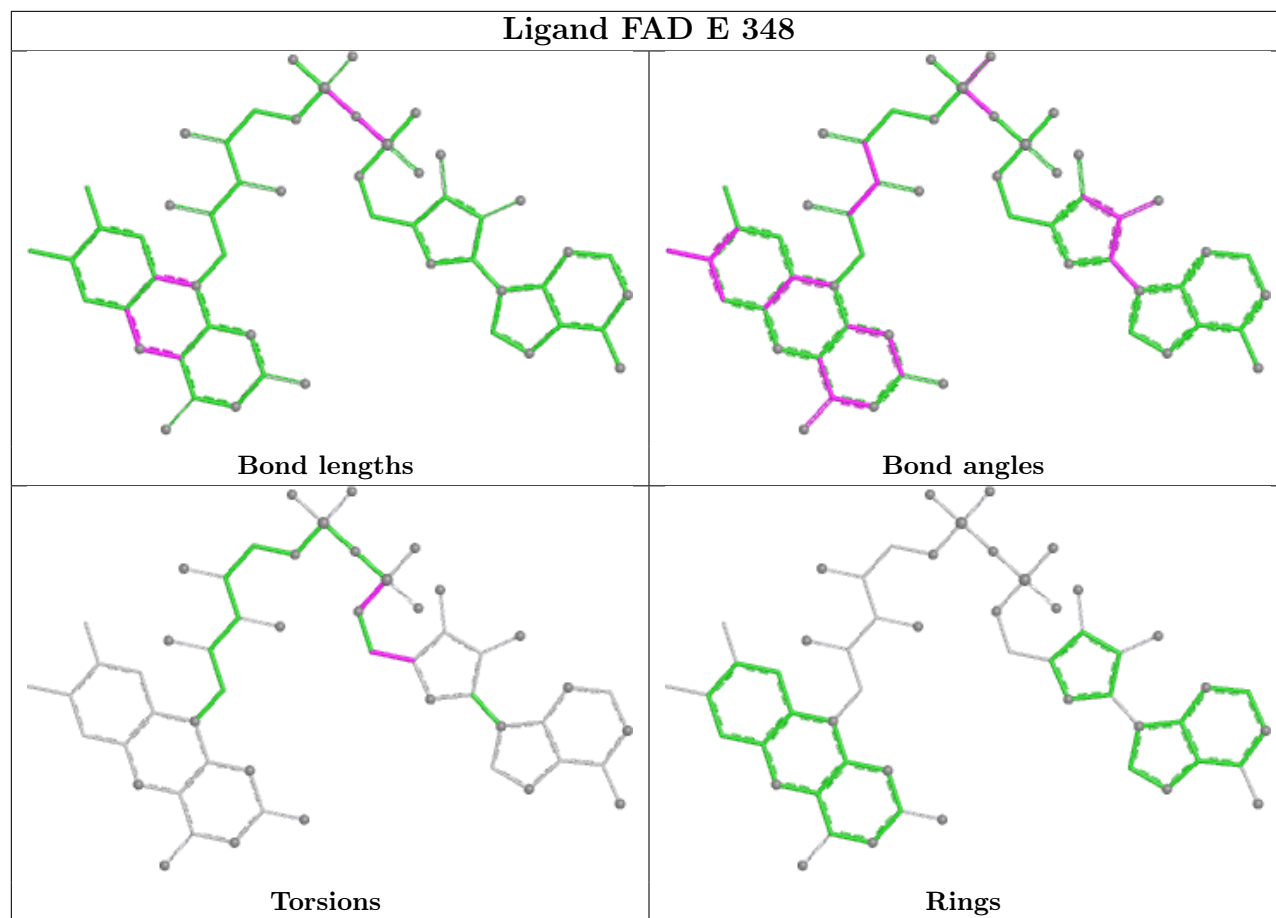
11 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 348 | FAD  | 4       | 0            |
| 2   | E     | 348 | FAD  | 2       | 0            |
| 2   | F     | 348 | FAD  | 4       | 0            |
| 2   | D     | 348 | FAD  | 4       | 0            |
| 2   | G     | 348 | FAD  | 5       | 0            |
| 2   | H     | 348 | FAD  | 5       | 0            |
| 3   | F     | 349 | ITR  | 1       | 0            |
| 2   | A     | 348 | FAD  | 5       | 0            |
| 2   | B     | 348 | FAD  | 3       | 0            |
| 4   | E     | 350 | DTR  | 7       | 0            |
| 4   | F     | 350 | DTR  | 3       | 0            |

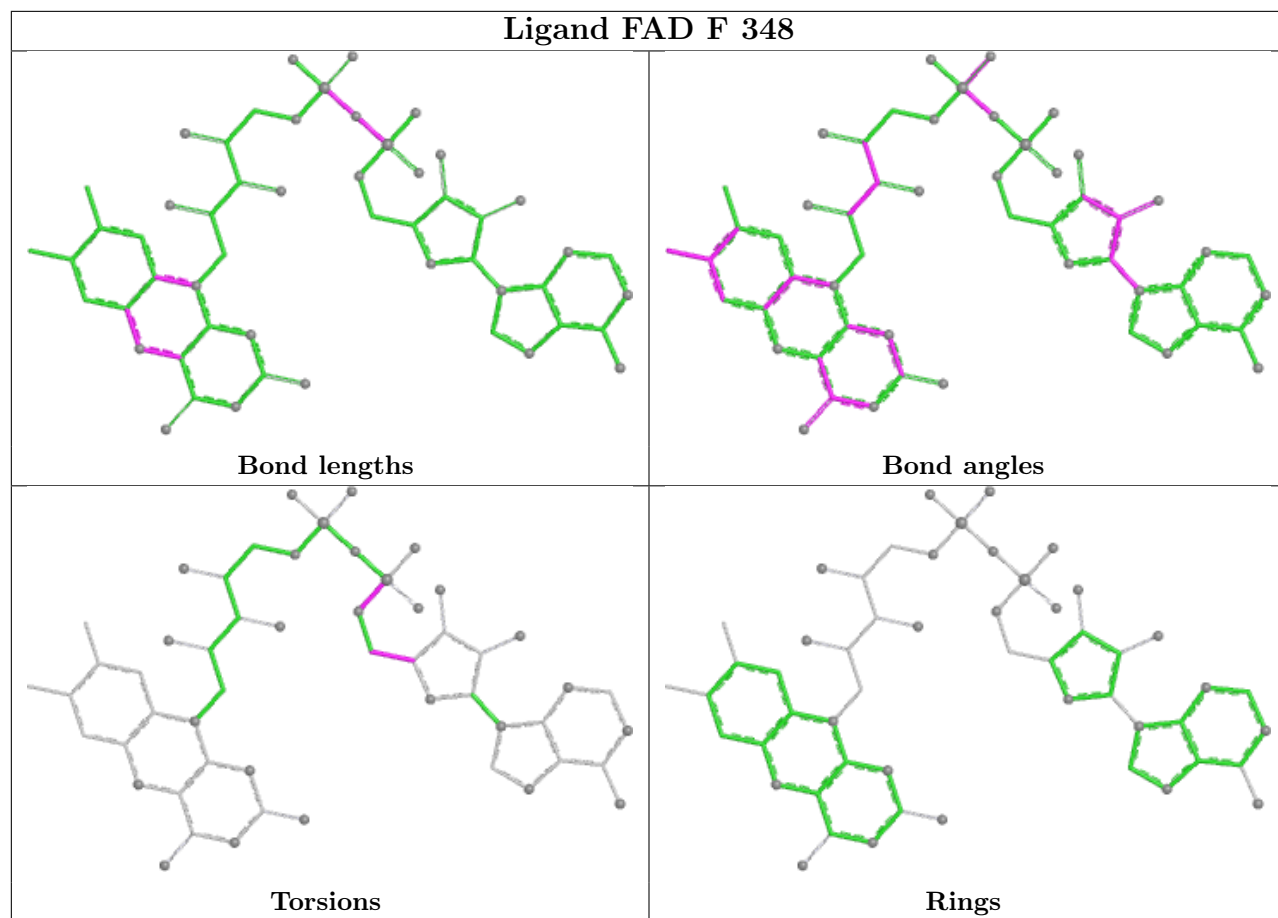
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



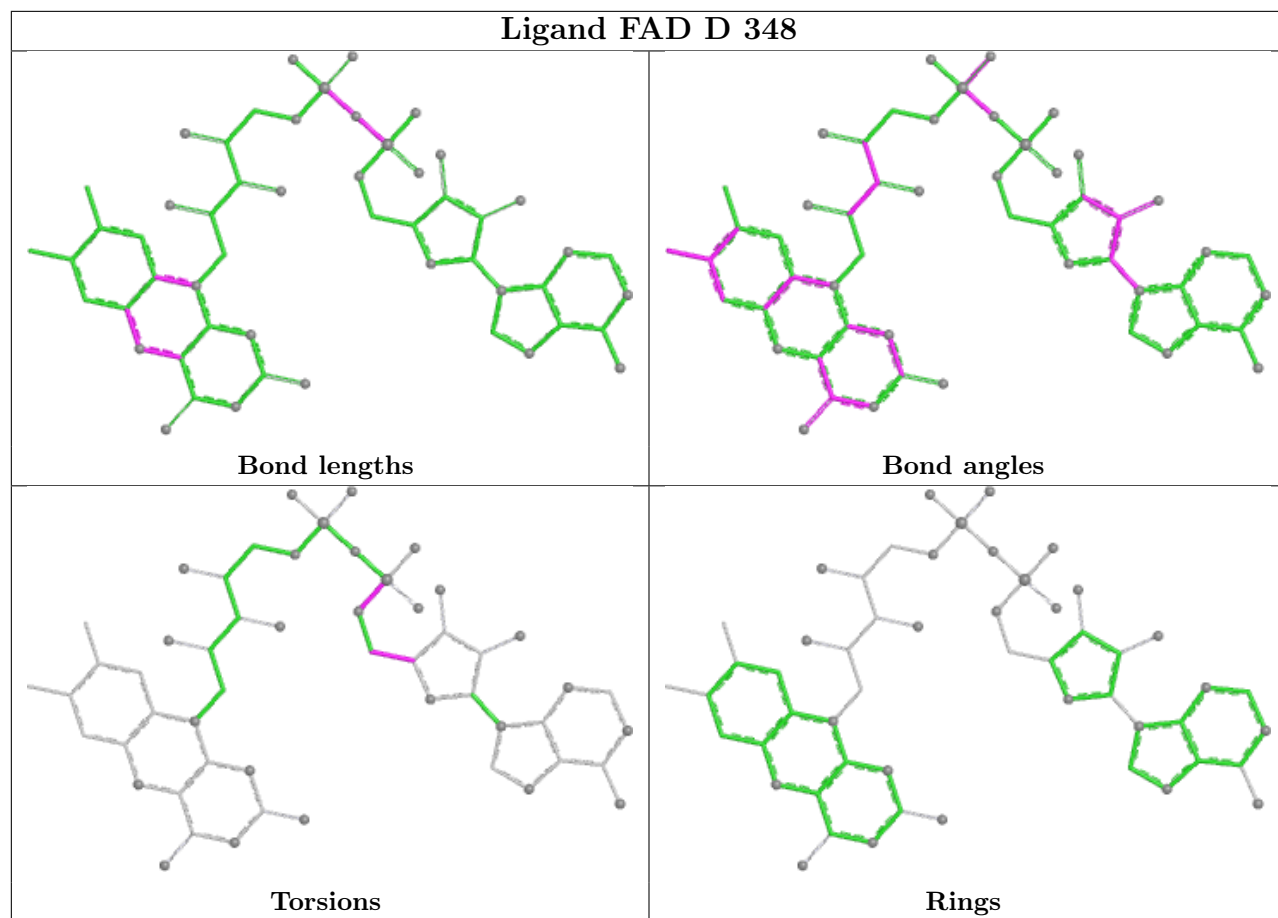
## Ligand FAD E 348

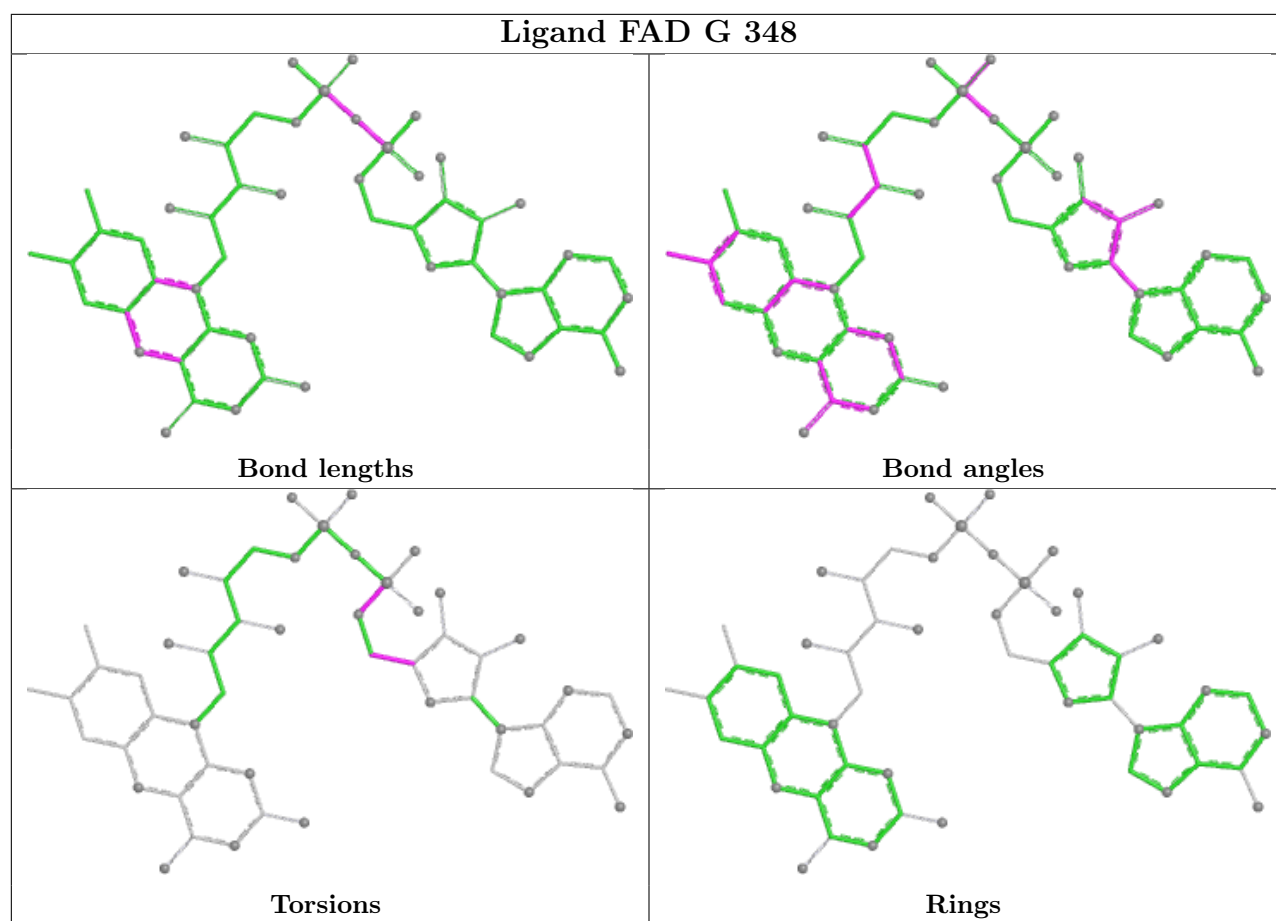


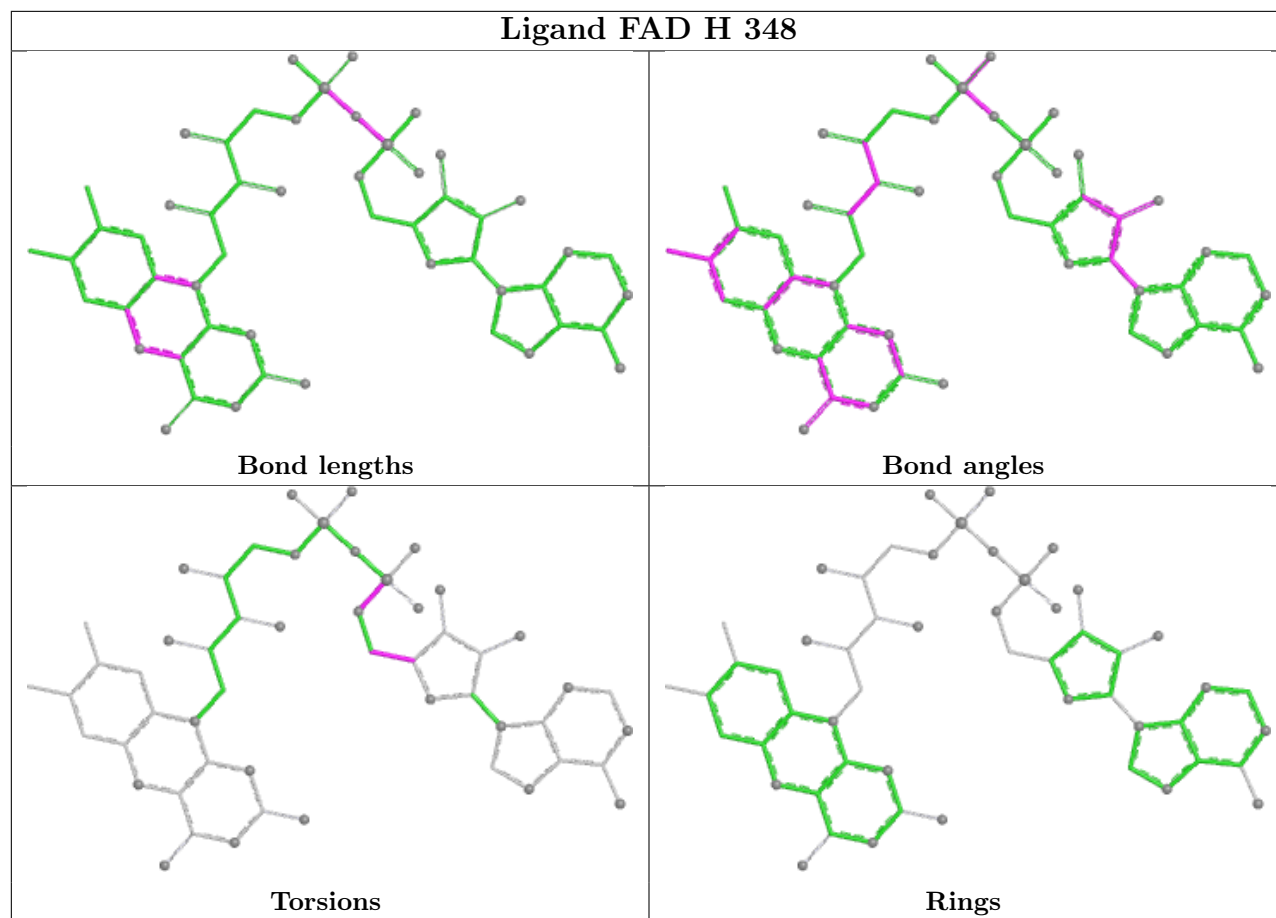
## Ligand FAD F 348



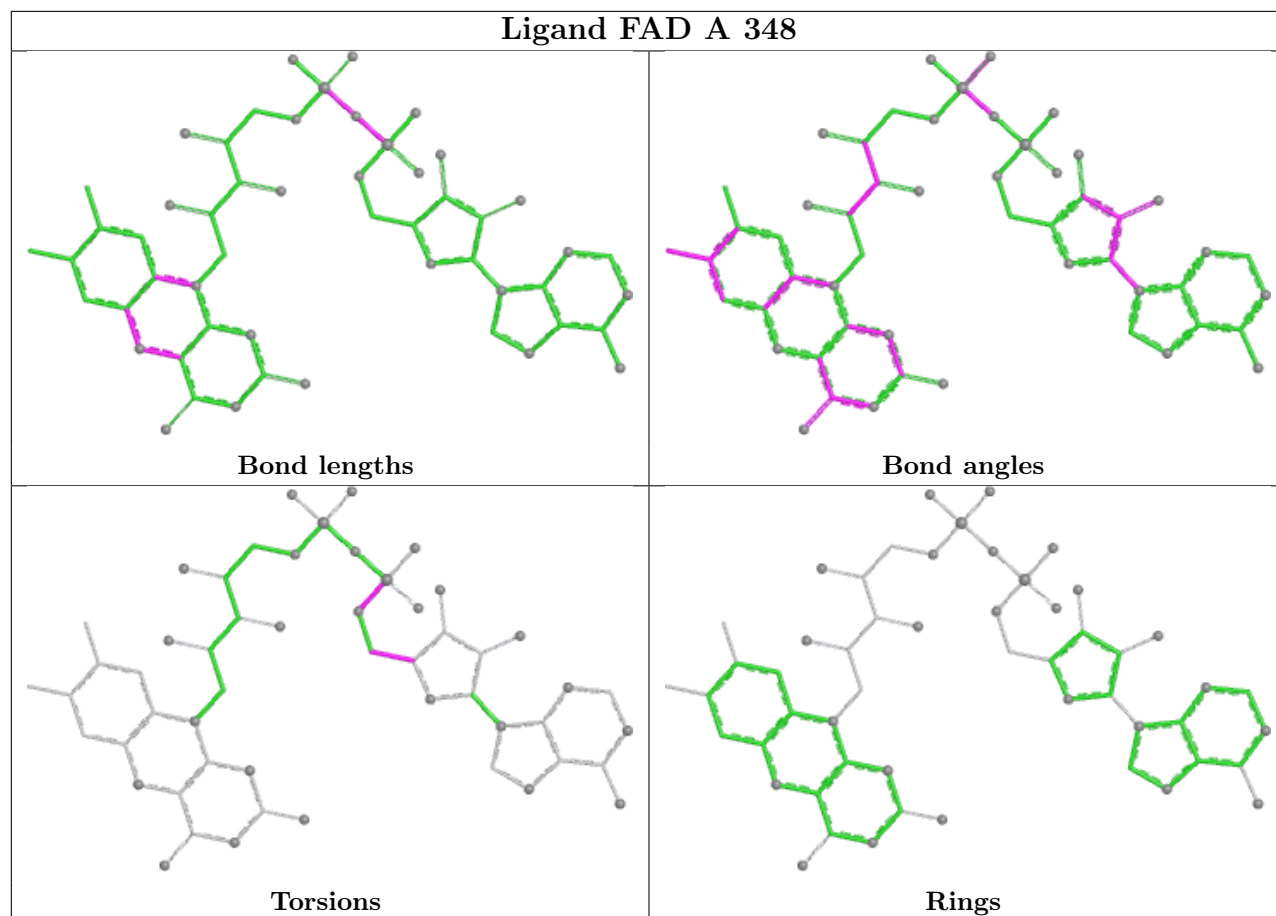
## Ligand FAD D 348

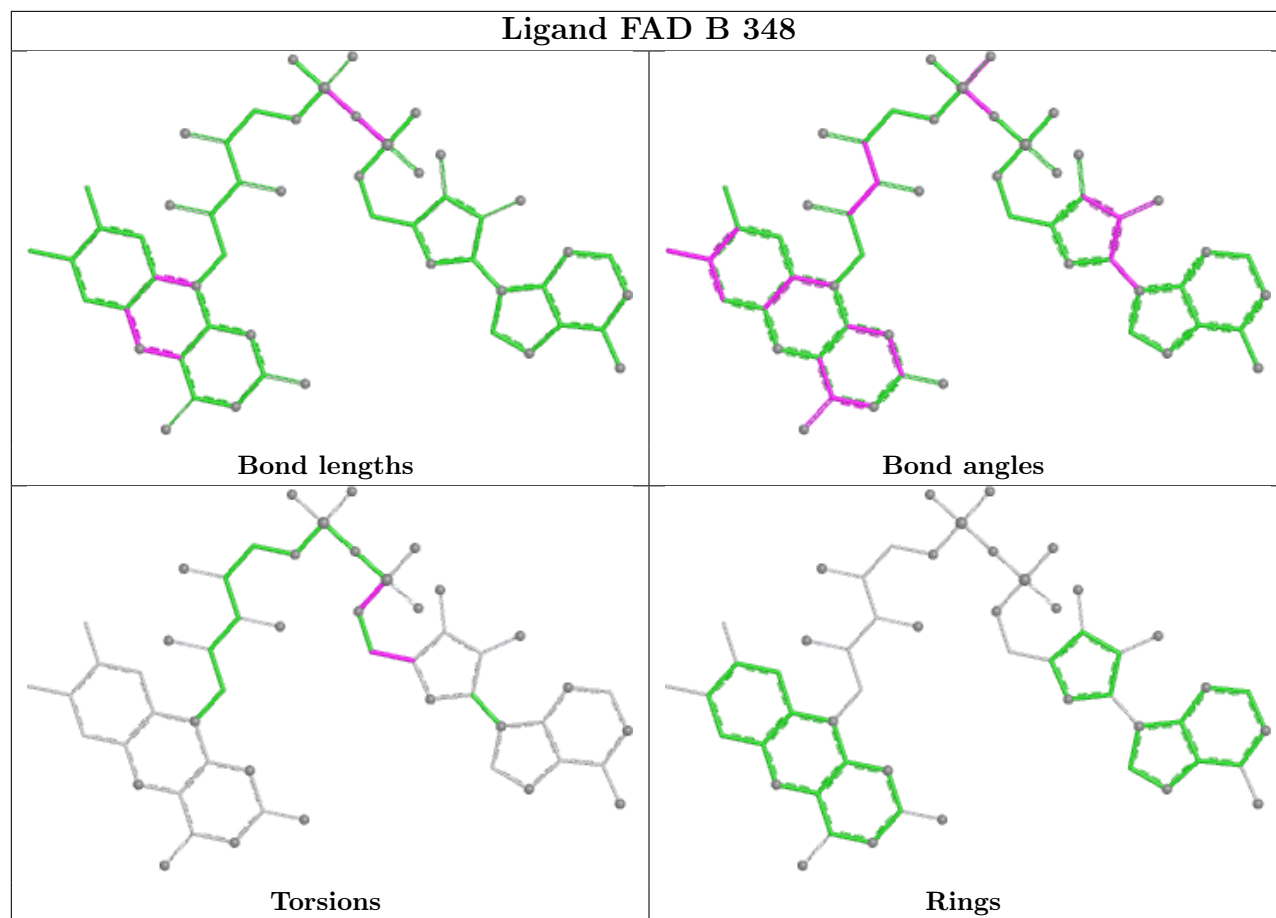






## Ligand FAD A 348





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9  |
|-----|-------|-----------------|--------|-----------|----|----|-----------------------|----------|
| 1   | A     | 330/347 (95%)   | 0.48   | 17 (5%)   | 33 | 17 | 12, 34, 67, 100       | 23 (6%)  |
| 1   | B     | 328/347 (94%)   | 0.52   | 22 (6%)   | 24 | 13 | 13, 35, 70, 100       | 24 (7%)  |
| 1   | C     | 331/347 (95%)   | 0.45   | 17 (5%)   | 33 | 18 | 13, 35, 71, 100       | 26 (7%)  |
| 1   | D     | 332/347 (95%)   | 0.49   | 24 (7%)   | 21 | 11 | 12, 35, 67, 100       | 19 (5%)  |
| 1   | E     | 331/347 (95%)   | 0.41   | 19 (5%)   | 29 | 16 | 13, 35, 69, 100       | 26 (7%)  |
| 1   | F     | 329/347 (94%)   | 0.38   | 13 (3%)   | 42 | 23 | 13, 35, 68, 100       | 19 (5%)  |
| 1   | G     | 327/347 (94%)   | 0.67   | 24 (7%)   | 21 | 11 | 8, 35, 79, 100        | 26 (7%)  |
| 1   | H     | 329/347 (94%)   | 0.45   | 19 (5%)   | 29 | 16 | 13, 35, 69, 100       | 22 (6%)  |
| All | All   | 2637/2776 (94%) | 0.48   | 155 (5%)  | 28 | 15 | 8, 35, 70, 100        | 185 (7%) |

All (155) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 303 | THR  | 6.5  |
| 1   | D     | 299 | GLY  | 6.4  |
| 1   | H     | 221 | ARG  | 5.7  |
| 1   | G     | 60  | SER  | 5.4  |
| 1   | C     | 224 | TYR  | 5.3  |
| 1   | D     | 57  | SER  | 4.9  |
| 1   | B     | 24  | HIS  | 4.9  |
| 1   | F     | 335 | GLU  | 4.6  |
| 1   | E     | 335 | GLU  | 4.5  |
| 1   | A     | 337 | ARG  | 4.4  |
| 1   | F     | 301 | SER  | 4.3  |
| 1   | D     | 224 | TYR  | 4.2  |
| 1   | G     | 301 | SER  | 4.2  |
| 1   | C     | 60  | SER  | 3.9  |
| 1   | G     | 288 | GLN  | 3.6  |
| 1   | C     | 24  | HIS  | 3.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 58  | GLU  | 3.5  |
| 1   | C     | 61  | ASN  | 3.4  |
| 1   | D     | 300 | SER  | 3.4  |
| 1   | G     | 300 | SER  | 3.4  |
| 1   | C     | 221 | ARG  | 3.4  |
| 1   | D     | 221 | ARG  | 3.3  |
| 1   | E     | 162 | ARG  | 3.3  |
| 1   | D     | 298 | PHE  | 3.3  |
| 1   | H     | 337 | ARG  | 3.3  |
| 1   | E     | 301 | SER  | 3.3  |
| 1   | D     | 295 | GLN  | 3.3  |
| 1   | G     | 303 | THR  | 3.2  |
| 1   | F     | 224 | TYR  | 3.2  |
| 1   | G     | 335 | GLU  | 3.2  |
| 1   | H     | 118 | THR  | 3.2  |
| 1   | E     | 27  | LEU  | 3.2  |
| 1   | A     | 335 | GLU  | 3.2  |
| 1   | D     | 119 | PRO  | 3.2  |
| 1   | G     | 299 | GLY  | 3.1  |
| 1   | G     | 24  | HIS  | 3.1  |
| 1   | H     | 100 | GLU  | 3.0  |
| 1   | A     | 300 | SER  | 3.0  |
| 1   | G     | 62  | PRO  | 3.0  |
| 1   | C     | 57  | SER  | 3.0  |
| 1   | D     | 126 | PRO  | 2.9  |
| 1   | G     | 224 | TYR  | 2.9  |
| 1   | G     | 295 | GLN  | 2.9  |
| 1   | D     | 337 | ARG  | 2.9  |
| 1   | A     | 331 | GLY  | 2.9  |
| 1   | D     | 62  | PRO  | 2.9  |
| 1   | E     | 336 | GLU  | 2.9  |
| 1   | B     | 335 | GLU  | 2.9  |
| 1   | H     | 297 | ARG  | 2.8  |
| 1   | C     | 100 | GLU  | 2.8  |
| 1   | D     | 335 | GLU  | 2.8  |
| 1   | F     | 336 | GLU  | 2.8  |
| 1   | G     | 298 | PHE  | 2.8  |
| 1   | E     | 24  | HIS  | 2.7  |
| 1   | G     | 327 | ALA  | 2.7  |
| 1   | H     | 172 | ARG  | 2.7  |
| 1   | B     | 224 | TYR  | 2.7  |
| 1   | D     | 296 | LEU  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 223 | ILE  | 2.7  |
| 1   | H     | 335 | GLU  | 2.7  |
| 1   | C     | 297 | ARG  | 2.7  |
| 1   | C     | 299 | GLY  | 2.7  |
| 1   | E     | 221 | ARG  | 2.7  |
| 1   | E     | 240 | GLY  | 2.7  |
| 1   | H     | 99  | ARG  | 2.6  |
| 1   | H     | 173 | GLY  | 2.6  |
| 1   | A     | 297 | ARG  | 2.6  |
| 1   | G     | 173 | GLY  | 2.6  |
| 1   | B     | 56  | THR  | 2.6  |
| 1   | C     | 118 | THR  | 2.6  |
| 1   | F     | 300 | SER  | 2.6  |
| 1   | A     | 103 | PRO  | 2.6  |
| 1   | E     | 225 | ASN  | 2.6  |
| 1   | A     | 292 | GLU  | 2.6  |
| 1   | E     | 56  | THR  | 2.6  |
| 1   | D     | 272 | ASP  | 2.5  |
| 1   | B     | 160 | PHE  | 2.5  |
| 1   | B     | 60  | SER  | 2.5  |
| 1   | D     | 301 | SER  | 2.5  |
| 1   | H     | 295 | GLN  | 2.5  |
| 1   | G     | 66  | ASN  | 2.5  |
| 1   | G     | 118 | THR  | 2.5  |
| 1   | C     | 298 | PHE  | 2.5  |
| 1   | B     | 57  | SER  | 2.5  |
| 1   | D     | 168 | GLU  | 2.5  |
| 1   | D     | 248 | ASN  | 2.5  |
| 1   | F     | 337 | ARG  | 2.5  |
| 1   | C     | 175 | ALA  | 2.4  |
| 1   | A     | 25  | SER  | 2.4  |
| 1   | E     | 298 | PHE  | 2.4  |
| 1   | E     | 123 | ASP  | 2.4  |
| 1   | D     | 222 | GLY  | 2.4  |
| 1   | E     | 253 | ILE  | 2.4  |
| 1   | B     | 300 | SER  | 2.4  |
| 1   | C     | 220 | GLU  | 2.4  |
| 1   | F     | 168 | GLU  | 2.4  |
| 1   | D     | 66  | ASN  | 2.4  |
| 1   | B     | 174 | GLY  | 2.4  |
| 1   | B     | 334 | LEU  | 2.4  |
| 1   | G     | 177 | VAL  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 248 | ASN  | 2.4  |
| 1   | B     | 2   | ARG  | 2.4  |
| 1   | A     | 154 | GLU  | 2.3  |
| 1   | B     | 21  | GLU  | 2.3  |
| 1   | B     | 337 | ARG  | 2.3  |
| 1   | B     | 123 | ASP  | 2.3  |
| 1   | A     | 27  | LEU  | 2.3  |
| 1   | B     | 299 | GLY  | 2.3  |
| 1   | F     | 279 | TYR  | 2.3  |
| 1   | A     | 298 | PHE  | 2.3  |
| 1   | H     | 298 | PHE  | 2.3  |
| 1   | A     | 325 | GLU  | 2.3  |
| 1   | E     | 247 | TRP  | 2.3  |
| 1   | E     | 60  | SER  | 2.3  |
| 1   | H     | 299 | GLY  | 2.3  |
| 1   | A     | 166 | SER  | 2.3  |
| 1   | F     | 123 | ASP  | 2.3  |
| 1   | H     | 218 | ASP  | 2.3  |
| 1   | A     | 227 | PRO  | 2.2  |
| 1   | H     | 303 | THR  | 2.2  |
| 1   | G     | 305 | VAL  | 2.2  |
| 1   | H     | 61  | ASN  | 2.2  |
| 1   | C     | 154 | GLU  | 2.2  |
| 1   | F     | 298 | PHE  | 2.2  |
| 1   | B     | 303 | THR  | 2.2  |
| 1   | D     | 118 | THR  | 2.2  |
| 1   | H     | 24  | HIS  | 2.2  |
| 1   | B     | 66  | ASN  | 2.2  |
| 1   | B     | 252 | ASN  | 2.2  |
| 1   | F     | 303 | THR  | 2.2  |
| 1   | G     | 254 | GLN  | 2.2  |
| 1   | D     | 21  | GLU  | 2.2  |
| 1   | A     | 303 | THR  | 2.1  |
| 1   | B     | 119 | PRO  | 2.1  |
| 1   | E     | 252 | ASN  | 2.1  |
| 1   | G     | 287 | PRO  | 2.1  |
| 1   | B     | 176 | ASP  | 2.1  |
| 1   | E     | 218 | ASP  | 2.1  |
| 1   | H     | 169 | GLU  | 2.1  |
| 1   | C     | 190 | GLN  | 2.1  |
| 1   | G     | 243 | GLN  | 2.1  |
| 1   | D     | 60  | SER  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 252 | ASN  | 2.1  |
| 1   | H     | 294 | GLU  | 2.1  |
| 1   | B     | 301 | SER  | 2.1  |
| 1   | E     | 25  | SER  | 2.1  |
| 1   | E     | 337 | ARG  | 2.1  |
| 1   | B     | 240 | GLY  | 2.1  |
| 1   | F     | 299 | GLY  | 2.1  |
| 1   | D     | 100 | GLU  | 2.1  |
| 1   | G     | 242 | PHE  | 2.1  |
| 1   | F     | 118 | THR  | 2.0  |
| 1   | C     | 300 | SER  | 2.0  |
| 1   | A     | 252 | ASN  | 2.0  |
| 1   | C     | 66  | ASN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | ITR  | E     | 349 | 15/15 | 0.77 | 0.21 | 45,52,58,72                 | 0     |
| 3   | ITR  | C     | 349 | 15/15 | 0.82 | 0.23 | 45,52,58,72                 | 0     |
| 3   | ITR  | H     | 349 | 15/15 | 0.82 | 0.23 | 45,52,58,72                 | 0     |
| 3   | ITR  | G     | 349 | 15/15 | 0.83 | 0.20 | 45,52,58,72                 | 0     |
| 3   | ITR  | D     | 349 | 15/15 | 0.84 | 0.20 | 45,52,58,72                 | 0     |
| 3   | ITR  | F     | 349 | 15/15 | 0.85 | 0.20 | 45,52,58,72                 | 0     |
| 3   | ITR  | B     | 349 | 15/15 | 0.89 | 0.16 | 45,52,58,72                 | 0     |
| 4   | DTR  | E     | 350 | 15/15 | 0.89 | 0.15 | 9,42,100,100                | 0     |
| 2   | FAD  | G     | 348 | 53/53 | 0.91 | 0.14 | 20,27,42,43                 | 0     |
| 3   | ITR  | A     | 349 | 15/15 | 0.91 | 0.16 | 45,52,58,72                 | 0     |

*Continued on next page...*

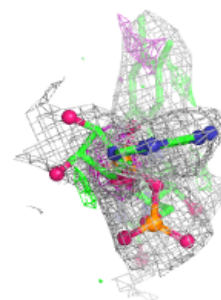
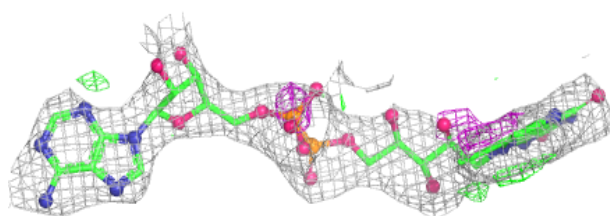
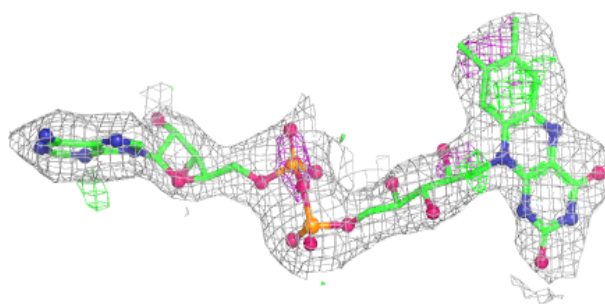
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | FAD  | B     | 348 | 53/53 | 0.93 | 0.12 | 20,27,42,43                 | 0     |
| 4   | DTR  | F     | 350 | 15/15 | 0.93 | 0.17 | 1,49,100,100                | 0     |
| 2   | FAD  | F     | 348 | 53/53 | 0.94 | 0.12 | 20,27,42,43                 | 0     |
| 2   | FAD  | C     | 348 | 53/53 | 0.94 | 0.12 | 20,27,42,43                 | 0     |
| 2   | FAD  | E     | 348 | 53/53 | 0.94 | 0.11 | 20,27,42,43                 | 0     |
| 2   | FAD  | A     | 348 | 53/53 | 0.95 | 0.10 | 20,27,42,43                 | 0     |
| 2   | FAD  | D     | 348 | 53/53 | 0.96 | 0.10 | 20,27,42,43                 | 0     |
| 2   | FAD  | H     | 348 | 53/53 | 0.96 | 0.09 | 20,27,42,43                 | 0     |

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

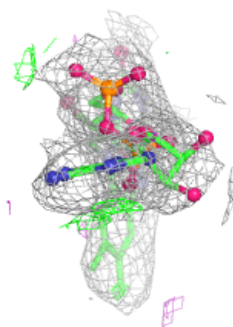
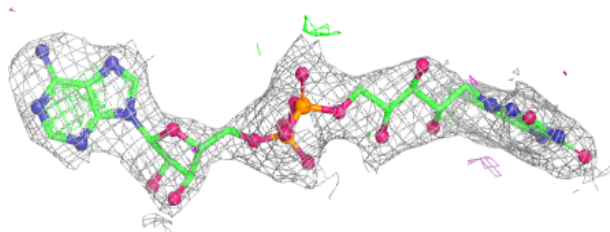
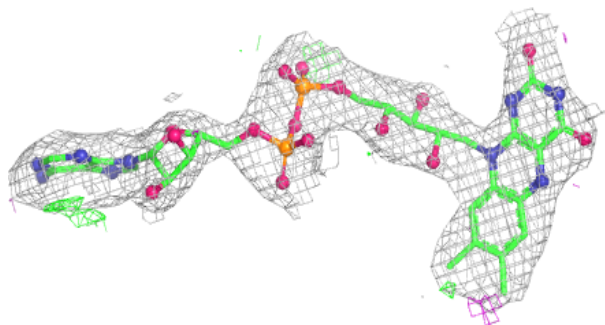
**Electron density around FAD G 348:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

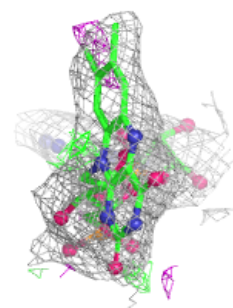
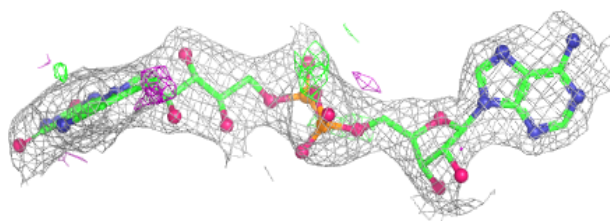
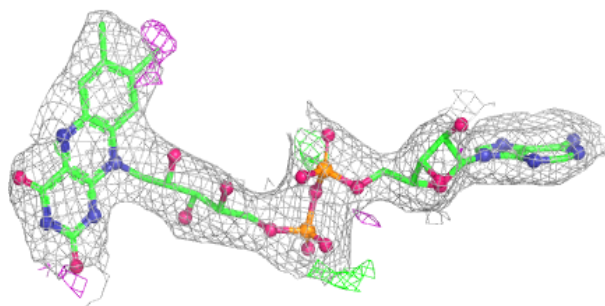


**Electron density around FAD B 348:**

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

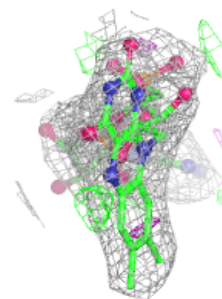
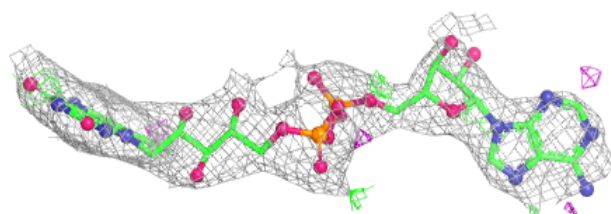
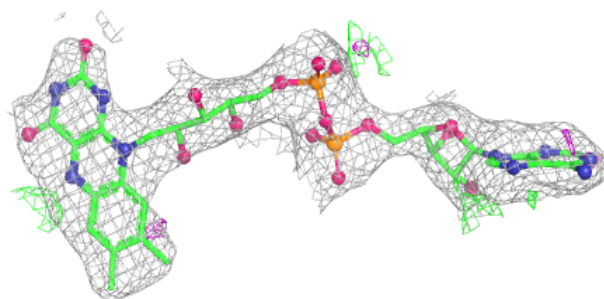
**Electron density around FAD F 348:**

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

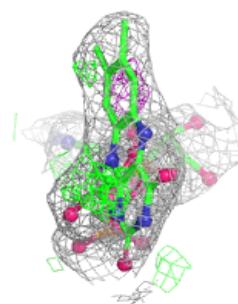
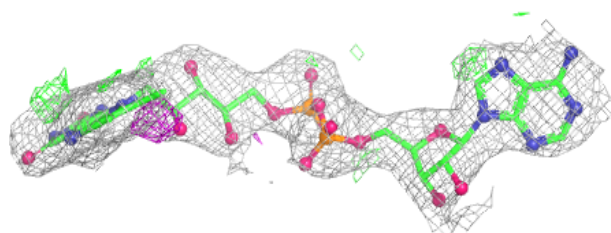
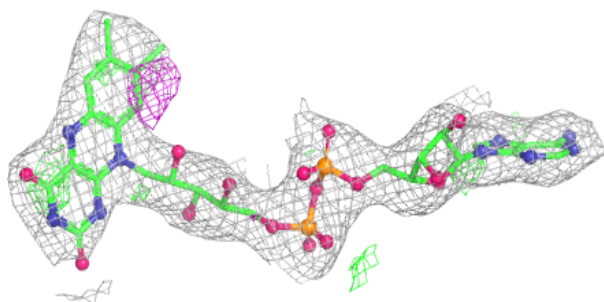


**Electron density around FAD C 348:**

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

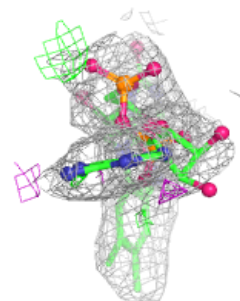
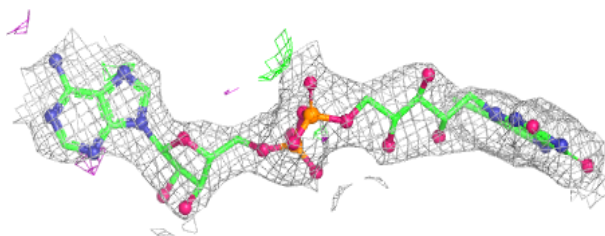
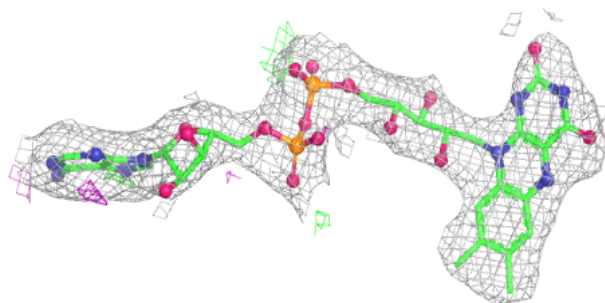
**Electron density around FAD E 348:**

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

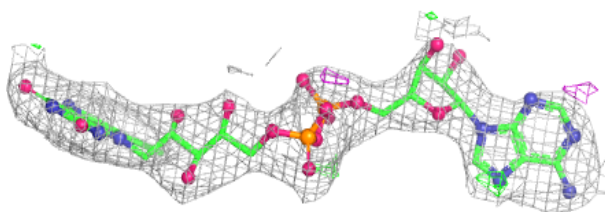
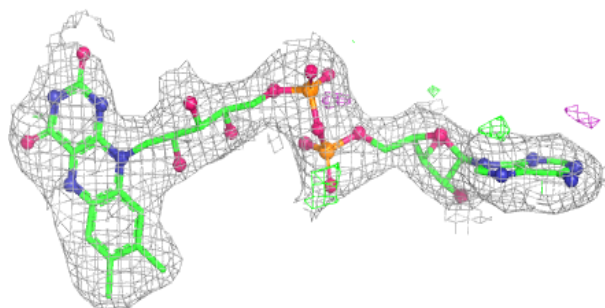


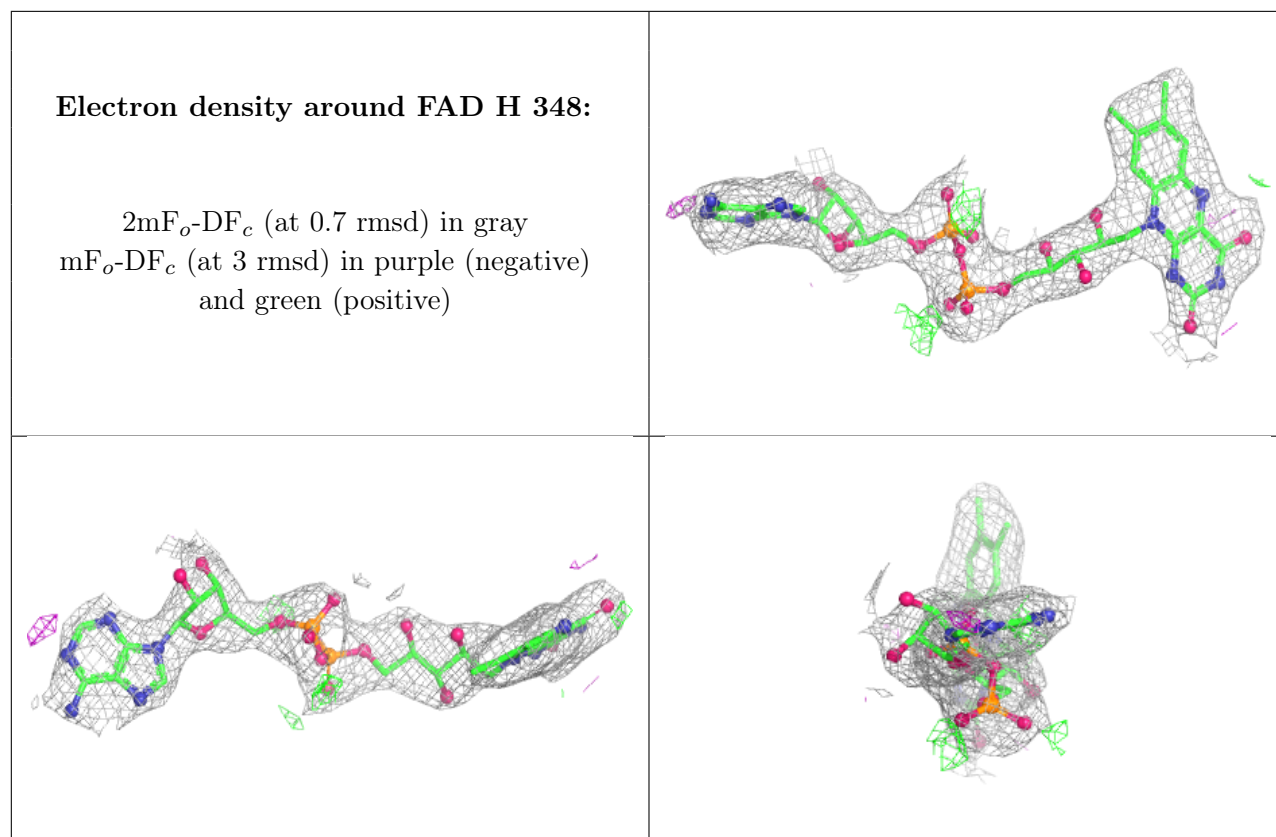
**Electron density around FAD A 348:**

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

**Electron density around FAD D 348:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.