



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:03 PM EDT

PDB ID : 1BCC / pdb\_00001bcc  
Title : CYTOCHROME BC1 COMPLEX FROM CHICKEN  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.-I.; Kim, K.K.; Hung, L.-W.;  
Crofts, A.R.; Berry, E.A.; Kim, S.-H.  
Deposited on : 1998-03-23  
Resolution : 3.16 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 : 9.0.015 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

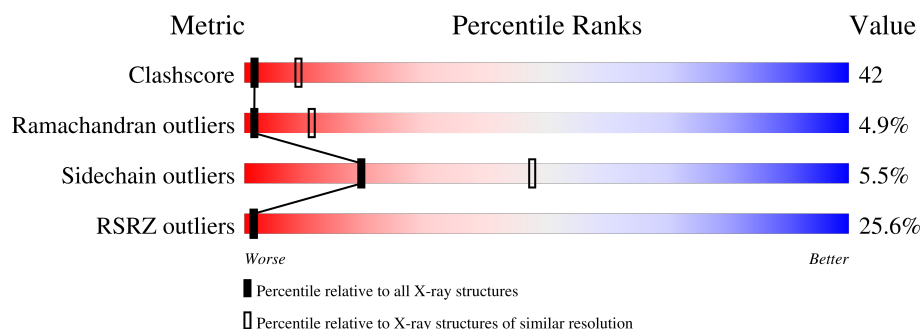
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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                      | 2486 (3.20-3.12)                                      |
| Ramachandran outliers | 187476                      | 2405 (3.20-3.12)                                      |
| Sidechain outliers    | 187428                      | 2404 (3.20-3.12)                                      |
| RSRZ outliers         | 180081                      | 2361 (3.20-3.12)                                      |

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     | 446    | <div> <div>25%</div> <div>38%</div> <div>52%</div> <div>9%</div> <div>.</div> </div>               |
| 2   | B     | 422    | <div> <div>27%</div> <div>37%</div> <div>49%</div> <div>10%</div> <div>.</div> </div>              |
| 3   | C     | 380    | <div> <div>12%</div> <div>39%</div> <div>51%</div> <div>9%</div> <div>.</div> </div>               |
| 4   | D     | 241    | <div> <div>16%</div> <div>40%</div> <div>52%</div> <div>8%</div> </div>                            |
| 5   | E     | 196    | <div> <div>58%</div> <div>33%</div> <div>53%</div> <div>13%</div> <div>.</div> </div>              |
| 6   | F     | 109    | <div> <div>15%</div> <div>49%</div> <div>38%</div> <div>5%</div> <div>8%</div> <div>.</div> </div> |
| 7   | G     | 81     | <div> <div>22%</div> <div>38%</div> <div>48%</div> <div>9%</div> <div>.</div> </div>               |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | H     | 78     |                  |
| 9   | I     | 33     |                  |
| 10  | J     | 62     |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | PEE  | C     | 384 | X         | -        | -       | -                |
| 13  | PEE  | E     | 198 | X         | -        | -       | -                |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15719 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 442      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3423  | 2147 | 601 | 657 | 18 |         |         |       |

There are 45 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 3       | TYR      | THR    | conflict | UNP P13272 |
| A     | 23      | VAL      | LEU    | conflict | UNP P13272 |
| A     | 59      | LEU      | VAL    | conflict | UNP P13272 |
| A     | 72      | GLN      | GLY    | conflict | UNP P13272 |
| A     | 91      | SER      | THR    | conflict | UNP P13272 |
| A     | 106     | VAL      | LEU    | conflict | UNP P13272 |
| A     | 135     | VAL      | LEU    | conflict | UNP P13272 |
| A     | 136     | ARG      | GLN    | conflict | UNP P13272 |
| A     | 147     | GLU      | ASP    | conflict | UNP P13272 |
| A     | 162     | GLY      | PRO    | conflict | UNP P13272 |
| A     | 174     | ILE      | VAL    | conflict | UNP P13272 |
| A     | 188     | THR      | ARG    | conflict | UNP P13272 |
| A     | 191     | THR      | LYS    | conflict | UNP P13272 |
| A     | 203     | VAL      | LEU    | conflict | UNP P13272 |
| A     | 206     | GLN      | ARG    | conflict | UNP P13272 |
| A     | 210     | GLU      | ASP    | conflict | UNP P13272 |
| A     | 217     | GLY      | SER    | conflict | UNP P13272 |
| A     | 219     | VAL      | LEU    | conflict | UNP P13272 |
| A     | 220     | PRO      | SER    | conflict | UNP P13272 |
| A     | 221     | PHE      | GLY    | conflict | UNP P13272 |
| A     | 225     | ASP      | GLU    | conflict | UNP P13272 |
| A     | 233     | LYS      | PRO    | conflict | UNP P13272 |
| A     | 242     | ARG      | CYS    | conflict | UNP P13272 |
| A     | 267     | LEU      | ASN    | conflict | UNP P13272 |
| A     | 282     | ARG      | CYS    | conflict | UNP P13272 |
| A     | 288     | LEU      | ALA    | conflict | UNP P13272 |
| A     | 290     | SER      | LEU    | conflict | UNP P13272 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 299     | VAL      | ALA    | conflict | UNP P13272 |
| A     | 311     | SER      | ASN    | conflict | UNP P13272 |
| A     | 315     | SER      | ALA    | conflict | UNP P13272 |
| A     | 316     | GLU      | ASP    | conflict | UNP P13272 |
| A     | 320     | PHE      | LEU    | conflict | UNP P13272 |
| A     | 322     | PHE      | ALA    | conflict | UNP P13272 |
| A     | 323     | TYR      | HIS    | conflict | UNP P13272 |
| A     | 328     | ARG      | HIS    | conflict | UNP P13272 |
| A     | 349     | ILE      | ALA    | conflict | UNP P13272 |
| A     | 350     | SER      | THR    | conflict | UNP P13272 |
| A     | 360     | PHE      | LEU    | conflict | UNP P13272 |
| A     | 382     | GLU      | SER    | conflict | UNP P13272 |
| A     | 393     | GLU      | ALA    | conflict | UNP P13272 |
| A     | 397     | GLU      | SER    | conflict | UNP P13272 |
| A     | 399     | LEU      | ILE    | conflict | UNP P13272 |
| A     | 406     | MET      | VAL    | conflict | UNP P13272 |
| A     | 415     | ILE      | PHE    | conflict | UNP P13272 |
| A     | 425     | PRO      | PHE    | conflict | UNP P13272 |

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 406      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2994  | 1878 | 518 | 591 | 7 |         |         |       |

There are 37 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 26      | ILE      | PHE    | conflict | UNP P23004 |
| B     | 28      | LYS      | ARG    | conflict | UNP P23004 |
| B     | 42      | SER      | ALA    | conflict | UNP P23004 |
| B     | 44      | GLY      | ALA    | conflict | UNP P23004 |
| B     | 46      | THR      | ARG    | conflict | UNP P23004 |
| B     | 49      | VAL      | LEU    | conflict | UNP P23004 |
| B     | 61      | SER      | ASN    | conflict | UNP P23004 |
| B     | 99      | GLU      | THR    | conflict | UNP P23004 |
| B     | 117     | GLU      | ASP    | conflict | UNP P23004 |
| B     | 134     | PRO      | ARG    | conflict | UNP P23004 |
| B     | 139     | ASP      | ALA    | conflict | UNP P23004 |
| B     | 145     | LYS      | ARG    | conflict | UNP P23004 |
| B     | 152     | PHE      | LEU    | conflict | UNP P23004 |
| B     | 157     | THR      | ALA    | conflict | UNP P23004 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 174     | ASP      | ASN    | conflict | UNP P23004 |
| B     | 188     | SER      | PRO    | conflict | UNP P23004 |
| B     | 194     | PHE      | TYR    | conflict | UNP P23004 |
| B     | 207     | VAL      | ILE    | conflict | UNP P23004 |
| B     | 218     | ASN      | GLN    | conflict | UNP P23004 |
| B     | 223     | LEU      | PHE    | conflict | UNP P23004 |
| B     | 240     | ARG      | HIS    | conflict | UNP P23004 |
| B     | 257     | ILE      | LEU    | conflict | UNP P23004 |
| B     | 266     | GLY      | SER    | conflict | UNP P23004 |
| B     | 282     | ASN      | GLY    | conflict | UNP P23004 |
| B     | 321     | LEU      | SER    | conflict | UNP P23004 |
| B     | 332     | TYR      | SER    | conflict | UNP P23004 |
| B     | 335     | GLN      | ASP    | conflict | UNP P23004 |
| B     | 352     | VAL      | LEU    | conflict | UNP P23004 |
| B     | 355     | GLU      | PRO    | conflict | UNP P23004 |
| B     | 356     | ASN      | ASP    | conflict | UNP P23004 |
| B     | 367     | LYS      | GLY    | conflict | UNP P23004 |
| B     | 380     | GLU      | ASP    | conflict | UNP P23004 |
| B     | 393     | ASN      | THR    | conflict | UNP P23004 |
| B     | 412     | LYS      | ASN    | conflict | UNP P23004 |
| B     | 420     | ARG      | GLY    | conflict | UNP P23004 |
| B     | 421     | GLN      | ARG    | conflict | UNP P23004 |
| B     | 436     | VAL      | ILE    | conflict | UNP P23004 |

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 379      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3002  | 2013 | 473 | 504 | 12 |         |         |       |

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 241      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1899  | 1214 | 326 | 345 | 14 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 17      | PRO      | LEU    | conflict | UNP P00125 |
| D     | 143     | VAL      | LEU    | conflict | UNP P00125 |
| D     | 167     | ASP      | GLU    | conflict | UNP P00125 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 216     | VAL      | LEU    | conflict | UNP P00125 |
| D     | 221     | TYR      | ALA    | conflict | UNP P00125 |

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1512  | 953 | 266 | 285 | 8 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 9       | ASN      | ASP    | conflict | UNP P13272 |
| E     | 17      | PRO      | GLU    | conflict | UNP P13272 |
| E     | 18      | ASP      | VAL    | conflict | UNP P13272 |
| E     | 19      | ASP      | LEU    | conflict | UNP P13272 |
| E     | 20      | TYR      | ASP    | conflict | UNP P13272 |
| E     | 26      | ARG      | LYS    | conflict | UNP P13272 |
| E     | 29      | ASP      | SER    | conflict | UNP P13272 |
| E     | 30      | PRO      | GLU    | conflict | UNP P13272 |
| E     | 31      | SER      | ALA    | conflict | UNP P13272 |
| E     | 42      | VAL      | THR    | conflict | UNP P13272 |
| E     | 45      | LEU      | VAL    | conflict | UNP P13272 |
| E     | 56      | THR      | SER    | conflict | UNP P13272 |

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 875   | 557 | 153 | 162 | 3 |         |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 29      | TYR      | LEU    | conflict | UNP P00129 |
| F     | 38      | TYR      | HIS    | conflict | UNP P00129 |
| F     | 59      | MET      | VAL    | conflict | UNP P00129 |
| F     | 69      | ASN      | SER    | conflict | UNP P00129 |
| F     | 87      | VAL      | LYS    | conflict | UNP P00129 |
| F     | 88      | PRO      | SER    | conflict | UNP P00129 |
| F     | 108     | ASP      | ALA    | conflict | UNP P00129 |

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 626   | 411 | 114 | 100 | 1 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| G     | 13      | LEU      | VAL    | conflict | UNP P13271 |
| G     | 25      | PRO      | ALA    | conflict | UNP P13271 |
| G     | 34      | VAL      | ILE    | conflict | UNP P13271 |
| G     | 38      | TRP      | LEU    | conflict | UNP P13271 |
| G     | 41      | LEU      | THR    | conflict | UNP P13271 |
| G     | 53      | LEU      | VAL    | conflict | UNP P13271 |
| G     | 58      | LEU      | VAL    | conflict | UNP P13271 |
| G     | 78      | VAL      | GLU    | conflict | UNP P13271 |

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | H     | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 490   | 301 | 88 | 96 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| H     | 59      | PHE      | LEU    | conflict | UNP P00126 |

- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

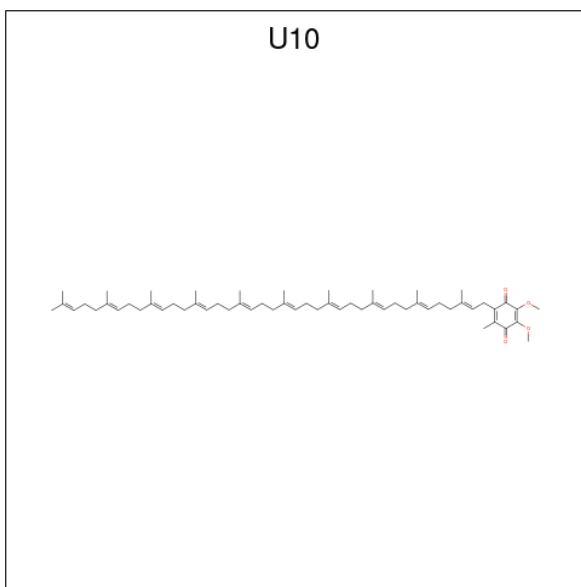
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 9   | I     | 33       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 159   | 92 | 33 | 34 |         |         |       |

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10  | J     | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 459   | 299 | 78 | 82 |         |         |       |

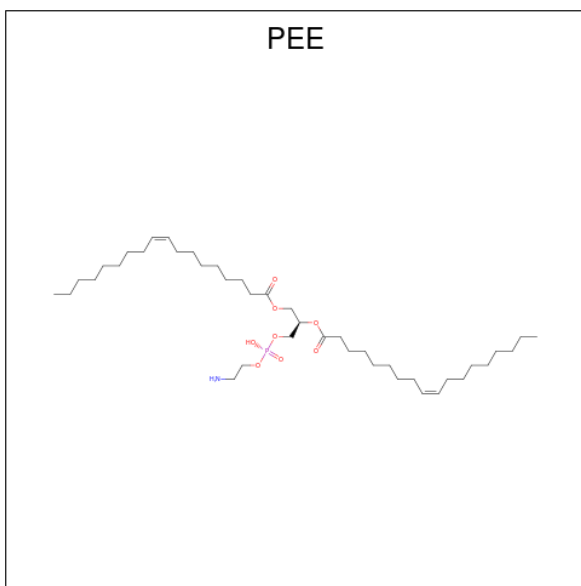
There is a discrepancy between the modelled and reference sequences:





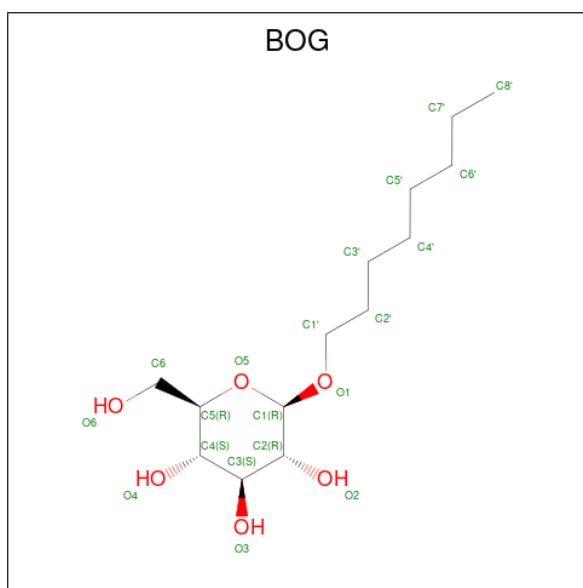
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 12  | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 29    | 25 | 4 |         |         |

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



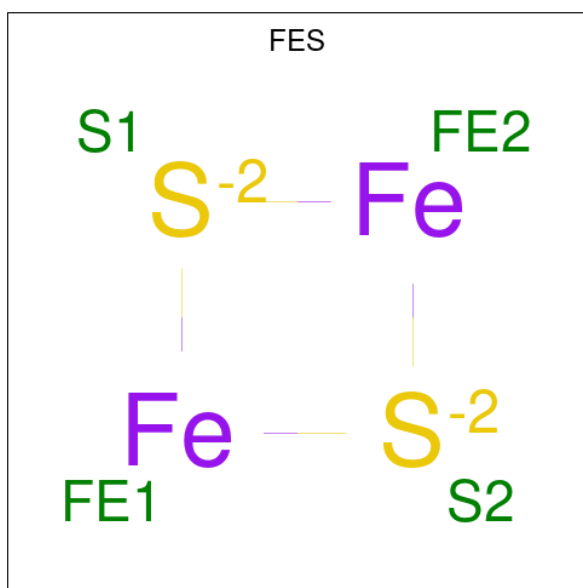
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 13  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |
| 13  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |         |

- Molecule 14 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula:  $C_{14}H_{28}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 14  | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).

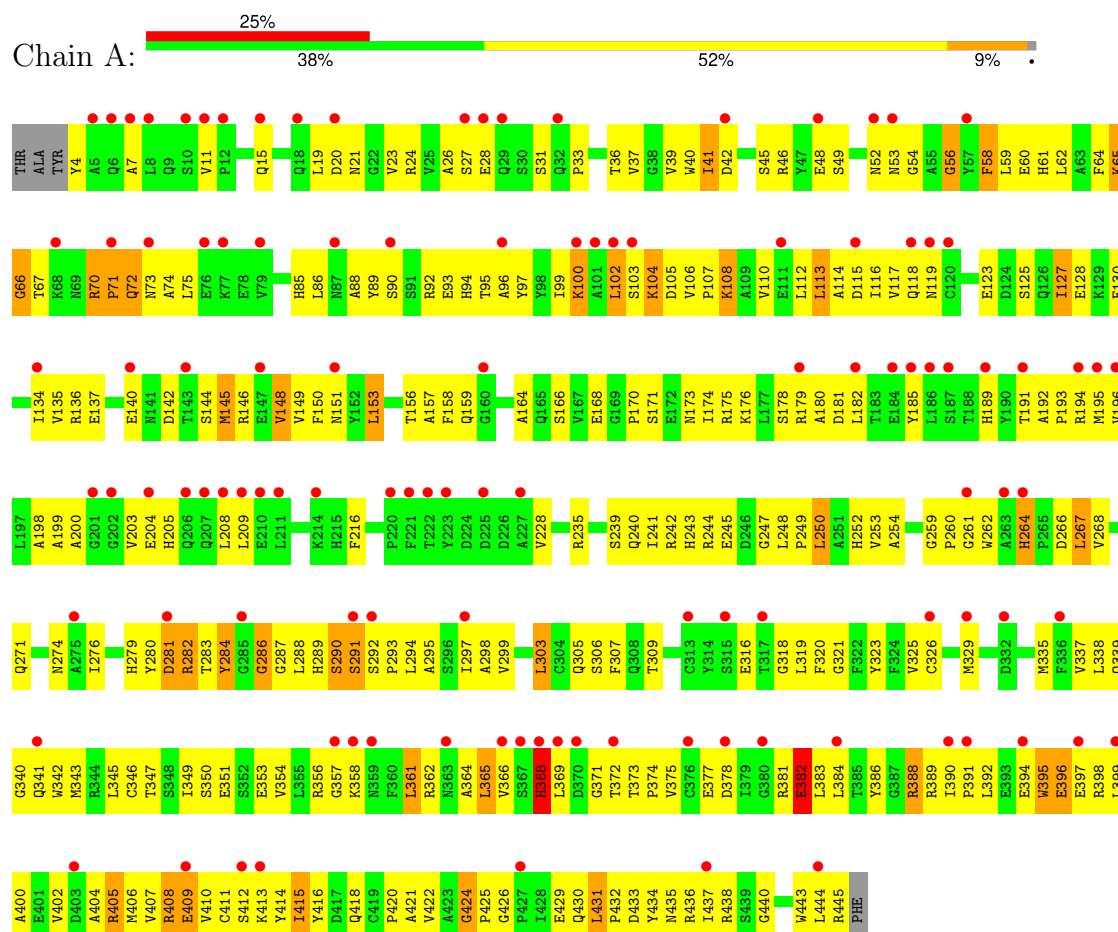


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 15  | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

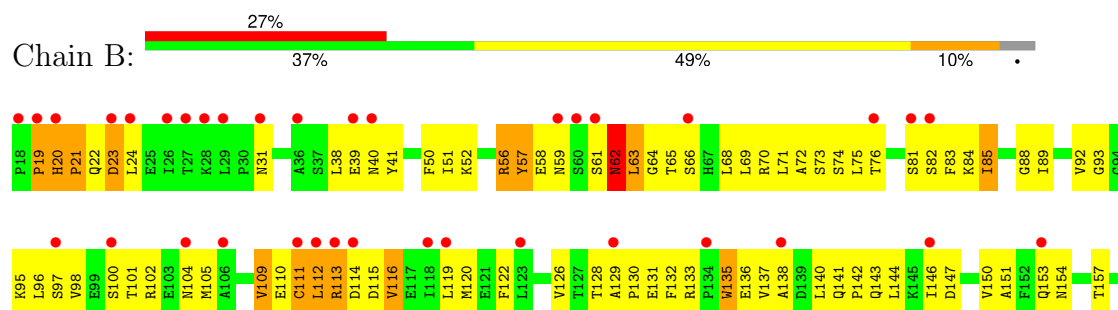
### 3 Residue-property plots

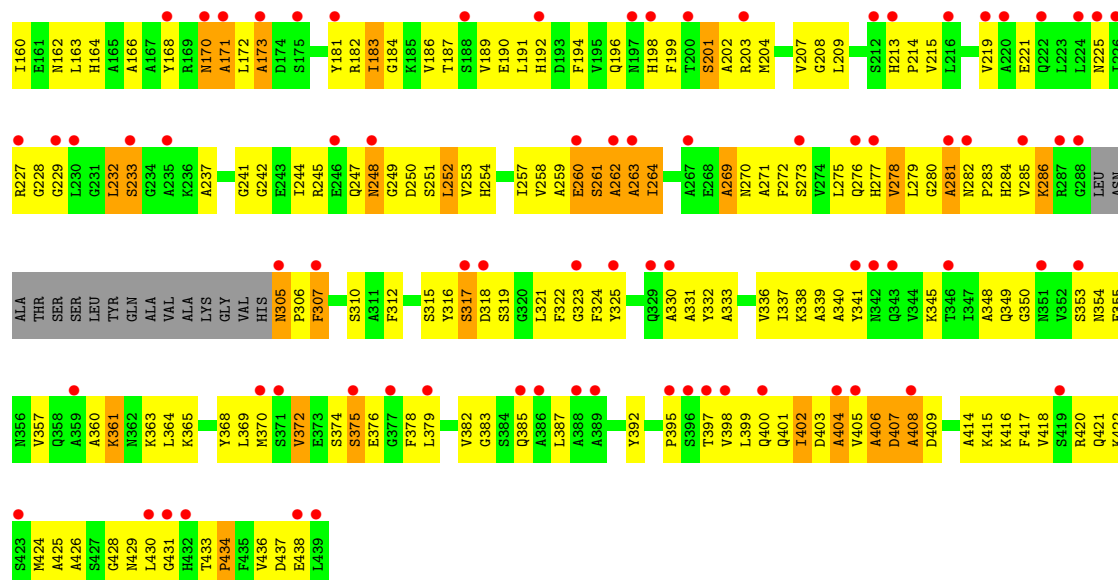
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

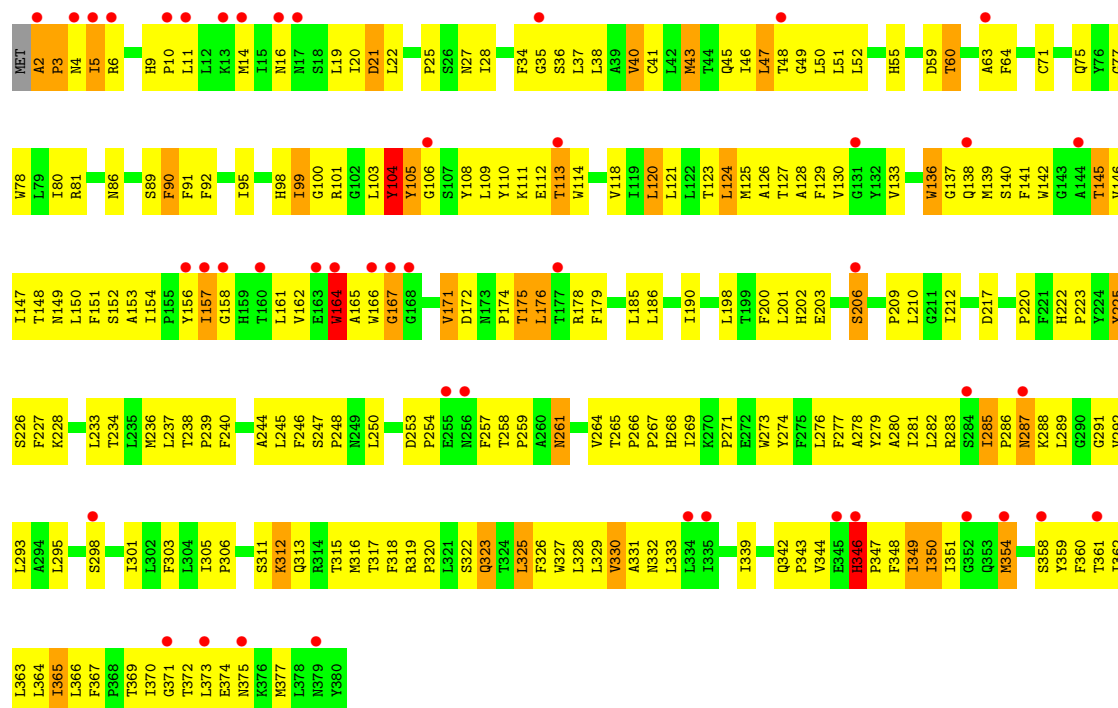


#### • Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



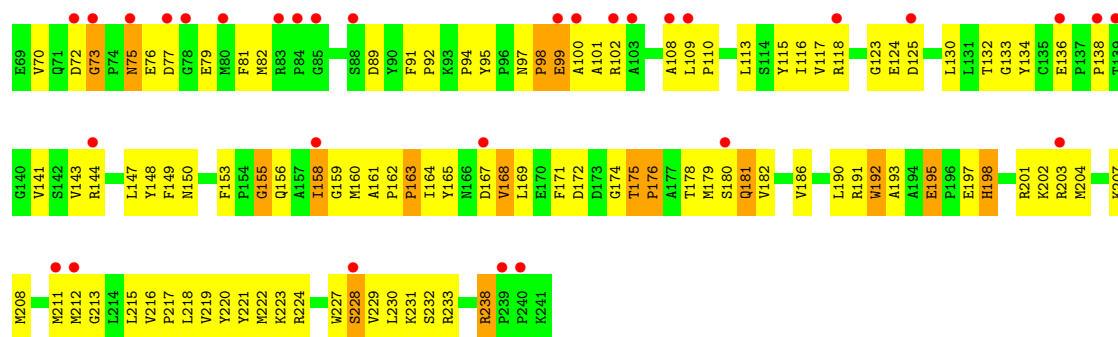


• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

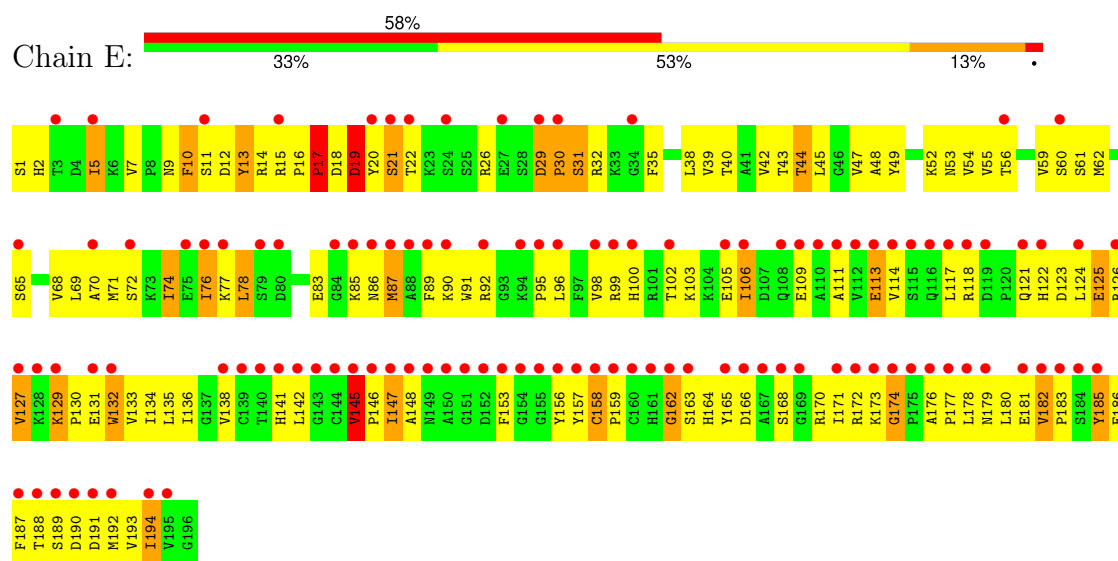


• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

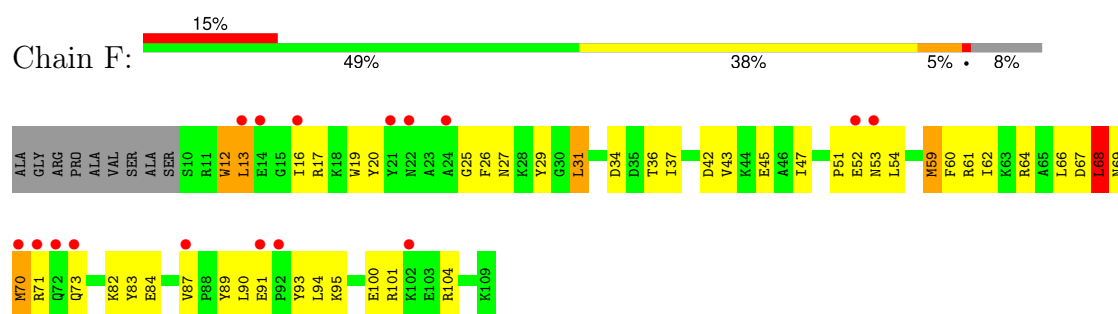




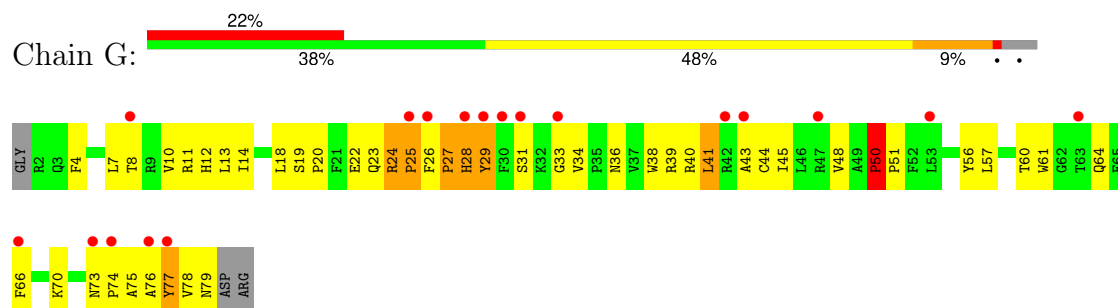
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



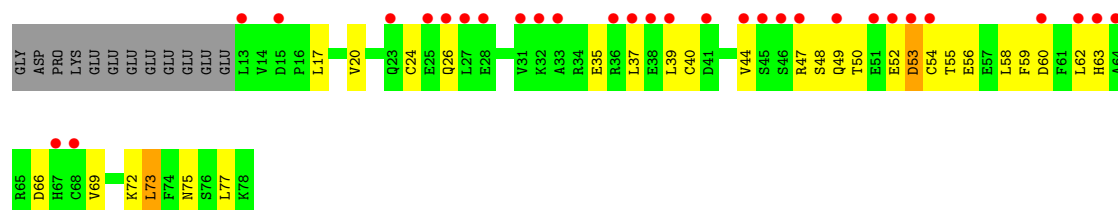
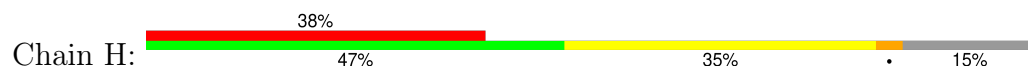
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



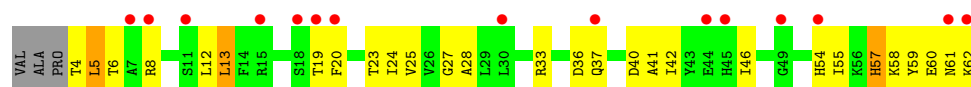
- Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



- Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



- Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 169.59Å 182.52Å 240.57Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 12.00 – 3.16<br>12.00 – 3.16                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 85.5 (12.00-3.16)<br>89.4 (12.00-3.16)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.40 (at 3.17Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 0.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.270 , 0.310<br>0.285 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 90.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.543                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 70.0                                                 | 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                                                  | 0.68                                                        | EDS              |
| Total number of atoms                                                   | 15719                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 80.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: HEM, U10, BOG, PEE, FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.60         | 0/3495      | 1.14        | 29/4742 (0.6%)   |
| 2   | B     | 0.54         | 0/3046      | 1.03        | 9/4132 (0.2%)    |
| 3   | C     | 0.69         | 0/3104      | 1.13        | 25/4252 (0.6%)   |
| 4   | D     | 0.65         | 0/1960      | 1.17        | 15/2665 (0.6%)   |
| 5   | E     | 0.72         | 0/1548      | 1.30        | 31/2095 (1.5%)   |
| 6   | F     | 0.62         | 0/896       | 1.10        | 5/1206 (0.4%)    |
| 7   | G     | 0.62         | 0/648       | 1.15        | 8/882 (0.9%)     |
| 8   | H     | 0.54         | 0/495       | 0.93        | 1/669 (0.1%)     |
| 10  | J     | 0.57         | 0/470       | 1.04        | 4/635 (0.6%)     |
| All | All   | 0.63         | 0/15662     | 1.13        | 127/21278 (0.6%) |

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

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

There are no bond length outliers.

All (127) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | D     | 76  | GLU  | N-CA-C | -12.69 | 97.77       | 113.38   |
| 3   | C     | 365 | ILE  | N-CA-C | 10.05  | 120.04      | 111.90   |
| 1   | A     | 287 | GLY  | N-CA-C | -9.82  | 98.83       | 115.62   |
| 6   | F     | 13  | LEU  | N-CA-C | -9.27  | 101.05      | 111.71   |
| 1   | A     | 104 | LYS  | N-CA-C | -9.16  | 101.63      | 113.17   |
| 1   | A     | 248 | LEU  | CA-C-N | 8.81   | 128.83      | 119.05   |
| 1   | A     | 248 | LEU  | C-N-CA | 8.81   | 128.83      | 119.05   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 20  | ASP  | N-CA-C | -8.44 | 102.88      | 113.01   |
| 5   | E     | 158 | CYS  | CA-C-N | 8.32  | 127.97      | 119.82   |
| 5   | E     | 158 | CYS  | C-N-CA | 8.32  | 127.97      | 119.82   |
| 1   | A     | 424 | GLY  | CA-C-N | 8.31  | 130.23      | 119.84   |
| 1   | A     | 424 | GLY  | C-N-CA | 8.31  | 130.23      | 119.84   |
| 3   | C     | 105 | TYR  | N-CA-C | -8.12 | 100.10      | 113.50   |
| 7   | G     | 78  | VAL  | N-CA-C | -8.01 | 103.44      | 111.77   |
| 10  | J     | 60  | GLU  | N-CA-C | -8.01 | 98.42       | 109.71   |
| 1   | A     | 58  | PHE  | N-CA-C | -7.88 | 102.69      | 111.28   |
| 3   | C     | 285 | ILE  | CA-C-N | 7.83  | 127.38      | 119.24   |
| 3   | C     | 285 | ILE  | C-N-CA | 7.83  | 127.38      | 119.24   |
| 5   | E     | 30  | PRO  | N-CA-C | -7.73 | 104.19      | 113.86   |
| 5   | E     | 185 | TYR  | N-CA-C | 7.47  | 117.75      | 107.73   |
| 1   | A     | 259 | GLY  | CA-C-N | 7.46  | 126.73      | 118.97   |
| 1   | A     | 259 | GLY  | C-N-CA | 7.46  | 126.73      | 118.97   |
| 1   | A     | 66  | GLY  | N-CA-C | 7.45  | 121.47      | 111.72   |
| 5   | E     | 132 | TRP  | N-CA-C | 7.21  | 120.16      | 108.41   |
| 5   | E     | 129 | LYS  | CA-C-N | 7.17  | 127.01      | 119.05   |
| 5   | E     | 129 | LYS  | C-N-CA | 7.17  | 127.01      | 119.05   |
| 7   | G     | 24  | ARG  | CA-C-N | 7.16  | 128.79      | 119.84   |
| 7   | G     | 24  | ARG  | C-N-CA | 7.16  | 128.79      | 119.84   |
| 5   | E     | 111 | ALA  | N-CA-C | 7.14  | 121.22      | 112.23   |
| 3   | C     | 226 | SER  | N-CA-C | -7.06 | 103.27      | 110.97   |
| 6   | F     | 87  | VAL  | N-CA-C | 6.98  | 114.46      | 107.55   |
| 4   | D     | 175 | THR  | CA-C-N | 6.98  | 128.56      | 119.84   |
| 4   | D     | 175 | THR  | C-N-CA | 6.98  | 128.56      | 119.84   |
| 3   | C     | 346 | HIS  | N-CA-C | 6.94  | 125.15      | 109.81   |
| 3   | C     | 176 | LEU  | N-CA-C | -6.93 | 103.73      | 111.28   |
| 2   | B     | 253 | VAL  | N-CA-C | 6.82  | 118.49      | 109.21   |
| 5   | E     | 26  | ARG  | N-CA-C | 6.82  | 119.73      | 111.82   |
| 1   | A     | 140 | GLU  | N-CA-C | -6.77 | 104.65      | 113.12   |
| 3   | C     | 129 | PHE  | N-CA-C | -6.77 | 102.51      | 111.24   |
| 5   | E     | 125 | GLU  | N-CA-C | -6.59 | 104.47      | 113.30   |
| 4   | D     | 195 | GLU  | CA-C-N | 6.48  | 127.94      | 119.84   |
| 4   | D     | 195 | GLU  | C-N-CA | 6.48  | 127.94      | 119.84   |
| 1   | A     | 119 | ASN  | N-CA-C | 6.43  | 119.25      | 110.06   |
| 6   | F     | 68  | LEU  | N-CA-C | -6.35 | 104.05      | 110.97   |
| 4   | D     | 44  | ASP  | N-CA-C | 6.32  | 119.84      | 111.75   |
| 5   | E     | 10  | PHE  | N-CA-C | -6.29 | 104.87      | 113.30   |
| 5   | E     | 5   | ILE  | N-CA-C | 6.25  | 117.11      | 108.12   |
| 3   | C     | 206 | SER  | N-CA-C | -6.24 | 99.54       | 109.59   |
| 5   | E     | 113 | GLU  | N-CA-C | 6.15  | 119.18      | 109.96   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 90  | PHE  | N-CA-C | -6.14 | 103.89      | 111.33   |
| 1   | A     | 415 | ILE  | N-CA-C | 6.14  | 116.84      | 111.56   |
| 4   | D     | 159 | GLY  | N-CA-C | -6.10 | 107.96      | 114.67   |
| 1   | A     | 329 | MET  | N-CA-C | 6.08  | 120.77      | 113.23   |
| 3   | C     | 104 | TYR  | N-CA-C | 6.04  | 121.11      | 111.81   |
| 4   | D     | 203 | ARG  | N-CA-C | -6.02 | 104.78      | 111.71   |
| 2   | B     | 281 | ALA  | N-CA-C | -5.95 | 104.13      | 111.33   |
| 3   | C     | 164 | TRP  | N-CA-C | -5.95 | 105.94      | 113.43   |
| 1   | A     | 364 | ALA  | N-CA-C | -5.92 | 104.46      | 111.03   |
| 3   | C     | 99  | ILE  | N-CA-C | -5.90 | 104.57      | 110.30   |
| 5   | E     | 162 | GLY  | N-CA-C | 5.89  | 124.26      | 114.48   |
| 3   | C     | 6   | ARG  | N-CA-C | -5.86 | 105.89      | 114.39   |
| 8   | H     | 53  | ASP  | N-CA-C | -5.85 | 100.60      | 109.85   |
| 10  | J     | 13  | LEU  | N-CA-C | 5.85  | 120.92      | 113.55   |
| 5   | E     | 114 | VAL  | N-CA-C | 5.83  | 116.57      | 110.62   |
| 5   | E     | 19  | ASP  | N-CA-C | 5.81  | 120.03      | 107.49   |
| 7   | G     | 19  | SER  | CA-C-N | 5.80  | 125.48      | 119.56   |
| 7   | G     | 19  | SER  | C-N-CA | 5.80  | 125.48      | 119.56   |
| 2   | B     | 74  | SER  | N-CA-C | 5.80  | 120.35      | 113.16   |
| 10  | J     | 57  | HIS  | N-CA-C | 5.77  | 118.31      | 111.33   |
| 3   | C     | 35  | GLY  | N-CA-C | -5.74 | 105.84      | 112.50   |
| 7   | G     | 50  | PRO  | N-CA-C | 5.71  | 117.67      | 110.70   |
| 1   | A     | 45  | SER  | N-CA-C | -5.69 | 105.06      | 112.23   |
| 5   | E     | 182 | VAL  | CA-C-N | 5.67  | 125.62      | 119.78   |
| 5   | E     | 182 | VAL  | C-N-CA | 5.67  | 125.62      | 119.78   |
| 5   | E     | 44  | THR  | N-CA-C | -5.66 | 105.11      | 111.28   |
| 5   | E     | 127 | VAL  | N-CA-C | 5.64  | 118.06      | 108.86   |
| 5   | E     | 147 | ILE  | N-CA-C | 5.62  | 117.09      | 108.71   |
| 3   | C     | 185 | LEU  | N-CA-C | 5.62  | 117.26      | 111.03   |
| 3   | C     | 2   | ALA  | CA-C-N | 5.60  | 126.84      | 119.84   |
| 3   | C     | 2   | ALA  | C-N-CA | 5.60  | 126.84      | 119.84   |
| 1   | A     | 368 | HIS  | N-CA-C | -5.58 | 105.73      | 112.54   |
| 3   | C     | 267 | PRO  | N-CA-C | -5.58 | 101.74      | 112.01   |
| 3   | C     | 279 | TYR  | N-CA-C | -5.58 | 105.30      | 111.71   |
| 2   | B     | 438 | GLU  | N-CA-C | -5.53 | 105.89      | 113.30   |
| 6   | F     | 100 | GLU  | N-CA-C | -5.51 | 105.27      | 111.28   |
| 5   | E     | 145 | VAL  | N-CA-C | 5.50  | 114.01      | 107.73   |
| 6   | F     | 45  | GLU  | N-CA-C | -5.49 | 105.19      | 111.07   |
| 1   | A     | 284 | TYR  | N-CA-C | 5.49  | 120.48      | 113.18   |
| 1   | A     | 176 | LYS  | N-CA-C | 5.46  | 122.51      | 113.89   |
| 4   | D     | 155 | GLY  | N-CA-C | -5.45 | 108.20      | 114.69   |
| 5   | E     | 174 | GLY  | CA-C-N | 5.40  | 125.12      | 119.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | E     | 174 | GLY  | C-N-CA  | 5.40  | 125.12      | 119.82   |
| 5   | E     | 29  | ASP  | CA-C-N  | -5.38 | 114.13      | 119.56   |
| 5   | E     | 29  | ASP  | C-N-CA  | -5.38 | 114.13      | 119.56   |
| 1   | A     | 290 | SER  | N-CA-C  | -5.37 | 102.67      | 110.24   |
| 5   | E     | 31  | SER  | N-CA-C  | -5.37 | 105.08      | 111.69   |
| 4   | D     | 238 | ARG  | N-CA-C  | 5.36  | 118.37      | 109.79   |
| 2   | B     | 116 | VAL  | N-CA-C  | -5.34 | 105.64      | 110.82   |
| 4   | D     | 110 | PRO  | CA-C-N  | 5.32  | 125.61      | 119.92   |
| 4   | D     | 110 | PRO  | C-N-CA  | 5.32  | 125.61      | 119.92   |
| 2   | B     | 93  | GLY  | N-CA-C  | -5.27 | 106.43      | 115.08   |
| 1   | A     | 426 | GLY  | CA-C-N  | 5.25  | 126.40      | 119.84   |
| 1   | A     | 426 | GLY  | C-N-CA  | 5.25  | 126.40      | 119.84   |
| 2   | B     | 278 | VAL  | N-CA-C  | -5.24 | 104.50      | 111.05   |
| 2   | B     | 98  | VAL  | N-CA-C  | 5.23  | 116.03      | 107.24   |
| 10  | J     | 8   | ARG  | N-CA-C  | -5.21 | 105.50      | 111.07   |
| 1   | A     | 416 | TYR  | N-CA-C  | 5.18  | 117.86      | 110.24   |
| 1   | A     | 70  | ARG  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 1   | A     | 70  | ARG  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 7   | G     | 8   | THR  | N-CA-C  | 5.17  | 116.70      | 108.79   |
| 5   | E     | 65  | SER  | N-CA-C  | 5.16  | 117.51      | 110.55   |
| 1   | A     | 264 | HIS  | N-CA-C  | 5.13  | 116.16      | 109.64   |
| 3   | C     | 312 | LYS  | N-CA-C  | -5.13 | 107.09      | 113.19   |
| 5   | E     | 76  | ILE  | N-CA-C  | 5.12  | 115.28      | 108.11   |
| 3   | C     | 111 | LYS  | N-CA-C  | 5.12  | 119.77      | 111.37   |
| 5   | E     | 29  | ASP  | N-CA-C  | 5.12  | 121.12      | 109.81   |
| 4   | D     | 45  | TYR  | N-CA-C  | 5.11  | 119.51      | 113.28   |
| 7   | G     | 76  | ALA  | N-CA-C  | -5.11 | 106.74      | 112.87   |
| 1   | A     | 41  | ILE  | N-CA-C  | 5.08  | 117.15      | 109.12   |
| 4   | D     | 158 | ILE  | CB-CA-C | -5.08 | 103.81      | 110.98   |
| 5   | E     | 74  | ILE  | N-CA-C  | 5.06  | 115.41      | 108.12   |
| 3   | C     | 317 | THR  | N-CA-C  | -5.04 | 105.69      | 111.14   |
| 4   | D     | 24  | THR  | N-CA-C  | -5.03 | 105.80      | 111.28   |
| 3   | C     | 261 | ASN  | CA-C-N  | 5.03  | 126.12      | 119.84   |
| 3   | C     | 261 | ASN  | C-N-CA  | 5.03  | 126.12      | 119.84   |
| 1   | A     | 303 | LEU  | N-CA-C  | 5.02  | 119.12      | 112.89   |
| 2   | B     | 173 | ALA  | N-CA-C  | -5.01 | 106.94      | 113.16   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | C     | 225 | 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     | 3423  | 0        | 3286     | 308     | 0            |
| 2   | B     | 2994  | 0        | 2906     | 297     | 0            |
| 3   | C     | 3002  | 0        | 3036     | 273     | 0            |
| 4   | D     | 1899  | 0        | 1822     | 166     | 0            |
| 5   | E     | 1512  | 0        | 1485     | 164     | 0            |
| 6   | F     | 875   | 0        | 839      | 55      | 0            |
| 7   | G     | 626   | 0        | 591      | 54      | 0            |
| 8   | H     | 490   | 0        | 445      | 39      | 0            |
| 9   | I     | 159   | 0        | 42       | 19      | 0            |
| 10  | J     | 459   | 0        | 424      | 23      | 0            |
| 11  | C     | 86    | 0        | 60       | 12      | 0            |
| 11  | D     | 43    | 0        | 30       | 0       | 0            |
| 12  | C     | 29    | 0        | 33       | 2       | 0            |
| 13  | C     | 49    | 0        | 70       | 2       | 0            |
| 13  | E     | 49    | 0        | 70       | 1       | 0            |
| 14  | D     | 20    | 0        | 28       | 3       | 0            |
| 15  | E     | 4     | 0        | 0        | 1       | 0            |
| All | All   | 15719 | 0        | 15167    | 1283    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (1283) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:158:ILE:HG22 | 4:D:160:MET:H     | 1.07                     | 1.15              |
| 1:A:282:ARG:NH1  | 9:I:202:UNK:H     | 1.47                     | 1.11              |
| 2:B:168:TYR:HB2  | 2:B:173:ALA:HB2   | 1.33                     | 1.10              |
| 3:C:27:ASN:HD22  | 6:F:69:ASN:ND2    | 1.56                     | 1.02              |
| 2:B:76:THR:HG22  | 2:B:82:SER:H      | 1.23                     | 1.01              |
| 1:A:88:ALA:HB1   | 1:A:96:ALA:O      | 1.62                     | 1.00              |
| 2:B:241:GLY:HA3  | 2:B:421:GLN:HE21  | 1.26                     | 0.99              |
| 2:B:280:GLY:H    | 2:B:283:PRO:HD2   | 1.30                     | 0.96              |
| 5:E:62:MET:HE3   | 5:E:62:MET:HA     | 1.46                     | 0.96              |
| 3:C:99:ILE:HD13  | 11:C:382:HEM:HBC2 | 1.49                     | 0.95              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:42:ASP:HB3   | 1:A:194:ARG:HB3   | 1.48                     | 0.93              |
| 3:C:167:GLY:H    | 3:C:175:THR:HG22  | 1.34                     | 0.93              |
| 1:A:49:SER:H     | 1:A:52:ASN:HB3    | 1.35                     | 0.91              |
| 3:C:139:MET:HE1  | 3:C:269:ILE:HA    | 1.49                     | 0.91              |
| 5:E:164:HIS:HB2  | 5:E:173:LYS:HB3   | 1.53                     | 0.89              |
| 2:B:258:VAL:HG11 | 2:B:321:LEU:HB3   | 1.54                     | 0.89              |
| 2:B:20:HIS:N     | 2:B:21:PRO:HD3    | 1.85                     | 0.89              |
| 2:B:162:ASN:HB3  | 2:B:244:ILE:HD11  | 1.54                     | 0.88              |
| 8:H:47:ARG:HD3   | 8:H:48:SER:H      | 1.38                     | 0.88              |
| 2:B:120:MET:HE2  | 2:B:219:VAL:HG11  | 1.56                     | 0.88              |
| 4:D:32:VAL:O     | 4:D:36:VAL:HG13   | 1.73                     | 0.87              |
| 4:D:130:LEU:HD11 | 4:D:158:ILE:HD11  | 1.57                     | 0.87              |
| 6:F:59:MET:HE3   | 6:F:59:MET:HA     | 1.57                     | 0.86              |
| 3:C:238:THR:HG23 | 3:C:239:PRO:HD3   | 1.57                     | 0.86              |
| 4:D:164:ILE:HD11 | 4:D:182:VAL:HG13  | 1.57                     | 0.85              |
| 2:B:199:PHE:C    | 2:B:204:MET:HE3   | 2.01                     | 0.85              |
| 3:C:104:TYR:CE2  | 3:C:316:MET:HB2   | 2.11                     | 0.85              |
| 4:D:158:ILE:HG22 | 4:D:160:MET:N     | 1.92                     | 0.85              |
| 3:C:342:GLN:HE21 | 3:C:343:PRO:HD2   | 1.40                     | 0.85              |
| 1:A:88:ALA:HB2   | 1:A:97:TYR:HA     | 1.59                     | 0.83              |
| 1:A:282:ARG:NH1  | 9:I:202:UNK:N     | 2.26                     | 0.83              |
| 1:A:36:THR:HG22  | 1:A:100:LYS:HB3   | 1.58                     | 0.83              |
| 1:A:286:GLY:HA3  | 1:A:289:HIS:CD2   | 2.13                     | 0.83              |
| 5:E:14:ARG:HG2   | 5:E:14:ARG:HH11   | 1.42                     | 0.83              |
| 1:A:291:SER:HB2  | 1:A:356:ARG:NH2   | 1.94                     | 0.83              |
| 2:B:128:THR:C    | 2:B:130:PRO:HD3   | 2.04                     | 0.83              |
| 5:E:121:GLN:HB3  | 5:E:126:ARG:HD2   | 1.59                     | 0.82              |
| 6:F:43:VAL:O     | 6:F:47:ILE:HG13   | 1.80                     | 0.81              |
| 1:A:361:LEU:HD13 | 1:A:399:LEU:HD22  | 1.61                     | 0.81              |
| 2:B:129:ALA:N    | 2:B:130:PRO:HD3   | 1.93                     | 0.81              |
| 5:E:166:ASP:OD2  | 5:E:170:ARG:HB2   | 1.80                     | 0.80              |
| 3:C:99:ILE:CD1   | 11:C:382:HEM:HBC2 | 2.10                     | 0.80              |
| 5:E:11:SER:HA    | 5:E:15:ARG:HD2    | 1.62                     | 0.80              |
| 4:D:43:MET:HE3   | 4:D:46:VAL:HG21   | 1.61                     | 0.80              |
| 3:C:27:ASN:HB2   | 6:F:69:ASN:ND2    | 1.97                     | 0.80              |
| 1:A:94:HIS:NE2   | 1:A:381:ARG:HG2   | 1.97                     | 0.80              |
| 4:D:98:PRO:HG2   | 4:D:99:GLU:OE2    | 1.81                     | 0.80              |
| 1:A:433:ASP:OD2  | 1:A:435:ASN:HB2   | 1.82                     | 0.80              |
| 5:E:45:LEU:HD21  | 10:J:27:GLY:C     | 2.07                     | 0.79              |
| 4:D:54:VAL:HG21  | 4:D:192:TRP:CZ3   | 2.18                     | 0.79              |
| 2:B:232:LEU:HG   | 2:B:233:SER:H     | 1.49                     | 0.78              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:325:LEU:HD11 | 3:C:366:LEU:HB3   | 1.66                     | 0.78              |
| 1:A:281:ASP:O    | 1:A:283:THR:N     | 2.17                     | 0.78              |
| 3:C:27:ASN:HD22  | 6:F:69:ASN:HD22   | 1.32                     | 0.78              |
| 3:C:123:THR:O    | 3:C:127:THR:HG23  | 1.84                     | 0.77              |
| 5:E:157:TYR:HE1  | 5:E:162:GLY:HA2   | 1.48                     | 0.77              |
| 3:C:238:THR:OG1  | 4:D:212:MET:HG3   | 1.84                     | 0.77              |
| 4:D:167:ASP:C    | 4:D:169:LEU:H     | 1.92                     | 0.77              |
| 8:H:50:THR:HG22  | 8:H:52:GLU:H      | 1.50                     | 0.77              |
| 3:C:92:PHE:HA    | 3:C:95:ILE:HG22   | 1.65                     | 0.76              |
| 1:A:37:VAL:HG12  | 1:A:199:ALA:CB    | 2.16                     | 0.76              |
| 1:A:145:MET:HA   | 1:A:148:VAL:CG1   | 2.16                     | 0.76              |
| 2:B:227:ARG:O    | 2:B:229:GLY:N     | 2.18                     | 0.76              |
| 1:A:282:ARG:HH12 | 9:I:202:UNK:H     | 1.32                     | 0.76              |
| 5:E:136:ILE:HG13 | 5:E:181:GLU:HG2   | 1.67                     | 0.76              |
| 2:B:69:LEU:HD12  | 2:B:105:MET:HE1   | 1.68                     | 0.75              |
| 5:E:45:LEU:HD21  | 10:J:28:ALA:N     | 2.00                     | 0.75              |
| 2:B:51:ILE:HG12  | 2:B:204:MET:HG2   | 1.67                     | 0.75              |
| 3:C:325:LEU:HD22 | 3:C:362:ILE:HG23  | 1.66                     | 0.75              |
| 1:A:362:ARG:HG3  | 1:A:399:LEU:HD11  | 1.68                     | 0.75              |
| 3:C:172:ASP:O    | 3:C:175:THR:HG23  | 1.85                     | 0.75              |
| 5:E:60:SER:C     | 5:E:62:MET:H      | 1.93                     | 0.75              |
| 1:A:85:HIS:HB2   | 1:A:100:LYS:CG    | 2.17                     | 0.75              |
| 10:J:42:ILE:O    | 10:J:46:ILE:HG13  | 1.87                     | 0.75              |
| 5:E:11:SER:O     | 5:E:13:TYR:N      | 2.19                     | 0.75              |
| 5:E:83:GLU:HA    | 5:E:100:HIS:HB3   | 1.68                     | 0.75              |
| 5:E:122:HIS:O    | 5:E:125:GLU:HG2   | 1.87                     | 0.75              |
| 2:B:181:TYR:CE1  | 2:B:182:ARG:HG3   | 2.20                     | 0.75              |
| 5:E:123:ASP:HB2  | 5:E:170:ARG:NH2   | 2.02                     | 0.75              |
| 1:A:39:VAL:HG11  | 1:A:117:VAL:HG11  | 1.68                     | 0.74              |
| 4:D:211:MET:HG3  | 14:D:242:BOG:H5'1 | 1.69                     | 0.74              |
| 3:C:43:MET:HE2   | 3:C:43:MET:HA     | 1.68                     | 0.74              |
| 2:B:399:LEU:HA   | 2:B:402:ILE:HG22  | 1.69                     | 0.74              |
| 3:C:127:THR:HG22 | 3:C:186:LEU:HB3   | 1.69                     | 0.74              |
| 5:E:171:ILE:HD13 | 5:E:176:ALA:HB3   | 1.67                     | 0.74              |
| 7:G:36:ASN:O     | 7:G:40:ARG:HG3    | 1.87                     | 0.74              |
| 1:A:85:HIS:HB2   | 1:A:100:LYS:HG3   | 1.69                     | 0.74              |
| 1:A:23:VAL:HG23  | 1:A:192:ALA:HB1   | 1.70                     | 0.73              |
| 1:A:178:SER:HB2  | 1:A:181:ASP:OD1   | 1.87                     | 0.73              |
| 1:A:291:SER:HB2  | 1:A:356:ARG:HH22  | 1.52                     | 0.73              |
| 4:D:167:ASP:O    | 4:D:169:LEU:N     | 2.21                     | 0.73              |
| 3:C:360:PHE:O    | 3:C:364:LEU:HB2   | 1.89                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:164:HIS:CD2  | 5:E:173:LYS:HD3  | 2.24                     | 0.72              |
| 2:B:241:GLY:HA3  | 2:B:421:GLN:NE2  | 2.04                     | 0.72              |
| 1:A:106:VAL:HG21 | 1:A:203:VAL:HG13 | 1.70                     | 0.72              |
| 2:B:405:VAL:HG12 | 2:B:406:ALA:H    | 1.54                     | 0.72              |
| 2:B:257:ILE:HD11 | 2:B:424:MET:HE2  | 1.71                     | 0.72              |
| 3:C:52:LEU:HD13  | 3:C:80:ILE:HG22  | 1.70                     | 0.72              |
| 3:C:167:GLY:H    | 3:C:175:THR:CG2  | 2.00                     | 0.72              |
| 10:J:12:LEU:O    | 10:J:19:THR:HG21 | 1.89                     | 0.72              |
| 1:A:102:LEU:HD12 | 1:A:102:LEU:N    | 2.05                     | 0.72              |
| 2:B:63:LEU:HB2   | 2:B:182:ARG:HD3  | 1.71                     | 0.72              |
| 2:B:111:CYS:SG   | 2:B:119:LEU:HD22 | 2.30                     | 0.72              |
| 2:B:280:GLY:N    | 2:B:283:PRO:HD2  | 2.03                     | 0.71              |
| 4:D:32:VAL:HG11  | 4:D:186:VAL:HG22 | 1.70                     | 0.71              |
| 3:C:148:THR:HG22 | 3:C:162:VAL:HG13 | 1.72                     | 0.71              |
| 1:A:295:ALA:O    | 1:A:299:VAL:HG23 | 1.90                     | 0.71              |
| 1:A:354:VAL:O    | 1:A:358:LYS:HG3  | 1.90                     | 0.71              |
| 3:C:238:THR:CG2  | 3:C:239:PRO:HD3  | 2.20                     | 0.71              |
| 2:B:280:GLY:H    | 2:B:283:PRO:CD   | 2.02                     | 0.71              |
| 4:D:21:LEU:HD13  | 4:D:26:ILE:HD11  | 1.73                     | 0.71              |
| 5:E:47:VAL:HG21  | 13:E:198:PEE:H24 | 1.73                     | 0.71              |
| 5:E:86:ASN:HD22  | 5:E:148:ALA:HB2  | 1.55                     | 0.71              |
| 1:A:243:HIS:O    | 1:A:425:PRO:HA   | 1.91                     | 0.71              |
| 1:A:282:ARG:HH11 | 9:I:202:UNK:H    | 1.39                     | 0.71              |
| 2:B:407:ASP:C    | 2:B:409:ASP:H    | 1.98                     | 0.71              |
| 4:D:212:MET:O    | 4:D:216:VAL:HG22 | 1.90                     | 0.71              |
| 1:A:267:LEU:O    | 1:A:271:GLN:HB2  | 1.91                     | 0.71              |
| 1:A:382:GLU:HG2  | 1:A:389:ARG:HA   | 1.73                     | 0.71              |
| 2:B:81:SER:O     | 2:B:85:ILE:HG22  | 1.90                     | 0.71              |
| 2:B:264:ILE:HG12 | 2:B:316:TYR:O    | 1.91                     | 0.70              |
| 1:A:37:VAL:HG12  | 1:A:199:ALA:HB2  | 1.73                     | 0.70              |
| 4:D:116:ILE:HG23 | 4:D:117:VAL:N    | 2.07                     | 0.70              |
| 7:G:50:PRO:HG2   | 7:G:51:PRO:HD2   | 1.73                     | 0.70              |
| 1:A:4:TYR:HB2    | 2:B:113:ARG:HB3  | 1.73                     | 0.70              |
| 2:B:92:VAL:CG1   | 2:B:115:ASP:HB3  | 2.20                     | 0.70              |
| 3:C:320:PRO:HA   | 3:C:323:GLN:HE21 | 1.55                     | 0.70              |
| 1:A:106:VAL:O    | 1:A:110:VAL:HG23 | 1.90                     | 0.70              |
| 2:B:56:ARG:HH11  | 2:B:56:ARG:HG3   | 1.57                     | 0.70              |
| 3:C:370:ILE:O    | 3:C:374:GLU:HB2  | 1.91                     | 0.70              |
| 1:A:281:ASP:HB3  | 1:A:284:TYR:CE1  | 2.27                     | 0.70              |
| 2:B:353:SER:C    | 2:B:355:GLU:H    | 1.99                     | 0.70              |
| 2:B:248:ASN:C    | 2:B:248:ASN:HD22 | 1.99                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:95:LYS:O     | 2:B:109:VAL:HA    | 1.92                     | 0.69              |
| 4:D:224:ARG:HH21 | 7:G:26:PHE:HA     | 1.56                     | 0.69              |
| 1:A:399:LEU:O    | 1:A:399:LEU:HD12  | 1.93                     | 0.69              |
| 1:A:282:ARG:HB2  | 9:I:203:UNK:CB    | 2.23                     | 0.69              |
| 2:B:132:PHE:CE2  | 2:B:191:LEU:HB3   | 2.28                     | 0.69              |
| 2:B:109:VAL:HG22 | 2:B:119:LEU:HD21  | 1.73                     | 0.69              |
| 3:C:142:TRP:CH2  | 3:C:265:THR:HG22  | 2.27                     | 0.69              |
| 4:D:30:PHE:CE2   | 4:D:64:LEU:HD21   | 2.28                     | 0.69              |
| 6:F:70:MET:HE2   | 6:F:70:MET:C      | 2.18                     | 0.68              |
| 7:G:28:HIS:HB3   | 7:G:31:SER:HB2    | 1.75                     | 0.68              |
| 3:C:27:ASN:ND2   | 6:F:69:ASN:ND2    | 2.36                     | 0.68              |
| 5:E:17:PRO:HD3   | 7:G:24:ARG:HE     | 1.59                     | 0.68              |
| 1:A:64:PHE:O     | 1:A:75:LEU:HD23   | 1.93                     | 0.68              |
| 2:B:76:THR:CG2   | 2:B:82:SER:H      | 2.04                     | 0.68              |
| 2:B:132:PHE:CD2  | 2:B:191:LEU:HB3   | 2.28                     | 0.68              |
| 2:B:209:LEU:HG   | 2:B:379:LEU:HD23  | 1.76                     | 0.68              |
| 5:E:13:TYR:O     | 5:E:14:ARG:HD3    | 1.93                     | 0.68              |
| 4:D:229:VAL:CG2  | 7:G:20:PRO:HG3    | 2.24                     | 0.68              |
| 2:B:424:MET:HG2  | 2:B:425:ALA:N     | 2.08                     | 0.68              |
| 1:A:40:TRP:CH2   | 1:A:377:GLU:HA    | 2.28                     | 0.67              |
| 4:D:165:TYR:CE2  | 4:D:168:VAL:HG22  | 2.30                     | 0.67              |
| 1:A:292:SER:N    | 1:A:293:PRO:HD3   | 2.07                     | 0.67              |
| 3:C:316:MET:SD   | 3:C:319:ARG:NE    | 2.67                     | 0.67              |
| 2:B:395:PRO:O    | 2:B:398:VAL:HG12  | 1.94                     | 0.67              |
| 3:C:198:LEU:HD21 | 11:C:382:HEM:HMA1 | 1.75                     | 0.67              |
| 3:C:332:ASN:C    | 3:C:332:ASN:HD22  | 2.03                     | 0.67              |
| 1:A:58:PHE:HB3   | 1:A:182:LEU:HD11  | 1.77                     | 0.67              |
| 2:B:258:VAL:HG12 | 2:B:259:ALA:N     | 2.09                     | 0.67              |
| 3:C:110:TYR:HB3  | 3:C:113:THR:CG2   | 2.24                     | 0.67              |
| 3:C:238:THR:CB   | 4:D:212:MET:HG3   | 2.25                     | 0.67              |
| 5:E:157:TYR:CE1  | 5:E:162:GLY:HA2   | 2.29                     | 0.67              |
| 1:A:23:VAL:HG23  | 1:A:192:ALA:CB    | 2.25                     | 0.67              |
| 1:A:371:GLY:O    | 1:A:375:VAL:HG23  | 1.95                     | 0.67              |
| 2:B:38:LEU:HD23  | 2:B:378:PHE:HZ    | 1.60                     | 0.67              |
| 1:A:205:HIS:NE2  | 1:A:209:LEU:HD21  | 2.09                     | 0.67              |
| 3:C:127:THR:HG22 | 3:C:186:LEU:CB    | 2.25                     | 0.67              |
| 5:E:15:ARG:HH11  | 5:E:19:ASP:HB3    | 1.58                     | 0.67              |
| 5:E:43:THR:O     | 5:E:47:VAL:HG23   | 1.95                     | 0.67              |
| 3:C:354:MET:HE2  | 3:C:354:MET:HA    | 1.78                     | 0.66              |
| 1:A:36:THR:HG22  | 1:A:100:LYS:CB    | 2.26                     | 0.66              |
| 1:A:110:VAL:HA   | 1:A:113:LEU:HD12  | 1.77                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:162:ASN:HB3  | 2:B:244:ILE:CD1  | 2.23                     | 0.66              |
| 2:B:333:ALA:O    | 2:B:337:ILE:HG13 | 1.95                     | 0.66              |
| 5:E:86:ASN:HB3   | 5:E:148:ALA:HB1  | 1.77                     | 0.66              |
| 6:F:13:LEU:O     | 6:F:17:ARG:HG3   | 1.95                     | 0.66              |
| 4:D:132:THR:HA   | 4:D:179:MET:HE2  | 1.77                     | 0.66              |
| 3:C:27:ASN:ND2   | 6:F:69:ASN:HD22  | 1.93                     | 0.66              |
| 2:B:154:ASN:O    | 2:B:157:THR:HG22 | 1.96                     | 0.66              |
| 2:B:405:VAL:HG12 | 2:B:406:ALA:N    | 2.11                     | 0.66              |
| 3:C:28:ILE:HD12  | 3:C:225:TYR:CZ   | 2.30                     | 0.66              |
| 3:C:167:GLY:HA3  | 3:C:174:PRO:HG2  | 1.77                     | 0.66              |
| 3:C:222:HIS:O    | 3:C:223:PRO:C    | 2.38                     | 0.66              |
| 7:G:60:THR:HG22  | 7:G:64:GLN:HE21  | 1.61                     | 0.66              |
| 7:G:79:ASN:O     | 8:H:47:ARG:NH1   | 2.29                     | 0.65              |
| 2:B:111:CYS:SG   | 2:B:116:VAL:HA   | 2.37                     | 0.65              |
| 5:E:136:ILE:HG12 | 5:E:183:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:134:ILE:HG21 | 1:A:174:ILE:HD13 | 1.76                     | 0.65              |
| 3:C:5:ILE:O      | 3:C:5:ILE:HG22   | 1.97                     | 0.65              |
| 3:C:146:VAL:O    | 3:C:150:LEU:HD13 | 1.96                     | 0.65              |
| 1:A:102:LEU:HD12 | 1:A:102:LEU:H    | 1.62                     | 0.65              |
| 1:A:288:LEU:HD22 | 2:B:83:PHE:HD1   | 1.61                     | 0.65              |
| 2:B:357:VAL:HG12 | 2:B:361:LYS:HD2  | 1.77                     | 0.65              |
| 4:D:164:ILE:HD11 | 4:D:182:VAL:CG1  | 2.27                     | 0.65              |
| 3:C:104:TYR:CE2  | 3:C:316:MET:CB   | 2.80                     | 0.64              |
| 5:E:16:PRO:HD2   | 7:G:22:GLU:O     | 1.96                     | 0.64              |
| 2:B:89:ILE:HD13  | 2:B:96:LEU:HB2   | 1.77                     | 0.64              |
| 3:C:120:LEU:HG   | 11:C:382:HEM:HAB | 1.79                     | 0.64              |
| 5:E:171:ILE:HG22 | 5:E:179:ASN:OD1  | 1.96                     | 0.64              |
| 2:B:100:SER:O    | 9:I:106:UNK:HA   | 1.97                     | 0.64              |
| 4:D:192:TRP:CD1  | 4:D:193:ALA:N    | 2.65                     | 0.64              |
| 1:A:362:ARG:HH22 | 2:B:113:ARG:NH1  | 1.95                     | 0.64              |
| 5:E:62:MET:HA    | 5:E:62:MET:CE    | 2.22                     | 0.64              |
| 3:C:198:LEU:HD21 | 11:C:382:HEM:CMA | 2.27                     | 0.64              |
| 13:C:384:PEE:O5  | 7:G:48:VAL:HG21  | 1.98                     | 0.64              |
| 4:D:51:LEU:O     | 4:D:54:VAL:HG12  | 1.98                     | 0.64              |
| 8:H:72:LYS:HA    | 8:H:75:ASN:ND2   | 2.12                     | 0.64              |
| 2:B:357:VAL:HG11 | 2:B:406:ALA:HB1  | 1.80                     | 0.64              |
| 3:C:104:TYR:CZ   | 3:C:316:MET:HG3  | 2.33                     | 0.64              |
| 4:D:195:GLU:HG3  | 4:D:195:GLU:O    | 1.97                     | 0.64              |
| 5:E:162:GLY:O    | 5:E:164:HIS:HD2  | 1.81                     | 0.64              |
| 5:E:142:LEU:HB2  | 15:E:197:FES:S2  | 2.37                     | 0.64              |
| 4:D:238:ARG:HD2  | 5:E:5:ILE:HD11   | 1.79                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:310:SER:O    | 2:B:324:PHE:HB2  | 1.99                     | 0.63              |
| 2:B:96:LEU:HD23  | 2:B:97:SER:N     | 2.12                     | 0.63              |
| 2:B:272:PHE:O    | 2:B:276:GLN:N    | 2.26                     | 0.63              |
| 3:C:236:MET:O    | 3:C:239:PRO:HD2  | 1.99                     | 0.63              |
| 5:E:109:GLU:OE1  | 5:E:166:ASP:HB2  | 1.98                     | 0.63              |
| 2:B:39:GLU:HG3   | 2:B:41:TYR:CE1   | 2.34                     | 0.63              |
| 3:C:103:LEU:O    | 3:C:103:LEU:HD13 | 1.99                     | 0.63              |
| 4:D:216:VAL:HG23 | 4:D:217:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:53:ASN:HD22  | 1:A:54:GLY:N     | 1.97                     | 0.63              |
| 1:A:378:ASP:O    | 1:A:382:GLU:HB2  | 1.98                     | 0.63              |
| 1:A:429:GLU:OE2  | 7:G:7:LEU:HB2    | 1.99                     | 0.63              |
| 2:B:70:ARG:HD3   | 2:B:100:SER:HB3  | 1.78                     | 0.63              |
| 2:B:133:ARG:HD3  | 2:B:135:TRP:CH2  | 2.34                     | 0.63              |
| 3:C:34:PHE:HD1   | 3:C:37:LEU:HD12  | 1.63                     | 0.63              |
| 1:A:245:GLU:HG3  | 7:G:11:ARG:HG2   | 1.80                     | 0.62              |
| 2:B:62:ASN:O     | 2:B:65:THR:HG22  | 1.99                     | 0.62              |
| 5:E:122:HIS:CE1  | 5:E:124:LEU:HB2  | 2.34                     | 0.62              |
| 5:E:45:LEU:C     | 5:E:45:LEU:HD13  | 2.24                     | 0.62              |
| 1:A:108:LYS:HE3  | 1:A:108:LYS:HA   | 1.80                     | 0.62              |
| 3:C:142:TRP:CD1  | 3:C:266:PRO:HD3  | 2.34                     | 0.62              |
| 5:E:78:LEU:HG    | 5:E:191:ASP:C    | 2.23                     | 0.62              |
| 1:A:343:MET:HE2  | 1:A:343:MET:HA   | 1.81                     | 0.62              |
| 2:B:31:ASN:HB3   | 2:B:201:SER:HB2  | 1.81                     | 0.62              |
| 2:B:202:ALA:HB3  | 2:B:229:GLY:O    | 2.00                     | 0.62              |
| 5:E:44:THR:HB    | 10:J:24:ILE:HD12 | 1.80                     | 0.62              |
| 2:B:71:LEU:HD12  | 2:B:144:LEU:HD23 | 1.80                     | 0.62              |
| 4:D:149:PHE:HA   | 4:D:156:GLN:O    | 2.00                     | 0.62              |
| 5:E:147:ILE:O    | 5:E:156:TYR:HA   | 2.00                     | 0.62              |
| 1:A:245:GLU:HG2  | 1:A:247:GLY:H    | 1.64                     | 0.62              |
| 4:D:155:GLY:C    | 4:D:156:GLN:NE2  | 2.58                     | 0.62              |
| 4:D:218:LEU:HD11 | 5:E:42:VAL:HG12  | 1.82                     | 0.62              |
| 5:E:16:PRO:HD3   | 7:G:23:GLN:HA    | 1.81                     | 0.62              |
| 3:C:167:GLY:N    | 3:C:175:THR:HG22 | 2.12                     | 0.62              |
| 1:A:284:TYR:CE1  | 9:I:112:UNK:O    | 2.53                     | 0.62              |
| 2:B:163:LEU:HD21 | 2:B:258:VAL:HG21 | 1.80                     | 0.61              |
| 3:C:247:SER:HB3  | 3:C:250:LEU:HB2  | 1.82                     | 0.61              |
| 8:H:50:THR:HG22  | 8:H:52:GLU:N     | 2.15                     | 0.61              |
| 3:C:25:PRO:HD2   | 3:C:28:ILE:HD11  | 1.82                     | 0.61              |
| 5:E:123:ASP:HB2  | 5:E:170:ARG:CZ   | 2.30                     | 0.61              |
| 1:A:342:TRP:O    | 1:A:345:LEU:HB3  | 1.99                     | 0.61              |
| 2:B:92:VAL:HG11  | 2:B:115:ASP:HB3  | 1.81                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:124:LEU:O    | 3:C:124:LEU:HD22 | 2.00                     | 0.61              |
| 1:A:62:LEU:HD11  | 1:A:127:ILE:HG12 | 1.82                     | 0.61              |
| 2:B:207:VAL:HG12 | 2:B:208:GLY:N    | 2.15                     | 0.61              |
| 5:E:99:ARG:HB3   | 5:E:133:VAL:CG1  | 2.30                     | 0.61              |
| 5:E:183:PRO:O    | 5:E:185:TYR:HD1  | 1.84                     | 0.61              |
| 1:A:56:GLY:HA2   | 1:A:185:TYR:CE2  | 2.35                     | 0.61              |
| 2:B:360:ALA:O    | 2:B:363:LYS:N    | 2.31                     | 0.61              |
| 3:C:104:TYR:OH   | 3:C:322:SER:HB2  | 1.99                     | 0.61              |
| 5:E:14:ARG:O     | 7:G:24:ARG:HG3   | 2.00                     | 0.61              |
| 1:A:250:LEU:C    | 1:A:250:LEU:HD22 | 2.25                     | 0.61              |
| 3:C:166:TRP:HB2  | 3:C:175:THR:HG21 | 1.81                     | 0.61              |
| 3:C:125:MET:O    | 3:C:128:ALA:N    | 2.33                     | 0.61              |
| 3:C:238:THR:HG23 | 3:C:239:PRO:CD   | 2.31                     | 0.61              |
| 1:A:102:LEU:C    | 1:A:104:LYS:H    | 2.09                     | 0.61              |
| 5:E:102:THR:O    | 5:E:106:ILE:HG13 | 2.01                     | 0.61              |
| 2:B:122:PHE:O    | 2:B:126:VAL:HG23 | 2.01                     | 0.60              |
| 2:B:166:ALA:HB1  | 2:B:242:GLY:HA3  | 1.82                     | 0.60              |
| 2:B:170:ASN:HD21 | 2:B:237:ALA:HA   | 1.66                     | 0.60              |
| 3:C:142:TRP:O    | 3:C:146:VAL:HG22 | 2.01                     | 0.60              |
| 3:C:209:PRO:O    | 3:C:315:THR:HG21 | 2.01                     | 0.60              |
| 3:C:212:ILE:HD12 | 6:F:62:ILE:HG23  | 1.83                     | 0.60              |
| 2:B:395:PRO:HA   | 2:B:398:VAL:HG12 | 1.82                     | 0.60              |
| 2:B:260:GLU:O    | 2:B:261:SER:HB3  | 2.01                     | 0.60              |
| 3:C:112:GLU:N    | 3:C:112:GLU:OE1  | 2.34                     | 0.60              |
| 5:E:59:VAL:HG12  | 5:E:59:VAL:O     | 2.01                     | 0.60              |
| 5:E:99:ARG:H     | 5:E:133:VAL:HG12 | 1.65                     | 0.60              |
| 3:C:49:GLY:C     | 11:C:381:HEM:HAC | 2.27                     | 0.60              |
| 3:C:278:ALA:HB1  | 3:C:295:LEU:CD1  | 2.31                     | 0.60              |
| 4:D:167:ASP:C    | 4:D:169:LEU:N    | 2.59                     | 0.60              |
| 5:E:78:LEU:HD12  | 5:E:190:ASP:O    | 2.02                     | 0.60              |
| 1:A:252:HIS:CE1  | 1:A:325:VAL:HG22 | 2.37                     | 0.59              |
| 2:B:52:LYS:O     | 2:B:203:ARG:NH2  | 2.27                     | 0.59              |
| 2:B:101:THR:HG22 | 2:B:102:ARG:N    | 2.17                     | 0.59              |
| 2:B:405:VAL:O    | 2:B:406:ALA:HB2  | 2.02                     | 0.59              |
| 4:D:32:VAL:CG1   | 4:D:186:VAL:HG22 | 2.31                     | 0.59              |
| 4:D:167:ASP:O    | 4:D:169:LEU:HD23 | 2.02                     | 0.59              |
| 1:A:279:HIS:HA   | 1:A:307:PHE:CE1  | 2.36                     | 0.59              |
| 2:B:24:LEU:H     | 2:B:24:LEU:HD23  | 1.67                     | 0.59              |
| 2:B:258:VAL:CG1  | 2:B:321:LEU:HB3  | 2.29                     | 0.59              |
| 3:C:110:TYR:HB3  | 3:C:113:THR:HG23 | 1.83                     | 0.59              |
| 4:D:116:ILE:CG2  | 4:D:117:VAL:N    | 2.65                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:171:ILE:CD1  | 5:E:176:ALA:HB3  | 2.31                     | 0.59              |
| 2:B:95:LYS:HB2   | 2:B:110:GLU:CG   | 2.32                     | 0.59              |
| 3:C:27:ASN:HD22  | 6:F:69:ASN:HD21  | 1.43                     | 0.59              |
| 3:C:136:TRP:CD1  | 3:C:176:LEU:HD13 | 2.37                     | 0.59              |
| 4:D:12:TRP:CZ2   | 4:D:124:GLU:HB2  | 2.37                     | 0.59              |
| 1:A:102:LEU:O    | 1:A:104:LYS:N    | 2.35                     | 0.59              |
| 1:A:381:ARG:O    | 1:A:382:GLU:C    | 2.46                     | 0.59              |
| 1:A:61:HIS:CD2   | 1:A:134:ILE:HG12 | 2.37                     | 0.59              |
| 2:B:101:THR:HB   | 2:B:104:ASN:OD1  | 2.02                     | 0.59              |
| 2:B:207:VAL:HG11 | 2:B:382:VAL:HG23 | 1.83                     | 0.59              |
| 3:C:45:GLN:CB    | 11:C:381:HEM:HAB | 2.32                     | 0.59              |
| 3:C:301:ILE:HD11 | 3:C:364:LEU:HD11 | 1.85                     | 0.59              |
| 5:E:16:PRO:HD3   | 7:G:23:GLN:CA    | 2.33                     | 0.59              |
| 2:B:406:ALA:O    | 2:B:408:ALA:N    | 2.35                     | 0.59              |
| 3:C:106:GLY:HA2  | 3:C:108:TYR:CE2  | 2.38                     | 0.59              |
| 1:A:252:HIS:ND1  | 1:A:325:VAL:HG22 | 2.18                     | 0.59              |
| 3:C:120:LEU:CG   | 11:C:382:HEM:HAB | 2.33                     | 0.59              |
| 3:C:328:LEU:HD12 | 7:G:51:PRO:HB3   | 1.84                     | 0.59              |
| 4:D:227:TRP:O    | 4:D:229:VAL:N    | 2.36                     | 0.59              |
| 10:J:13:LEU:HA   | 10:J:19:THR:HG21 | 1.85                     | 0.58              |
| 2:B:341:TYR:OH   | 2:B:422:LYS:HE3  | 2.02                     | 0.58              |
| 2:B:361:LYS:HA   | 2:B:402:ILE:HD11 | 1.85                     | 0.58              |
| 4:D:182:VAL:O    | 4:D:186:VAL:HG23 | 2.03                     | 0.58              |
| 2:B:353:SER:C    | 2:B:355:GLU:N    | 2.59                     | 0.58              |
| 3:C:175:THR:HA   | 3:C:178:ARG:HG2  | 1.86                     | 0.58              |
| 3:C:225:TYR:HA   | 3:C:228:LYS:HB3  | 1.86                     | 0.58              |
| 3:C:346:HIS:O    | 3:C:350:ILE:HG12 | 2.02                     | 0.58              |
| 5:E:96:LEU:HD12  | 5:E:135:LEU:O    | 2.04                     | 0.58              |
| 2:B:171:ALA:C    | 2:B:173:ALA:H    | 2.10                     | 0.58              |
| 3:C:45:GLN:HB3   | 11:C:381:HEM:HAB | 1.86                     | 0.58              |
| 5:E:12:ASP:O     | 5:E:13:TYR:C     | 2.46                     | 0.58              |
| 1:A:151:ASN:ND2  | 5:E:2:HIS:NE2    | 2.51                     | 0.58              |
| 2:B:95:LYS:HB2   | 2:B:110:GLU:HG2  | 1.85                     | 0.58              |
| 3:C:347:PRO:HG3  | 7:G:66:PHE:HB2   | 1.86                     | 0.58              |
| 2:B:357:VAL:HG12 | 2:B:361:LYS:CD   | 2.34                     | 0.58              |
| 2:B:395:PRO:HA   | 2:B:398:VAL:CG1  | 2.33                     | 0.57              |
| 3:C:64:PHE:CD2   | 3:C:259:PRO:HG3  | 2.39                     | 0.57              |
| 4:D:171:PHE:HE2  | 4:D:181:GLN:HE22 | 1.50                     | 0.57              |
| 5:E:76:ILE:O     | 5:E:193:VAL:HG12 | 2.04                     | 0.57              |
| 2:B:146:ILE:HG13 | 2:B:147:ASP:N    | 2.19                     | 0.57              |
| 5:E:85:LYS:HD2   | 5:E:87:MET:SD    | 2.44                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:ALA:O      | 1:A:11:VAL:HG23  | 2.04                     | 0.57              |
| 3:C:220:PRO:HG2  | 3:C:223:PRO:HG2  | 1.86                     | 0.57              |
| 2:B:112:LEU:HD23 | 2:B:112:LEU:N    | 2.19                     | 0.57              |
| 3:C:313:GLN:NE2  | 6:F:36:THR:OG1   | 2.36                     | 0.57              |
| 4:D:2:ASP:OD2    | 7:G:70:LYS:HE2   | 2.04                     | 0.57              |
| 1:A:88:ALA:CB    | 1:A:97:TYR:HA    | 2.32                     | 0.57              |
| 1:A:196:VAL:HG11 | 1:A:383:LEU:HD12 | 1.85                     | 0.57              |
| 2:B:258:VAL:HG13 | 2:B:322:PHE:H    | 1.68                     | 0.57              |
| 1:A:356:ARG:O    | 1:A:357:GLY:C    | 2.47                     | 0.57              |
| 3:C:89:SER:O     | 3:C:90:PHE:C     | 2.47                     | 0.57              |
| 1:A:4:TYR:CB     | 2:B:113:ARG:HB3  | 2.35                     | 0.57              |
| 1:A:130:GLU:O    | 1:A:134:ILE:HG13 | 2.04                     | 0.57              |
| 2:B:19:PRO:C     | 2:B:21:PRO:HD3   | 2.29                     | 0.57              |
| 4:D:3:LEU:HD23   | 4:D:4:GLU:N      | 2.20                     | 0.57              |
| 4:D:165:TYR:O    | 4:D:168:VAL:HG23 | 2.05                     | 0.57              |
| 1:A:37:VAL:HG12  | 1:A:199:ALA:HB1  | 1.87                     | 0.57              |
| 3:C:245:LEU:O    | 4:D:201:ARG:HD3  | 2.04                     | 0.57              |
| 3:C:330:VAL:CG2  | 3:C:331:ALA:N    | 2.68                     | 0.57              |
| 4:D:116:ILE:HG21 | 4:D:190:LEU:HD13 | 1.87                     | 0.57              |
| 4:D:232:SER:CB   | 7:G:23:GLN:HE22  | 2.17                     | 0.57              |
| 7:G:77:TYR:CE1   | 8:H:52:GLU:HB2   | 2.39                     | 0.57              |
| 1:A:297:ILE:HG21 | 1:A:337:VAL:HG11 | 1.85                     | 0.56              |
| 4:D:30:PHE:HE2   | 4:D:64:LEU:HD21  | 1.68                     | 0.56              |
| 5:E:17:PRO:HD3   | 7:G:24:ARG:NE    | 2.20                     | 0.56              |
| 5:E:78:LEU:HB3   | 5:E:132:TRP:CZ2  | 2.40                     | 0.56              |
| 6:F:51:PRO:HD2   | 6:F:54:LEU:HD12  | 1.86                     | 0.56              |
| 3:C:95:ILE:O     | 3:C:99:ILE:HG12  | 2.05                     | 0.56              |
| 1:A:250:LEU:HD13 | 1:A:250:LEU:N    | 2.20                     | 0.56              |
| 1:A:395:TRP:HA   | 1:A:395:TRP:CE3  | 2.40                     | 0.56              |
| 2:B:248:ASN:HD21 | 2:B:428:GLY:HA2  | 1.69                     | 0.56              |
| 2:B:307:PHE:CD1  | 2:B:307:PHE:C    | 2.83                     | 0.56              |
| 2:B:357:VAL:O    | 2:B:361:LYS:HG3  | 2.05                     | 0.56              |
| 3:C:64:PHE:CE2   | 3:C:259:PRO:HG3  | 2.40                     | 0.56              |
| 3:C:81:ARG:NH1   | 11:C:381:HEM:O1D | 2.38                     | 0.56              |
| 4:D:32:VAL:HG21  | 4:D:186:VAL:CG2  | 2.35                     | 0.56              |
| 8:H:35:GLU:O     | 8:H:39:LEU:HD13  | 2.05                     | 0.56              |
| 1:A:205:HIS:O    | 1:A:208:LEU:HB3  | 2.06                     | 0.56              |
| 2:B:257:ILE:O    | 2:B:323:GLY:HA3  | 2.05                     | 0.56              |
| 3:C:146:VAL:HG23 | 3:C:147:ILE:N    | 2.21                     | 0.56              |
| 1:A:48:GLU:CD    | 1:A:53:ASN:HA    | 2.31                     | 0.56              |
| 1:A:388:ARG:HG3  | 1:A:388:ARG:HH11 | 1.70                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:395:PRO:C    | 2:B:398:VAL:HG12 | 2.31                     | 0.56              |
| 6:F:67:ASP:O     | 6:F:71:ARG:HG3   | 2.06                     | 0.56              |
| 2:B:56:ARG:HB2   | 2:B:102:ARG:O    | 2.06                     | 0.56              |
| 1:A:61:HIS:HD2   | 1:A:134:ILE:HG12 | 1.69                     | 0.56              |
| 1:A:346:CYS:HB3  | 1:A:411:CYS:HB2  | 1.87                     | 0.56              |
| 2:B:20:HIS:N     | 2:B:21:PRO:CD    | 2.64                     | 0.56              |
| 2:B:101:THR:HG22 | 2:B:102:ARG:H    | 1.70                     | 0.56              |
| 2:B:258:VAL:HA   | 2:B:322:PHE:O    | 2.06                     | 0.56              |
| 3:C:156:TYR:C    | 3:C:158:GLY:H    | 2.13                     | 0.56              |
| 3:C:293:LEU:N    | 3:C:293:LEU:HD22 | 2.21                     | 0.56              |
| 3:C:373:LEU:HD23 | 3:C:373:LEU:O    | 2.05                     | 0.56              |
| 6:F:12:TRP:HA    | 6:F:12:TRP:CE3   | 2.41                     | 0.56              |
| 1:A:33:PRO:HG3   | 2:B:369:LEU:HD22 | 1.87                     | 0.56              |
| 2:B:109:VAL:CG2  | 2:B:119:LEU:HD11 | 2.35                     | 0.56              |
| 2:B:372:VAL:HG12 | 2:B:372:VAL:O    | 2.06                     | 0.56              |
| 2:B:397:THR:O    | 2:B:401:GLN:HG2  | 2.05                     | 0.56              |
| 3:C:20:ILE:C     | 3:C:22:LEU:H     | 2.14                     | 0.55              |
| 3:C:157:ILE:HG12 | 3:C:157:ILE:O    | 2.06                     | 0.55              |
| 2:B:140:LEU:C    | 2:B:142:PRO:HD2  | 2.30                     | 0.55              |
| 2:B:250:ASP:O    | 2:B:251:SER:HB3  | 2.05                     | 0.55              |
| 3:C:209:PRO:HG2  | 6:F:69:ASN:HD21  | 1.71                     | 0.55              |
| 3:C:319:ARG:HH12 | 3:C:371:GLY:HA2  | 1.72                     | 0.55              |
| 1:A:354:VAL:HG11 | 1:A:404:ALA:HA   | 1.87                     | 0.55              |
| 3:C:167:GLY:HA3  | 3:C:174:PRO:CG   | 2.36                     | 0.55              |
| 4:D:207:LYS:O    | 4:D:211:MET:HG2  | 2.06                     | 0.55              |
| 5:E:100:HIS:CD2  | 5:E:131:GLU:HB2  | 2.42                     | 0.55              |
| 9:I:310:UNK:O    | 9:I:311:UNK:C    | 2.54                     | 0.55              |
| 3:C:261:ASN:HD21 | 3:C:264:VAL:HG23 | 1.71                     | 0.55              |
| 4:D:68:VAL:HG11  | 4:D:92:PRO:HG2   | 1.89                     | 0.55              |
| 1:A:39:VAL:HA    | 1:A:196:VAL:O    | 2.06                     | 0.55              |
| 1:A:108:LYS:O    | 1:A:112:LEU:HG   | 2.06                     | 0.55              |
| 2:B:126:VAL:O    | 2:B:130:PRO:HG3  | 2.06                     | 0.55              |
| 3:C:105:TYR:CD1  | 3:C:209:PRO:HA   | 2.41                     | 0.55              |
| 3:C:246:PHE:C    | 3:C:248:PRO:HD3  | 2.32                     | 0.55              |
| 5:E:98:VAL:HA    | 5:E:133:VAL:O    | 2.05                     | 0.55              |
| 2:B:76:THR:HG22  | 2:B:82:SER:N     | 2.07                     | 0.55              |
| 3:C:273:TRP:HA   | 3:C:276:LEU:HG   | 1.88                     | 0.55              |
| 3:C:293:LEU:HD22 | 3:C:293:LEU:H    | 1.72                     | 0.55              |
| 4:D:75:ASN:HB2   | 4:D:77:ASP:H     | 1.70                     | 0.55              |
| 4:D:213:GLY:O    | 4:D:217:PRO:CD   | 2.54                     | 0.55              |
| 4:D:215:LEU:O    | 4:D:219:VAL:HG22 | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:11:ARG:O     | 7:G:12:HIS:HB2   | 2.07                     | 0.55              |
| 1:A:291:SER:CB   | 1:A:356:ARG:HH22 | 2.17                     | 0.55              |
| 1:A:307:PHE:CD1  | 1:A:307:PHE:C    | 2.84                     | 0.55              |
| 2:B:248:ASN:HD22 | 2:B:249:GLY:N    | 2.05                     | 0.55              |
| 3:C:20:ILE:HG22  | 3:C:21:ASP:OD1   | 2.07                     | 0.55              |
| 3:C:342:GLN:NE2  | 3:C:343:PRO:HD2  | 2.16                     | 0.55              |
| 4:D:130:LEU:HD11 | 4:D:158:ILE:CD1  | 2.35                     | 0.55              |
| 6:F:12:TRP:HA    | 6:F:12:TRP:HE3   | 1.72                     | 0.55              |
| 6:F:91:GLU:O     | 6:F:95:LYS:HG3   | 2.07                     | 0.55              |
| 2:B:407:ASP:C    | 2:B:409:ASP:N    | 2.64                     | 0.55              |
| 3:C:27:ASN:HB2   | 6:F:69:ASN:HD22  | 1.71                     | 0.55              |
| 1:A:280:TYR:CG   | 1:A:281:ASP:N    | 2.75                     | 0.55              |
| 1:A:291:SER:O    | 1:A:292:SER:C    | 2.48                     | 0.55              |
| 3:C:3:PRO:HG2    | 3:C:4:ASN:H      | 1.71                     | 0.55              |
| 5:E:77:LYS:HA    | 5:E:191:ASP:O    | 2.07                     | 0.55              |
| 10:J:36:ASP:O    | 10:J:37:GLN:C    | 2.50                     | 0.55              |
| 1:A:26:ALA:O     | 1:A:198:ALA:HA   | 2.07                     | 0.54              |
| 1:A:346:CYS:HB3  | 1:A:411:CYS:CB   | 2.36                     | 0.54              |
| 3:C:293:LEU:H    | 3:C:293:LEU:CD2  | 2.21                     | 0.54              |
| 4:D:94:PRO:HB2   | 4:D:95:TYR:CD1   | 2.42                     | 0.54              |
| 10:J:13:LEU:HA   | 10:J:19:THR:CG2  | 2.37                     | 0.54              |
| 10:J:55:ILE:HG22 | 10:J:59:TYR:HE1  | 1.73                     | 0.54              |
| 1:A:290:SER:O    | 1:A:291:SER:C    | 2.49                     | 0.54              |
| 1:A:349:ILE:HD12 | 1:A:407:VAL:HG11 | 1.89                     | 0.54              |
| 2:B:143:GLN:O    | 2:B:144:LEU:C    | 2.49                     | 0.54              |
| 3:C:358:SER:O    | 3:C:362:ILE:HG13 | 2.06                     | 0.54              |
| 4:D:181:GLN:CB   | 8:H:77:LEU:HD22  | 2.37                     | 0.54              |
| 5:E:103:LYS:HA   | 5:E:106:ILE:HD12 | 1.89                     | 0.54              |
| 1:A:58:PHE:CE1   | 1:A:127:ILE:HG23 | 2.42                     | 0.54              |
| 1:A:85:HIS:O     | 1:A:99:ILE:HA    | 2.07                     | 0.54              |
| 1:A:266:ASP:C    | 1:A:268:VAL:H    | 2.15                     | 0.54              |
| 1:A:284:TYR:HE1  | 9:I:112:UNK:O    | 1.90                     | 0.54              |
| 1:A:374:PRO:O    | 1:A:377:GLU:HB3  | 2.07                     | 0.54              |
| 2:B:57:TYR:CE2   | 2:B:203:ARG:NH2  | 2.70                     | 0.54              |
| 5:E:189:SER:OG   | 5:E:192:MET:HB2  | 2.08                     | 0.54              |
| 3:C:166:TRP:HB2  | 3:C:175:THR:CG2  | 2.38                     | 0.54              |
| 3:C:289:LEU:O    | 3:C:293:LEU:HD23 | 2.07                     | 0.54              |
| 4:D:216:VAL:HG23 | 4:D:217:PRO:CD   | 2.37                     | 0.54              |
| 5:E:48:ALA:O     | 5:E:49:TYR:C     | 2.51                     | 0.54              |
| 2:B:414:ALA:O    | 2:B:417:PHE:HB3  | 2.08                     | 0.54              |
| 2:B:109:VAL:HG22 | 2:B:119:LEU:HD11 | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:62:LYS:O     | 4:D:66:GLU:HG2   | 2.07                     | 0.54              |
| 3:C:133:VAL:HA   | 3:C:140:SER:HB3  | 1.90                     | 0.54              |
| 5:E:52:LYS:C     | 5:E:52:LYS:HD3   | 2.33                     | 0.54              |
| 2:B:400:GLN:O    | 2:B:404:ALA:HB2  | 2.06                     | 0.54              |
| 4:D:165:TYR:CD2  | 4:D:168:VAL:HG22 | 2.43                     | 0.54              |
| 7:G:60:THR:O     | 7:G:61:TRP:C     | 2.50                     | 0.54              |
| 1:A:15:GLN:HB3   | 1:A:205:HIS:ND1  | 2.22                     | 0.54              |
| 1:A:394:GLU:O    | 1:A:395:TRP:C    | 2.51                     | 0.54              |
| 2:B:143:GLN:OE1  | 2:B:146:ILE:HD11 | 2.07                     | 0.54              |
| 3:C:105:TYR:CE1  | 3:C:209:PRO:HA   | 2.43                     | 0.54              |
| 3:C:151:PHE:HB2  | 3:C:162:VAL:HG22 | 1.89                     | 0.54              |
| 5:E:76:ILE:HB    | 5:E:193:VAL:CG1  | 2.38                     | 0.54              |
| 5:E:164:HIS:CB   | 5:E:173:LYS:HB3  | 2.34                     | 0.54              |
| 8:H:47:ARG:CD    | 8:H:48:SER:H     | 2.14                     | 0.54              |
| 2:B:56:ARG:HG3   | 2:B:56:ARG:NH1   | 2.23                     | 0.54              |
| 4:D:148:TYR:N    | 4:D:148:TYR:CD1  | 2.76                     | 0.54              |
| 5:E:147:ILE:HD12 | 5:E:159:PRO:HD3  | 1.90                     | 0.54              |
| 1:A:318:GLY:O    | 1:A:319:LEU:HD23 | 2.08                     | 0.53              |
| 2:B:129:ALA:N    | 2:B:130:PRO:CD   | 2.69                     | 0.53              |
| 3:C:34:PHE:CD1   | 3:C:37:LEU:HD12  | 2.42                     | 0.53              |
| 4:D:117:VAL:O    | 4:D:123:GLY:HA2  | 2.08                     | 0.53              |
| 6:F:59:MET:HA    | 6:F:59:MET:CE    | 2.34                     | 0.53              |
| 1:A:40:TRP:CD1   | 1:A:40:TRP:N     | 2.77                     | 0.53              |
| 2:B:59:ASN:C     | 2:B:61:SER:N     | 2.65                     | 0.53              |
| 10:J:13:LEU:HG   | 10:J:23:THR:HG21 | 1.90                     | 0.53              |
| 1:A:46:ARG:NH1   | 1:A:93:GLU:OE2   | 2.41                     | 0.53              |
| 1:A:350:SER:HG   | 1:A:353:GLU:HG3  | 1.74                     | 0.53              |
| 1:A:362:ARG:HH22 | 2:B:113:ARG:HH12 | 1.56                     | 0.53              |
| 3:C:127:THR:CG2  | 3:C:186:LEU:HB3  | 2.37                     | 0.53              |
| 2:B:213:HIS:N    | 2:B:214:PRO:HD2  | 2.24                     | 0.53              |
| 2:B:305:ASN:CB   | 2:B:306:PRO:HD2  | 2.38                     | 0.53              |
| 3:C:20:ILE:O     | 3:C:22:LEU:N     | 2.42                     | 0.53              |
| 4:D:134:TYR:CG   | 4:D:162:PRO:HG3  | 2.44                     | 0.53              |
| 6:F:71:ARG:O     | 6:F:73:GLN:HG2   | 2.09                     | 0.53              |
| 1:A:40:TRP:CZ3   | 1:A:377:GLU:CD   | 2.87                     | 0.53              |
| 1:A:250:LEU:HD21 | 1:A:325:VAL:HG13 | 1.91                     | 0.53              |
| 2:B:348:ALA:C    | 2:B:350:GLY:H    | 2.17                     | 0.53              |
| 3:C:19:LEU:C     | 3:C:20:ILE:HG13  | 2.33                     | 0.53              |
| 4:D:75:ASN:ND2   | 4:D:79:GLU:O     | 2.42                     | 0.53              |
| 4:D:75:ASN:H     | 4:D:79:GLU:H     | 1.57                     | 0.53              |
| 1:A:189:HIS:CD2  | 1:A:194:ARG:HH12 | 2.26                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:402:ILE:HD13 | 2:B:402:ILE:C     | 2.33                     | 0.53              |
| 5:E:177:PRO:O    | 5:E:178:LEU:HD23  | 2.09                     | 0.53              |
| 1:A:242:ARG:O    | 7:G:14:ILE:HA     | 2.09                     | 0.52              |
| 2:B:109:VAL:HG13 | 2:B:119:LEU:HD21  | 1.91                     | 0.52              |
| 2:B:353:SER:O    | 2:B:355:GLU:N     | 2.42                     | 0.52              |
| 2:B:424:MET:HE3  | 2:B:436:VAL:HG13  | 1.90                     | 0.52              |
| 4:D:32:VAL:HG21  | 4:D:186:VAL:HG22  | 1.91                     | 0.52              |
| 6:F:16:ILE:O     | 6:F:19:TRP:HB3    | 2.09                     | 0.52              |
| 6:F:91:GLU:HG2   | 6:F:95:LYS:HE3    | 1.89                     | 0.52              |
| 1:A:253:VAL:O    | 1:A:323:TYR:HD1   | 1.92                     | 0.52              |
| 2:B:361:LYS:NZ   | 2:B:403:ASP:HA    | 2.25                     | 0.52              |
| 3:C:342:GLN:HE21 | 3:C:342:GLN:HA    | 1.73                     | 0.52              |
| 1:A:88:ALA:CB    | 1:A:96:ALA:O      | 2.48                     | 0.52              |
| 3:C:103:LEU:HD13 | 3:C:103:LEU:C     | 2.34                     | 0.52              |
| 5:E:78:LEU:CD1   | 5:E:187:PHE:HE1   | 2.21                     | 0.52              |
| 8:H:47:ARG:HD3   | 8:H:48:SER:N      | 2.17                     | 0.52              |
| 1:A:114:ALA:HB2  | 1:A:216:PHE:CE1   | 2.45                     | 0.52              |
| 1:A:281:ASP:C    | 1:A:283:THR:H     | 2.17                     | 0.52              |
| 1:A:293:PRO:O    | 1:A:297:ILE:N     | 2.37                     | 0.52              |
| 2:B:40:ASN:O     | 2:B:41:TYR:HB2    | 2.09                     | 0.52              |
| 1:A:274:ASN:O    | 1:A:309:THR:HG21  | 2.09                     | 0.52              |
| 2:B:66:SER:O     | 2:B:69:LEU:HB3    | 2.09                     | 0.52              |
| 2:B:199:PHE:CA   | 2:B:204:MET:HE3   | 2.39                     | 0.52              |
| 2:B:248:ASN:C    | 2:B:248:ASN:ND2   | 2.67                     | 0.52              |
| 2:B:280:GLY:O    | 2:B:283:PRO:HG2   | 2.08                     | 0.52              |
| 3:C:157:ILE:O    | 3:C:161:LEU:HG    | 2.09                     | 0.52              |
| 3:C:206:SER:HB2  | 12:C:383:U10:H3M1 | 1.92                     | 0.52              |
| 1:A:286:GLY:HA3  | 1:A:289:HIS:NE2   | 2.24                     | 0.52              |
| 1:A:297:ILE:HG22 | 1:A:303:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:366:VAL:C    | 1:A:368:HIS:H     | 2.17                     | 0.52              |
| 2:B:202:ALA:HB2  | 2:B:229:GLY:HA2   | 1.92                     | 0.52              |
| 2:B:144:LEU:HB2  | 2:B:183:ILE:HD12  | 1.92                     | 0.52              |
| 10:J:58:LYS:HB2  | 10:J:59:TYR:CE1   | 2.44                     | 0.52              |
| 1:A:250:LEU:HB2  | 1:A:326:CYS:O     | 2.10                     | 0.52              |
| 2:B:258:VAL:CG1  | 2:B:259:ALA:N     | 2.71                     | 0.52              |
| 2:B:264:ILE:HG12 | 2:B:316:TYR:C     | 2.35                     | 0.52              |
| 3:C:261:ASN:ND2  | 3:C:264:VAL:HG23  | 2.25                     | 0.52              |
| 5:E:118:ARG:HB3  | 5:E:118:ARG:HH11  | 1.75                     | 0.52              |
| 2:B:63:LEU:HB2   | 2:B:182:ARG:CD    | 2.38                     | 0.52              |
| 1:A:171:SER:O    | 1:A:175:ARG:HG3   | 2.10                     | 0.52              |
| 1:A:431:LEU:HD23 | 1:A:432:PRO:HD2   | 1.91                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:ASP:C    | 1:A:268:VAL:N    | 2.66                     | 0.51              |
| 1:A:350:SER:OG   | 1:A:353:GLU:HG3  | 2.09                     | 0.51              |
| 3:C:164:TRP:CD1  | 3:C:165:ALA:N    | 2.78                     | 0.51              |
| 4:D:12:TRP:HB3   | 4:D:14:HIS:CE1   | 2.46                     | 0.51              |
| 7:G:77:TYR:CZ    | 8:H:52:GLU:HB2   | 2.45                     | 0.51              |
| 2:B:113:ARG:HG3  | 2:B:114:ASP:H    | 1.75                     | 0.51              |
| 2:B:150:VAL:HG23 | 2:B:151:ALA:N    | 2.24                     | 0.51              |
| 2:B:399:LEU:CA   | 2:B:402:ILE:HG22 | 2.40                     | 0.51              |
| 3:C:3:PRO:O      | 3:C:5:ILE:HG13   | 2.10                     | 0.51              |
| 4:D:149:PHE:CE1  | 4:D:156:GLN:HB3  | 2.46                     | 0.51              |
| 4:D:221:TYR:CD2  | 5:E:39:VAL:HG11  | 2.46                     | 0.51              |
| 4:D:231:LYS:HA   | 6:F:70:MET:HE1   | 1.91                     | 0.51              |
| 4:D:117:VAL:HG23 | 4:D:190:LEU:HB3  | 1.92                     | 0.51              |
| 6:F:16:ILE:O     | 6:F:19:TRP:N     | 2.43                     | 0.51              |
| 1:A:60:GLU:OE2   | 1:A:89:TYR:HA    | 2.11                     | 0.51              |
| 1:A:178:SER:O    | 1:A:182:LEU:HD23 | 2.11                     | 0.51              |
| 2:B:259:ALA:O    | 2:B:260:GLU:C    | 2.53                     | 0.51              |
| 1:A:102:LEU:C    | 1:A:104:LYS:N    | 2.67                     | 0.51              |
| 2:B:262:ALA:O    | 2:B:263:ALA:HB2  | 2.10                     | 0.51              |
| 3:C:233:LEU:O    | 3:C:237:LEU:HB2  | 2.10                     | 0.51              |
| 4:D:29:GLY:O     | 4:D:32:VAL:HG13  | 2.11                     | 0.51              |
| 5:E:86:ASN:ND2   | 5:E:156:TYR:HE2  | 2.09                     | 0.51              |
| 1:A:250:LEU:CD2  | 1:A:325:VAL:HG13 | 2.40                     | 0.51              |
| 1:A:438:ARG:C    | 1:A:440:GLY:H    | 2.19                     | 0.51              |
| 2:B:132:PHE:CD2  | 2:B:191:LEU:CB   | 2.94                     | 0.51              |
| 3:C:48:THR:O     | 3:C:52:LEU:HB2   | 2.11                     | 0.51              |
| 4:D:3:LEU:HD22   | 8:H:59:PHE:HE2   | 1.75                     | 0.51              |
| 4:D:5:LEU:HB2    | 8:H:59:PHE:CD1   | 2.46                     | 0.51              |
| 1:A:86:LEU:O     | 9:I:312:UNK:O    | 2.28                     | 0.51              |
| 1:A:382:GLU:HG2  | 1:A:389:ARG:HD2  | 1.91                     | 0.51              |
| 1:A:388:ARG:HG2  | 1:A:389:ARG:N    | 2.26                     | 0.51              |
| 4:D:37:CYS:O     | 4:D:39:SER:N     | 2.43                     | 0.51              |
| 4:D:57:THR:HB    | 4:D:60:GLU:HB2   | 1.93                     | 0.51              |
| 1:A:343:MET:O    | 1:A:347:THR:HG22 | 2.11                     | 0.51              |
| 1:A:444:LEU:O    | 1:A:445:ARG:O    | 2.28                     | 0.51              |
| 2:B:162:ASN:CB   | 2:B:244:ILE:HD11 | 2.34                     | 0.51              |
| 2:B:166:ALA:HB1  | 2:B:242:GLY:C    | 2.36                     | 0.51              |
| 3:C:328:LEU:CD1  | 7:G:51:PRO:HB3   | 2.41                     | 0.51              |
| 3:C:342:GLN:NE2  | 3:C:342:GLN:HA   | 2.26                     | 0.51              |
| 1:A:19:LEU:C     | 1:A:21:ASN:H     | 2.18                     | 0.51              |
| 1:A:321:GLY:HA2  | 1:A:342:TRP:HZ2  | 1.76                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:278:VAL:O    | 2:B:282:ASN:ND2  | 2.44                     | 0.51              |
| 3:C:372:THR:O    | 3:C:375:ASN:N    | 2.43                     | 0.51              |
| 3:C:373:LEU:HD23 | 3:C:373:LEU:C    | 2.36                     | 0.51              |
| 4:D:94:PRO:HB2   | 4:D:95:TYR:CE1   | 2.46                     | 0.51              |
| 5:E:78:LEU:HD21  | 5:E:193:VAL:HB   | 1.93                     | 0.51              |
| 5:E:166:ASP:OD1  | 5:E:168:SER:HB3  | 2.11                     | 0.51              |
| 1:A:100:LYS:HE3  | 2:B:370:MET:CE   | 2.41                     | 0.50              |
| 1:A:444:LEU:C    | 1:A:445:ARG:O    | 2.54                     | 0.50              |
| 2:B:245:ARG:HB3  | 2:B:430:LEU:HD13 | 1.93                     | 0.50              |
| 3:C:142:TRP:HA   | 3:C:145:THR:OG1  | 2.11                     | 0.50              |
| 3:C:146:VAL:HG23 | 3:C:147:ILE:H    | 1.76                     | 0.50              |
| 4:D:72:ASP:O     | 4:D:73:GLY:O     | 2.29                     | 0.50              |
| 10:J:4:THR:O     | 10:J:5:LEU:C     | 2.53                     | 0.50              |
| 1:A:42:ASP:CB    | 1:A:194:ARG:HB3  | 2.30                     | 0.50              |
| 1:A:134:ILE:CG2  | 1:A:174:ILE:HD13 | 2.41                     | 0.50              |
| 1:A:153:LEU:HD23 | 1:A:153:LEU:C    | 2.36                     | 0.50              |
| 1:A:252:HIS:HB2  | 1:A:425:PRO:HD2  | 1.93                     | 0.50              |
| 2:B:207:VAL:HG12 | 2:B:208:GLY:H    | 1.76                     | 0.50              |
| 3:C:281:ILE:HG22 | 3:C:281:ILE:O    | 2.10                     | 0.50              |
| 10:J:59:TYR:CD1  | 10:J:59:TYR:N    | 2.78                     | 0.50              |
| 1:A:351:GLU:HA   | 1:A:354:VAL:HG22 | 1.94                     | 0.50              |
| 3:C:95:ILE:HD13  | 3:C:121:LEU:HD13 | 1.93                     | 0.50              |
| 3:C:377:MET:HE2  | 6:F:20:TYR:CG    | 2.46                     | 0.50              |
| 5:E:117:LEU:HD12 | 5:E:121:GLN:H    | 1.74                     | 0.50              |
| 4:D:28:ARG:HD2   | 4:D:171:PHE:CE2  | 2.46                     | 0.50              |
| 4:D:181:GLN:HG2  | 8:H:77:LEU:HD22  | 1.93                     | 0.50              |
| 5:E:38:LEU:O     | 5:E:42:VAL:HG23  | 2.12                     | 0.50              |
| 1:A:4:TYR:HB2    | 2:B:113:ARG:CB   | 2.40                     | 0.50              |
| 1:A:106:VAL:HG21 | 1:A:203:VAL:CG1  | 2.40                     | 0.50              |
| 1:A:106:VAL:CG2  | 1:A:203:VAL:HG22 | 2.41                     | 0.50              |
| 2:B:109:VAL:HG13 | 2:B:109:VAL:O    | 2.11                     | 0.50              |
| 2:B:368:TYR:O    | 2:B:372:VAL:HG23 | 2.12                     | 0.50              |
| 4:D:227:TRP:O    | 4:D:228:SER:C    | 2.52                     | 0.50              |
| 5:E:99:ARG:HB3   | 5:E:133:VAL:HG12 | 1.93                     | 0.50              |
| 1:A:15:GLN:HB3   | 1:A:205:HIS:CE1  | 2.47                     | 0.50              |
| 1:A:49:SER:N     | 1:A:52:ASN:HB3   | 2.16                     | 0.50              |
| 1:A:253:VAL:HG11 | 1:A:335:MET:CE   | 2.41                     | 0.50              |
| 2:B:135:TRP:H    | 2:B:135:TRP:CD1  | 2.30                     | 0.50              |
| 5:E:12:ASP:N     | 5:E:20:TYR:HE2   | 2.10                     | 0.50              |
| 8:H:73:LEU:C     | 8:H:73:LEU:CD2   | 2.84                     | 0.50              |
| 1:A:245:GLU:C    | 1:A:247:GLY:H    | 2.18                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:232:LEU:HG   | 2:B:233:SER:N    | 2.23                     | 0.50              |
| 3:C:86:ASN:OD1   | 3:C:244:ALA:HA   | 2.12                     | 0.50              |
| 1:A:95:THR:HG22  | 1:A:96:ALA:N     | 2.27                     | 0.50              |
| 1:A:444:LEU:HD12 | 1:A:444:LEU:H    | 1.76                     | 0.50              |
| 2:B:62:ASN:O     | 2:B:65:THR:CG2   | 2.59                     | 0.50              |
| 5:E:9:ASN:HD21   | 5:E:11:SER:HB3   | 1.76                     | 0.50              |
| 5:E:14:ARG:HG2   | 5:E:14:ARG:NH1   | 2.17                     | 0.50              |
| 9:I:313:UNK:CB   | 9:I:314:UNK:CD   | 2.90                     | 0.50              |
| 2:B:131:GLU:O    | 2:B:131:GLU:HG3  | 2.11                     | 0.49              |
| 1:A:292:SER:N    | 1:A:293:PRO:CD   | 2.71                     | 0.49              |
| 4:D:37:CYS:C     | 4:D:39:SER:H     | 2.20                     | 0.49              |
| 5:E:136:ILE:HG22 | 5:E:138:VAL:HG23 | 1.92                     | 0.49              |
| 6:F:25:GLY:C     | 6:F:27:ASN:H     | 2.21                     | 0.49              |
| 7:G:24:ARG:HB2   | 7:G:27:PRO:HB3   | 1.94                     | 0.49              |
| 10:J:57:HIS:HB2  | 10:J:62:LYS:CB   | 2.42                     | 0.49              |
| 1:A:106:VAL:HB   | 1:A:107:PRO:CD   | 2.42                     | 0.49              |
| 1:A:339:GLN:OE1  | 1:A:437:ILE:O    | 2.30                     | 0.49              |
| 3:C:9:HIS:HD2    | 3:C:10:PRO:CD    | 2.23                     | 0.49              |
| 4:D:43:MET:CE    | 4:D:46:VAL:HG21  | 2.37                     | 0.49              |
| 4:D:150:ASN:O    | 4:D:156:GLN:HA   | 2.13                     | 0.49              |
| 1:A:391:PRO:O    | 1:A:392:LEU:C    | 2.53                     | 0.49              |
| 3:C:342:GLN:HE21 | 3:C:343:PRO:CD   | 2.18                     | 0.49              |
| 1:A:349:ILE:HG22 | 1:A:408:ARG:HG3  | 1.93                     | 0.49              |
| 1:A:395:TRP:HA   | 1:A:395:TRP:HE3  | 1.75                     | 0.49              |
| 4:D:27:ARG:CZ    | 10:J:59:TYR:CE2  | 2.95                     | 0.49              |
| 4:D:180:SER:HB2  | 8:H:17:LEU:HB2   | 1.94                     | 0.49              |
| 5:E:135:LEU:HD13 | 5:E:180:LEU:HD12 | 1.95                     | 0.49              |
| 5:E:147:ILE:HD11 | 5:E:159:PRO:HG3  | 1.94                     | 0.49              |
| 8:H:73:LEU:C     | 8:H:73:LEU:HD23  | 2.38                     | 0.49              |
| 3:C:369:THR:C    | 3:C:371:GLY:N    | 2.67                     | 0.49              |
| 5:E:29:ASP:OD1   | 5:E:32:ARG:HB2   | 2.13                     | 0.49              |
| 5:E:60:SER:C     | 5:E:62:MET:N     | 2.61                     | 0.49              |
| 5:E:109:GLU:CD   | 5:E:166:ASP:HB2  | 2.38                     | 0.49              |
| 1:A:106:VAL:N    | 1:A:107:PRO:HD2  | 2.27                     | 0.49              |
| 1:A:338:LEU:O    | 1:A:341:GLN:N    | 2.45                     | 0.49              |
| 2:B:170:ASN:H    | 2:B:170:ASN:HD22 | 1.60                     | 0.49              |
| 3:C:112:GLU:CD   | 3:C:112:GLU:H    | 2.13                     | 0.49              |
| 3:C:227:PHE:HE1  | 4:D:222:MET:HE2  | 1.77                     | 0.49              |
| 3:C:318:PHE:CG   | 6:F:26:PHE:HB3   | 2.48                     | 0.49              |
| 3:C:377:MET:CE   | 6:F:20:TYR:HB2   | 2.43                     | 0.49              |
| 1:A:48:GLU:CD    | 1:A:54:GLY:H     | 2.20                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:ASP:O    | 1:A:106:VAL:C    | 2.55                     | 0.49              |
| 2:B:56:ARG:O     | 2:B:56:ARG:HD3   | 2.13                     | 0.49              |
| 2:B:372:VAL:O    | 2:B:378:PHE:HB2  | 2.13                     | 0.49              |
| 3:C:141:PHE:HE1  | 3:C:171:VAL:O    | 1.96                     | 0.49              |
| 3:C:147:ILE:HD11 | 3:C:271:PRO:HB3  | 1.94                     | 0.49              |
| 8:H:49:GLN:O     | 8:H:49:GLN:HG2   | 2.11                     | 0.49              |
| 2:B:24:LEU:HD23  | 2:B:24:LEU:N     | 2.27                     | 0.49              |
| 2:B:72:ALA:HB1   | 2:B:75:LEU:HD12  | 1.95                     | 0.49              |
| 3:C:120:LEU:CD1  | 3:C:190:ILE:HG23 | 2.43                     | 0.49              |
| 5:E:42:VAL:O     | 5:E:45:LEU:HB3   | 2.13                     | 0.49              |
| 5:E:136:ILE:HG13 | 5:E:181:GLU:CG   | 2.41                     | 0.49              |
| 6:F:42:ASP:OD2   | 6:F:101:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:74:ALA:O     | 1:A:75:LEU:C     | 2.55                     | 0.48              |
| 1:A:240:GLN:OE1  | 1:A:434:TYR:HB2  | 2.13                     | 0.48              |
| 1:A:320:PHE:CE2  | 1:A:415:ILE:HD11 | 2.48                     | 0.48              |
| 2:B:58:GLU:OE2   | 2:B:65:THR:HG22  | 2.13                     | 0.48              |
| 3:C:130:VAL:HG13 | 3:C:179:PHE:CG   | 2.48                     | 0.48              |
| 4:D:97:ASN:O     | 4:D:100:ALA:HB3  | 2.12                     | 0.48              |
| 5:E:15:ARG:NH1   | 5:E:19:ASP:HB3   | 2.28                     | 0.48              |
| 7:G:73:ASN:O     | 7:G:75:ALA:N     | 2.46                     | 0.48              |
| 2:B:61:SER:O     | 2:B:62:ASN:OD1   | 2.31                     | 0.48              |
| 3:C:125:MET:O    | 3:C:126:ALA:C    | 2.57                     | 0.48              |
| 3:C:130:VAL:HG13 | 3:C:179:PHE:CB   | 2.42                     | 0.48              |
| 3:C:283:ARG:NH2  | 3:C:339:ILE:O    | 2.46                     | 0.48              |
| 4:D:181:GLN:C    | 4:D:181:GLN:NE2  | 2.71                     | 0.48              |
| 1:A:288:LEU:HD22 | 2:B:83:PHE:CD1   | 2.45                     | 0.48              |
| 1:A:305:GLN:O    | 1:A:306:SER:HB3  | 2.13                     | 0.48              |
| 2:B:187:THR:OG1  | 2:B:190:GLU:HG3  | 2.13                     | 0.48              |
| 2:B:429:ASN:O    | 2:B:430:LEU:HB2  | 2.13                     | 0.48              |
| 4:D:21:LEU:CD1   | 4:D:26:ILE:HD11  | 2.42                     | 0.48              |
| 5:E:19:ASP:C     | 5:E:20:TYR:CD1   | 2.91                     | 0.48              |
| 8:H:37:LEU:HD13  | 8:H:37:LEU:C     | 2.37                     | 0.48              |
| 2:B:89:ILE:CD1   | 2:B:96:LEU:HB2   | 2.44                     | 0.48              |
| 3:C:220:PRO:HG2  | 3:C:223:PRO:CG   | 2.43                     | 0.48              |
| 3:C:327:TRP:CE2  | 7:G:48:VAL:HG22  | 2.48                     | 0.48              |
| 3:C:333:LEU:HD11 | 3:C:359:TYR:CE1  | 2.48                     | 0.48              |
| 7:G:29:TYR:CD1   | 7:G:29:TYR:N     | 2.80                     | 0.48              |
| 1:A:19:LEU:C     | 1:A:21:ASN:N     | 2.69                     | 0.48              |
| 1:A:40:TRP:HZ3   | 1:A:377:GLU:CD   | 2.21                     | 0.48              |
| 1:A:431:LEU:HD23 | 1:A:432:PRO:CD   | 2.43                     | 0.48              |
| 2:B:399:LEU:O    | 2:B:402:ILE:HG22 | 2.13                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:110:TYR:CB   | 3:C:113:THR:HG23  | 2.44                     | 0.48              |
| 3:C:344:VAL:HG23 | 3:C:344:VAL:O     | 2.12                     | 0.48              |
| 4:D:229:VAL:HG23 | 7:G:20:PRO:HG3    | 1.95                     | 0.48              |
| 5:E:21:SER:O     | 5:E:22:THR:OG1    | 2.23                     | 0.48              |
| 5:E:35:PHE:O     | 5:E:38:LEU:HB3    | 2.13                     | 0.48              |
| 6:F:13:LEU:N     | 6:F:13:LEU:HD12   | 2.28                     | 0.48              |
| 8:H:62:LEU:O     | 8:H:66:ASP:OD1    | 2.32                     | 0.48              |
| 1:A:391:PRO:O    | 1:A:394:GLU:N     | 2.40                     | 0.48              |
| 2:B:72:ALA:O     | 2:B:73:SER:C      | 2.56                     | 0.48              |
| 3:C:312:LYS:HG2  | 3:C:375:ASN:OD1   | 2.13                     | 0.48              |
| 4:D:153:PHE:CG   | 4:D:158:ILE:HG12  | 2.49                     | 0.48              |
| 4:D:211:MET:CG   | 14:D:242:BOG:H5'1 | 2.42                     | 0.48              |
| 5:E:11:SER:CA    | 5:E:15:ARG:HD2    | 2.40                     | 0.48              |
| 1:A:288:LEU:HD13 | 2:B:83:PHE:HA     | 1.96                     | 0.48              |
| 1:A:366:VAL:C    | 1:A:368:HIS:N     | 2.71                     | 0.48              |
| 1:A:408:ARG:O    | 1:A:409:GLU:C     | 2.56                     | 0.48              |
| 2:B:75:LEU:HD22  | 2:B:136:GLU:HB3   | 1.96                     | 0.48              |
| 2:B:112:LEU:O    | 2:B:113:ARG:C     | 2.57                     | 0.48              |
| 3:C:329:LEU:O    | 3:C:330:VAL:C     | 2.57                     | 0.48              |
| 2:B:232:LEU:CG   | 2:B:233:SER:H     | 2.20                     | 0.48              |
| 2:B:63:LEU:C     | 2:B:65:THR:H      | 2.22                     | 0.48              |
| 3:C:27:ASN:ND2   | 3:C:209:PRO:HG2   | 2.29                     | 0.48              |
| 4:D:68:VAL:HG11  | 4:D:92:PRO:CG     | 2.44                     | 0.48              |
| 4:D:220:TYR:O    | 4:D:224:ARG:HG2   | 2.13                     | 0.48              |
| 5:E:86:ASN:HD22  | 5:E:148:ALA:CB    | 2.24                     | 0.48              |
| 1:A:65:LYS:HZ3   | 9:I:311:UNK:HA    | 1.78                     | 0.48              |
| 2:B:39:GLU:HG3   | 2:B:41:TYR:CD1    | 2.48                     | 0.48              |
| 2:B:141:GLN:N    | 2:B:142:PRO:HD2   | 2.29                     | 0.48              |
| 2:B:360:ALA:O    | 2:B:361:LYS:C     | 2.57                     | 0.48              |
| 3:C:280:ALA:C    | 3:C:282:LEU:N     | 2.71                     | 0.48              |
| 4:D:29:GLY:O     | 4:D:30:PHE:C      | 2.57                     | 0.48              |
| 8:H:50:THR:CG2   | 8:H:52:GLU:H      | 2.23                     | 0.48              |
| 1:A:59:LEU:HD12  | 1:A:59:LEU:O      | 2.14                     | 0.47              |
| 1:A:444:LEU:HD12 | 1:A:444:LEU:N     | 2.29                     | 0.47              |
| 2:B:430:LEU:O    | 2:B:433:THR:N     | 2.36                     | 0.47              |
| 4:D:220:TYR:CZ   | 4:D:224:ARG:HD3   | 2.49                     | 0.47              |
| 5:E:29:ASP:N     | 5:E:30:PRO:HD2    | 2.28                     | 0.47              |
| 7:G:38:TRP:C     | 7:G:40:ARG:N      | 2.69                     | 0.47              |
| 1:A:146:ARG:HG3  | 1:A:323:TYR:OH    | 2.15                     | 0.47              |
| 2:B:166:ALA:HB1  | 2:B:242:GLY:CA    | 2.44                     | 0.47              |
| 2:B:214:PRO:HG2  | 2:B:215:VAL:H     | 1.79                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:337:ILE:HD12 | 2:B:434:PRO:HD2  | 1.94                     | 0.47              |
| 3:C:285:ILE:HG23 | 3:C:291:GLY:HA2  | 1.97                     | 0.47              |
| 4:D:141:VAL:HG21 | 8:H:55:THR:HG23  | 1.95                     | 0.47              |
| 4:D:222:MET:CE   | 5:E:40:THR:HG23  | 2.45                     | 0.47              |
| 8:H:20:VAL:HG12  | 8:H:20:VAL:O     | 2.13                     | 0.47              |
| 1:A:373:THR:N    | 1:A:374:PRO:HD2  | 2.29                     | 0.47              |
| 2:B:114:ASP:C    | 2:B:116:VAL:H    | 2.22                     | 0.47              |
| 8:H:72:LYS:O     | 8:H:73:LEU:C     | 2.56                     | 0.47              |
| 1:A:254:ALA:O    | 1:A:422:VAL:HA   | 2.14                     | 0.47              |
| 1:A:292:SER:O    | 1:A:295:ALA:N    | 2.44                     | 0.47              |
| 1:A:349:ILE:CD1  | 1:A:407:VAL:HG11 | 2.44                     | 0.47              |
| 1:A:397:GLU:O    | 1:A:398:ARG:C    | 2.57                     | 0.47              |
| 2:B:133:ARG:HD3  | 2:B:135:TRP:CZ2  | 2.49                     | 0.47              |
| 2:B:395:PRO:CA   | 2:B:398:VAL:HG12 | 2.44                     | 0.47              |
| 3:C:108:TYR:HB3  | 3:C:114:TRP:CE3  | 2.48                     | 0.47              |
| 3:C:118:VAL:HB   | 3:C:303:PHE:CE1  | 2.49                     | 0.47              |
| 8:H:59:PHE:O     | 8:H:60:ASP:C     | 2.57                     | 0.47              |
| 1:A:65:LYS:NZ    | 9:I:311:UNK:N    | 2.63                     | 0.47              |
| 2:B:31:ASN:HB3   | 2:B:201:SER:CB   | 2.43                     | 0.47              |
| 3:C:138:GLN:OE1  | 3:C:138:GLN:HA   | 2.15                     | 0.47              |
| 3:C:148:THR:HG21 | 3:C:166:TRP:CE3  | 2.50                     | 0.47              |
| 3:C:326:PHE:O    | 3:C:329:LEU:HB3  | 2.15                     | 0.47              |
| 7:G:57:LEU:HD22  | 7:G:57:LEU:H     | 1.79                     | 0.47              |
| 1:A:418:GLN:O    | 1:A:420:PRO:HD3  | 2.14                     | 0.47              |
| 2:B:75:LEU:HD11  | 2:B:140:LEU:HD22 | 1.96                     | 0.47              |
| 2:B:258:VAL:HG11 | 2:B:321:LEU:CB   | 2.37                     | 0.47              |
| 3:C:325:LEU:CD2  | 3:C:362:ILE:HG23 | 2.42                     | 0.47              |
| 3:C:342:GLN:HE21 | 3:C:342:GLN:CA   | 2.27                     | 0.47              |
| 4:D:204:MET:HE2  | 14:D:242:BOG:H1  | 1.96                     | 0.47              |
| 5:E:123:ASP:HA   | 5:E:126:ARG:HD3  | 1.97                     | 0.47              |
| 2:B:24:LEU:HD11  | 2:B:392:TYR:CG   | 2.50                     | 0.47              |
| 2:B:170:ASN:H    | 2:B:170:ASN:ND2  | 2.13                     | 0.47              |
| 2:B:361:LYS:O    | 2:B:365:LYS:HG3  | 2.14                     | 0.47              |
| 3:C:78:TRP:CG    | 4:D:197:GLU:HG2  | 2.50                     | 0.47              |
| 3:C:292:VAL:O    | 3:C:295:LEU:HB3  | 2.15                     | 0.47              |
| 3:C:342:GLN:HB3  | 3:C:343:PRO:HD2  | 1.97                     | 0.47              |
| 5:E:14:ARG:NH1   | 5:E:14:ARG:CG    | 2.74                     | 0.47              |
| 5:E:124:LEU:HA   | 5:E:127:VAL:HG22 | 1.96                     | 0.47              |
| 5:E:170:ARG:HA   | 5:E:179:ASN:HB3  | 1.97                     | 0.47              |
| 7:G:41:LEU:O     | 7:G:41:LEU:HD13  | 2.15                     | 0.47              |
| 1:A:149:VAL:HG13 | 1:A:150:PHE:N    | 2.30                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:PHE:O    | 1:A:164:ALA:HB2  | 2.15                     | 0.47              |
| 1:A:178:SER:C    | 1:A:180:ALA:N    | 2.68                     | 0.47              |
| 4:D:102:ARG:HG2  | 4:D:109:LEU:HB2  | 1.96                     | 0.47              |
| 4:D:165:TYR:O    | 4:D:168:VAL:CG2  | 2.63                     | 0.47              |
| 2:B:252:LEU:HD23 | 2:B:252:LEU:N    | 2.29                     | 0.47              |
| 2:B:317:SER:OG   | 2:B:318:ASP:N    | 2.47                     | 0.47              |
| 3:C:51:LEU:HG    | 3:C:80:ILE:HD13  | 1.97                     | 0.47              |
| 3:C:278:ALA:HB1  | 3:C:295:LEU:HD12 | 1.96                     | 0.47              |
| 4:D:3:LEU:HD22   | 8:H:59:PHE:CE2   | 2.49                     | 0.47              |
| 6:F:82:LYS:O     | 6:F:83:TYR:C     | 2.57                     | 0.47              |
| 10:J:5:LEU:O     | 10:J:6:THR:C     | 2.57                     | 0.47              |
| 1:A:240:GLN:NE2  | 1:A:242:ARG:HE   | 2.13                     | 0.47              |
| 2:B:281:ALA:O    | 2:B:285:VAL:HB   | 2.15                     | 0.47              |
| 3:C:103:LEU:HD12 | 3:C:326:PHE:CE1  | 2.50                     | 0.47              |
| 4:D:75:ASN:CB    | 4:D:77:ASP:H     | 2.27                     | 0.47              |
| 7:G:25:PRO:C     | 7:G:27:PRO:HD3   | 2.40                     | 0.47              |
| 1:A:40:TRP:HZ3   | 1:A:377:GLU:OE2  | 1.97                     | 0.46              |
| 2:B:323:GLY:O    | 2:B:324:PHE:HB3  | 2.15                     | 0.46              |
| 2:B:338:LYS:O    | 2:B:341:TYR:HB3  | 2.16                     | 0.46              |
| 5:E:10:PHE:CD1   | 7:G:18:LEU:HD21  | 2.51                     | 0.46              |
| 5:E:16:PRO:O     | 5:E:18:ASP:N     | 2.47                     | 0.46              |
| 6:F:60:PHE:CD1   | 7:G:13:LEU:HD22  | 2.49                     | 0.46              |
| 1:A:382:GLU:HA   | 1:A:386:TYR:HD2  | 1.79                     | 0.46              |
| 2:B:68:LEU:HD23  | 2:B:186:VAL:HG11 | 1.96                     | 0.46              |
| 4:D:28:ARG:O     | 4:D:29:GLY:C     | 2.58                     | 0.46              |
| 4:D:197:GLU:O    | 4:D:198:HIS:C    | 2.58                     | 0.46              |
| 5:E:17:PRO:HD3   | 7:G:24:ARG:HH21  | 1.80                     | 0.46              |
| 1:A:144:SER:O    | 1:A:146:ARG:N    | 2.48                     | 0.46              |
| 2:B:70:ARG:HD3   | 2:B:100:SER:CB   | 2.45                     | 0.46              |
| 2:B:146:ILE:O    | 2:B:147:ASP:C    | 2.57                     | 0.46              |
| 3:C:38:LEU:HD11  | 3:C:95:ILE:HA    | 1.97                     | 0.46              |
| 3:C:330:VAL:HG23 | 3:C:331:ALA:N    | 2.30                     | 0.46              |
| 4:D:54:VAL:HG11  | 4:D:192:TRP:CH2  | 2.50                     | 0.46              |
| 4:D:178:THR:O    | 4:D:179:MET:C    | 2.57                     | 0.46              |
| 6:F:52:GLU:O     | 6:F:53:ASN:C     | 2.58                     | 0.46              |
| 1:A:27:SER:HA    | 1:A:199:ALA:O    | 2.15                     | 0.46              |
| 2:B:84:LYS:O     | 2:B:88:GLY:N     | 2.48                     | 0.46              |
| 4:D:221:TYR:CE1  | 7:G:25:PRO:HG2   | 2.51                     | 0.46              |
| 5:E:99:ARG:HB3   | 5:E:133:VAL:HG11 | 1.96                     | 0.46              |
| 5:E:129:LYS:HA   | 5:E:130:PRO:HD3  | 1.73                     | 0.46              |
| 5:E:163:SER:OG   | 5:E:176:ALA:HB2  | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:48:GLU:OE1   | 1:A:53:ASN:ND2   | 2.49                     | 0.46              |
| 2:B:57:TYR:N     | 2:B:57:TYR:CD1   | 2.84                     | 0.46              |
| 2:B:379:LEU:O    | 2:B:382:VAL:HG22 | 2.16                     | 0.46              |
| 3:C:346:HIS:ND1  | 3:C:346:HIS:C    | 2.72                     | 0.46              |
| 5:E:86:ASN:HB2   | 5:E:99:ARG:HE    | 1.80                     | 0.46              |
| 2:B:71:LEU:CD1   | 2:B:144:LEU:HD23 | 2.45                     | 0.46              |
| 2:B:102:ARG:NE   | 2:B:164:HIS:CD2  | 2.84                     | 0.46              |
| 2:B:170:ASN:HD22 | 2:B:170:ASN:C    | 2.24                     | 0.46              |
| 2:B:433:THR:HG23 | 2:B:434:PRO:HD2  | 1.98                     | 0.46              |
| 3:C:150:LEU:O    | 3:C:151:PHE:C    | 2.59                     | 0.46              |
| 1:A:72:GLN:O     | 1:A:73:ASN:C     | 2.59                     | 0.46              |
| 1:A:268:VAL:CG1  | 1:A:399:LEU:HB3  | 2.45                     | 0.46              |
| 1:A:362:ARG:NH2  | 2:B:113:ARG:NH1  | 2.63                     | 0.46              |
| 2:B:258:VAL:HG12 | 2:B:259:ALA:H    | 1.80                     | 0.46              |
| 2:B:258:VAL:HG13 | 2:B:322:PHE:N    | 2.30                     | 0.46              |
| 2:B:405:VAL:CG1  | 2:B:406:ALA:H    | 2.26                     | 0.46              |
| 5:E:163:SER:HA   | 5:E:174:GLY:HA3  | 1.97                     | 0.46              |
| 6:F:62:ILE:O     | 6:F:66:LEU:HG    | 2.15                     | 0.46              |
| 8:H:73:LEU:HD23  | 8:H:73:LEU:O     | 2.16                     | 0.46              |
| 3:C:350:ILE:HD13 | 3:C:350:ILE:N    | 2.31                     | 0.46              |
| 1:A:24:ARG:HG3   | 1:A:24:ARG:HH11  | 1.81                     | 0.46              |
| 1:A:156:THR:HG23 | 1:A:157:ALA:N    | 2.30                     | 0.46              |
| 1:A:410:VAL:O    | 1:A:411:CYS:C    | 2.59                     | 0.46              |
| 2:B:282:ASN:HB2  | 2:B:283:PRO:CD   | 2.46                     | 0.46              |
| 5:E:141:HIS:HA   | 5:E:177:PRO:HD2  | 1.97                     | 0.46              |
| 1:A:48:GLU:OE2   | 1:A:54:GLY:N     | 2.44                     | 0.46              |
| 2:B:59:ASN:C     | 2:B:61:SER:H     | 2.22                     | 0.46              |
| 3:C:280:ALA:C    | 3:C:282:LEU:H    | 2.24                     | 0.46              |
| 3:C:301:ILE:HD11 | 3:C:364:LEU:CD1  | 2.45                     | 0.46              |
| 3:C:348:PHE:O    | 3:C:349:ILE:C    | 2.59                     | 0.46              |
| 3:C:377:MET:HE2  | 6:F:20:TYR:CD1   | 2.51                     | 0.46              |
| 4:D:91:PHE:HA    | 4:D:92:PRO:HD3   | 1.84                     | 0.46              |
| 4:D:124:GLU:O    | 4:D:125:ASP:C    | 2.59                     | 0.46              |
| 4:D:132:THR:HG21 | 4:D:180:SER:HA   | 1.97                     | 0.46              |
| 5:E:123:ASP:H    | 5:E:170:ARG:NH1  | 2.14                     | 0.46              |
| 8:H:59:PHE:O     | 8:H:62:LEU:N     | 2.49                     | 0.46              |
| 2:B:168:TYR:CE2  | 2:B:172:LEU:HD23 | 2.50                     | 0.45              |
| 2:B:258:VAL:HG11 | 2:B:321:LEU:HD22 | 1.98                     | 0.45              |
| 2:B:397:THR:HA   | 2:B:400:GLN:CB   | 2.46                     | 0.45              |
| 4:D:98:PRO:O     | 4:D:101:ALA:N    | 2.48                     | 0.45              |
| 5:E:17:PRO:HG3   | 7:G:24:ARG:HH21  | 1.81                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:36:THR:CG2   | 1:A:100:LYS:HB3  | 2.38                     | 0.45              |
| 1:A:65:LYS:HD2   | 1:A:65:LYS:N     | 2.30                     | 0.45              |
| 2:B:137:VAL:CG2  | 2:B:138:ALA:N    | 2.78                     | 0.45              |
| 3:C:359:TYR:HD2  | 3:C:360:PHE:CD1  | 2.35                     | 0.45              |
| 4:D:75:ASN:OD1   | 4:D:79:GLU:HB2   | 2.16                     | 0.45              |
| 5:E:52:LYS:O     | 5:E:56:THR:HG23  | 2.17                     | 0.45              |
| 1:A:430:GLN:O    | 1:A:430:GLN:HG2  | 2.15                     | 0.45              |
| 2:B:258:VAL:CG1  | 2:B:259:ALA:H    | 2.30                     | 0.45              |
| 3:C:164:TRP:O    | 3:C:165:ALA:C    | 2.60                     | 0.45              |
| 3:C:366:LEU:O    | 3:C:367:PHE:C    | 2.60                     | 0.45              |
| 4:D:43:MET:HE3   | 4:D:46:VAL:CG2   | 2.40                     | 0.45              |
| 4:D:231:LYS:HD3  | 6:F:70:MET:HE1   | 1.97                     | 0.45              |
| 1:A:116:ILE:C    | 1:A:118:GLN:H    | 2.25                     | 0.45              |
| 1:A:192:ALA:N    | 1:A:193:PRO:HD2  | 2.31                     | 0.45              |
| 1:A:249:PRO:HG2  | 1:A:250:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:298:ALA:HA   | 1:A:303:LEU:HB2  | 1.98                     | 0.45              |
| 2:B:130:PRO:HB3  | 2:B:132:PHE:CE1  | 2.51                     | 0.45              |
| 2:B:361:LYS:HZ1  | 2:B:403:ASP:HA   | 1.79                     | 0.45              |
| 3:C:137:GLY:H    | 3:C:140:SER:HB2  | 1.81                     | 0.45              |
| 3:C:327:TRP:HZ2  | 13:C:384:PEE:H7  | 1.81                     | 0.45              |
| 5:E:12:ASP:N     | 5:E:20:TYR:CE2   | 2.84                     | 0.45              |
| 5:E:78:LEU:HD11  | 5:E:187:PHE:HE1  | 1.80                     | 0.45              |
| 1:A:261:GLY:O    | 1:A:262:TRP:C    | 2.60                     | 0.45              |
| 1:A:405:ARG:CA   | 1:A:408:ARG:HH21 | 2.30                     | 0.45              |
| 2:B:171:ALA:C    | 2:B:173:ALA:N    | 2.75                     | 0.45              |
| 3:C:20:ILE:C     | 3:C:22:LEU:N     | 2.74                     | 0.45              |
| 3:C:210:LEU:O    | 3:C:212:ILE:HG23 | 2.16                     | 0.45              |
| 3:C:287:ASN:O    | 3:C:288:LYS:C    | 2.58                     | 0.45              |
| 4:D:164:ILE:O    | 4:D:179:MET:HG3  | 2.17                     | 0.45              |
| 3:C:40:VAL:HG21  | 3:C:233:LEU:HD21 | 1.98                     | 0.45              |
| 4:D:28:ARG:O     | 4:D:31:GLN:HB2   | 2.17                     | 0.45              |
| 5:E:11:SER:C     | 5:E:13:TYR:N     | 2.75                     | 0.45              |
| 7:G:36:ASN:HA    | 7:G:39:ARG:HB2   | 1.99                     | 0.45              |
| 1:A:178:SER:O    | 1:A:179:ARG:C    | 2.58                     | 0.45              |
| 1:A:250:LEU:C    | 1:A:250:LEU:CD2  | 2.90                     | 0.45              |
| 1:A:306:SER:HB2  | 9:I:206:UNK:CB   | 2.47                     | 0.45              |
| 1:A:365:LEU:HD22 | 1:A:365:LEU:O    | 2.17                     | 0.45              |
| 3:C:27:ASN:CB    | 6:F:69:ASN:HD22  | 2.29                     | 0.45              |
| 4:D:1:SER:C      | 4:D:3:LEU:H      | 2.24                     | 0.45              |
| 7:G:38:TRP:C     | 7:G:40:ARG:H     | 2.23                     | 0.45              |
| 4:D:118:ARG:HD3  | 4:D:191:ARG:HH12 | 1.82                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:181:GLN:CG   | 8:H:77:LEU:HD22  | 2.47                     | 0.45              |
| 5:E:78:LEU:HD11  | 5:E:187:PHE:CE1  | 2.52                     | 0.45              |
| 5:E:91:TRP:CE2   | 5:E:92:ARG:HG3   | 2.51                     | 0.45              |
| 5:E:121:GLN:OE1  | 5:E:126:ARG:NH1  | 2.44                     | 0.45              |
| 1:A:36:THR:HG23  | 1:A:372:THR:OG1  | 2.17                     | 0.45              |
| 1:A:92:ARG:HH12  | 1:A:166:SER:HA   | 1.81                     | 0.45              |
| 1:A:170:PRO:HG2  | 1:A:173:ASN:HB2  | 1.97                     | 0.45              |
| 3:C:59:ASP:O     | 3:C:60:THR:C     | 2.60                     | 0.45              |
| 3:C:295:LEU:O    | 3:C:298:SER:OG   | 2.32                     | 0.45              |
| 10:J:33:ARG:O    | 10:J:37:GLN:HG3  | 2.17                     | 0.45              |
| 1:A:62:LEU:CD1   | 1:A:127:ILE:HG12 | 2.45                     | 0.45              |
| 1:A:239:SER:O    | 1:A:421:ALA:HA   | 2.16                     | 0.45              |
| 1:A:245:GLU:C    | 1:A:247:GLY:N    | 2.73                     | 0.45              |
| 1:A:396:GLU:O    | 1:A:400:ALA:N    | 2.50                     | 0.45              |
| 2:B:137:VAL:HG23 | 2:B:138:ALA:N    | 2.30                     | 0.45              |
| 3:C:261:ASN:ND2  | 3:C:264:VAL:CG2  | 2.80                     | 0.45              |
| 4:D:81:PHE:CD1   | 4:D:81:PHE:C     | 2.95                     | 0.45              |
| 4:D:231:LYS:HD3  | 6:F:70:MET:CE    | 2.47                     | 0.45              |
| 5:E:9:ASN:OD1    | 5:E:11:SER:HB2   | 2.17                     | 0.45              |
| 5:E:182:VAL:HA   | 5:E:183:PRO:HD2  | 1.83                     | 0.45              |
| 6:F:34:ASP:OD2   | 6:F:90:LEU:HB3   | 2.17                     | 0.45              |
| 1:A:281:ASP:C    | 1:A:283:THR:N    | 2.75                     | 0.44              |
| 2:B:232:LEU:O    | 2:B:233:SER:HB3  | 2.16                     | 0.44              |
| 3:C:27:ASN:CB    | 6:F:69:ASN:ND2   | 2.77                     | 0.44              |
| 3:C:319:ARG:NH1  | 3:C:374:GLU:HB3  | 2.32                     | 0.44              |
| 4:D:116:ILE:CG2  | 4:D:190:LEU:HD13 | 2.47                     | 0.44              |
| 4:D:223:LYS:HD2  | 4:D:227:TRP:CD1  | 2.52                     | 0.44              |
| 5:E:69:LEU:O     | 5:E:72:SER:HB3   | 2.17                     | 0.44              |
| 1:A:410:VAL:O    | 1:A:413:LYS:N    | 2.49                     | 0.44              |
| 2:B:65:THR:O     | 2:B:69:LEU:HB2   | 2.17                     | 0.44              |
| 2:B:70:ARG:NE    | 9:I:107:UNK:CB   | 2.80                     | 0.44              |
| 2:B:399:LEU:HA   | 2:B:402:ILE:CG2  | 2.43                     | 0.44              |
| 3:C:145:THR:O    | 3:C:149:ASN:HB2  | 2.18                     | 0.44              |
| 3:C:361:THR:HA   | 3:C:365:ILE:HG22 | 2.00                     | 0.44              |
| 4:D:32:VAL:CG2   | 4:D:186:VAL:HG22 | 2.47                     | 0.44              |
| 4:D:138:PRO:HB3  | 8:H:58:LEU:HD22  | 1.99                     | 0.44              |
| 5:E:59:VAL:O     | 5:E:59:VAL:CG1   | 2.66                     | 0.44              |
| 1:A:365:LEU:CD1  | 1:A:392:LEU:HD22 | 2.47                     | 0.44              |
| 2:B:24:LEU:HD11  | 2:B:392:TYR:CD1  | 2.52                     | 0.44              |
| 2:B:59:ASN:O     | 2:B:61:SER:O     | 2.35                     | 0.44              |
| 2:B:89:ILE:HD11  | 2:B:96:LEU:HD12  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:104:TYR:CD2  | 3:C:316:MET:HB2  | 2.52                     | 0.44              |
| 3:C:212:ILE:CD1  | 6:F:62:ILE:HG23  | 2.45                     | 0.44              |
| 5:E:55:VAL:O     | 5:E:59:VAL:HG23  | 2.17                     | 0.44              |
| 5:E:121:GLN:NE2  | 5:E:126:ARG:HG3  | 2.32                     | 0.44              |
| 1:A:65:LYS:NZ    | 9:I:311:UNK:HA   | 2.32                     | 0.44              |
| 1:A:114:ALA:CB   | 1:A:216:PHE:CE1  | 3.01                     | 0.44              |
| 1:A:153:LEU:C    | 1:A:153:LEU:CD2  | 2.90                     | 0.44              |
| 1:A:369:LEU:HD21 | 1:A:378:ASP:OD2  | 2.18                     | 0.44              |
| 2:B:61:SER:C     | 2:B:63:LEU:H     | 2.26                     | 0.44              |
| 2:B:402:ILE:HD13 | 2:B:402:ILE:O    | 2.17                     | 0.44              |
| 3:C:150:LEU:C    | 3:C:152:SER:N    | 2.76                     | 0.44              |
| 6:F:93:TYR:O     | 6:F:94:LEU:C     | 2.60                     | 0.44              |
| 1:A:123:GLU:HG3  | 1:A:125:SER:OG   | 2.18                     | 0.44              |
| 1:A:349:ILE:HG22 | 1:A:408:ARG:CD   | 2.47                     | 0.44              |
| 2:B:96:LEU:HD23  | 2:B:96:LEU:C     | 2.42                     | 0.44              |
| 2:B:143:GLN:O    | 2:B:146:ILE:HG12 | 2.18                     | 0.44              |
| 3:C:41:CYS:SG    | 3:C:91:PHE:HA    | 2.57                     | 0.44              |
| 3:C:377:MET:HE2  | 6:F:20:TYR:HB2   | 1.99                     | 0.44              |
| 4:D:178:THR:O    | 4:D:182:VAL:HG12 | 2.17                     | 0.44              |
| 1:A:266:ASP:O    | 1:A:268:VAL:N    | 2.50                     | 0.44              |
| 2:B:207:VAL:HG21 | 2:B:383:GLY:HA2  | 1.98                     | 0.44              |
| 4:D:57:THR:HG22  | 4:D:58:GLU:N     | 2.32                     | 0.44              |
| 4:D:175:THR:HA   | 4:D:176:PRO:HD3  | 1.73                     | 0.44              |
| 5:E:171:ILE:HG12 | 5:E:176:ALA:O    | 2.18                     | 0.44              |
| 6:F:29:TYR:HB2   | 6:F:31:LEU:CD2   | 2.48                     | 0.44              |
| 7:G:24:ARG:HA    | 7:G:25:PRO:HD3   | 1.68                     | 0.44              |
| 1:A:114:ALA:HA   | 1:A:216:PHE:HE1  | 1.82                     | 0.44              |
| 2:B:170:ASN:HD22 | 2:B:170:ASN:N    | 2.15                     | 0.44              |
| 3:C:161:LEU:O    | 3:C:164:TRP:HD1  | 2.00                     | 0.44              |
| 3:C:227:PHE:CE1  | 4:D:222:MET:HE2  | 2.53                     | 0.44              |
| 4:D:55:CYS:SG    | 4:D:56:TYR:HD2   | 2.40                     | 0.44              |
| 4:D:116:ILE:CG2  | 4:D:117:VAL:H    | 2.30                     | 0.44              |
| 8:H:63:HIS:O     | 8:H:63:HIS:ND1   | 2.51                     | 0.44              |
| 1:A:67:THR:HG21  | 1:A:115:ASP:OD2  | 2.18                     | 0.44              |
| 1:A:276:ILE:CD1  | 1:A:349:ILE:HD11 | 2.48                     | 0.44              |
| 1:A:346:CYS:HB2  | 1:A:412:SER:N    | 2.33                     | 0.44              |
| 3:C:92:PHE:O     | 3:C:95:ILE:HG22  | 2.18                     | 0.44              |
| 3:C:273:TRP:HA   | 3:C:276:LEU:CD1  | 2.47                     | 0.44              |
| 3:C:311:SER:CB   | 3:C:316:MET:HE1  | 2.47                     | 0.44              |
| 3:C:327:TRP:NE1  | 7:G:48:VAL:HG22  | 2.33                     | 0.44              |
| 3:C:359:TYR:HD2  | 3:C:360:PHE:CE1  | 2.36                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:51:LEU:C     | 4:D:54:VAL:HG12  | 2.42                     | 0.44              |
| 4:D:147:LEU:HD22 | 4:D:147:LEU:N    | 2.32                     | 0.44              |
| 5:E:145:VAL:HA   | 5:E:146:PRO:HD3  | 1.83                     | 0.44              |
| 1:A:64:PHE:O     | 1:A:66:GLY:N     | 2.51                     | 0.44              |
| 1:A:85:HIS:ND1   | 2:B:370:MET:HE1  | 2.33                     | 0.44              |
| 1:A:228:VAL:O    | 1:A:228:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:281:ASP:O    | 1:A:284:TYR:CD1  | 2.71                     | 0.44              |
| 1:A:373:THR:HB   | 1:A:374:PRO:CD   | 2.47                     | 0.44              |
| 2:B:332:TYR:O    | 2:B:336:VAL:HG23 | 2.18                     | 0.44              |
| 3:C:311:SER:HB2  | 3:C:316:MET:HE1  | 1.99                     | 0.44              |
| 2:B:241:GLY:CA   | 2:B:421:GLN:HE21 | 2.12                     | 0.43              |
| 2:B:250:ASP:O    | 2:B:251:SER:CB   | 2.66                     | 0.43              |
| 2:B:424:MET:HG2  | 2:B:425:ALA:H    | 1.78                     | 0.43              |
| 3:C:329:LEU:O    | 3:C:332:ASN:HB3  | 2.18                     | 0.43              |
| 3:C:346:HIS:ND1  | 3:C:347:PRO:N    | 2.65                     | 0.43              |
| 5:E:16:PRO:HG3   | 5:E:32:ARG:HH11  | 1.82                     | 0.43              |
| 5:E:134:ILE:HD12 | 5:E:185:TYR:CE2  | 2.53                     | 0.43              |
| 5:E:136:ILE:HG12 | 5:E:181:GLU:O    | 2.17                     | 0.43              |
| 7:G:36:ASN:HA    | 7:G:39:ARG:CB    | 2.48                     | 0.43              |
| 1:A:284:TYR:HD2  | 1:A:289:HIS:CE1  | 2.37                     | 0.43              |
| 1:A:349:ILE:CG2  | 1:A:408:ARG:HG3  | 2.48                     | 0.43              |
| 2:B:150:VAL:CG2  | 2:B:151:ALA:N    | 2.81                     | 0.43              |
| 2:B:194:PHE:O    | 2:B:198:HIS:ND1  | 2.40                     | 0.43              |
| 3:C:121:LEU:HD11 | 3:C:125:MET:HE3  | 2.00                     | 0.43              |
| 3:C:344:VAL:O    | 3:C:349:ILE:HD11 | 2.18                     | 0.43              |
| 4:D:28:ARG:O     | 4:D:31:GLN:N     | 2.51                     | 0.43              |
| 5:E:29:ASP:C     | 5:E:31:SER:N     | 2.72                     | 0.43              |
| 6:F:70:MET:HE2   | 6:F:71:ARG:N     | 2.32                     | 0.43              |
| 1:A:41:ILE:HD12  | 1:A:195:MET:SD   | 2.59                     | 0.43              |
| 1:A:438:ARG:C    | 1:A:438:ARG:HD3  | 2.43                     | 0.43              |
| 2:B:150:VAL:HA   | 2:B:153:GLN:HE21 | 1.84                     | 0.43              |
| 4:D:181:GLN:C    | 4:D:181:GLN:HE21 | 2.26                     | 0.43              |
| 6:F:101:ARG:HG3  | 6:F:104:ARG:HH21 | 1.82                     | 0.43              |
| 1:A:410:VAL:O    | 1:A:413:LYS:HB3  | 2.18                     | 0.43              |
| 2:B:24:LEU:H     | 2:B:24:LEU:CD2   | 2.29                     | 0.43              |
| 3:C:166:TRP:O    | 3:C:167:GLY:C    | 2.61                     | 0.43              |
| 5:E:53:ASN:O     | 5:E:54:VAL:C     | 2.60                     | 0.43              |
| 8:H:35:GLU:C     | 8:H:37:LEU:N     | 2.76                     | 0.43              |
| 2:B:260:GLU:O    | 2:B:261:SER:CB   | 2.66                     | 0.43              |
| 2:B:405:VAL:CG1  | 2:B:406:ALA:N    | 2.81                     | 0.43              |
| 4:D:21:LEU:HB3   | 4:D:26:ILE:HD11  | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:230:LEU:HB3  | 6:F:70:MET:SD    | 2.58                     | 0.43              |
| 5:E:118:ARG:HH11 | 5:E:118:ARG:CB   | 2.31                     | 0.43              |
| 1:A:24:ARG:HG3   | 1:A:24:ARG:NH1   | 2.33                     | 0.43              |
| 2:B:109:VAL:HG13 | 2:B:119:LEU:CD2  | 2.49                     | 0.43              |
| 3:C:285:ILE:CG2  | 3:C:291:GLY:HA2  | 2.48                     | 0.43              |
| 3:C:319:ARG:CZ   | 3:C:374:GLU:OE1  | 2.66                     | 0.43              |
| 1:A:293:PRO:O    | 1:A:294:LEU:C    | 2.61                     | 0.43              |
| 2:B:89:ILE:CD1   | 2:B:96:LEU:HD12  | 2.49                     | 0.43              |
| 2:B:192:HIS:O    | 2:B:196:GLN:HG3  | 2.19                     | 0.43              |
| 3:C:9:HIS:HA     | 3:C:10:PRO:HD2   | 1.90                     | 0.43              |
| 4:D:102:ARG:HA   | 4:D:108:ALA:O    | 2.18                     | 0.43              |
| 10:J:12:LEU:C    | 10:J:13:LEU:HD12 | 2.43                     | 0.43              |
| 1:A:53:ASN:ND2   | 1:A:53:ASN:C     | 2.77                     | 0.43              |
| 3:C:153:ALA:O    | 3:C:154:ILE:C    | 2.61                     | 0.43              |
| 7:G:56:TYR:O     | 7:G:57:LEU:C     | 2.61                     | 0.43              |
| 7:G:75:ALA:C     | 7:G:77:TYR:N     | 2.75                     | 0.43              |
| 1:A:149:VAL:HG13 | 1:A:150:PHE:H    | 1.84                     | 0.43              |
| 1:A:153:LEU:HD23 | 1:A:157:ALA:HB2  | 2.01                     | 0.43              |
| 3:C:51:LEU:HD11  | 5:E:61:SER:OG    | 2.19                     | 0.43              |
| 3:C:55:HIS:HE1   | 5:E:61:SER:O     | 2.01                     | 0.43              |
| 3:C:101:ARG:HD2  | 3:C:101:ARG:C    | 2.43                     | 0.43              |
| 3:C:103:LEU:HD13 | 3:C:104:TYR:HD1  | 1.84                     | 0.43              |
| 3:C:234:THR:OG1  | 4:D:216:VAL:HG12 | 2.18                     | 0.43              |
| 4:D:10:TYR:N     | 4:D:10:TYR:CD1   | 2.87                     | 0.43              |
| 5:E:45:LEU:HD21  | 10:J:28:ALA:CA   | 2.49                     | 0.43              |
| 5:E:52:LYS:C     | 5:E:52:LYS:CD    | 2.92                     | 0.43              |
| 5:E:118:ARG:CB   | 5:E:118:ARG:NH1  | 2.82                     | 0.43              |
| 5:E:166:ASP:OD1  | 5:E:168:SER:N    | 2.50                     | 0.43              |
| 2:B:50:PHE:HZ    | 2:B:379:LEU:HD13 | 1.84                     | 0.43              |
| 2:B:135:TRP:CD1  | 2:B:135:TRP:N    | 2.87                     | 0.43              |
| 2:B:170:ASN:O    | 2:B:171:ALA:O    | 2.36                     | 0.43              |
| 2:B:202:ALA:HB3  | 2:B:229:GLY:C    | 2.44                     | 0.43              |
| 3:C:201:LEU:O    | 3:C:203:GLU:N    | 2.52                     | 0.43              |
| 1:A:65:LYS:HZ3   | 9:I:311:UNK:CA   | 2.32                     | 0.42              |
| 1:A:93:GLU:O     | 1:A:94:HIS:HB2   | 2.19                     | 0.42              |
| 1:A:320:PHE:HE2  | 1:A:415:ILE:HD11 | 1.83                     | 0.42              |
| 2:B:113:ARG:HG3  | 2:B:114:ASP:N    | 2.34                     | 0.42              |
| 2:B:353:SER:OG   | 2:B:355:GLU:HB3  | 2.19                     | 0.42              |
| 4:D:32:VAL:HG21  | 4:D:186:VAL:HG21 | 2.01                     | 0.42              |
| 5:E:45:LEU:HA    | 5:E:45:LEU:HD22  | 1.83                     | 0.42              |
| 7:G:26:PHE:HE1   | 7:G:29:TYR:HB3   | 1.84                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:85:HIS:HB2   | 1:A:100:LYS:HG2 | 1.97                     | 0.42              |
| 1:A:123:GLU:OE1  | 1:A:123:GLU:HA  | 2.19                     | 0.42              |
| 1:A:159:GLN:NE2  | 5:E:7:VAL:HG11  | 2.33                     | 0.42              |
| 1:A:250:LEU:CD2  | 1:A:325:VAL:CG1 | 2.97                     | 0.42              |
| 1:A:321:GLY:HA2  | 1:A:342:TRP:CZ2 | 2.54                     | 0.42              |
| 2:B:22:GLN:O     | 2:B:23:ASP:C    | 2.63                     | 0.42              |
| 2:B:339:ALA:O    | 2:B:340:ALA:C   | 2.62                     | 0.42              |
| 2:B:415:LYS:O    | 2:B:416:LYS:C   | 2.61                     | 0.42              |
| 3:C:350:ILE:O    | 3:C:351:ILE:C   | 2.62                     | 0.42              |
| 3:C:369:THR:C    | 3:C:371:GLY:H   | 2.27                     | 0.42              |
| 4:D:102:ARG:HH11 | 4:D:109:LEU:HB2 | 1.84                     | 0.42              |
| 4:D:132:THR:HA   | 4:D:179:MET:CE  | 2.46                     | 0.42              |
| 5:E:17:PRO:CD    | 7:G:24:ARG:HH21 | 2.32                     | 0.42              |
| 5:E:45:LEU:C     | 5:E:45:LEU:CD1  | 2.91                     | 0.42              |
| 5:E:105:GLU:O    | 5:E:109:GLU:HG2 | 2.19                     | 0.42              |
| 1:A:15:GLN:O     | 1:A:26:ALA:HA   | 2.19                     | 0.42              |
| 1:A:338:LEU:C    | 1:A:340:GLY:N   | 2.76                     | 0.42              |
| 1:A:383:LEU:HD23 | 1:A:388:ARG:HA  | 2.01                     | 0.42              |
| 2:B:198:HIS:NE2  | 2:B:232:LEU:CD2 | 2.83                     | 0.42              |
| 3:C:92:PHE:HA    | 3:C:95:ILE:CG2  | 2.43                     | 0.42              |
| 3:C:101:ARG:O    | 3:C:105:TYR:HD2 | 2.02                     | 0.42              |
| 3:C:104:TYR:OH   | 3:C:316:MET:HG3 | 2.19                     | 0.42              |
| 3:C:109:LEU:HD23 | 3:C:109:LEU:HA  | 1.82                     | 0.42              |
| 3:C:237:LEU:HD12 | 3:C:240:PHE:HD2 | 1.83                     | 0.42              |
| 3:C:293:LEU:N    | 3:C:293:LEU:CD2 | 2.81                     | 0.42              |
| 3:C:362:ILE:HA   | 3:C:366:LEU:HB2 | 2.01                     | 0.42              |
| 5:E:17:PRO:HA    | 5:E:20:TYR:HE1  | 1.83                     | 0.42              |
| 2:B:312:PHE:H    | 2:B:324:PHE:HA  | 1.84                     | 0.42              |
| 2:B:385:GLN:NE2  | 2:B:392:TYR:HA  | 2.35                     | 0.42              |
| 2:B:405:VAL:O    | 2:B:406:ALA:CB  | 2.67                     | 0.42              |
| 3:C:75:GLN:C     | 3:C:77:GLY:N    | 2.78                     | 0.42              |
| 3:C:145:THR:HG23 | 3:C:171:VAL:HB  | 2.00                     | 0.42              |
| 4:D:46:VAL:HG12  | 4:D:47:ALA:N    | 2.34                     | 0.42              |
| 5:E:12:ASP:CA    | 5:E:20:TYR:OH   | 2.67                     | 0.42              |
| 5:E:153:PHE:CE2  | 5:E:172:ARG:NH1 | 2.87                     | 0.42              |
| 1:A:65:LYS:N     | 1:A:65:LYS:CD   | 2.83                     | 0.42              |
| 1:A:134:ILE:C    | 1:A:136:ARG:N   | 2.76                     | 0.42              |
| 1:A:339:GLN:HG2  | 1:A:440:GLY:O   | 2.20                     | 0.42              |
| 1:A:434:TYR:O    | 1:A:435:ASN:C   | 2.61                     | 0.42              |
| 2:B:75:LEU:HD11  | 2:B:140:LEU:CD2 | 2.50                     | 0.42              |
| 2:B:135:TRP:O    | 2:B:136:GLU:C   | 2.62                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:364:LEU:O    | 2:B:365:LYS:C    | 2.63                     | 0.42              |
| 4:D:55:CYS:O     | 4:D:56:TYR:CD2   | 2.72                     | 0.42              |
| 7:G:44:CYS:O     | 7:G:45:ILE:C     | 2.62                     | 0.42              |
| 2:B:56:ARG:O     | 2:B:171:ALA:HB1  | 2.19                     | 0.42              |
| 2:B:272:PHE:O    | 2:B:273:SER:C    | 2.62                     | 0.42              |
| 3:C:130:VAL:HG13 | 3:C:179:PHE:HB3  | 2.01                     | 0.42              |
| 4:D:54:VAL:HG13  | 4:D:55:CYS:N     | 2.34                     | 0.42              |
| 5:E:86:ASN:HB2   | 5:E:99:ARG:NE    | 2.35                     | 0.42              |
| 6:F:31:LEU:HD23  | 6:F:31:LEU:H     | 1.84                     | 0.42              |
| 1:A:274:ASN:ND2  | 1:A:320:PHE:CZ   | 2.88                     | 0.42              |
| 3:C:268:HIS:CD2  | 3:C:268:HIS:N    | 2.87                     | 0.42              |
| 3:C:332:ASN:C    | 3:C:332:ASN:ND2  | 2.74                     | 0.42              |
| 10:J:20:PHE:CE1  | 10:J:24:ILE:HD11 | 2.55                     | 0.42              |
| 1:A:343:MET:HE2  | 1:A:343:MET:CA   | 2.49                     | 0.42              |
| 2:B:284:HIS:O    | 2:B:286:LYS:N    | 2.48                     | 0.42              |
| 3:C:2:ALA:HB1    | 3:C:3:PRO:HD2    | 2.01                     | 0.42              |
| 8:H:40:CYS:C     | 8:H:54:CYS:SG    | 3.03                     | 0.42              |
| 8:H:72:LYS:HA    | 8:H:75:ASN:HD21  | 1.85                     | 0.42              |
| 1:A:48:GLU:HB3   | 1:A:53:ASN:HA    | 2.02                     | 0.42              |
| 1:A:61:HIS:NE2   | 1:A:137:GLU:OE1  | 2.40                     | 0.42              |
| 1:A:282:ARG:HD3  | 9:I:203:UNK:CB   | 2.50                     | 0.42              |
| 1:A:365:LEU:HD13 | 1:A:392:LEU:HD22 | 2.02                     | 0.42              |
| 3:C:98:HIS:HD2   | 11:C:382:HEM:C1C | 2.38                     | 0.42              |
| 4:D:98:PRO:O     | 4:D:99:GLU:C     | 2.61                     | 0.42              |
| 9:I:107:UNK:HA   | 9:I:115:UNK:O    | 2.19                     | 0.42              |
| 1:A:64:PHE:C     | 1:A:66:GLY:H     | 2.28                     | 0.42              |
| 1:A:244:ARG:NE   | 7:G:10:VAL:HB    | 2.35                     | 0.42              |
| 1:A:250:LEU:HD21 | 1:A:325:VAL:CG1  | 2.49                     | 0.42              |
| 2:B:374:SER:O    | 2:B:375:SER:C    | 2.62                     | 0.42              |
| 3:C:46:ILE:O     | 3:C:50:LEU:HB2   | 2.19                     | 0.42              |
| 4:D:218:LEU:HD22 | 5:E:39:VAL:HG13  | 2.02                     | 0.42              |
| 1:A:134:ILE:O    | 1:A:135:VAL:C    | 2.61                     | 0.41              |
| 1:A:424:GLY:HA2  | 1:A:425:PRO:HD3  | 1.73                     | 0.41              |
| 2:B:275:LEU:O    | 2:B:279:LEU:HB2  | 2.19                     | 0.41              |
| 3:C:99:ILE:O     | 3:C:100:GLY:C    | 2.63                     | 0.41              |
| 3:C:238:THR:HB   | 4:D:212:MET:HG3  | 2.01                     | 0.41              |
| 3:C:276:LEU:O    | 3:C:277:PHE:C    | 2.62                     | 0.41              |
| 1:A:102:LEU:H    | 1:A:102:LEU:CD1  | 2.31                     | 0.41              |
| 3:C:9:HIS:HD2    | 3:C:10:PRO:HG2   | 1.86                     | 0.41              |
| 3:C:250:LEU:HD13 | 3:C:250:LEU:O    | 2.20                     | 0.41              |
| 4:D:75:ASN:ND2   | 4:D:81:PHE:HD2   | 2.19                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:176:ALA:HA   | 5:E:177:PRO:HD2  | 1.85                     | 0.41              |
| 1:A:391:PRO:HG2  | 1:A:394:GLU:HB2  | 2.02                     | 0.41              |
| 1:A:399:LEU:HD12 | 1:A:399:LEU:C    | 2.44                     | 0.41              |
| 2:B:189:VAL:O    | 2:B:192:HIS:N    | 2.53                     | 0.41              |
| 2:B:258:VAL:HG13 | 2:B:322:PHE:O    | 2.21                     | 0.41              |
| 2:B:424:MET:HE3  | 2:B:436:VAL:CG1  | 2.50                     | 0.41              |
| 3:C:92:PHE:CA    | 3:C:95:ILE:HG22  | 2.43                     | 0.41              |
| 12:C:383:U10:H8  | 12:C:383:U10:C1M | 2.50                     | 0.41              |
| 4:D:70:VAL:HG21  | 4:D:89:ASP:OD2   | 2.20                     | 0.41              |
| 4:D:208:MET:SD   | 4:D:208:MET:C    | 3.03                     | 0.41              |
| 5:E:32:ARG:HD2   | 5:E:32:ARG:HA    | 1.76                     | 0.41              |
| 1:A:142:ASP:OD2  | 5:E:1:SER:HA     | 2.20                     | 0.41              |
| 1:A:145:MET:HA   | 1:A:148:VAL:HG13 | 2.00                     | 0.41              |
| 5:E:177:PRO:C    | 5:E:178:LEU:HD23 | 2.46                     | 0.41              |
| 1:A:28:GLU:O     | 1:A:200:ALA:HA   | 2.21                     | 0.41              |
| 1:A:70:ARG:HA    | 1:A:71:PRO:HD2   | 1.73                     | 0.41              |
| 1:A:86:LEU:HD13  | 1:A:99:ILE:CG1   | 2.50                     | 0.41              |
| 1:A:189:HIS:HD2  | 1:A:194:ARG:HH12 | 1.69                     | 0.41              |
| 1:A:394:GLU:C    | 1:A:396:GLU:N    | 2.77                     | 0.41              |
| 1:A:433:ASP:OD1  | 1:A:436:ARG:HG2  | 2.20                     | 0.41              |
| 2:B:264:ILE:HG23 | 2:B:315:SER:O    | 2.20                     | 0.41              |
| 3:C:5:ILE:O      | 3:C:5:ILE:CG2    | 2.66                     | 0.41              |
| 3:C:16:ASN:OD1   | 3:C:16:ASN:O     | 2.39                     | 0.41              |
| 3:C:285:ILE:HA   | 3:C:286:PRO:HD3  | 1.83                     | 0.41              |
| 3:C:311:SER:C    | 3:C:313:GLN:H    | 2.27                     | 0.41              |
| 4:D:41:HIS:HB3   | 4:D:113:LEU:HD13 | 2.02                     | 0.41              |
| 4:D:144:ARG:HG3  | 4:D:147:LEU:HD23 | 2.02                     | 0.41              |
| 4:D:232:SER:OG   | 5:E:14:ARG:HG3   | 2.20                     | 0.41              |
| 5:E:68:VAL:C     | 5:E:70:ALA:N     | 2.76                     | 0.41              |
| 6:F:84:GLU:H     | 6:F:84:GLU:CD    | 2.29                     | 0.41              |
| 10:J:25:VAL:O    | 10:J:28:ALA:N    | 2.52                     | 0.41              |
| 10:J:54:HIS:CD2  | 10:J:54:HIS:N    | 2.88                     | 0.41              |
| 1:A:123:GLU:C    | 1:A:125:SER:N    | 2.77                     | 0.41              |
| 1:A:191:THR:C    | 1:A:193:PRO:HD2  | 2.46                     | 0.41              |
| 1:A:241:ILE:O    | 1:A:241:ILE:HG23 | 2.19                     | 0.41              |
| 1:A:250:LEU:N    | 1:A:250:LEU:CD1  | 2.83                     | 0.41              |
| 2:B:280:GLY:C    | 2:B:283:PRO:HD2  | 2.45                     | 0.41              |
| 2:B:407:ASP:OD1  | 2:B:408:ALA:N    | 2.52                     | 0.41              |
| 3:C:101:ARG:C    | 3:C:101:ARG:CD   | 2.93                     | 0.41              |
| 4:D:161:ALA:O    | 4:D:163:PRO:HD3  | 2.21                     | 0.41              |
| 2:B:269:ALA:C    | 2:B:271:ALA:N    | 2.79                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:70:MET:CE    | 6:F:71:ARG:HG2   | 2.50                     | 0.41              |
| 1:A:260:PRO:HD3  | 1:A:414:TYR:CE2  | 2.55                     | 0.41              |
| 1:A:402:VAL:HA   | 1:A:406:MET:SD   | 2.61                     | 0.41              |
| 2:B:50:PHE:CD1   | 2:B:50:PHE:N     | 2.89                     | 0.41              |
| 2:B:189:VAL:C    | 2:B:191:LEU:N    | 2.78                     | 0.41              |
| 2:B:318:ASP:O    | 2:B:319:SER:HB2  | 2.20                     | 0.41              |
| 2:B:385:GLN:C    | 2:B:387:LEU:H    | 2.27                     | 0.41              |
| 3:C:166:TRP:O    | 3:C:167:GLY:O    | 2.39                     | 0.41              |
| 3:C:348:PHE:O    | 3:C:350:ILE:N    | 2.54                     | 0.41              |
| 6:F:60:PHE:O     | 6:F:61:ARG:C     | 2.62                     | 0.41              |
| 1:A:90:SER:HB3   | 1:A:95:THR:HG23  | 2.03                     | 0.41              |
| 1:A:108:LYS:HA   | 1:A:108:LYS:CE   | 2.50                     | 0.41              |
| 1:A:289:HIS:O    | 1:A:290:SER:C    | 2.63                     | 0.41              |
| 2:B:269:ALA:O    | 2:B:271:ALA:N    | 2.54                     | 0.41              |
| 2:B:277:HIS:C    | 2:B:279:LEU:N    | 2.78                     | 0.41              |
| 2:B:374:SER:O    | 2:B:376:GLU:N    | 2.54                     | 0.41              |
| 3:C:151:PHE:HB2  | 3:C:162:VAL:CG2  | 2.51                     | 0.41              |
| 3:C:156:TYR:O    | 3:C:158:GLY:N    | 2.51                     | 0.41              |
| 3:C:200:PHE:O    | 3:C:201:LEU:C    | 2.62                     | 0.41              |
| 3:C:257:PHE:HD2  | 4:D:115:TYR:HB3  | 1.86                     | 0.41              |
| 3:C:273:TRP:CD2  | 3:C:274:TYR:N    | 2.89                     | 0.41              |
| 3:C:305:ILE:HB   | 3:C:306:PRO:HD3  | 2.02                     | 0.41              |
| 4:D:17:PRO:O     | 4:D:202:LYS:HD3  | 2.21                     | 0.41              |
| 5:E:17:PRO:HD3   | 7:G:24:ARG:NH2   | 2.35                     | 0.41              |
| 5:E:74:ILE:O     | 5:E:194:ILE:HA   | 2.21                     | 0.41              |
| 5:E:86:ASN:OD1   | 5:E:99:ARG:HB2   | 2.21                     | 0.41              |
| 5:E:158:CYS:HA   | 5:E:159:PRO:HD2  | 1.76                     | 0.41              |
| 6:F:26:PHE:C     | 6:F:26:PHE:CD1   | 2.99                     | 0.41              |
| 6:F:89:TYR:CD1   | 6:F:89:TYR:C     | 2.98                     | 0.41              |
| 1:A:144:SER:C    | 1:A:146:ARG:H    | 2.29                     | 0.41              |
| 1:A:264:HIS:HD2  | 1:A:266:ASP:HB2  | 1.86                     | 0.41              |
| 2:B:254:HIS:O    | 2:B:426:ALA:HA   | 2.20                     | 0.41              |
| 2:B:414:ALA:O    | 2:B:418:VAL:HG23 | 2.20                     | 0.41              |
| 3:C:120:LEU:HA   | 3:C:120:LEU:HD13 | 1.87                     | 0.41              |
| 3:C:166:TRP:CD1  | 3:C:166:TRP:C    | 2.99                     | 0.41              |
| 3:C:253:ASP:HA   | 3:C:254:PRO:HD2  | 1.90                     | 0.41              |
| 3:C:258:THR:O    | 3:C:259:PRO:C    | 2.63                     | 0.41              |
| 3:C:325:LEU:HD22 | 3:C:362:ILE:CG2  | 2.44                     | 0.41              |
| 8:H:24:CYS:C     | 8:H:26:GLN:H     | 2.28                     | 0.41              |
| 8:H:69:VAL:O     | 8:H:73:LEU:HB2   | 2.21                     | 0.41              |
| 1:A:389:ARG:HD2  | 1:A:390:ILE:H    | 1.86                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:LEU:HG    | 2:B:24:LEU:O     | 2.21                     | 0.40              |
| 2:B:160:ILE:HG23 | 2:B:164:HIS:CE1  | 2.57                     | 0.40              |
| 3:C:75:GLN:C     | 3:C:77:GLY:H     | 2.29                     | 0.40              |
| 3:C:305:ILE:HD11 | 3:C:363:LEU:HD22 | 2.03                     | 0.40              |
| 11:C:381:HEM:HHA | 11:C:381:HEM:O2D | 2.20                     | 0.40              |
| 4:D:172:ASP:C    | 4:D:174:GLY:N    | 2.79                     | 0.40              |
| 1:A:53:ASN:ND2   | 1:A:54:GLY:N     | 2.67                     | 0.40              |
| 1:A:245:GLU:HA   | 7:G:11:ARG:HA    | 2.04                     | 0.40              |
| 2:B:183:ILE:HG22 | 2:B:184:GLY:N    | 2.36                     | 0.40              |
| 2:B:399:LEU:C    | 2:B:401:GLN:N    | 2.79                     | 0.40              |
| 3:C:37:LEU:O     | 3:C:41:CYS:HB2   | 2.21                     | 0.40              |
| 3:C:105:TYR:HA   | 3:C:315:THR:HG22 | 2.03                     | 0.40              |
| 3:C:239:PRO:O    | 3:C:240:PHE:C    | 2.63                     | 0.40              |
| 5:E:89:PHE:O     | 5:E:95:PRO:HA    | 2.20                     | 0.40              |
| 5:E:165:TYR:HE2  | 5:E:179:ASN:HA   | 1.86                     | 0.40              |
| 6:F:64:ARG:O     | 6:F:68:LEU:HD13  | 2.21                     | 0.40              |
| 1:A:349:ILE:HG12 | 1:A:350:SER:N    | 2.36                     | 0.40              |
| 2:B:92:VAL:O     | 2:B:92:VAL:HG12  | 2.21                     | 0.40              |
| 2:B:95:LYS:HB2   | 2:B:110:GLU:HG3  | 2.01                     | 0.40              |
| 2:B:109:VAL:O    | 2:B:109:VAL:CG1  | 2.69                     | 0.40              |
| 2:B:273:SER:O    | 2:B:276:GLN:HB3  | 2.21                     | 0.40              |
| 2:B:382:VAL:HG23 | 2:B:383:GLY:N    | 2.36                     | 0.40              |
| 3:C:71:CYS:SG    | 3:C:81:ARG:HD3   | 2.62                     | 0.40              |
| 3:C:150:LEU:O    | 3:C:152:SER:N    | 2.55                     | 0.40              |
| 4:D:118:ARG:NH1  | 4:D:195:GLU:OE1  | 2.54                     | 0.40              |
| 8:H:40:CYS:O     | 8:H:44:VAL:HG23  | 2.22                     | 0.40              |
| 10:J:40:ASP:O    | 10:J:41:ALA:C    | 2.65                     | 0.40              |
| 1:A:89:TYR:CD1   | 1:A:89:TYR:C     | 3.00                     | 0.40              |
| 1:A:235:ARG:NH1  | 5:E:15:ARG:CZ    | 2.84                     | 0.40              |
| 2:B:51:ILE:HG22  | 2:B:52:LYS:N     | 2.35                     | 0.40              |
| 3:C:101:ARG:HD2  | 3:C:101:ARG:O    | 2.21                     | 0.40              |
| 4:D:99:GLU:CD    | 4:D:99:GLU:H     | 2.28                     | 0.40              |
| 4:D:141:VAL:HG23 | 8:H:53:ASP:HB3   | 2.03                     | 0.40              |
| 4:D:161:ALA:O    | 4:D:162:PRO:C    | 2.64                     | 0.40              |
| 4:D:218:LEU:O    | 4:D:222:MET:HG3  | 2.21                     | 0.40              |
| 5:E:100:HIS:HD2  | 5:E:131:GLU:O    | 2.04                     | 0.40              |
| 8:H:55:THR:O     | 8:H:56:GLU:C     | 2.64                     | 0.40              |
| 1:A:182:LEU:N    | 1:A:182:LEU:HD22 | 2.36                     | 0.40              |
| 3:C:11:LEU:O     | 3:C:14:MET:HB2   | 2.22                     | 0.40              |
| 4:D:164:ILE:O    | 4:D:164:ILE:HG23 | 2.22                     | 0.40              |
| 5:E:19:ASP:O     | 5:E:20:TYR:CG    | 2.74                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 5:E:83:GLU:HA | 5:E:100:HIS:CB  | 2.46                     | 0.40              |
| 7:G:29:TYR:O  | 7:G:34:VAL:HG23 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 440/446 (99%)   | 348 (79%)  | 73 (17%)  | 19 (4%)  | 2           | 13  |
| 2   | B     | 404/422 (96%)   | 291 (72%)  | 74 (18%)  | 39 (10%) | 0           | 2   |
| 3   | C     | 377/380 (99%)   | 299 (79%)  | 64 (17%)  | 14 (4%)  | 2           | 15  |
| 4   | D     | 239/241 (99%)   | 195 (82%)  | 31 (13%)  | 13 (5%)  | 1           | 9   |
| 5   | E     | 194/196 (99%)   | 167 (86%)  | 23 (12%)  | 4 (2%)   | 5           | 26  |
| 6   | F     | 98/109 (90%)    | 83 (85%)   | 15 (15%)  | 0        | 100         | 100 |
| 7   | G     | 76/81 (94%)     | 61 (80%)   | 10 (13%)  | 5 (7%)   | 1           | 6   |
| 8   | H     | 64/78 (82%)     | 50 (78%)   | 14 (22%)  | 0        | 100         | 100 |
| 10  | J     | 57/62 (92%)     | 43 (75%)   | 12 (21%)  | 2 (4%)   | 3           | 16  |
| All | All   | 1949/2015 (97%) | 1537 (79%) | 316 (16%) | 96 (5%)  | 1           | 11  |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | SER  |
| 1   | A     | 65  | LYS  |
| 1   | A     | 103 | SER  |
| 1   | A     | 282 | ARG  |
| 1   | A     | 291 | SER  |
| 2   | B     | 113 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 171 | ALA  |
| 2   | B     | 183 | ILE  |
| 2   | B     | 228 | GLY  |
| 2   | B     | 263 | ALA  |
| 2   | B     | 286 | LYS  |
| 2   | B     | 330 | ALA  |
| 2   | B     | 375 | SER  |
| 2   | B     | 407 | ASP  |
| 4   | D     | 73  | GLY  |
| 4   | D     | 198 | HIS  |
| 4   | D     | 228 | SER  |
| 4   | D     | 233 | ARG  |
| 5   | E     | 21  | SER  |
| 1   | A     | 145 | MET  |
| 2   | B     | 23  | ASP  |
| 2   | B     | 109 | VAL  |
| 2   | B     | 111 | CYS  |
| 2   | B     | 233 | SER  |
| 2   | B     | 404 | ALA  |
| 2   | B     | 431 | GLY  |
| 3   | C     | 21  | ASP  |
| 3   | C     | 157 | ILE  |
| 3   | C     | 167 | GLY  |
| 3   | C     | 171 | VAL  |
| 3   | C     | 202 | HIS  |
| 4   | D     | 8   | PRO  |
| 4   | D     | 38  | SER  |
| 4   | D     | 75  | ASN  |
| 5   | E     | 17  | PRO  |
| 5   | E     | 106 | ILE  |
| 7   | G     | 43  | ALA  |
| 10  | J     | 5   | LEU  |
| 1   | A     | 71  | PRO  |
| 1   | A     | 128 | GLU  |
| 2   | B     | 21  | PRO  |
| 2   | B     | 63  | LEU  |
| 2   | B     | 261 | SER  |
| 2   | B     | 270 | ASN  |
| 2   | B     | 317 | SER  |
| 2   | B     | 345 | LYS  |
| 2   | B     | 349 | GLN  |
| 2   | B     | 354 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 406 | ALA  |
| 2   | B     | 408 | ALA  |
| 2   | B     | 420 | ARG  |
| 3   | C     | 63  | ALA  |
| 3   | C     | 346 | HIS  |
| 3   | C     | 349 | ILE  |
| 4   | D     | 168 | VAL  |
| 10  | J     | 61  | ASN  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 281 | ASP  |
| 1   | A     | 382 | GLU  |
| 1   | A     | 396 | GLU  |
| 1   | A     | 408 | ARG  |
| 2   | B     | 201 | SER  |
| 2   | B     | 269 | ALA  |
| 2   | B     | 361 | LYS  |
| 2   | B     | 372 | VAL  |
| 3   | C     | 60  | THR  |
| 3   | C     | 287 | ASN  |
| 4   | D     | 9   | SER  |
| 4   | D     | 67  | GLU  |
| 4   | D     | 176 | PRO  |
| 5   | E     | 13  | TYR  |
| 1   | A     | 405 | ARG  |
| 2   | B     | 19  | PRO  |
| 2   | B     | 20  | HIS  |
| 2   | B     | 260 | GLU  |
| 2   | B     | 262 | ALA  |
| 2   | B     | 331 | ALA  |
| 3   | C     | 47  | LEU  |
| 7   | G     | 25  | PRO  |
| 7   | G     | 50  | PRO  |
| 1   | A     | 56  | GLY  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 267 | LEU  |
| 2   | B     | 62  | ASN  |
| 2   | B     | 232 | LEU  |
| 3   | C     | 3   | PRO  |
| 3   | C     | 36  | SER  |
| 7   | G     | 74  | PRO  |
| 1   | A     | 127 | ILE  |
| 1   | A     | 286 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 64  | GLY  |
| 3   | C     | 5   | ILE  |
| 4   | D     | 133 | GLY  |
| 7   | G     | 33  | GLY  |
| 4   | D     | 98  | PRO  |
| 2   | B     | 305 | ASN  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 359/376 (96%)   | 340 (95%)  | 19 (5%)  | 20          | 49  |
| 2   | B     | 307/336 (91%)   | 289 (94%)  | 18 (6%)  | 18          | 45  |
| 3   | C     | 326/329 (99%)   | 309 (95%)  | 17 (5%)  | 21          | 49  |
| 4   | D     | 201/207 (97%)   | 191 (95%)  | 10 (5%)  | 22          | 50  |
| 5   | E     | 165/169 (98%)   | 154 (93%)  | 11 (7%)  | 15          | 42  |
| 6   | F     | 90/98 (92%)     | 84 (93%)   | 6 (7%)   | 15          | 42  |
| 7   | G     | 60/72 (83%)     | 54 (90%)   | 6 (10%)  | 7           | 27  |
| 8   | H     | 51/74 (69%)     | 50 (98%)   | 1 (2%)   | 48          | 68  |
| 10  | J     | 41/52 (79%)     | 41 (100%)  | 0        | 100         | 100 |
| All | All   | 1600/1713 (93%) | 1512 (94%) | 88 (6%)  | 19          | 47  |

All (88) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 100 | LYS  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 108 | LYS  |
| 1   | A     | 148 | VAL  |
| 1   | A     | 153 | LEU  |
| 1   | A     | 168 | GLU  |
| 1   | A     | 204 | GLU  |
| 1   | A     | 250 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 316 | GLU  |
| 1   | A     | 361 | LEU  |
| 1   | A     | 365 | LEU  |
| 1   | A     | 368 | HIS  |
| 1   | A     | 382 | GLU  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 388 | ARG  |
| 1   | A     | 395 | TRP  |
| 1   | A     | 409 | GLU  |
| 1   | A     | 431 | LEU  |
| 1   | A     | 443 | TRP  |
| 2   | B     | 56  | ARG  |
| 2   | B     | 57  | TYR  |
| 2   | B     | 62  | ASN  |
| 2   | B     | 85  | ILE  |
| 2   | B     | 112 | LEU  |
| 2   | B     | 135 | TRP  |
| 2   | B     | 170 | ASN  |
| 2   | B     | 221 | GLU  |
| 2   | B     | 225 | ASN  |
| 2   | B     | 247 | GLN  |
| 2   | B     | 248 | ASN  |
| 2   | B     | 252 | LEU  |
| 2   | B     | 264 | ILE  |
| 2   | B     | 307 | PHE  |
| 2   | B     | 325 | TYR  |
| 2   | B     | 402 | ILE  |
| 2   | B     | 434 | PRO  |
| 2   | B     | 437 | ASP  |
| 3   | C     | 40  | VAL  |
| 3   | C     | 43  | MET  |
| 3   | C     | 47  | LEU  |
| 3   | C     | 104 | TYR  |
| 3   | C     | 113 | THR  |
| 3   | C     | 120 | LEU  |
| 3   | C     | 124 | LEU  |
| 3   | C     | 136 | TRP  |
| 3   | C     | 145 | THR  |
| 3   | C     | 164 | TRP  |
| 3   | C     | 175 | THR  |
| 3   | C     | 217 | ASP  |
| 3   | C     | 323 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 325 | LEU  |
| 3   | C     | 330 | VAL  |
| 3   | C     | 350 | ILE  |
| 3   | C     | 354 | MET  |
| 4   | D     | 24  | THR  |
| 4   | D     | 32  | VAL  |
| 4   | D     | 36  | VAL  |
| 4   | D     | 82  | MET  |
| 4   | D     | 99  | GLU  |
| 4   | D     | 136 | GLU  |
| 4   | D     | 143 | VAL  |
| 4   | D     | 163 | PRO  |
| 4   | D     | 181 | GLN  |
| 4   | D     | 192 | TRP  |
| 5   | E     | 17  | PRO  |
| 5   | E     | 19  | ASP  |
| 5   | E     | 71  | MET  |
| 5   | E     | 78  | LEU  |
| 5   | E     | 87  | MET  |
| 5   | E     | 90  | LYS  |
| 5   | E     | 113 | GLU  |
| 5   | E     | 145 | VAL  |
| 5   | E     | 186 | GLU  |
| 5   | E     | 188 | THR  |
| 5   | E     | 194 | ILE  |
| 6   | F     | 12  | TRP  |
| 6   | F     | 31  | LEU  |
| 6   | F     | 37  | ILE  |
| 6   | F     | 59  | MET  |
| 6   | F     | 68  | LEU  |
| 6   | F     | 70  | MET  |
| 7   | G     | 4   | PHE  |
| 7   | G     | 27  | PRO  |
| 7   | G     | 28  | HIS  |
| 7   | G     | 29  | TYR  |
| 7   | G     | 41  | LEU  |
| 7   | G     | 77  | TYR  |
| 8   | H     | 73  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | GLN  |
| 1   | A     | 53  | ASN  |
| 1   | A     | 69  | ASN  |
| 1   | A     | 118 | GLN  |
| 1   | A     | 141 | ASN  |
| 1   | A     | 151 | ASN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 207 | GLN  |
| 1   | A     | 240 | GLN  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 289 | HIS  |
| 1   | A     | 339 | GLN  |
| 1   | A     | 341 | GLN  |
| 1   | A     | 363 | ASN  |
| 1   | A     | 435 | ASN  |
| 2   | B     | 22  | GLN  |
| 2   | B     | 31  | ASN  |
| 2   | B     | 141 | GLN  |
| 2   | B     | 153 | GLN  |
| 2   | B     | 170 | ASN  |
| 2   | B     | 196 | GLN  |
| 2   | B     | 225 | ASN  |
| 2   | B     | 248 | ASN  |
| 2   | B     | 282 | ASN  |
| 2   | B     | 343 | GLN  |
| 2   | B     | 349 | GLN  |
| 2   | B     | 351 | ASN  |
| 2   | B     | 356 | ASN  |
| 2   | B     | 393 | ASN  |
| 2   | B     | 401 | GLN  |
| 2   | B     | 421 | GLN  |
| 2   | B     | 429 | ASN  |
| 3   | C     | 4   | ASN  |
| 3   | C     | 9   | HIS  |
| 3   | C     | 55  | HIS  |
| 3   | C     | 73  | ASN  |
| 3   | C     | 82  | ASN  |
| 3   | C     | 261 | ASN  |
| 3   | C     | 287 | ASN  |
| 3   | C     | 313 | GLN  |
| 3   | C     | 323 | GLN  |
| 3   | C     | 342 | GLN  |
| 3   | C     | 379 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 35  | GLN  |
| 4   | D     | 75  | ASN  |
| 4   | D     | 156 | GLN  |
| 4   | D     | 181 | GLN  |
| 5   | E     | 86  | ASN  |
| 5   | E     | 122 | HIS  |
| 5   | E     | 164 | HIS  |
| 6   | F     | 69  | ASN  |
| 6   | F     | 72  | GLN  |
| 7   | G     | 12  | HIS  |
| 7   | G     | 23  | GLN  |
| 7   | G     | 64  | GLN  |
| 8   | H     | 75  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 11  | HEM  | C     | 381 | 3    | 50,50,50     | 1.54 | 11 (22%)    | 67,82,82    | 2.26 | 21 (31%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | PEE  | E     | 198 | -    | 48,48,50     | 2.51 | 11 (22%) | 51,53,55    | 4.34 | 17 (33%) |
| 13  | PEE  | C     | 384 | -    | 48,48,50     | 2.57 | 12 (25%) | 51,53,55    | 4.31 | 18 (35%) |
| 12  | U10  | C     | 383 | -    | 29,29,63     | 2.30 | 8 (27%)  | 36,38,79    | 1.73 | 11 (30%) |
| 15  | FES  | E     | 197 | 5    | 0,4,4        | -    | -        | -           | -    | -        |
| 11  | HEM  | C     | 382 | 3    | 50,50,50     | 1.81 | 12 (24%) | 67,82,82    | 2.37 | 22 (32%) |
| 14  | BOG  | D     | 242 | -    | 20,20,20     | 0.74 | 0        | 25,25,25    | 0.94 | 1 (4%)   |
| 11  | HEM  | D     | 243 | 4    | 50,50,50     | 1.80 | 12 (24%) | 67,82,82    | 2.18 | 24 (35%) |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 13  | PEE  | E     | 198 | -    | 1/1/4/8 | 27/52/52/54 | -       |
| 11  | HEM  | C     | 381 | 3    | -       | 5/14/54/54  | -       |
| 13  | PEE  | C     | 384 | -    | 1/1/4/8 | 21/52/52/54 | -       |
| 12  | U10  | C     | 383 | -    | -       | 8/23/47/87  | 0/1/1/1 |
| 15  | FES  | E     | 197 | 5    | -       | -           | 0/1/1/1 |
| 11  | HEM  | C     | 382 | 3    | -       | 7/14/54/54  | -       |
| 14  | BOG  | D     | 242 | -    | -       | 5/11/31/31  | 0/1/1/1 |
| 11  | HEM  | D     | 243 | 4    | -       | 8/14/54/54  | -       |

All (66) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | E     | 198 | PEE  | O5-C30  | 11.44 | 1.56        | 1.22     |
| 13  | C     | 384 | PEE  | O5-C30  | 11.17 | 1.55        | 1.22     |
| 12  | C     | 383 | U10  | C6-C1   | 7.62  | 1.48        | 1.35     |
| 11  | C     | 382 | HEM  | FE-ND   | -5.60 | 1.77        | 1.94     |
| 11  | D     | 243 | HEM  | FE-ND   | -5.13 | 1.79        | 1.94     |
| 13  | C     | 384 | PEE  | C18-C19 | 5.03  | 1.60        | 1.31     |
| 13  | E     | 198 | PEE  | O2-C10  | 5.02  | 1.48        | 1.34     |
| 13  | C     | 384 | PEE  | C39-C38 | 5.01  | 1.60        | 1.31     |
| 12  | C     | 383 | U10  | C7-C6   | 4.92  | 1.60        | 1.51     |
| 13  | E     | 198 | PEE  | C39-C38 | 4.76  | 1.58        | 1.31     |
| 13  | E     | 198 | PEE  | C18-C19 | 4.72  | 1.58        | 1.31     |
| 13  | C     | 384 | PEE  | O2-C10  | 4.44  | 1.46        | 1.34     |
| 11  | D     | 243 | HEM  | CBB-CAB | 4.41  | 1.51        | 1.30     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 11  | C     | 382 | HEM  | CHA-C1A | -4.40 | 1.29        | 1.39     |
| 11  | D     | 243 | HEM  | CBC-CAC | 4.19  | 1.50        | 1.30     |
| 11  | C     | 381 | HEM  | FE-NB   | -4.16 | 1.82        | 1.94     |
| 13  | C     | 384 | PEE  | C11-C10 | 3.96  | 1.62        | 1.50     |
| 13  | E     | 198 | PEE  | C21-C22 | -3.66 | 1.33        | 1.51     |
| 12  | C     | 383 | U10  | C18-C19 | 3.62  | 1.41        | 1.33     |
| 13  | E     | 198 | PEE  | C42-C41 | -3.57 | 1.34        | 1.51     |
| 11  | C     | 381 | HEM  | CAB-C3B | -3.56 | 1.37        | 1.47     |
| 13  | E     | 198 | PEE  | C11-C10 | 3.48  | 1.60        | 1.50     |
| 13  | C     | 384 | PEE  | C21-C22 | -3.46 | 1.34        | 1.51     |
| 13  | C     | 384 | PEE  | C42-C41 | -3.39 | 1.34        | 1.51     |
| 13  | C     | 384 | PEE  | C1-C2   | 3.39  | 1.61        | 1.50     |
| 11  | C     | 381 | HEM  | FE-NA   | -3.34 | 1.84        | 1.95     |
| 12  | C     | 383 | U10  | C13-C14 | 3.15  | 1.40        | 1.33     |
| 13  | E     | 198 | PEE  | C31-C30 | -3.07 | 1.41        | 1.50     |
| 11  | C     | 382 | HEM  | FE-NC   | -3.04 | 1.85        | 1.95     |
| 11  | C     | 382 | HEM  | CHB-C1B | -3.03 | 1.32        | 1.38     |
| 11  | C     | 382 | HEM  | CHA-C4D | -2.88 | 1.32        | 1.38     |
| 11  | D     | 243 | HEM  | FE-NA   | -2.87 | 1.85        | 1.95     |
| 11  | C     | 382 | HEM  | CAC-C3C | -2.84 | 1.39        | 1.47     |
| 13  | C     | 384 | PEE  | C31-C30 | -2.84 | 1.42        | 1.50     |
| 13  | C     | 384 | PEE  | P-O3P   | 2.81  | 1.70        | 1.59     |
| 11  | D     | 243 | HEM  | CHB-C4A | -2.67 | 1.33        | 1.39     |
| 11  | C     | 381 | HEM  | FE-NC   | -2.62 | 1.86        | 1.95     |
| 12  | C     | 383 | U10  | C3-C2   | -2.61 | 1.41        | 1.48     |
| 11  | C     | 381 | HEM  | CHD-C4C | -2.56 | 1.33        | 1.38     |
| 11  | D     | 243 | HEM  | C1B-NB  | -2.56 | 1.35        | 1.40     |
| 11  | C     | 382 | HEM  | CAB-C3B | -2.53 | 1.40        | 1.47     |
| 11  | D     | 243 | HEM  | CHB-C1B | -2.52 | 1.33        | 1.38     |
| 12  | C     | 383 | U10  | C8-C9   | 2.51  | 1.38        | 1.33     |
| 11  | D     | 243 | HEM  | C2A-C3A | -2.39 | 1.32        | 1.38     |
| 13  | C     | 384 | PEE  | O2-C2   | -2.37 | 1.41        | 1.46     |
| 11  | C     | 382 | HEM  | C1A-NA  | -2.37 | 1.35        | 1.39     |
| 11  | D     | 243 | HEM  | CHD-C1D | -2.36 | 1.33        | 1.39     |
| 12  | C     | 383 | U10  | O4-C4M  | -2.29 | 1.40        | 1.45     |
| 11  | C     | 381 | HEM  | CAC-C3C | -2.28 | 1.41        | 1.47     |
| 11  | C     | 382 | HEM  | C4D-ND  | -2.23 | 1.36        | 1.40     |
| 11  | D     | 243 | HEM  | C3C-C2C | -2.23 | 1.32        | 1.37     |
| 11  | C     | 381 | HEM  | CHA-C4D | -2.20 | 1.34        | 1.38     |
| 11  | C     | 382 | HEM  | FE-NA   | -2.20 | 1.87        | 1.95     |
| 11  | C     | 381 | HEM  | C2A-C3A | -2.19 | 1.33        | 1.38     |
| 11  | C     | 381 | HEM  | CHA-C1A | -2.19 | 1.34        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | C     | 384 | PEE  | C23-C24 | 2.17  | 1.62        | 1.51     |
| 11  | D     | 243 | HEM  | CHA-C1A | -2.13 | 1.34        | 1.39     |
| 13  | E     | 198 | PEE  | O2-C2   | -2.13 | 1.41        | 1.46     |
| 11  | D     | 243 | HEM  | FE-NC   | -2.13 | 1.88        | 1.95     |
| 13  | E     | 198 | PEE  | C1-C2   | 2.12  | 1.57        | 1.50     |
| 12  | C     | 383 | U10  | C16-C14 | 2.11  | 1.55        | 1.51     |
| 11  | C     | 381 | HEM  | CHD-C1D | -2.10 | 1.34        | 1.39     |
| 13  | E     | 198 | PEE  | C5-C4   | 2.07  | 1.58        | 1.49     |
| 11  | C     | 382 | HEM  | C3D-C2D | -2.04 | 1.32        | 1.36     |
| 11  | C     | 381 | HEM  | CHC-C4B | -2.03 | 1.34        | 1.39     |
| 11  | C     | 382 | HEM  | CBC-CAC | 2.02  | 1.40        | 1.30     |

All (114) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 13  | E     | 198 | PEE  | O4-C10-C11  | -18.60 | 51.02       | 123.78   |
| 13  | C     | 384 | PEE  | O4-C10-C11  | -18.58 | 51.11       | 123.78   |
| 13  | E     | 198 | PEE  | O3-C30-C31  | 13.17  | 151.98      | 111.83   |
| 13  | C     | 384 | PEE  | O3-C30-C31  | 12.89  | 151.15      | 111.83   |
| 13  | C     | 384 | PEE  | O3-C30-O5   | -11.49 | 94.89       | 123.63   |
| 13  | E     | 198 | PEE  | O3-C30-O5   | -11.34 | 95.27       | 123.63   |
| 13  | E     | 198 | PEE  | O2-C2-C3    | 7.95   | 136.86      | 108.34   |
| 13  | C     | 384 | PEE  | O2-C2-C3    | 7.84   | 136.47      | 108.34   |
| 13  | E     | 198 | PEE  | O2-C10-C11  | 7.16   | 126.96      | 111.48   |
| 13  | C     | 384 | PEE  | O2-C10-O4   | -6.66  | 108.13      | 123.70   |
| 11  | C     | 382 | HEM  | C2A-C1A-NA  | 6.45   | 117.31      | 110.15   |
| 13  | E     | 198 | PEE  | C12-C11-C10 | -6.44  | 90.09       | 113.69   |
| 13  | C     | 384 | PEE  | O2-C10-C11  | 6.43   | 125.40      | 111.48   |
| 13  | E     | 198 | PEE  | O2-C10-O4   | -6.42  | 108.69      | 123.70   |
| 11  | D     | 243 | HEM  | C3B-C4B-NB  | 6.14   | 113.88      | 109.47   |
| 11  | C     | 381 | HEM  | C3B-C4B-NB  | 6.05   | 113.81      | 109.47   |
| 13  | C     | 384 | PEE  | C12-C11-C10 | -5.95  | 91.91       | 113.69   |
| 11  | C     | 382 | HEM  | C3D-C4D-ND  | 5.65   | 116.37      | 110.17   |
| 11  | C     | 382 | HEM  | C2B-C1B-NB  | 5.63   | 116.32      | 109.84   |
| 11  | C     | 382 | HEM  | C4D-ND-C1D  | -5.58  | 98.60       | 105.21   |
| 11  | C     | 381 | HEM  | CAD-C3D-C4D | 5.42   | 134.14      | 124.70   |
| 13  | C     | 384 | PEE  | O3-C3-C2    | 5.09   | 123.07      | 108.40   |
| 11  | D     | 243 | HEM  | CMA-C3A-C4A | 5.09   | 133.16      | 125.42   |
| 11  | C     | 381 | HEM  | CAD-C3D-C2D | -5.08  | 118.36      | 127.87   |
| 13  | E     | 198 | PEE  | O3-C3-C2    | 4.70   | 121.94      | 108.40   |
| 11  | D     | 243 | HEM  | CAD-C3D-C4D | 4.58   | 132.68      | 124.70   |
| 11  | C     | 382 | HEM  | C4A-NA-C1A  | -4.55  | 98.40       | 105.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | C     | 382 | HEM  | CBD-CAD-C3D | 4.52  | 125.04      | 112.53   |
| 11  | C     | 381 | HEM  | C4C-C3C-C2C | -4.36 | 103.03      | 106.81   |
| 12  | C     | 383 | U10  | C1-C6-C5    | -4.25 | 115.49      | 119.62   |
| 11  | C     | 382 | HEM  | CBA-CAA-C2A | 4.18  | 124.09      | 112.53   |
| 11  | D     | 243 | HEM  | C2B-C1B-NB  | 4.16  | 114.62      | 109.84   |
| 11  | C     | 382 | HEM  | C3B-C2B-C1B | -4.15 | 103.30      | 106.41   |
| 11  | C     | 381 | HEM  | C2D-C1D-ND  | 4.08  | 114.62      | 109.90   |
| 11  | C     | 381 | HEM  | C4D-ND-C1D  | -4.01 | 100.45      | 105.21   |
| 11  | D     | 243 | HEM  | C1B-NB-C4B  | -3.98 | 100.49      | 105.21   |
| 11  | C     | 381 | HEM  | C2A-C1A-NA  | 3.86  | 114.44      | 110.15   |
| 12  | C     | 383 | U10  | C10-C9-C8   | -3.83 | 113.79      | 123.63   |
| 11  | C     | 382 | HEM  | C1B-NB-C4B  | -3.83 | 100.67      | 105.21   |
| 11  | C     | 382 | HEM  | C3B-C4B-NB  | 3.75  | 112.16      | 109.47   |
| 11  | C     | 381 | HEM  | C4C-NC-C1C  | -3.68 | 99.83       | 105.82   |
| 11  | D     | 243 | HEM  | CMD-C2D-C1D | 3.59  | 130.64      | 125.03   |
| 14  | D     | 242 | BOG  | C1'-O1-C1   | 3.58  | 119.79      | 113.68   |
| 11  | C     | 381 | HEM  | C3B-C2B-C1B | -3.53 | 103.76      | 106.41   |
| 11  | D     | 243 | HEM  | C4D-ND-C1D  | -3.53 | 101.03      | 105.21   |
| 11  | C     | 382 | HEM  | C2D-C1D-ND  | 3.50  | 113.95      | 109.90   |
| 13  | C     | 384 | PEE  | C42-C41-C40 | 3.44  | 130.40      | 113.86   |
| 13  | E     | 198 | PEE  | C22-C21-C20 | 3.41  | 130.27      | 113.86   |
| 11  | D     | 243 | HEM  | CAD-C3D-C2D | -3.41 | 121.48      | 127.87   |
| 11  | D     | 243 | HEM  | CBB-CAB-C3B | -3.40 | 110.52      | 127.53   |
| 11  | C     | 382 | HEM  | CHD-C1D-ND  | -3.38 | 120.79      | 124.42   |
| 11  | C     | 381 | HEM  | CMB-C2B-C1B | 3.36  | 130.29      | 125.03   |
| 13  | E     | 198 | PEE  | C42-C41-C40 | 3.36  | 130.01      | 113.86   |
| 11  | C     | 381 | HEM  | C2B-C1B-NB  | 3.28  | 113.62      | 109.84   |
| 11  | C     | 381 | HEM  | C1B-NB-C4B  | -3.28 | 101.33      | 105.21   |
| 13  | C     | 384 | PEE  | C22-C21-C20 | 3.24  | 129.43      | 113.86   |
| 11  | D     | 243 | HEM  | C3D-C4D-ND  | 3.19  | 113.67      | 110.17   |
| 13  | E     | 198 | PEE  | C33-C32-C31 | 3.11  | 124.56      | 113.13   |
| 11  | D     | 243 | HEM  | C2D-C1D-ND  | 3.10  | 113.49      | 109.90   |
| 11  | C     | 381 | HEM  | CBA-CAA-C2A | 3.10  | 121.10      | 112.53   |
| 11  | D     | 243 | HEM  | CMC-C2C-C1C | 3.05  | 130.09      | 124.73   |
| 13  | E     | 198 | PEE  | C34-C33-C32 | -3.04 | 99.00       | 114.37   |
| 11  | C     | 381 | HEM  | C4A-NA-C1A  | -3.03 | 100.88      | 105.82   |
| 13  | C     | 384 | PEE  | C12-C13-C14 | -3.03 | 99.07       | 114.37   |
| 11  | C     | 382 | HEM  | C1A-C2A-C3A | -3.03 | 102.19      | 106.87   |
| 11  | C     | 381 | HEM  | CMD-C2D-C1D | 2.95  | 129.64      | 125.03   |
| 13  | C     | 384 | PEE  | C33-C32-C31 | 2.91  | 123.81      | 113.13   |
| 11  | D     | 243 | HEM  | C4A-NA-C1A  | -2.88 | 101.13      | 105.82   |
| 12  | C     | 383 | U10  | C15-C14-C13 | -2.87 | 116.26      | 123.63   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | C     | 384 | PEE  | C34-C33-C32 | -2.84 | 99.99       | 114.37   |
| 13  | E     | 198 | PEE  | O5-C30-C31  | -2.82 | 112.74      | 123.78   |
| 11  | C     | 381 | HEM  | CHD-C4C-C3C | -2.76 | 120.55      | 125.21   |
| 11  | D     | 243 | HEM  | C4C-NC-C1C  | -2.71 | 101.39      | 105.82   |
| 11  | D     | 243 | HEM  | C2A-C1A-NA  | 2.69  | 113.14      | 110.15   |
| 12  | C     | 383 | U10  | C15-C14-C16 | 2.68  | 119.89      | 115.23   |
| 11  | D     | 243 | HEM  | CHD-C4C-NC  | -2.68 | 121.53      | 124.45   |
| 11  | C     | 382 | HEM  | CHA-C4D-C3D | -2.68 | 120.29      | 125.23   |
| 13  | E     | 198 | PEE  | C12-C13-C14 | -2.67 | 100.87      | 114.37   |
| 11  | C     | 381 | HEM  | C3D-C4D-ND  | 2.63  | 113.05      | 110.17   |
| 11  | C     | 382 | HEM  | C4C-NC-C1C  | -2.55 | 101.67      | 105.82   |
| 11  | C     | 382 | HEM  | CAA-C2A-C1A | 2.53  | 129.89      | 124.94   |
| 13  | C     | 384 | PEE  | O5-C30-C31  | -2.53 | 113.88      | 123.78   |
| 11  | C     | 381 | HEM  | C1D-C2D-C3D | -2.52 | 104.33      | 106.98   |
| 12  | C     | 383 | U10  | C10-C9-C11  | 2.52  | 119.60      | 115.23   |
| 11  | C     | 381 | HEM  | CHA-C4D-ND  | -2.43 | 121.36      | 124.37   |
| 12  | C     | 383 | U10  | C11-C9-C8   | 2.42  | 126.61      | 121.17   |
| 11  | D     | 243 | HEM  | CBD-CAD-C3D | 2.42  | 119.21      | 112.53   |
| 11  | D     | 243 | HEM  | CHC-C4B-NB  | -2.41 | 121.83      | 124.42   |
| 11  | C     | 382 | HEM  | CMD-C2D-C1D | 2.41  | 128.80      | 125.03   |
| 11  | C     | 382 | HEM  | CHD-C4C-NC  | -2.40 | 121.84      | 124.45   |
| 13  | C     | 384 | PEE  | O2-C2-C1    | 2.39  | 116.92      | 108.34   |
| 11  | C     | 381 | HEM  | C2C-C1C-NC  | 2.38  | 114.03      | 109.64   |
| 12  | C     | 383 | U10  | O2-C2-C3    | -2.38 | 116.00      | 121.03   |
| 11  | C     | 382 | HEM  | C4D-C3D-C2D | -2.38 | 103.43      | 106.89   |
| 11  | D     | 243 | HEM  | C3A-C4A-NA  | 2.36  | 113.93      | 110.14   |
| 13  | E     | 198 | PEE  | O2-C2-C1    | 2.34  | 116.73      | 108.34   |
| 11  | C     | 382 | HEM  | CMC-C2C-C1C | 2.32  | 128.81      | 124.73   |
| 13  | E     | 198 | PEE  | C3-C2-C1    | -2.31 | 106.40      | 111.78   |
| 11  | C     | 382 | HEM  | C3A-C4A-NA  | 2.28  | 113.80      | 110.14   |
| 11  | C     | 382 | HEM  | CHB-C1B-C2B | -2.27 | 120.48      | 126.95   |
| 11  | D     | 243 | HEM  | C4B-C3B-C2B | -2.27 | 105.19      | 107.28   |
| 11  | D     | 243 | HEM  | CMC-C2C-C3C | -2.25 | 122.98      | 128.43   |
| 12  | C     | 383 | U10  | C20-C19-C18 | -2.25 | 117.86      | 123.63   |
| 13  | C     | 384 | PEE  | C3-C2-C1    | -2.24 | 106.57      | 111.78   |
| 12  | C     | 383 | U10  | O5-C5-C4    | -2.23 | 116.30      | 121.03   |
| 11  | C     | 381 | HEM  | CAA-C2A-C1A | 2.21  | 129.26      | 124.94   |
| 11  | D     | 243 | HEM  | C4A-C3A-C2A | -2.20 | 104.30      | 106.82   |
| 13  | C     | 384 | PEE  | C3-O3-C30   | -2.20 | 109.09      | 117.12   |
| 11  | D     | 243 | HEM  | C4D-C3D-C2D | -2.19 | 103.70      | 106.89   |
| 12  | C     | 383 | U10  | C8-C7-C6    | 2.16  | 117.40      | 112.08   |
| 13  | C     | 384 | PEE  | C14-C15-C16 | -2.11 | 103.71      | 114.37   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | E     | 198 | PEE  | C36-C35-C34 | -2.09 | 103.81      | 114.37   |
| 12  | C     | 383 | U10  | C7-C8-C9    | 2.05  | 130.37      | 126.83   |
| 11  | D     | 243 | HEM  | CAA-C2A-C1A | 2.02  | 128.88      | 124.94   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13  | C     | 384 | PEE  | C2   |
| 13  | E     | 198 | PEE  | C2   |

All (81) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | C     | 381 | HEM  | C2B-C3B-CAB-CBB |
| 11  | C     | 381 | HEM  | C4B-C3B-CAB-CBB |
| 12  | C     | 383 | U10  | C5-C6-C7-C8     |
| 12  | C     | 383 | U10  | C14-C16-C17-C18 |
| 13  | C     | 384 | PEE  | O4-C10-O2-C2    |
| 13  | E     | 198 | PEE  | O4-C10-O2-C2    |
| 13  | E     | 198 | PEE  | O5-C30-O3-C3    |
| 13  | E     | 198 | PEE  | C31-C30-O3-C3   |
| 13  | C     | 384 | PEE  | O5-C30-O3-C3    |
| 12  | C     | 383 | U10  | C12-C11-C9-C10  |
| 13  | C     | 384 | PEE  | C37-C38-C39-C40 |
| 13  | E     | 198 | PEE  | C22-C23-C24-C25 |
| 11  | C     | 382 | HEM  | C4D-C3D-CAD-CBD |
| 13  | C     | 384 | PEE  | C22-C23-C24-C25 |
| 13  | C     | 384 | PEE  | C31-C30-O3-C3   |
| 13  | C     | 384 | PEE  | C17-C18-C19-C20 |
| 13  | E     | 198 | PEE  | C37-C38-C39-C40 |
| 12  | C     | 383 | U10  | C12-C11-C9-C8   |
| 14  | D     | 242 | BOG  | C2-C1-O1-C1'    |
| 13  | E     | 198 | PEE  | C30-C31-C32-C33 |
| 14  | D     | 242 | BOG  | O5-C1-O1-C1'    |
| 13  | C     | 384 | PEE  | C3-C2-O2-C10    |
| 13  | E     | 198 | PEE  | C17-C18-C19-C20 |
| 13  | E     | 198 | PEE  | C35-C36-C37-C38 |
| 13  | E     | 198 | PEE  | C12-C13-C14-C15 |
| 13  | E     | 198 | PEE  | C31-C32-C33-C34 |
| 13  | E     | 198 | PEE  | C21-C22-C23-C24 |
| 13  | C     | 384 | PEE  | C20-C21-C22-C23 |
| 13  | E     | 198 | PEE  | C14-C15-C16-C17 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | D     | 243 | HEM  | C2D-C3D-CAD-CBD |
| 12  | C     | 383 | U10  | C1-C6-C7-C8     |
| 13  | E     | 198 | PEE  | C33-C34-C35-C36 |
| 11  | D     | 243 | HEM  | C2B-C3B-CAB-CBB |
| 13  | C     | 384 | PEE  | C13-C14-C15-C16 |
| 14  | D     | 242 | BOG  | C2'-C3'-C4'-C5' |
| 13  | E     | 198 | PEE  | C39-C40-C41-C42 |
| 13  | E     | 198 | PEE  | C11-C12-C13-C14 |
| 14  | D     | 242 | BOG  | C3'-C4'-C5'-C6' |
| 13  | E     | 198 | PEE  | C1-C2-C3-O3     |
| 13  | E     | 198 | PEE  | C19-C20-C21-C22 |
| 13  | C     | 384 | PEE  | C12-C13-C14-C15 |
| 13  | C     | 384 | PEE  | C40-C41-C42-C43 |
| 13  | E     | 198 | PEE  | O3P-C1-C2-O2    |
| 13  | C     | 384 | PEE  | C39-C40-C41-C42 |
| 13  | C     | 384 | PEE  | C14-C15-C16-C17 |
| 13  | E     | 198 | PEE  | C41-C42-C43-C44 |
| 12  | C     | 383 | U10  | C9-C11-C12-C13  |
| 13  | C     | 384 | PEE  | C23-C24-C25-C26 |
| 13  | C     | 384 | PEE  | C41-C42-C43-C44 |
| 11  | C     | 382 | HEM  | C2C-C3C-CAC-CBC |
| 11  | D     | 243 | HEM  | C2C-C3C-CAC-CBC |
| 13  | C     | 384 | PEE  | O3P-C1-C2-O2    |
| 13  | C     | 384 | PEE  | O2-C2-C3-O3     |
| 13  | C     | 384 | PEE  | C4-O4P-P-O1P    |
| 13  | E     | 198 | PEE  | O4P-C4-C5-N     |
| 13  | E     | 198 | PEE  | C36-C37-C38-C39 |
| 13  | E     | 198 | PEE  | C40-C41-C42-C43 |
| 11  | C     | 382 | HEM  | C2B-C3B-CAB-CBB |
| 11  | C     | 382 | HEM  | CAA-CBA-CGA-O1A |
| 11  | C     | 381 | HEM  | CAA-CBA-CGA-O1A |
| 11  | C     | 382 | HEM  | CAA-CBA-CGA-O2A |
| 11  | C     | 381 | HEM  | CAA-CBA-CGA-O2A |
| 13  | C     | 384 | PEE  | C16-C17-C18-C19 |
| 13  | E     | 198 | PEE  | C20-C21-C22-C23 |
| 11  | C     | 382 | HEM  | CAD-CBD-CGD-O2D |
| 11  | C     | 382 | HEM  | CAD-CBD-CGD-O1D |
| 13  | C     | 384 | PEE  | C36-C37-C38-C39 |
| 13  | E     | 198 | PEE  | C42-C43-C44-C45 |
| 14  | D     | 242 | BOG  | C4'-C5'-C6'-C7' |
| 11  | D     | 243 | HEM  | CAA-CBA-CGA-O2A |
| 13  | E     | 198 | PEE  | C38-C39-C40-C41 |

*Continued on next page...*

*Continued from previous page...*

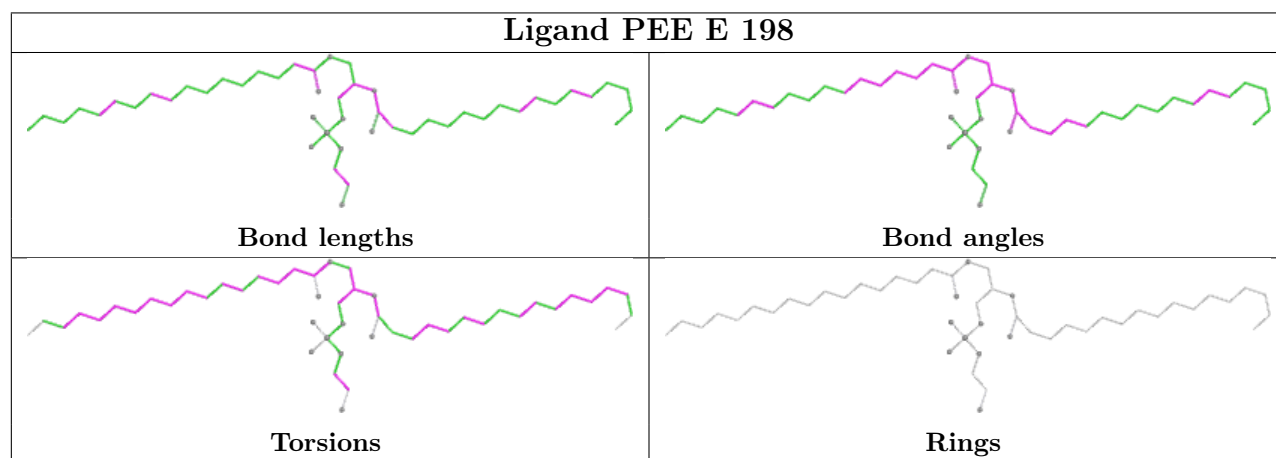
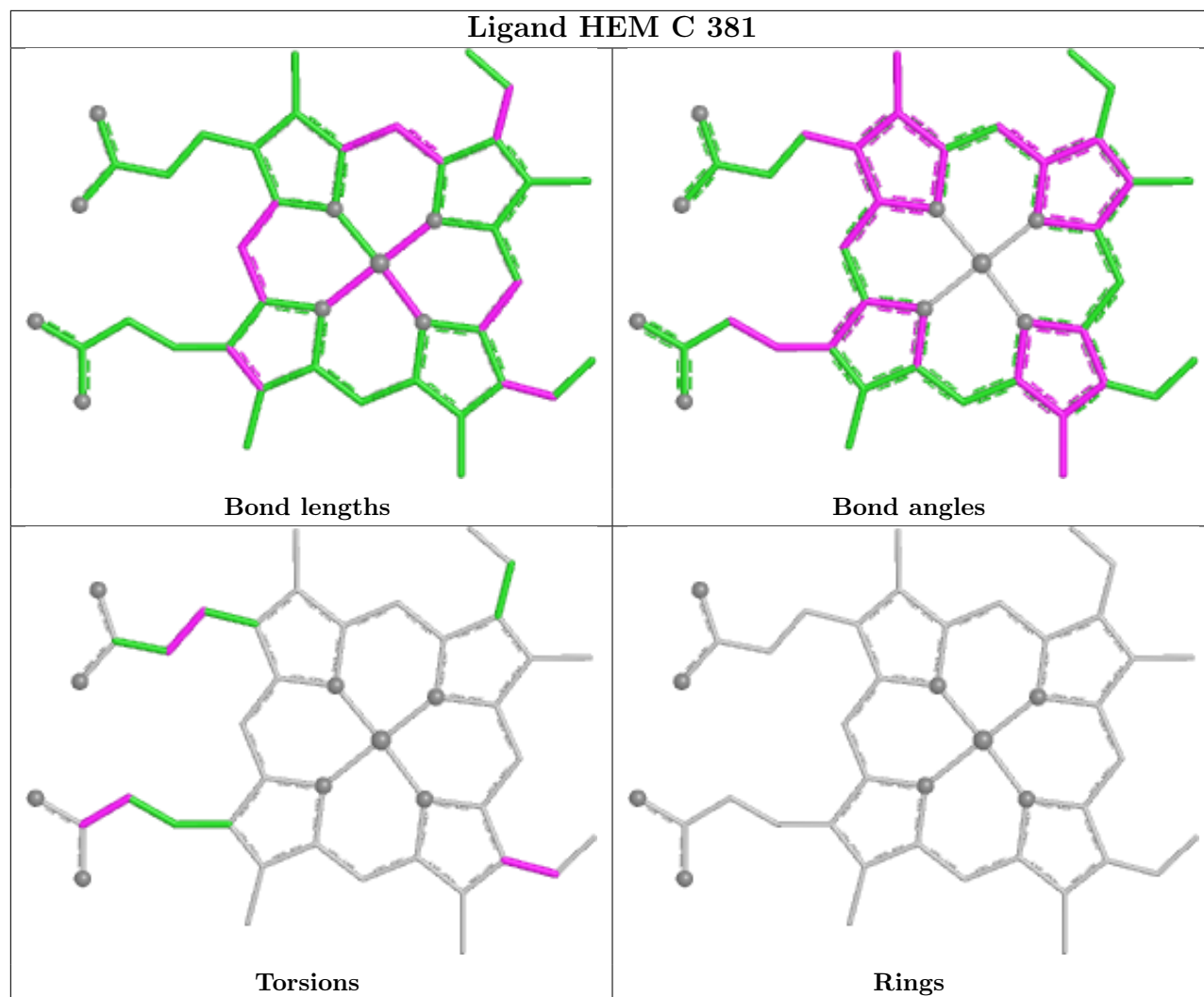
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | D     | 243 | HEM  | C4B-C3B-CAB-CBB |
| 11  | D     | 243 | HEM  | C4C-C3C-CAC-CBC |
| 11  | C     | 381 | HEM  | C3D-CAD-CBD-CGD |
| 13  | C     | 384 | PEE  | O3P-C1-C2-C3    |
| 11  | D     | 243 | HEM  | CAA-CBA-CGA-O1A |
| 13  | E     | 198 | PEE  | C3-C2-O2-C10    |
| 12  | C     | 383 | U10  | C6-C7-C8-C9     |
| 12  | C     | 383 | U10  | C16-C17-C18-C19 |
| 13  | E     | 198 | PEE  | O3-C30-C31-C32  |
| 11  | D     | 243 | HEM  | CAD-CBD-CGD-O2D |

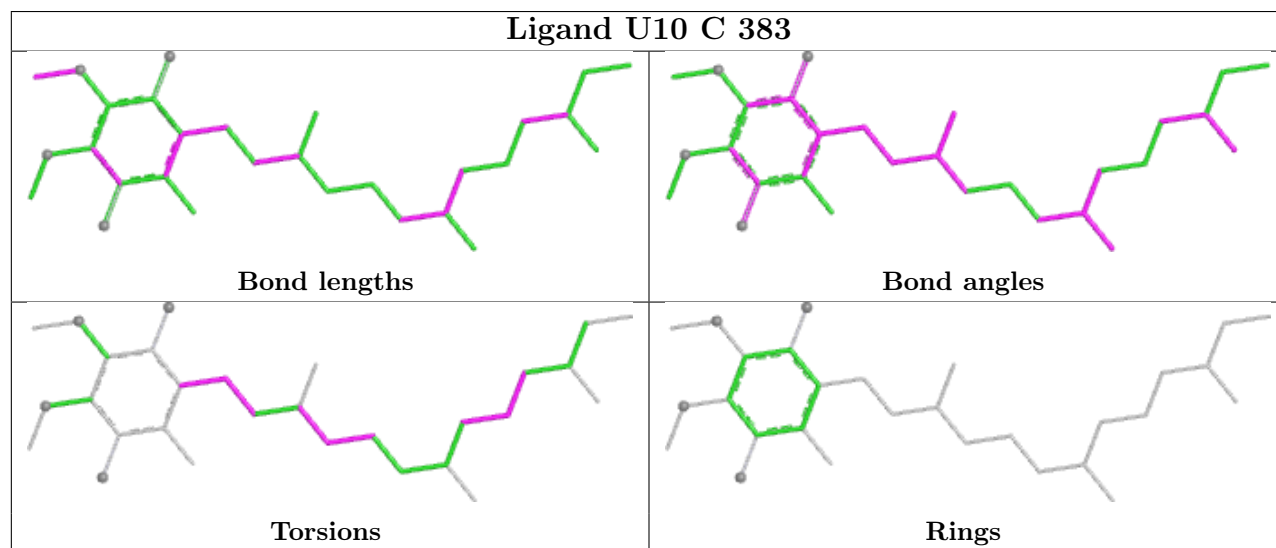
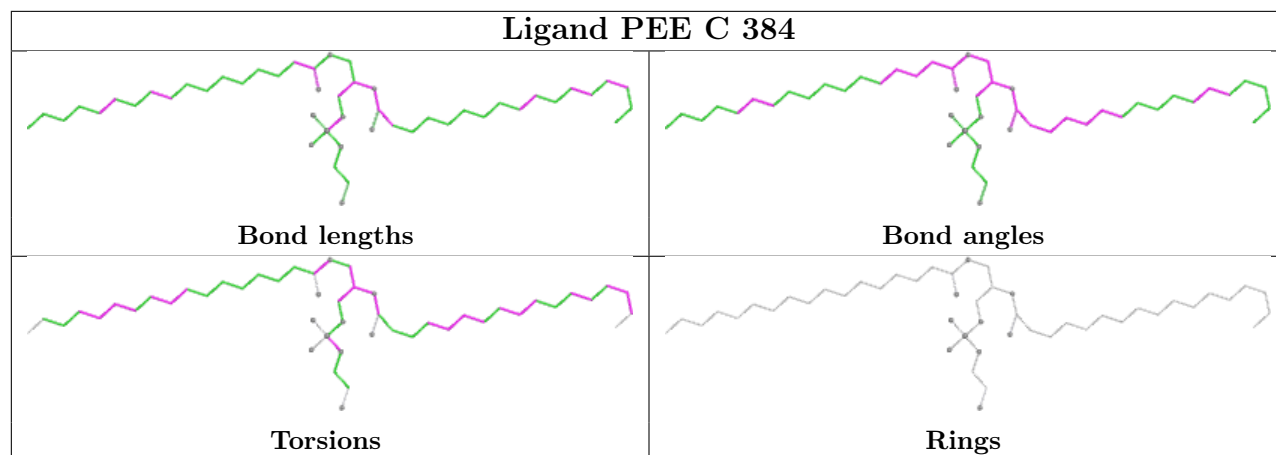
There are no ring outliers.

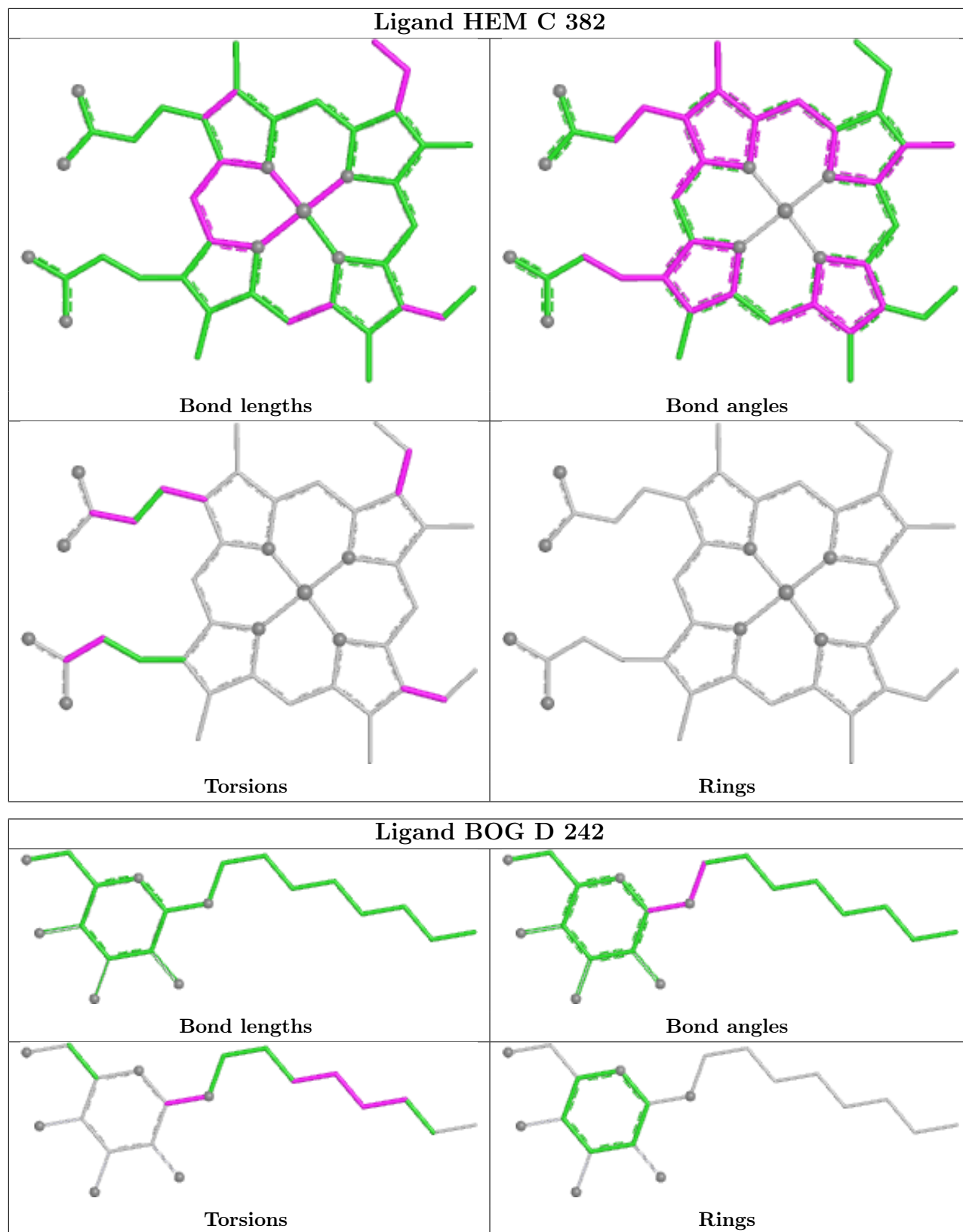
7 monomers are involved in 21 short contacts:

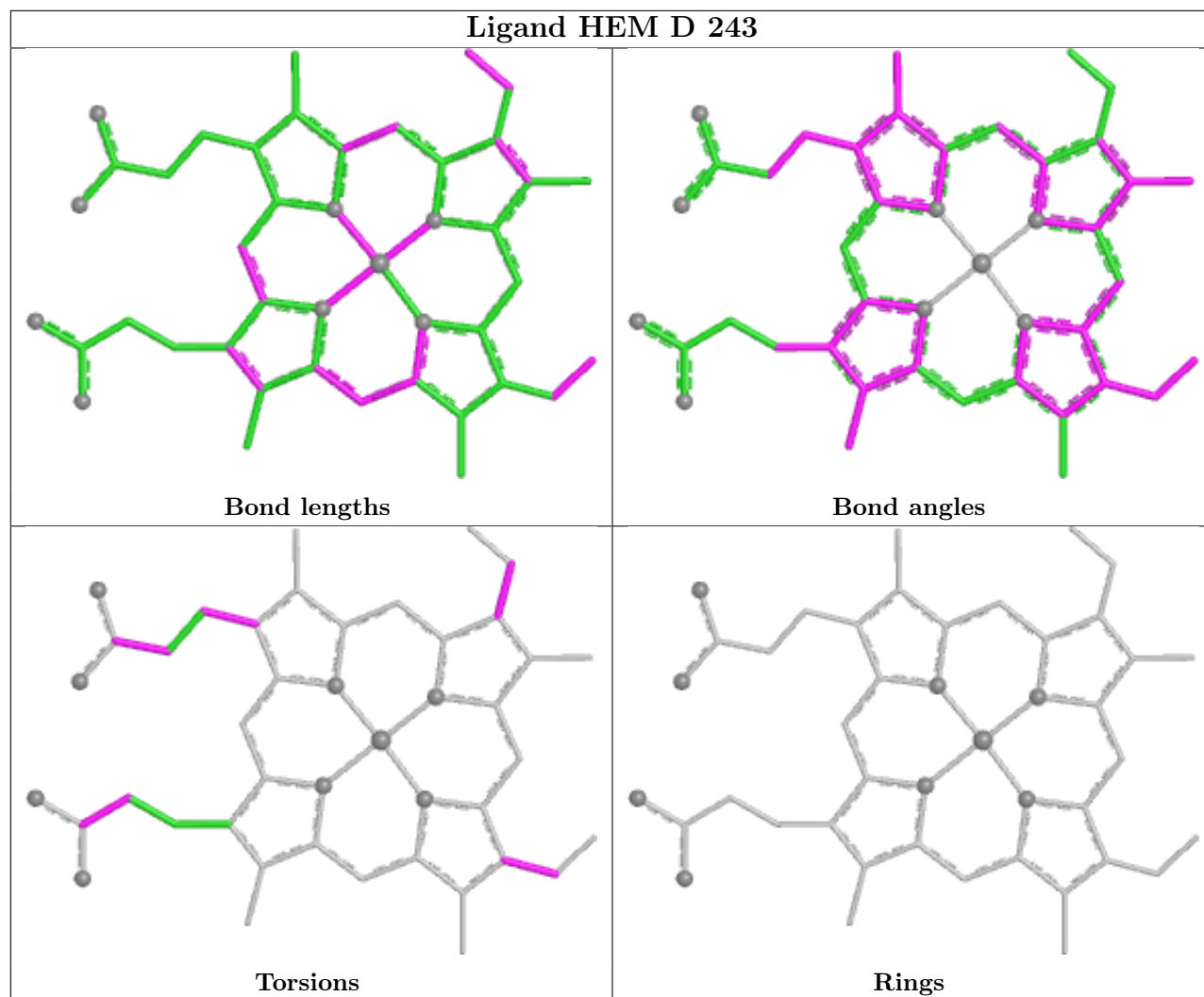
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | C     | 381 | HEM  | 5       | 0            |
| 13  | E     | 198 | PEE  | 1       | 0            |
| 13  | C     | 384 | PEE  | 2       | 0            |
| 12  | C     | 383 | U10  | 2       | 0            |
| 15  | E     | 197 | FES  | 1       | 0            |
| 11  | C     | 382 | HEM  | 7       | 0            |
| 14  | D     | 242 | BOG  | 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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9   | I     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I     | 210:UNK   | C      | 309:UNK   | N      | 33.23        |
| 1     | I     | 121:UNK   | C      | 202:UNK   | N      | 29.43        |

## 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     | 442/446 (99%)   | 1.38   | 113 (25%) <b>1</b> <b>1</b> | 47, 84, 100, 100      | 0     |
| 2   | B     | 406/422 (96%)   | 1.61   | 115 (28%) <b>1</b> <b>1</b> | 60, 93, 100, 100      | 0     |
| 3   | C     | 379/380 (99%)   | 0.89   | 46 (12%) <b>8</b> <b>5</b>  | 33, 64, 96, 100       | 0     |
| 4   | D     | 241/241 (100%)  | 1.16   | 38 (15%) <b>5</b> <b>3</b>  | 50, 76, 99, 100       | 0     |
| 5   | E     | 196/196 (100%)  | 2.43   | 113 (57%) <b>0</b> <b>0</b> | 54, 100, 100, 100     | 0     |
| 6   | F     | 100/109 (91%)   | 1.14   | 16 (16%) <b>5</b> <b>3</b>  | 50, 73, 98, 100       | 0     |
| 7   | G     | 78/81 (96%)     | 1.31   | 18 (23%) <b>2</b> <b>2</b>  | 51, 85, 100, 100      | 0     |
| 8   | H     | 66/78 (84%)     | 1.79   | 30 (45%) <b>0</b> <b>1</b>  | 76, 95, 99, 100       | 0     |
| 9   | I     | 0/33            | -      | -                           | -                     | -     |
| 10  | J     | 59/62 (95%)     | 1.47   | 15 (25%) <b>1</b> <b>1</b>  | 66, 80, 99, 100       | 0     |
| All | All   | 1967/2048 (96%) | 1.41   | 504 (25%) <b>1</b> <b>1</b> | 33, 83, 100, 100      | 0     |

All (504) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 163 | SER  | 7.7  |
| 5   | E     | 162 | GLY  | 7.6  |
| 5   | E     | 114 | VAL  | 7.5  |
| 4   | D     | 75  | ASN  | 6.8  |
| 5   | E     | 141 | HIS  | 6.5  |
| 5   | E     | 174 | GLY  | 6.3  |
| 5   | E     | 117 | LEU  | 6.2  |
| 1   | A     | 32  | GLN  | 6.2  |
| 1   | A     | 220 | PRO  | 6.2  |
| 5   | E     | 111 | ALA  | 6.1  |
| 5   | E     | 124 | LEU  | 5.9  |
| 5   | E     | 191 | ASP  | 5.9  |
| 5   | E     | 189 | SER  | 5.9  |
| 5   | E     | 115 | SER  | 5.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 23  | ASP  | 5.5  |
| 5   | E     | 84  | GLY  | 5.5  |
| 4   | D     | 72  | ASP  | 5.4  |
| 2   | B     | 114 | ASP  | 5.3  |
| 1   | A     | 202 | GLY  | 5.3  |
| 2   | B     | 222 | GLN  | 5.3  |
| 5   | E     | 121 | GLN  | 5.3  |
| 1   | A     | 380 | GLY  | 5.2  |
| 5   | E     | 150 | ALA  | 5.2  |
| 8   | H     | 26  | GLN  | 5.1  |
| 1   | A     | 96  | ALA  | 5.0  |
| 2   | B     | 423 | SER  | 4.9  |
| 2   | B     | 170 | ASN  | 4.9  |
| 5   | E     | 102 | THR  | 4.9  |
| 2   | B     | 305 | ASN  | 4.9  |
| 2   | B     | 212 | SER  | 4.8  |
| 5   | E     | 177 | PRO  | 4.8  |
| 5   | E     | 139 | CYS  | 4.8  |
| 5   | E     | 155 | GLY  | 4.8  |
| 2   | B     | 20  | HIS  | 4.8  |
| 1   | A     | 20  | ASP  | 4.8  |
| 10  | J     | 8   | ARG  | 4.7  |
| 10  | J     | 61  | ASN  | 4.7  |
| 5   | E     | 159 | PRO  | 4.7  |
| 5   | E     | 171 | ILE  | 4.7  |
| 2   | B     | 419 | SER  | 4.6  |
| 2   | B     | 40  | ASN  | 4.6  |
| 1   | A     | 101 | ALA  | 4.5  |
| 3   | C     | 35  | GLY  | 4.5  |
| 6   | F     | 91  | GLU  | 4.4  |
| 1   | A     | 412 | SER  | 4.4  |
| 2   | B     | 260 | GLU  | 4.4  |
| 7   | G     | 26  | PHE  | 4.4  |
| 4   | D     | 139 | THR  | 4.4  |
| 1   | A     | 120 | CYS  | 4.4  |
| 5   | E     | 98  | VAL  | 4.3  |
| 5   | E     | 87  | MET  | 4.3  |
| 5   | E     | 169 | GLY  | 4.3  |
| 1   | A     | 147 | GLU  | 4.3  |
| 4   | D     | 31  | GLN  | 4.2  |
| 5   | E     | 192 | MET  | 4.2  |
| 5   | E     | 161 | HIS  | 4.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 188 | THR  | 4.2  |
| 4   | D     | 228 | SER  | 4.2  |
| 2   | B     | 273 | SER  | 4.1  |
| 4   | D     | 65  | ALA  | 4.1  |
| 3   | C     | 158 | GLY  | 4.1  |
| 5   | E     | 165 | TYR  | 4.1  |
| 5   | E     | 158 | CYS  | 4.1  |
| 5   | E     | 146 | PRO  | 4.0  |
| 5   | E     | 110 | ALA  | 4.0  |
| 4   | D     | 180 | SER  | 3.9  |
| 5   | E     | 176 | ALA  | 3.9  |
| 2   | B     | 375 | SER  | 3.9  |
| 2   | B     | 18  | PRO  | 3.9  |
| 4   | D     | 239 | PRO  | 3.9  |
| 3   | C     | 48  | THR  | 3.8  |
| 8   | H     | 36  | ARG  | 3.8  |
| 5   | E     | 127 | VAL  | 3.8  |
| 2   | B     | 129 | ALA  | 3.8  |
| 4   | D     | 125 | ASP  | 3.8  |
| 5   | E     | 140 | THR  | 3.8  |
| 1   | A     | 437 | ILE  | 3.7  |
| 10  | J     | 19  | THR  | 3.7  |
| 5   | E     | 79  | SER  | 3.7  |
| 2   | B     | 181 | TYR  | 3.7  |
| 2   | B     | 397 | THR  | 3.7  |
| 5   | E     | 194 | ILE  | 3.7  |
| 5   | E     | 151 | GLY  | 3.7  |
| 5   | E     | 153 | PHE  | 3.7  |
| 4   | D     | 67  | GLU  | 3.6  |
| 5   | E     | 195 | VAL  | 3.6  |
| 5   | E     | 109 | GLU  | 3.6  |
| 1   | A     | 15  | GLN  | 3.6  |
| 3   | C     | 371 | GLY  | 3.6  |
| 5   | E     | 160 | CYS  | 3.6  |
| 7   | G     | 31  | SER  | 3.6  |
| 1   | A     | 223 | TYR  | 3.6  |
| 1   | A     | 118 | GLN  | 3.5  |
| 5   | E     | 112 | VAL  | 3.5  |
| 2   | B     | 224 | LEU  | 3.5  |
| 2   | B     | 226 | ILE  | 3.5  |
| 5   | E     | 108 | GLN  | 3.5  |
| 2   | B     | 281 | ALA  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | H     | 53  | ASP  | 3.5  |
| 5   | E     | 132 | TRP  | 3.5  |
| 3   | C     | 5   | ILE  | 3.5  |
| 2   | B     | 431 | GLY  | 3.5  |
| 4   | D     | 16  | GLY  | 3.5  |
| 5   | E     | 122 | HIS  | 3.5  |
| 5   | E     | 76  | ILE  | 3.4  |
| 5   | E     | 181 | GLU  | 3.4  |
| 2   | B     | 60  | SER  | 3.4  |
| 2   | B     | 100 | SER  | 3.4  |
| 2   | B     | 353 | SER  | 3.4  |
| 1   | A     | 403 | ASP  | 3.4  |
| 5   | E     | 113 | GLU  | 3.4  |
| 2   | B     | 200 | THR  | 3.4  |
| 3   | C     | 157 | ILE  | 3.4  |
| 5   | E     | 157 | TYR  | 3.4  |
| 1   | A     | 7   | ALA  | 3.4  |
| 3   | C     | 160 | THR  | 3.4  |
| 2   | B     | 370 | MET  | 3.4  |
| 1   | A     | 264 | HIS  | 3.4  |
| 3   | C     | 361 | THR  | 3.4  |
| 2   | B     | 197 | ASN  | 3.3  |
| 1   | A     | 281 | ASP  | 3.3  |
| 2   | B     | 439 | LEU  | 3.3  |
| 8   | H     | 15  | ASP  | 3.3  |
| 1   | A     | 52  | ASN  | 3.3  |
| 5   | E     | 96  | LEU  | 3.3  |
| 4   | D     | 80  | MET  | 3.3  |
| 2   | B     | 371 | SER  | 3.3  |
| 1   | A     | 119 | ASN  | 3.3  |
| 7   | G     | 77  | TYR  | 3.2  |
| 2   | B     | 19  | PRO  | 3.2  |
| 2   | B     | 134 | PRO  | 3.2  |
| 1   | A     | 8   | LEU  | 3.2  |
| 2   | B     | 408 | ALA  | 3.2  |
| 1   | A     | 187 | SER  | 3.2  |
| 4   | D     | 108 | ALA  | 3.2  |
| 5   | E     | 100 | HIS  | 3.2  |
| 2   | B     | 438 | GLU  | 3.2  |
| 5   | E     | 142 | LEU  | 3.2  |
| 6   | F     | 16  | ILE  | 3.2  |
| 10  | J     | 18  | SER  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 167 | ALA  | 3.2  |
| 8   | H     | 25  | GLU  | 3.1  |
| 1   | A     | 73  | ASN  | 3.1  |
| 5   | E     | 187 | PHE  | 3.1  |
| 2   | B     | 118 | ILE  | 3.1  |
| 4   | D     | 158 | ILE  | 3.1  |
| 6   | F     | 72  | GLN  | 3.1  |
| 5   | E     | 106 | ILE  | 3.1  |
| 2   | B     | 175 | SER  | 3.1  |
| 8   | H     | 23  | GLN  | 3.1  |
| 5   | E     | 72  | SER  | 3.1  |
| 1   | A     | 221 | PHE  | 3.1  |
| 1   | A     | 195 | MET  | 3.1  |
| 1   | A     | 390 | ILE  | 3.1  |
| 5   | E     | 86  | ASN  | 3.1  |
| 6   | F     | 22  | ASN  | 3.1  |
| 8   | H     | 46  | SER  | 3.1  |
| 1   | A     | 71  | PRO  | 3.1  |
| 2   | B     | 288 | GLY  | 3.0  |
| 1   | A     | 76  | GLU  | 3.0  |
| 2   | B     | 61  | SER  | 3.0  |
| 6   | F     | 14  | GLU  | 3.0  |
| 2   | B     | 263 | ALA  | 3.0  |
| 4   | D     | 100 | ALA  | 3.0  |
| 6   | F     | 21  | TYR  | 3.0  |
| 1   | A     | 151 | ASN  | 3.0  |
| 3   | C     | 17  | ASN  | 3.0  |
| 5   | E     | 85  | LYS  | 3.0  |
| 1   | A     | 140 | GLU  | 3.0  |
| 1   | A     | 102 | LEU  | 3.0  |
| 10  | J     | 49  | GLY  | 3.0  |
| 2   | B     | 26  | ILE  | 3.0  |
| 6   | F     | 70  | MET  | 3.0  |
| 4   | D     | 99  | GLU  | 3.0  |
| 5   | E     | 95  | PRO  | 3.0  |
| 5   | E     | 178 | LEU  | 3.0  |
| 10  | J     | 44  | GLU  | 3.0  |
| 7   | G     | 76  | ALA  | 3.0  |
| 10  | J     | 54  | HIS  | 3.0  |
| 1   | A     | 367 | SER  | 2.9  |
| 5   | E     | 173 | LYS  | 2.9  |
| 2   | B     | 235 | ALA  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 359 | ALA  | 2.9  |
| 1   | A     | 27  | SER  | 2.9  |
| 3   | C     | 156 | TYR  | 2.9  |
| 1   | A     | 42  | ASP  | 2.9  |
| 5   | E     | 29  | ASP  | 2.9  |
| 5   | E     | 80  | ASP  | 2.9  |
| 8   | H     | 31  | VAL  | 2.9  |
| 2   | B     | 119 | LEU  | 2.9  |
| 2   | B     | 123 | LEU  | 2.9  |
| 5   | E     | 152 | ASP  | 2.9  |
| 4   | D     | 203 | ARG  | 2.9  |
| 5   | E     | 128 | LYS  | 2.9  |
| 5   | E     | 60  | SER  | 2.8  |
| 5   | E     | 148 | ALA  | 2.8  |
| 2   | B     | 346 | THR  | 2.8  |
| 8   | H     | 52  | GLU  | 2.8  |
| 6   | F     | 24  | ALA  | 2.8  |
| 4   | D     | 84  | PRO  | 2.8  |
| 2   | B     | 398 | VAL  | 2.8  |
| 2   | B     | 29  | LEU  | 2.8  |
| 2   | B     | 198 | HIS  | 2.8  |
| 2   | B     | 396 | SER  | 2.8  |
| 4   | D     | 102 | ARG  | 2.8  |
| 2   | B     | 405 | VAL  | 2.8  |
| 1   | A     | 413 | LYS  | 2.8  |
| 4   | D     | 136 | GLU  | 2.8  |
| 10  | J     | 45  | HIS  | 2.8  |
| 1   | A     | 214 | LYS  | 2.8  |
| 1   | A     | 134 | ILE  | 2.8  |
| 1   | A     | 368 | HIS  | 2.8  |
| 2   | B     | 36  | ALA  | 2.8  |
| 1   | A     | 370 | ASP  | 2.7  |
| 8   | H     | 41  | ASP  | 2.7  |
| 6   | F     | 53  | ASN  | 2.7  |
| 4   | D     | 118 | ARG  | 2.7  |
| 6   | F     | 102 | LYS  | 2.7  |
| 1   | A     | 11  | VAL  | 2.7  |
| 1   | A     | 444 | LEU  | 2.7  |
| 5   | E     | 147 | ILE  | 2.7  |
| 3   | C     | 4   | ASN  | 2.7  |
| 5   | E     | 129 | LYS  | 2.7  |
| 10  | J     | 7   | ALA  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 204 | GLU  | 2.7  |
| 3   | C     | 168 | GLY  | 2.7  |
| 3   | C     | 6   | ARG  | 2.7  |
| 5   | E     | 190 | ASP  | 2.7  |
| 2   | B     | 341 | TYR  | 2.7  |
| 6   | F     | 87  | VAL  | 2.7  |
| 2   | B     | 400 | GLN  | 2.7  |
| 2   | B     | 111 | CYS  | 2.7  |
| 1   | A     | 103 | SER  | 2.7  |
| 2   | B     | 220 | ALA  | 2.7  |
| 5   | E     | 145 | VAL  | 2.7  |
| 8   | H     | 67  | HIS  | 2.7  |
| 2   | B     | 82  | SER  | 2.7  |
| 3   | C     | 206 | SER  | 2.7  |
| 2   | B     | 171 | ALA  | 2.7  |
| 8   | H     | 64  | ALA  | 2.7  |
| 1   | A     | 384 | LEU  | 2.7  |
| 2   | B     | 282 | ASN  | 2.7  |
| 1   | A     | 12  | PRO  | 2.6  |
| 2   | B     | 153 | GLN  | 2.6  |
| 5   | E     | 30  | PRO  | 2.6  |
| 5   | E     | 175 | PRO  | 2.6  |
| 5   | E     | 131 | GLU  | 2.6  |
| 1   | A     | 191 | THR  | 2.6  |
| 2   | B     | 330 | ALA  | 2.6  |
| 8   | H     | 33  | ALA  | 2.6  |
| 5   | E     | 166 | ASP  | 2.6  |
| 2   | B     | 104 | ASN  | 2.6  |
| 2   | B     | 395 | PRO  | 2.6  |
| 6   | F     | 92  | PRO  | 2.6  |
| 10  | J     | 62  | LYS  | 2.6  |
| 3   | C     | 131 | GLY  | 2.6  |
| 5   | E     | 143 | GLY  | 2.6  |
| 8   | H     | 28  | GLU  | 2.6  |
| 7   | G     | 63  | THR  | 2.6  |
| 1   | A     | 79  | VAL  | 2.6  |
| 2   | B     | 267 | ALA  | 2.6  |
| 2   | B     | 233 | SER  | 2.6  |
| 8   | H     | 45  | SER  | 2.6  |
| 5   | E     | 185 | TYR  | 2.6  |
| 6   | F     | 71  | ARG  | 2.6  |
| 2   | B     | 342 | ASN  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | E     | 179 | ASN  | 2.6  |
| 1   | A     | 261 | GLY  | 2.6  |
| 8   | H     | 51  | GLU  | 2.6  |
| 2   | B     | 106 | ALA  | 2.6  |
| 5   | E     | 168 | SER  | 2.6  |
| 7   | G     | 28  | HIS  | 2.6  |
| 4   | D     | 167 | ASP  | 2.6  |
| 1   | A     | 208 | LEU  | 2.6  |
| 1   | A     | 196 | VAL  | 2.6  |
| 2   | B     | 219 | VAL  | 2.6  |
| 5   | E     | 5   | ILE  | 2.6  |
| 4   | D     | 88  | SER  | 2.6  |
| 5   | E     | 183 | PRO  | 2.6  |
| 1   | A     | 206 | GLN  | 2.6  |
| 3   | C     | 379 | ASN  | 2.6  |
| 1   | A     | 394 | GLU  | 2.6  |
| 2   | B     | 404 | ALA  | 2.6  |
| 7   | G     | 30  | PHE  | 2.5  |
| 10  | J     | 20  | PHE  | 2.5  |
| 2   | B     | 386 | ALA  | 2.5  |
| 3   | C     | 335 | ILE  | 2.5  |
| 3   | C     | 346 | HIS  | 2.5  |
| 5   | E     | 156 | TYR  | 2.5  |
| 4   | D     | 5   | LEU  | 2.5  |
| 1   | A     | 263 | ALA  | 2.5  |
| 1   | A     | 378 | ASP  | 2.5  |
| 1   | A     | 409 | GLU  | 2.5  |
| 3   | C     | 2   | ALA  | 2.5  |
| 1   | A     | 329 | MET  | 2.5  |
| 4   | D     | 33  | TYR  | 2.5  |
| 8   | H     | 32  | LYS  | 2.5  |
| 5   | E     | 65  | SER  | 2.5  |
| 6   | F     | 73  | GLN  | 2.5  |
| 3   | C     | 63  | ALA  | 2.5  |
| 1   | A     | 111 | GLU  | 2.5  |
| 1   | A     | 87  | ASN  | 2.5  |
| 3   | C     | 287 | ASN  | 2.5  |
| 1   | A     | 57  | TYR  | 2.5  |
| 2   | B     | 192 | HIS  | 2.5  |
| 2   | B     | 227 | ARG  | 2.5  |
| 7   | G     | 29  | TYR  | 2.5  |
| 3   | C     | 138 | GLN  | 2.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 275 | ALA  | 2.5  |
| 2   | B     | 81  | SER  | 2.5  |
| 3   | C     | 255 | GLU  | 2.5  |
| 1   | A     | 332 | ASP  | 2.5  |
| 2   | B     | 31  | ASN  | 2.5  |
| 3   | C     | 13  | LYS  | 2.5  |
| 2   | B     | 66  | SER  | 2.4  |
| 1   | A     | 358 | LYS  | 2.4  |
| 2   | B     | 225 | ASN  | 2.4  |
| 5   | E     | 99  | ARG  | 2.4  |
| 5   | E     | 126 | ARG  | 2.4  |
| 2   | B     | 27  | THR  | 2.4  |
| 3   | C     | 10  | PRO  | 2.4  |
| 2   | B     | 323 | GLY  | 2.4  |
| 5   | E     | 154 | GLY  | 2.4  |
| 5   | E     | 11  | SER  | 2.4  |
| 7   | G     | 42  | ARG  | 2.4  |
| 3   | C     | 11  | LEU  | 2.4  |
| 7   | G     | 8   | THR  | 2.4  |
| 2   | B     | 213 | HIS  | 2.4  |
| 2   | B     | 285 | VAL  | 2.4  |
| 2   | B     | 389 | ALA  | 2.4  |
| 5   | E     | 88  | ALA  | 2.4  |
| 5   | E     | 172 | ARG  | 2.4  |
| 1   | A     | 211 | LEU  | 2.4  |
| 7   | G     | 73  | ASN  | 2.4  |
| 3   | C     | 106 | GLY  | 2.4  |
| 7   | G     | 33  | GLY  | 2.4  |
| 2   | B     | 39  | GLU  | 2.4  |
| 3   | C     | 373 | LEU  | 2.4  |
| 8   | H     | 27  | LEU  | 2.4  |
| 8   | H     | 62  | LEU  | 2.4  |
| 5   | E     | 24  | SER  | 2.4  |
| 1   | A     | 376 | CYS  | 2.4  |
| 8   | H     | 68  | CYS  | 2.4  |
| 1   | A     | 391 | PRO  | 2.4  |
| 2   | B     | 432 | HIS  | 2.4  |
| 4   | D     | 103 | ALA  | 2.4  |
| 8   | H     | 49  | GLN  | 2.4  |
| 2   | B     | 379 | LEU  | 2.4  |
| 8   | H     | 39  | LEU  | 2.4  |
| 1   | A     | 28  | GLU  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 10  | SER  | 2.4  |
| 1   | A     | 160 | GLY  | 2.3  |
| 1   | A     | 317 | THR  | 2.3  |
| 5   | E     | 3   | THR  | 2.3  |
| 2   | B     | 248 | ASN  | 2.3  |
| 2   | B     | 388 | ALA  | 2.3  |
| 1   | A     | 225 | ASP  | 2.3  |
| 1   | A     | 341 | GLN  | 2.3  |
| 2   | B     | 216 | LEU  | 2.3  |
| 5   | E     | 105 | GLU  | 2.3  |
| 6   | F     | 52  | GLU  | 2.3  |
| 1   | A     | 285 | GLY  | 2.3  |
| 4   | D     | 78  | GLY  | 2.3  |
| 1   | A     | 313 | CYS  | 2.3  |
| 2   | B     | 246 | GLU  | 2.3  |
| 1   | A     | 77  | LYS  | 2.3  |
| 4   | D     | 85  | GLY  | 2.3  |
| 4   | D     | 211 | MET  | 2.3  |
| 1   | A     | 186 | LEU  | 2.3  |
| 1   | A     | 369 | LEU  | 2.3  |
| 1   | A     | 399 | LEU  | 2.3  |
| 3   | C     | 256 | ASN  | 2.3  |
| 3   | C     | 375 | ASN  | 2.3  |
| 1   | A     | 29  | GLN  | 2.3  |
| 8   | H     | 44  | VAL  | 2.3  |
| 4   | D     | 144 | ARG  | 2.3  |
| 7   | G     | 47  | ARG  | 2.3  |
| 2   | B     | 229 | GLY  | 2.3  |
| 3   | C     | 358 | SER  | 2.3  |
| 2   | B     | 112 | LEU  | 2.3  |
| 8   | H     | 63  | HIS  | 2.3  |
| 5   | E     | 94  | LYS  | 2.3  |
| 1   | A     | 397 | GLU  | 2.3  |
| 5   | E     | 15  | ARG  | 2.3  |
| 1   | A     | 201 | GLY  | 2.3  |
| 2   | B     | 173 | ALA  | 2.3  |
| 6   | F     | 13  | LEU  | 2.3  |
| 7   | G     | 66  | PHE  | 2.3  |
| 1   | A     | 363 | ASN  | 2.3  |
| 1   | A     | 18  | GLN  | 2.3  |
| 1   | A     | 100 | LYS  | 2.3  |
| 2   | B     | 203 | ARG  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 329 | GLN  | 2.3  |
| 8   | H     | 60  | ASP  | 2.3  |
| 2   | B     | 377 | GLY  | 2.2  |
| 3   | C     | 167 | GLY  | 2.2  |
| 10  | J     | 30  | LEU  | 2.2  |
| 3   | C     | 284 | SER  | 2.2  |
| 1   | A     | 179 | ARG  | 2.2  |
| 4   | D     | 83  | ARG  | 2.2  |
| 8   | H     | 47  | ARG  | 2.2  |
| 1   | A     | 53  | ASN  | 2.2  |
| 1   | A     | 207 | GLN  | 2.2  |
| 2   | B     | 276 | GLN  | 2.2  |
| 3   | C     | 16  | ASN  | 2.2  |
| 5   | E     | 138 | VAL  | 2.2  |
| 1   | A     | 227 | ALA  | 2.2  |
| 8   | H     | 13  | LEU  | 2.2  |
| 8   | H     | 37  | LEU  | 2.2  |
| 2   | B     | 385 | GLN  | 2.2  |
| 5   | E     | 144 | CYS  | 2.2  |
| 2   | B     | 24  | LEU  | 2.2  |
| 4   | D     | 240 | PRO  | 2.2  |
| 7   | G     | 25  | PRO  | 2.2  |
| 1   | A     | 336 | PHE  | 2.2  |
| 2   | B     | 307 | PHE  | 2.2  |
| 1   | A     | 143 | THR  | 2.2  |
| 1   | A     | 222 | THR  | 2.2  |
| 3   | C     | 113 | THR  | 2.2  |
| 2   | B     | 325 | TYR  | 2.2  |
| 1   | A     | 366 | VAL  | 2.2  |
| 2   | B     | 59  | ASN  | 2.2  |
| 2   | B     | 430 | LEU  | 2.2  |
| 3   | C     | 163 | GLU  | 2.2  |
| 2   | B     | 318 | ASP  | 2.2  |
| 1   | A     | 189 | HIS  | 2.2  |
| 5   | E     | 182 | VAL  | 2.2  |
| 2   | B     | 146 | ILE  | 2.2  |
| 5   | E     | 116 | GLN  | 2.2  |
| 3   | C     | 334 | LEU  | 2.2  |
| 1   | A     | 48  | GLU  | 2.2  |
| 5   | E     | 70  | ALA  | 2.2  |
| 5   | E     | 149 | ASN  | 2.2  |
| 7   | G     | 43  | ALA  | 2.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 73  | GLY  | 2.2  |
| 5   | E     | 34  | GLY  | 2.2  |
| 5   | E     | 77  | LYS  | 2.2  |
| 5   | E     | 90  | LYS  | 2.2  |
| 5   | E     | 118 | ARG  | 2.2  |
| 8   | H     | 54  | CYS  | 2.2  |
| 1   | A     | 372 | THR  | 2.1  |
| 3   | C     | 177 | THR  | 2.1  |
| 5   | E     | 22  | THR  | 2.1  |
| 1   | A     | 90  | SER  | 2.1  |
| 1   | A     | 292 | SER  | 2.1  |
| 2   | B     | 28  | LYS  | 2.1  |
| 2   | B     | 188 | SER  | 2.1  |
| 1   | A     | 184 | GLU  | 2.1  |
| 1   | A     | 210 | GLU  | 2.1  |
| 2   | B     | 262 | ALA  | 2.1  |
| 2   | B     | 317 | SER  | 2.1  |
| 3   | C     | 345 | GLU  | 2.1  |
| 2   | B     | 351 | ASN  | 2.1  |
| 1   | A     | 115 | ASP  | 2.1  |
| 5   | E     | 56  | THR  | 2.1  |
| 4   | D     | 109 | LEU  | 2.1  |
| 1   | A     | 6   | GLN  | 2.1  |
| 2   | B     | 230 | LEU  | 2.1  |
| 3   | C     | 354 | MET  | 2.1  |
| 1   | A     | 5   | ALA  | 2.1  |
| 3   | C     | 144 | ALA  | 2.1  |
| 1   | A     | 291 | SER  | 2.1  |
| 2   | B     | 97  | SER  | 2.1  |
| 1   | A     | 359 | ASN  | 2.1  |
| 7   | G     | 53  | LEU  | 2.1  |
| 2   | B     | 343 | GLN  | 2.1  |
| 3   | C     | 352 | GLY  | 2.1  |
| 8   | H     | 38  | GLU  | 2.1  |
| 5   | E     | 21  | SER  | 2.1  |
| 2   | B     | 287 | ARG  | 2.1  |
| 3   | C     | 166 | TRP  | 2.1  |
| 10  | J     | 15  | ARG  | 2.1  |
| 5   | E     | 119 | ASP  | 2.1  |
| 2   | B     | 76  | THR  | 2.1  |
| 3   | C     | 14  | MET  | 2.1  |
| 5   | E     | 20  | TYR  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10  | J     | 37  | GLN  | 2.1  |
| 1   | A     | 427 | PRO  | 2.1  |
| 4   | D     | 138 | PRO  | 2.1  |
| 5   | E     | 27  | GLU  | 2.1  |
| 5   | E     | 75  | GLU  | 2.1  |
| 7   | G     | 74  | PRO  | 2.1  |
| 3   | C     | 298 | SER  | 2.0  |
| 2   | B     | 277 | HIS  | 2.0  |
| 4   | D     | 212 | MET  | 2.0  |
| 1   | A     | 185 | TYR  | 2.0  |
| 1   | A     | 357 | GLY  | 2.0  |
| 5   | E     | 89  | PHE  | 2.0  |
| 4   | D     | 58  | GLU  | 2.0  |
| 1   | A     | 194 | ARG  | 2.0  |
| 1   | A     | 209 | LEU  | 2.0  |
| 5   | E     | 92  | ARG  | 2.0  |
| 1   | A     | 315 | SER  | 2.0  |
| 5   | E     | 184 | SER  | 2.0  |
| 10  | J     | 11  | SER  | 2.0  |
| 3   | C     | 164 | TRP  | 2.0  |
| 2   | B     | 138 | ALA  | 2.0  |
| 2   | B     | 168 | TYR  | 2.0  |
| 4   | D     | 77  | ASP  | 2.0  |
| 1   | A     | 68  | LYS  | 2.0  |
| 1   | A     | 326 | CYS  | 2.0  |
| 2   | B     | 113 | ARG  | 2.0  |
| 1   | A     | 182 | LEU  | 2.0  |
| 1   | A     | 297 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

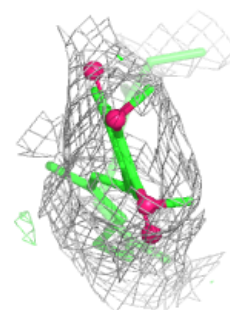
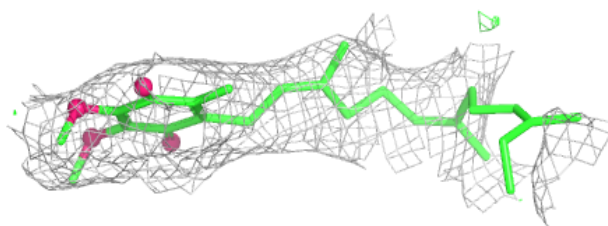
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 12  | U10  | C     | 383 | 29/63 | 0.63 | 0.21 | 77,83,100,100              | 29    |
| 13  | PEE  | E     | 198 | 49/51 | 0.76 | 0.18 | 24,45,64,65                | 49    |
| 14  | BOG  | D     | 242 | 20/20 | 0.81 | 0.13 | 37,59,70,72                | 20    |
| 13  | PEE  | C     | 384 | 49/51 | 0.84 | 0.12 | 20,39,54,55                | 49    |
| 11  | HEM  | C     | 382 | 43/43 | 0.94 | 0.13 | 43,46,59,62                | 0     |
| 11  | HEM  | C     | 381 | 43/43 | 0.95 | 0.10 | 43,51,59,62                | 0     |
| 11  | HEM  | D     | 243 | 43/43 | 0.95 | 0.10 | 46,58,69,74                | 0     |
| 15  | FES  | E     | 197 | 4/4   | 0.96 | 0.17 | 100,100,100,100            | 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.

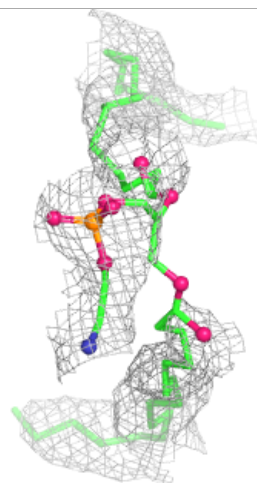
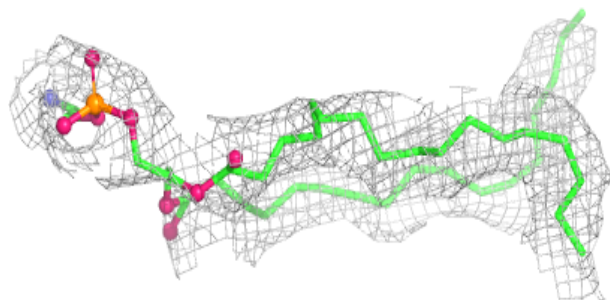
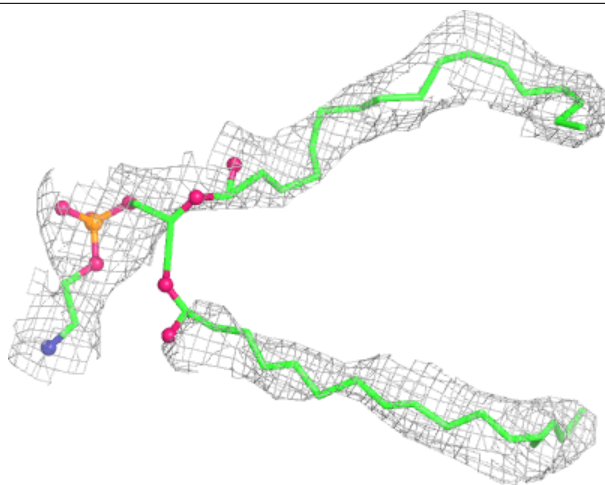
**Electron density around U10 C 383:**

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)



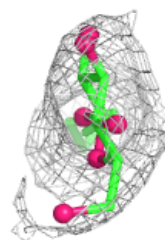
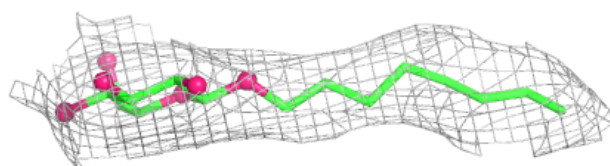
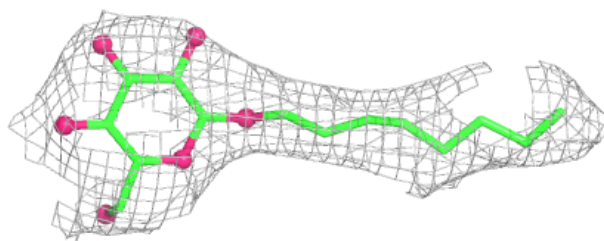
**Electron density around PEE E 198:**

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

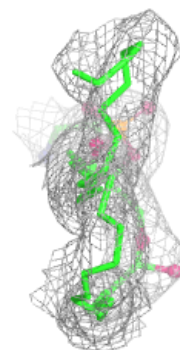
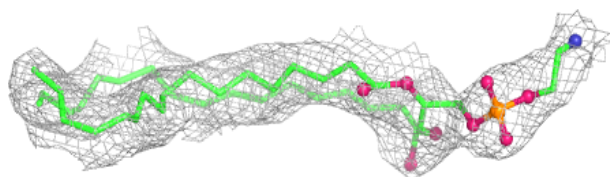
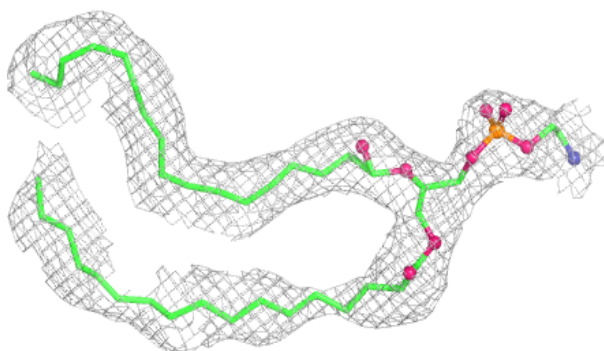


**Electron density around BOG D 242:**

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

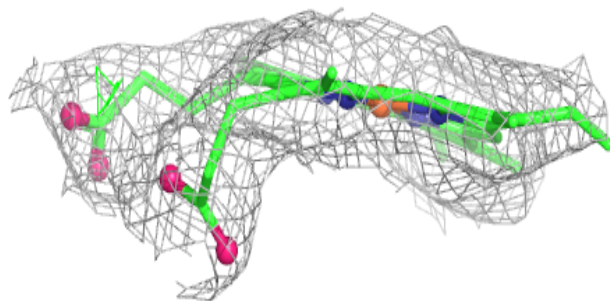
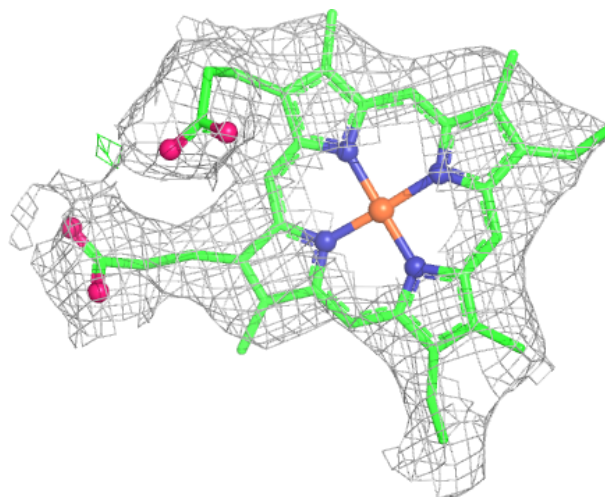
**Electron density around PEE C 384:**

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



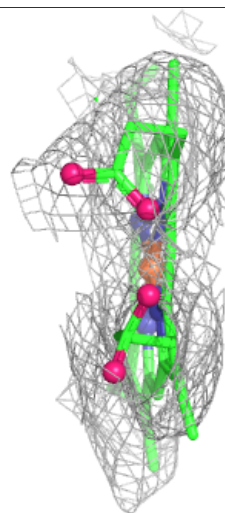
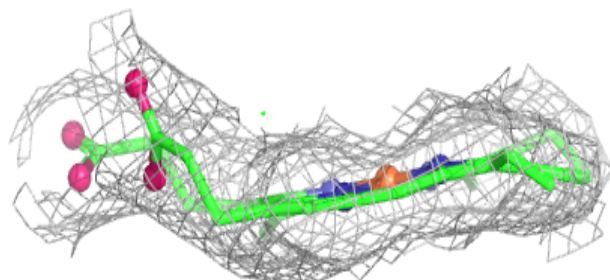
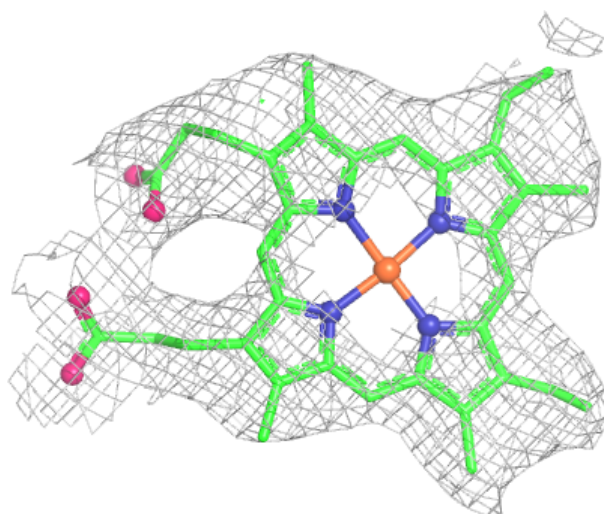
**Electron density around HEM C 382:**

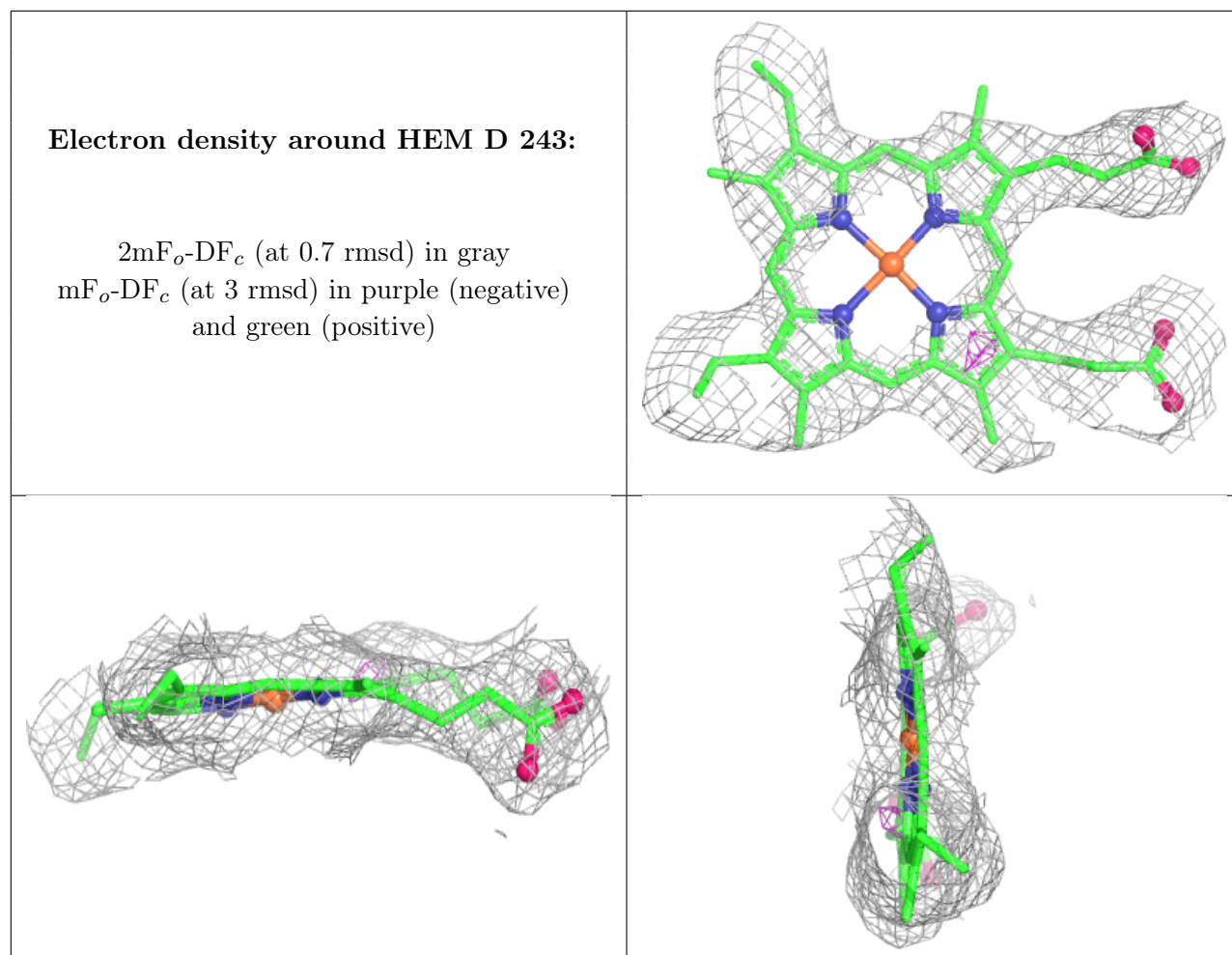
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 381:**

$2mF_o-DF_c$  (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.