



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:46 PM UTC

PDB ID : 1ND5 / pdb\_00001nd5  
Title : Crystal Structures of Human Prostatic Acid Phosphatase in Complex with a Phosphate Ion and alpha-Benzylaminobenzylphosphonic Acid Update the Mechanistic Picture and Offer New Insights into Inhibitor Design  
Authors : Ortlund, E.; LaCount, M.W.; Lebioda, L.  
Deposited on : 2002-12-07  
Resolution : 2.90 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)                                     |
| Xtrriage (Phenix)              | : | <b>NOT EXECUTED</b>                                              |
| EDS                            | : | <b>NOT EXECUTED</b>                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

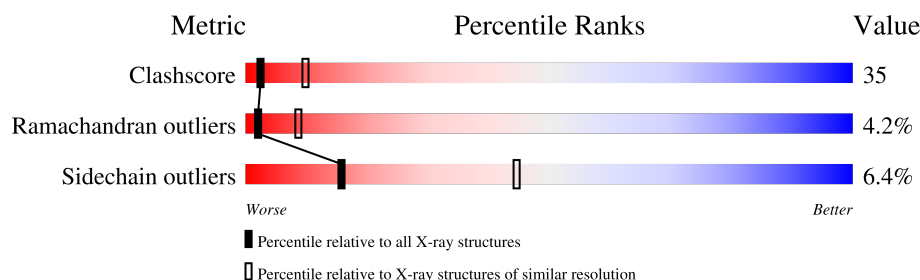
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 354    | 42% 47% 6% . .   |
| 1   | B     | 354    | 45% 43% 8% .     |
| 1   | C     | 354    | 40% 49% 8% . .   |
| 1   | D     | 354    | 38% 51% 7% . .   |
| 2   | E     | 2      | 50% 50%          |
| 2   | F     | 2      | 100%             |
| 2   | G     | 2      | 100%             |
| 2   | H     | 2      | 100%             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | I     | 3      |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | NAG  | E     | 2    | X         | -        | -       | -                |
| 2   | NAG  | F     | 1    | X         | -        | -       | -                |
| 2   | NAG  | G     | 1    | X         | -        | X       | -                |
| 2   | NAG  | H     | 1    | X         | -        | X       | -                |
| 2   | NAG  | H     | 2    | X         | -        | -       | -                |
| 3   | NAG  | I     | 1    | X         | -        | -       | -                |
| 4   | 2BF  | D     | 3402 | -         | X        | -       | -                |
| 6   | NDG  | B     | 1401 | -         | -        | X       | -                |
| 7   | NAG  | D     | 3401 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11727 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 prostatic acid phosphatase.

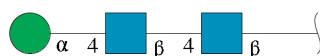
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2800  | 1807 | 461 | 516 | 16 |         |         |       |
| 1   | B     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2796  | 1802 | 461 | 517 | 16 |         |         |       |
| 1   | C     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2800  | 1807 | 461 | 516 | 16 |         |         |       |
| 1   | D     | 342      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2800  | 1807 | 461 | 516 | 16 |         |         |       |

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



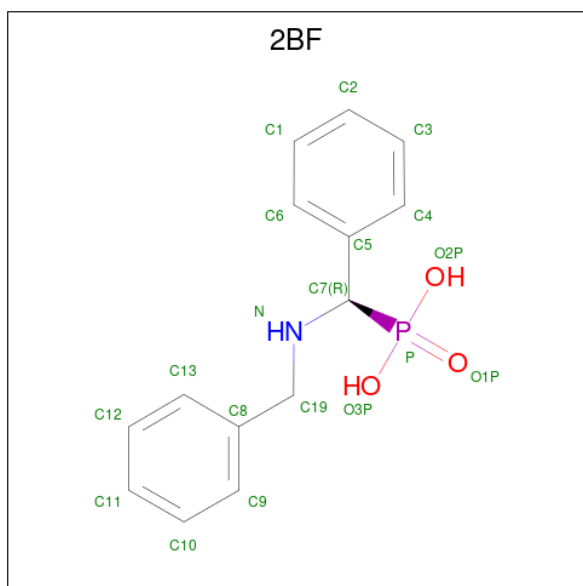
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 2   | E     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 30    | 16 | 2 | 12 |         |         |       |
| 2   | F     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 30    | 16 | 2 | 12 |         |         |       |
| 2   | G     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 30    | 16 | 2 | 12 |         |         |       |
| 2   | H     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 30    | 16 | 2 | 12 |         |         |       |

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 3   | I     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 42    | 22 | 2 | 18 |         |         |       |

- Molecule 4 is ALPHA-BENZYL-AMINOBENZYL-PHOSPHONIC ACID (CCD ID: 2BF) (formula:  $C_{14}H_{16}NO_3P$ ).



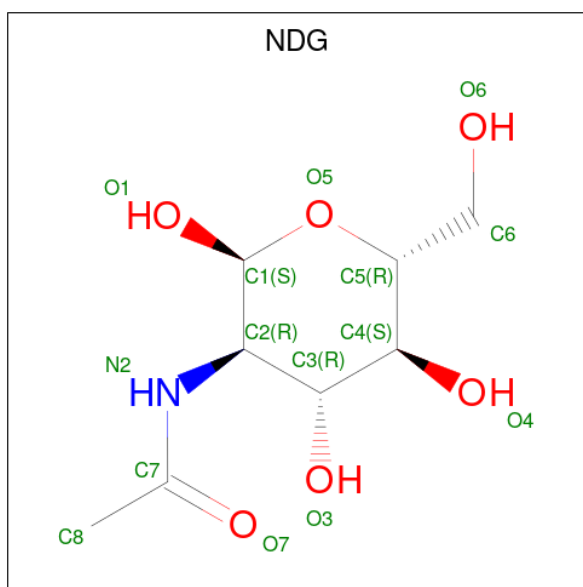
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 19    | 14 | 1 | 3 | 1 |         |         |
| 4   | B     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 19    | 14 | 1 | 3 | 1 |         |         |
| 4   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 19    | 14 | 1 | 3 | 1 |         |         |
| 4   | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 19    | 14 | 1 | 3 | 1 |         |         |

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 5   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | C     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 5   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 6   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 7   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |

- Molecule 8 is water.

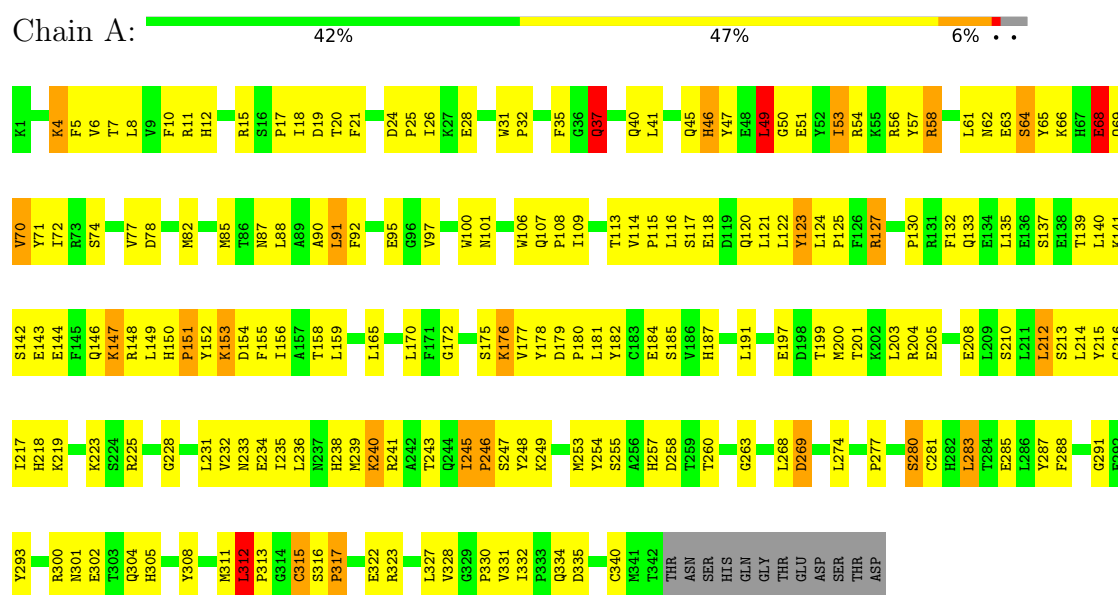
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 8   | A     | 45       | Total<br>45 | O<br>45 | 0       | 0       |
| 8   | B     | 35       | Total<br>35 | O<br>35 | 0       | 0       |
| 8   | C     | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 8   | D     | 33       | Total<br>33 | O<br>33 | 0       | 0       |

### 3 Residue-property plots

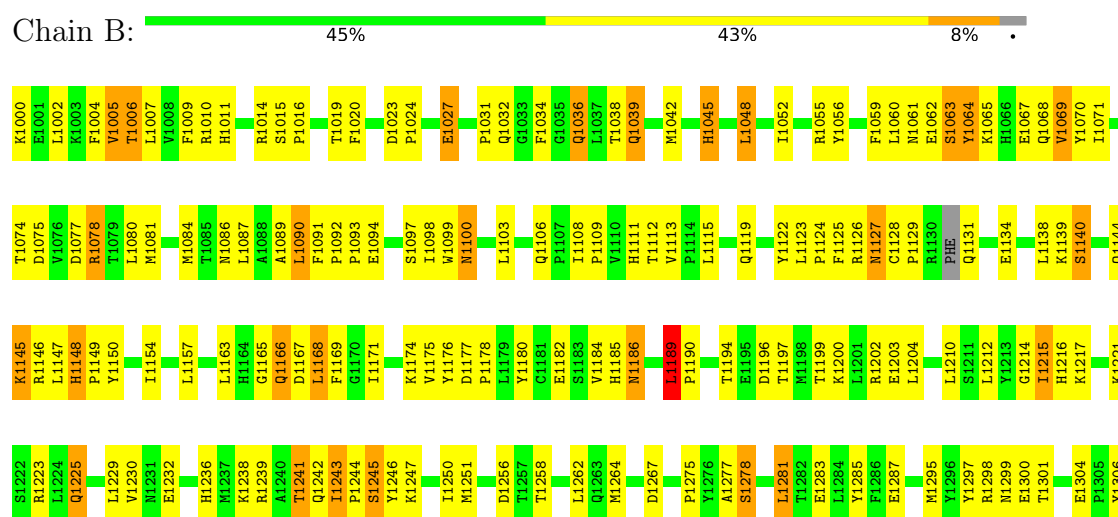
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

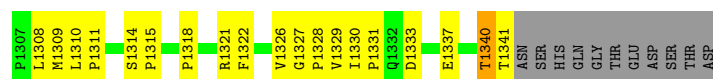
Note EDS was not executed.

- Molecule 1: prostatic acid phosphatase



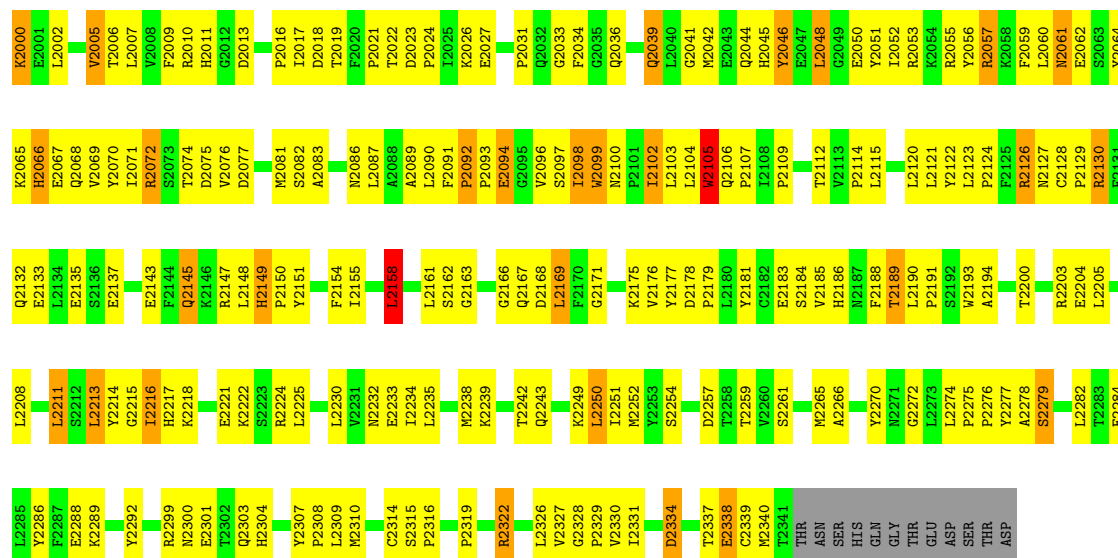
- Molecule 1: prostatic acid phosphatase





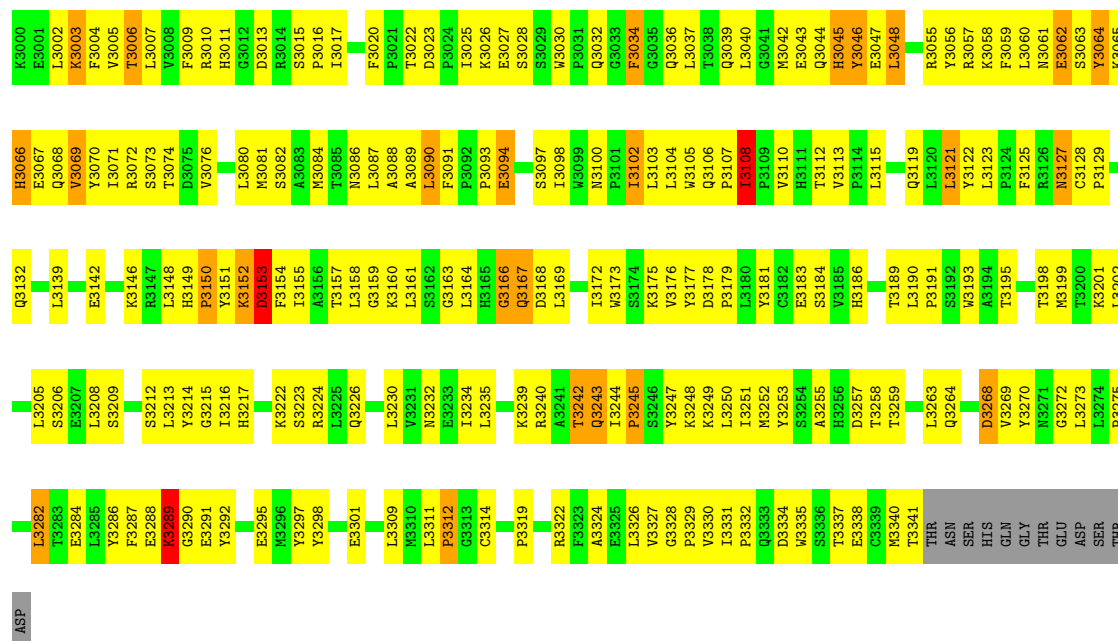
- Molecule 1: prostatic acid phosphatase

Chain C: 40% 49% 8% ..



- Molecule 1: prostatic acid phosphatase

Chain D: 38% 51% 7% ..

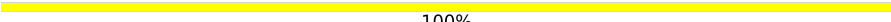


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

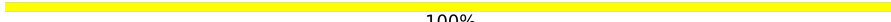
MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

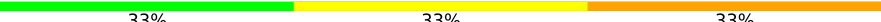
MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%

MAG1  
MAG2  
MAN3

## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 120.10Å 204.86Å 71.22Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 77.94 – 2.90                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 78.9 (77.94-2.90)                              | Depositor |
| $R_{merge}$                                              | 0.06                                           | Depositor |
| $R_{sym}$                                                | (Not available)                                | Depositor |
| Refinement program                                       | CNS                                            | Depositor |
| R, $R_{free}$                                            | 0.205 , 0.279                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 11727                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 29.0                                           | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, 1PE, MAN, 2BF

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     | 0.47         | 0/2882      | 0.99        | 11/3914 (0.3%)  |
| 1   | B     | 0.48         | 0/2876      | 0.99        | 14/3905 (0.4%)  |
| 1   | C     | 0.46         | 0/2882      | 0.97        | 8/3914 (0.2%)   |
| 1   | D     | 0.46         | 0/2882      | 0.97        | 8/3914 (0.2%)   |
| All | All   | 0.47         | 0/11522     | 0.98        | 41/15647 (0.3%) |

There are no bond length outliers.

All (41) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | B     | 1243 | ILE  | N-CA-C | 7.87  | 116.70      | 107.73   |
| 1   | C     | 2046 | TYR  | N-CA-C | -7.64 | 102.61      | 112.23   |
| 1   | B     | 1039 | GLN  | N-CA-C | -7.16 | 103.41      | 111.07   |
| 1   | A     | 47   | TYR  | N-CA-C | -7.14 | 102.69      | 111.40   |
| 1   | D     | 3030 | TRP  | CA-C-N | 7.06  | 126.58      | 119.24   |
| 1   | D     | 3030 | TRP  | C-N-CA | 7.06  | 126.58      | 119.24   |
| 1   | D     | 3245 | PRO  | N-CA-C | -6.78 | 101.73      | 111.22   |
| 1   | A     | 70   | VAL  | N-CA-C | 6.62  | 119.66      | 108.86   |
| 1   | D     | 3121 | LEU  | N-CA-C | 6.53  | 121.38      | 113.41   |
| 1   | B     | 1074 | THR  | N-CA-C | -6.46 | 101.82      | 110.55   |
| 1   | A     | 312  | LEU  | CA-C-N | -6.41 | 112.91      | 119.83   |
| 1   | A     | 312  | LEU  | C-N-CA | -6.41 | 112.91      | 119.83   |
| 1   | C     | 2092 | PRO  | CA-C-N | 6.31  | 126.68      | 119.93   |
| 1   | C     | 2092 | PRO  | C-N-CA | 6.31  | 126.68      | 119.93   |
| 1   | C     | 2279 | SER  | N-CA-C | -6.29 | 101.64      | 110.50   |
| 1   | A     | 176  | LYS  | N-CA-C | 6.15  | 120.05      | 112.54   |
| 1   | D     | 3046 | TYR  | N-CA-C | -6.13 | 105.07      | 112.54   |
| 1   | C     | 2222 | LYS  | N-CA-C | -6.04 | 104.70      | 111.28   |
| 1   | A     | 280  | SER  | N-CA-C | -6.01 | 101.38      | 110.28   |
| 1   | B     | 1225 | GLN  | N-CA-C | 5.91  | 117.52      | 108.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 68   | GLU  | N-CA-C | -5.87 | 105.61      | 112.89   |
| 1   | B     | 1278 | SER  | N-CA-C | -5.86 | 102.25      | 110.50   |
| 1   | B     | 1314 | SER  | CA-C-N | 5.72  | 125.58      | 119.28   |
| 1   | B     | 1314 | SER  | C-N-CA | 5.72  | 125.58      | 119.28   |
| 1   | B     | 1069 | VAL  | N-CA-C | 5.69  | 117.54      | 108.89   |
| 1   | D     | 3074 | THR  | N-CA-C | -5.59 | 101.43      | 110.32   |
| 1   | D     | 3017 | ILE  | N-CA-C | -5.56 | 106.92      | 113.42   |
| 1   | C     | 2039 | GLN  | N-CA-C | -5.35 | 105.34      | 111.07   |
| 1   | B     | 1100 | ASN  | CA-C-N | 5.34  | 125.81      | 120.04   |
| 1   | B     | 1100 | ASN  | C-N-CA | 5.34  | 125.81      | 120.04   |
| 1   | A     | 37   | GLN  | N-CA-C | 5.32  | 118.90      | 109.96   |
| 1   | B     | 1330 | ILE  | CA-C-N | 5.30  | 125.06      | 119.76   |
| 1   | B     | 1330 | ILE  | C-N-CA | 5.30  | 125.06      | 119.76   |
| 1   | C     | 2163 | GLY  | N-CA-C | -5.22 | 108.06      | 115.43   |
| 1   | A     | 49   | LEU  | N-CA-C | -5.19 | 105.52      | 111.07   |
| 1   | A     | 31   | TRP  | CA-C-N | 5.17  | 126.31      | 119.84   |
| 1   | A     | 31   | TRP  | C-N-CA | 5.17  | 126.31      | 119.84   |
| 1   | D     | 3034 | PHE  | N-CA-C | 5.15  | 118.10      | 110.48   |
| 1   | B     | 1186 | ASN  | N-CA-C | 5.10  | 119.35      | 113.38   |
| 1   | B     | 1189 | LEU  | N-CA-C | 5.05  | 117.25      | 110.29   |
| 1   | C     | 2158 | LEU  | N-CA-C | -5.03 | 106.24      | 112.38   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2800  | 0        | 2749     | 211     | 0            |
| 1   | B     | 2796  | 0        | 2745     | 182     | 0            |
| 1   | C     | 2800  | 0        | 2747     | 204     | 0            |
| 1   | D     | 2800  | 0        | 2746     | 213     | 0            |
| 2   | E     | 30    | 0        | 27       | 4       | 0            |
| 2   | F     | 30    | 0        | 28       | 4       | 0            |
| 2   | G     | 30    | 0        | 28       | 9       | 0            |
| 2   | H     | 30    | 0        | 27       | 8       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | I     | 42    | 0        | 38       | 4       | 0            |
| 4   | A     | 19    | 0        | 14       | 3       | 0            |
| 4   | B     | 19    | 0        | 14       | 2       | 0            |
| 4   | C     | 19    | 0        | 14       | 2       | 0            |
| 4   | D     | 19    | 0        | 14       | 0       | 0            |
| 5   | A     | 48    | 0        | 66       | 3       | 0            |
| 5   | B     | 32    | 0        | 44       | 5       | 0            |
| 5   | C     | 32    | 0        | 44       | 2       | 0            |
| 5   | D     | 16    | 0        | 22       | 1       | 0            |
| 6   | B     | 15    | 0        | 12       | 7       | 0            |
| 7   | D     | 15    | 0        | 14       | 6       | 0            |
| 8   | A     | 45    | 0        | 0        | 4       | 0            |
| 8   | B     | 35    | 0        | 0        | 4       | 0            |
| 8   | C     | 22    | 0        | 0        | 1       | 0            |
| 8   | D     | 33    | 0        | 0        | 8       | 0            |
| All | All   | 11727 | 0        | 11393    | 804     | 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 35.

All (804) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1:NAG:H61     | 3:I:2:NAG:H82     | 1.37                     | 1.07              |
| 1:B:1145:LYS:HA   | 1:B:1145:LYS:HE3  | 1.32                     | 1.05              |
| 1:B:1299:ASN:ND2  | 2:G:1:NAG:H1      | 1.74                     | 1.02              |
| 1:B:1299:ASN:HD21 | 2:G:1:NAG:H1      | 1.23                     | 0.98              |
| 1:C:2007:LEU:HD22 | 1:C:2282:LEU:HD22 | 1.43                     | 0.97              |
| 1:D:3100:ASN:HD21 | 1:D:3102:ILE:HB   | 1.29                     | 0.97              |
| 1:A:66:LYS:HD3    | 1:B:1032:GLN:HE22 | 1.30                     | 0.96              |
| 2:E:1:NAG:H61     | 2:E:2:NAG:H82     | 1.49                     | 0.94              |
| 1:B:1007:LEU:HD13 | 1:B:1052:ILE:HD13 | 1.50                     | 0.93              |
| 1:B:1199:THR:O    | 1:B:1203:GLU:HG3  | 1.68                     | 0.91              |
| 1:B:1299:ASN:HD21 | 2:G:1:NAG:C1      | 1.83                     | 0.91              |
| 1:C:2307:TYR:CE1  | 2:H:1:NAG:O1      | 2.24                     | 0.91              |
| 1:A:148:ARG:O     | 1:A:151:PRO:HD2   | 1.73                     | 0.89              |
| 1:B:1299:ASN:CG   | 2:G:1:NAG:H1      | 1.98                     | 0.89              |
| 1:A:150:HIS:HB3   | 1:A:151:PRO:HD3   | 1.55                     | 0.89              |
| 1:C:2337:THR:HA   | 1:C:2340:MET:HE3  | 1.53                     | 0.88              |
| 1:B:1127:ASN:HD22 | 1:B:1127:ASN:H    | 0.92                     | 0.88              |
| 1:B:1064:TYR:O    | 1:B:1065:LYS:HG3  | 1.75                     | 0.86              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2145:GLN:HE21 | 1:C:2145:GLN:HA   | 1.39                     | 0.86              |
| 1:A:180:PRO:O     | 1:A:184:GLU:HG3   | 1.73                     | 0.86              |
| 1:B:1127:ASN:H    | 1:B:1127:ASN:ND2  | 1.74                     | 0.86              |
| 1:D:3032:GLN:HB3  | 1:D:3036:GLN:HG2  | 1.56                     | 0.86              |
| 1:A:135:LEU:O     | 1:A:139:THR:HG23  | 1.77                     | 0.85              |
| 1:D:3087:LEU:HB3  | 1:D:3108:ILE:HD12 | 1.56                     | 0.84              |
| 1:B:1094:GLU:HA   | 1:B:1098:ILE:HD11 | 1.61                     | 0.83              |
| 1:B:1148:HIS:HB3  | 1:B:1149:PRO:HD3  | 1.61                     | 0.83              |
| 1:C:2288:GLU:HG3  | 1:C:2289:LYS:H    | 1.44                     | 0.83              |
| 1:C:2149:HIS:HB3  | 1:C:2150:PRO:HD3  | 1.61                     | 0.82              |
| 1:B:1299:ASN:OD1  | 2:G:1:NAG:H1      | 1.80                     | 0.82              |
| 1:C:2098:ILE:HG21 | 1:C:2104:LEU:HD22 | 1.61                     | 0.81              |
| 1:D:3065:LYS:HB2  | 1:D:3068:GLN:HG3  | 1.63                     | 0.80              |
| 1:C:2190:LEU:HB3  | 1:C:2191:PRO:HD2  | 1.63                     | 0.80              |
| 1:C:2288:GLU:HG3  | 1:C:2289:LYS:HG2  | 1.62                     | 0.80              |
| 1:B:1275:PRO:HD2  | 1:B:1278:SER:HB3  | 1.63                     | 0.80              |
| 1:B:1010:ARG:HD2  | 1:B:1256:ASP:HB3  | 1.61                     | 0.80              |
| 1:C:2050:GLU:HG3  | 1:C:2089:ALA:HB1  | 1.64                     | 0.79              |
| 1:A:56:ARG:HG2    | 1:A:57:TYR:CD2    | 2.18                     | 0.79              |
| 1:D:3003:LYS:HG3  | 1:D:3292:TYR:HE2  | 1.47                     | 0.79              |
| 1:D:3025:ILE:H    | 1:D:3025:ILE:HD12 | 1.47                     | 0.79              |
| 1:A:82:MET:HE2    | 1:B:1109:PRO:HD3  | 1.65                     | 0.79              |
| 1:A:311:MET:HE3   | 1:A:316:SER:HA    | 1.65                     | 0.79              |
| 1:B:1186:ASN:HD21 | 6:B:1401:NDG:C1   | 1.95                     | 0.79              |
| 1:B:1185:HIS:HA   | 6:B:1401:NDG:H8C3 | 1.62                     | 0.78              |
| 1:B:1125:PHE:H    | 1:B:1225:GLN:HE22 | 1.32                     | 0.78              |
| 1:C:2081:MET:HG2  | 1:D:3107:PRO:HB2  | 1.65                     | 0.78              |
| 1:A:139:THR:HG22  | 1:A:218:HIS:HB3   | 1.65                     | 0.78              |
| 1:C:2090:LEU:HD13 | 1:C:2091:PHE:CE1  | 2.19                     | 0.77              |
| 2:H:1:NAG:H61     | 2:H:2:NAG:H2      | 1.66                     | 0.76              |
| 1:D:3166:GLY:O    | 1:D:3168:ASP:N    | 2.17                     | 0.75              |
| 1:A:6:VAL:HG22    | 1:A:285:GLU:HG2   | 1.67                     | 0.75              |
| 1:A:245:ILE:HD12  | 1:A:246:PRO:CD    | 2.17                     | 0.75              |
| 1:A:8:LEU:HD23    | 1:A:283:LEU:HB3   | 1.69                     | 0.75              |
| 1:A:181:LEU:HD23  | 1:A:191:LEU:HD22  | 1.68                     | 0.75              |
| 1:D:3340:MET:HE2  | 1:D:3341:THR:HG22 | 1.68                     | 0.75              |
| 1:B:1267:ASP:OD2  | 1:B:1311:PRO:HG3  | 1.87                     | 0.74              |
| 7:D:3401:NAG:HO1  | 7:D:3401:NAG:C7   | 1.99                     | 0.74              |
| 1:A:41:LEU:O      | 1:A:45:GLN:HG3    | 1.88                     | 0.74              |
| 1:D:3149:HIS:HB3  | 1:D:3150:PRO:HD3  | 1.68                     | 0.74              |
| 1:B:1045:HIS:HD2  | 1:B:1086:ASN:HD22 | 1.35                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3155:ILE:HG21 | 1:D:3167:GLN:HG3  | 1.68                     | 0.74              |
| 1:C:2176:VAL:O    | 1:C:2179:PRO:HD2  | 1.87                     | 0.74              |
| 1:D:3289:LYS:H    | 1:D:3289:LYS:HD2  | 1.51                     | 0.74              |
| 1:D:3062:GLU:H    | 1:D:3062:GLU:CD   | 1.95                     | 0.73              |
| 1:D:3322:ARG:HH11 | 1:D:3322:ARG:HG2  | 1.53                     | 0.73              |
| 7:D:3401:NAG:O7   | 7:D:3401:NAG:O1   | 2.06                     | 0.73              |
| 1:A:61:LEU:O      | 1:A:63:GLU:N      | 2.21                     | 0.73              |
| 1:A:63:GLU:HG2    | 8:A:533:HOH:O     | 1.89                     | 0.73              |
| 1:C:2288:GLU:HG3  | 1:C:2289:LYS:N    | 2.04                     | 0.73              |
| 1:D:3169:LEU:O    | 8:D:3501:HOH:O    | 2.06                     | 0.72              |
| 1:B:1127:ASN:HD22 | 1:B:1127:ASN:N    | 1.73                     | 0.72              |
| 1:A:316:SER:HB2   | 1:A:317:PRO:HD2   | 1.70                     | 0.72              |
| 1:D:3004:PHE:HZ   | 1:D:3251:ILE:HD12 | 1.54                     | 0.72              |
| 1:C:2007:LEU:CD2  | 1:C:2282:LEU:HD22 | 2.20                     | 0.71              |
| 1:D:3115:LEU:HD22 | 1:D:3122:TYR:CE1  | 2.25                     | 0.71              |
| 1:C:2310:MET:HE3  | 1:C:2316:PRO:HD3  | 1.73                     | 0.71              |
| 1:C:2007:LEU:HD22 | 1:C:2282:LEU:CD2  | 2.20                     | 0.71              |
| 1:C:2145:GLN:HA   | 1:C:2145:GLN:NE2  | 2.06                     | 0.71              |
| 1:B:1281:LEU:HD23 | 1:B:1281:LEU:H    | 1.54                     | 0.70              |
| 1:A:66:LYS:CD     | 1:B:1032:GLN:HE22 | 2.02                     | 0.70              |
| 1:B:1163:LEU:HD11 | 1:B:1174:LYS:CB   | 2.21                     | 0.70              |
| 1:D:3172:ILE:N    | 8:D:3501:HOH:O    | 2.23                     | 0.70              |
| 1:A:212:LEU:HD12  | 1:A:217:ILE:HG13  | 1.72                     | 0.70              |
| 1:D:3268:ASP:HB3  | 1:D:3312:PRO:HG3  | 1.74                     | 0.70              |
| 1:D:3040:LEU:O    | 1:D:3044:GLN:HG3  | 1.92                     | 0.70              |
| 1:D:3125:PHE:H    | 1:D:3226:GLN:HE22 | 1.39                     | 0.70              |
| 1:B:1123:LEU:HD12 | 1:B:1258:THR:HA   | 1.75                     | 0.69              |
| 1:A:49:LEU:HD13   | 1:A:87:ASN:HD21   | 1.58                     | 0.69              |
| 1:B:1007:LEU:CD1  | 1:B:1052:ILE:HD13 | 2.21                     | 0.69              |
| 1:B:1077:ASP:O    | 1:B:1081:MET:HG3  | 1.93                     | 0.69              |
| 1:B:1239:ARG:HD2  | 1:B:1246:TYR:HE2  | 1.58                     | 0.69              |
| 1:C:2191:PRO:HG2  | 1:C:2194:ALA:HB2  | 1.74                     | 0.69              |
| 1:D:3340:MET:HE3  | 1:D:3341:THR:H    | 1.58                     | 0.68              |
| 1:B:1309:MET:HE2  | 1:B:1315:PRO:HG3  | 1.73                     | 0.68              |
| 1:B:1011:HIS:NE2  | 1:B:1078:ARG:HD2  | 2.08                     | 0.68              |
| 1:B:1306:TYR:CE2  | 2:G:1:NAG:H5      | 2.29                     | 0.68              |
| 1:D:3224:ARG:HA   | 1:D:3330:VAL:O    | 1.94                     | 0.68              |
| 1:D:3288:GLU:O    | 1:D:3290:GLY:N    | 2.25                     | 0.68              |
| 3:I:1:NAG:C6      | 3:I:2:NAG:H82     | 2.21                     | 0.68              |
| 1:B:1297:TYR:HB2  | 1:B:1308:LEU:HD11 | 1.76                     | 0.68              |
| 1:B:1045:HIS:CD2  | 1:B:1086:ASN:HD22 | 2.12                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1:NAG:H61     | 3:I:2:NAG:C8      | 2.21                     | 0.67              |
| 1:A:58:ARG:HH11   | 1:A:58:ARG:HG2    | 1.58                     | 0.67              |
| 1:C:2176:VAL:C    | 1:C:2179:PRO:HD2  | 2.20                     | 0.67              |
| 1:C:2319:PRO:HG2  | 1:C:2322:ARG:HB2  | 1.77                     | 0.67              |
| 1:D:3127:ASN:HD22 | 1:D:3127:ASN:H    | 1.42                     | 0.67              |
| 1:D:3169:LEU:HB3  | 1:D:3209:SER:HB2  | 1.76                     | 0.67              |
| 1:C:2120:LEU:HD23 | 1:C:2120:LEU:O    | 1.94                     | 0.66              |
| 1:D:3100:ASN:ND2  | 1:D:3102:ILE:HB   | 2.08                     | 0.66              |
| 1:C:2068:GLN:HG3  | 1:C:2249:LYS:HG3  | 1.78                     | 0.66              |
| 1:C:2310:MET:HE2  | 1:C:2315:SER:HA   | 1.76                     | 0.66              |
| 1:D:3055:ARG:HG2  | 1:D:3056:TYR:CE2  | 2.31                     | 0.66              |
| 1:B:1163:LEU:HD11 | 1:B:1174:LYS:HB2  | 1.78                     | 0.66              |
| 1:B:1119:GLN:HB3  | 5:B:1403:1PE:H142 | 1.78                     | 0.66              |
| 1:B:1281:LEU:HD23 | 1:B:1281:LEU:N    | 2.11                     | 0.66              |
| 1:C:2130:ARG:HD3  | 1:C:2221:GLU:OE2  | 1.95                     | 0.66              |
| 1:C:2005:VAL:HG22 | 1:C:2250:LEU:HD12 | 1.76                     | 0.65              |
| 1:D:3232:ASN:HB2  | 1:D:3331:ILE:HG23 | 1.78                     | 0.65              |
| 1:A:54:ARG:HG3    | 1:A:91:LEU:HD22   | 1.78                     | 0.65              |
| 1:D:3169:LEU:C    | 8:D:3501:HOH:O    | 2.39                     | 0.65              |
| 1:B:1015:SER:HB2  | 1:B:1016:PRO:HD2  | 1.79                     | 0.65              |
| 1:C:2086:ASN:HD22 | 1:C:2252:MET:HE1  | 1.61                     | 0.65              |
| 1:C:2200:THR:O    | 1:C:2204:GLU:HG3  | 1.96                     | 0.65              |
| 1:A:49:LEU:O      | 1:A:53:ILE:HG22   | 1.96                     | 0.65              |
| 1:A:108:PRO:C     | 1:A:109:ILE:HD12  | 2.22                     | 0.65              |
| 1:C:2232:ASN:HD22 | 1:C:2331:ILE:HD13 | 1.61                     | 0.65              |
| 1:B:1004:PHE:HZ   | 1:B:1250:ILE:HD12 | 1.62                     | 0.64              |
| 1:A:258:ASP:OD2   | 4:A:401:2BF:H7    | 1.97                     | 0.64              |
| 1:B:1011:HIS:CD2  | 1:B:1078:ARG:HD2  | 2.31                     | 0.64              |
| 1:B:1298:ARG:HH12 | 1:B:1301:THR:HG22 | 1.62                     | 0.64              |
| 1:A:10:PHE:HE2    | 1:A:253:MET:HE2   | 1.62                     | 0.64              |
| 1:D:3148:LEU:HD21 | 1:D:3167:GLN:NE2  | 2.13                     | 0.64              |
| 1:C:2086:ASN:ND2  | 1:C:2252:MET:HE1  | 2.13                     | 0.64              |
| 1:C:2098:ILE:HG22 | 1:C:2099:TRP:H    | 1.63                     | 0.64              |
| 1:A:283:LEU:N     | 1:A:283:LEU:HD23  | 2.13                     | 0.63              |
| 1:B:1129:PRO:O    | 1:B:1131:GLN:HB2  | 1.98                     | 0.63              |
| 1:D:3324:ALA:HA   | 1:D:3327:VAL:HG12 | 1.79                     | 0.63              |
| 1:B:1060:LEU:C    | 1:B:1062:GLU:H    | 2.06                     | 0.63              |
| 1:B:1139:LYS:O    | 1:B:1140:SER:C    | 2.41                     | 0.63              |
| 1:A:130:PRO:HD2   | 1:A:340:CYS:HB3   | 1.81                     | 0.62              |
| 1:C:2100:ASN:O    | 1:C:2104:LEU:HD23 | 1.97                     | 0.62              |
| 1:D:3322:ARG:HH21 | 1:D:3326:LEU:HD21 | 1.64                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1275:PRO:HD2  | 1:B:1278:SER:CB   | 2.29                     | 0.62              |
| 1:A:8:LEU:HD11    | 1:A:53:ILE:HD13   | 1.81                     | 0.62              |
| 1:A:74:SER:HB2    | 1:A:255:SER:HB3   | 1.82                     | 0.62              |
| 1:B:1009:PHE:HE2  | 1:B:1251:MET:HE3  | 1.65                     | 0.62              |
| 1:A:182:TYR:O     | 1:A:185:SER:HB3   | 1.98                     | 0.62              |
| 1:D:3242:THR:HG22 | 1:D:3243:GLN:HG2  | 1.81                     | 0.62              |
| 1:B:1078:ARG:NH2  | 4:B:1402:2BF:O3P  | 2.33                     | 0.62              |
| 1:B:1098:ILE:HG22 | 1:B:1098:ILE:O    | 1.99                     | 0.62              |
| 1:D:3172:ILE:HB   | 8:D:3501:HOH:O    | 2.00                     | 0.62              |
| 1:D:3224:ARG:HG2  | 1:D:3330:VAL:HA   | 1.81                     | 0.62              |
| 1:C:2114:PRO:HD3  | 1:D:3113:VAL:HG22 | 1.82                     | 0.61              |
| 1:C:2169:LEU:HD11 | 1:C:2208:LEU:HD23 | 1.81                     | 0.61              |
| 2:H:2:NAG:H3      | 2:H:2:NAG:H83     | 1.82                     | 0.61              |
| 1:A:177:VAL:C     | 1:A:180:PRO:HD2   | 2.24                     | 0.61              |
| 1:B:1056:TYR:HB3  | 1:B:1060:LEU:HD23 | 1.82                     | 0.61              |
| 1:C:2098:ILE:O    | 1:C:2099:TRP:HB3  | 2.00                     | 0.61              |
| 1:C:2178:ASP:HB3  | 1:C:2179:PRO:HD3  | 1.82                     | 0.61              |
| 1:C:2112:THR:HG22 | 1:D:3112:THR:HG22 | 1.80                     | 0.61              |
| 1:D:3107:PRO:C    | 1:D:3108:ILE:HG12 | 2.25                     | 0.61              |
| 1:A:139:THR:HG21  | 1:A:223:LYS:NZ    | 2.15                     | 0.61              |
| 1:C:2120:LEU:HD22 | 1:C:2121:LEU:HG   | 1.81                     | 0.61              |
| 1:D:3107:PRO:O    | 1:D:3108:ILE:HG23 | 1.99                     | 0.61              |
| 1:D:3289:LYS:HD2  | 1:D:3289:LYS:N    | 2.14                     | 0.61              |
| 1:D:3045:HIS:CD2  | 1:D:3086:ASN:HD22 | 2.18                     | 0.61              |
| 1:A:187:HIS:HA    | 2:E:1:NAG:H82     | 1.81                     | 0.61              |
| 1:A:312:LEU:HD23  | 1:A:327:LEU:HD12  | 1.80                     | 0.61              |
| 1:A:135:LEU:HD13  | 1:A:223:LYS:CG    | 2.30                     | 0.61              |
| 1:D:3158:LEU:HD23 | 1:D:3172:ILE:HD12 | 1.81                     | 0.61              |
| 1:A:159:LEU:C     | 1:A:159:LEU:HD13  | 2.26                     | 0.61              |
| 1:D:3322:ARG:NH2  | 1:D:3326:LEU:HD21 | 2.16                     | 0.61              |
| 1:D:3127:ASN:H    | 1:D:3127:ASN:ND2  | 1.99                     | 0.61              |
| 1:B:1340:THR:HG23 | 1:B:1341:THR:H    | 1.65                     | 0.60              |
| 1:C:2130:ARG:NH1  | 1:C:2221:GLU:OE1  | 2.34                     | 0.60              |
| 1:B:1196:ASP:HB2  | 8:B:1523:HOH:O    | 2.00                     | 0.60              |
| 1:C:2061:ASN:N    | 1:C:2061:ASN:HD22 | 1.99                     | 0.60              |
| 1:D:3282:LEU:N    | 1:D:3282:LEU:HD23 | 2.16                     | 0.60              |
| 1:A:225:ARG:HA    | 1:A:331:VAL:O     | 2.00                     | 0.60              |
| 1:D:3106:GLN:HB2  | 1:D:3107:PRO:HD2  | 1.83                     | 0.60              |
| 1:C:2018:ASP:OD2  | 1:C:2175:LYS:HD3  | 2.01                     | 0.60              |
| 1:D:3010:ARG:HD2  | 1:D:3257:ASP:HB3  | 1.84                     | 0.60              |
| 1:C:2328:GLY:N    | 1:C:2329:PRO:HD2  | 2.17                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:114:VAL:HG13  | 1:A:115:PRO:HD2   | 1.84                     | 0.59              |
| 1:A:155:PHE:HE1   | 1:A:199:THR:HG22  | 1.65                     | 0.59              |
| 1:B:1214:GLY:O    | 1:B:1215:ILE:HB   | 2.01                     | 0.59              |
| 1:C:2310:MET:HE3  | 1:C:2316:PRO:CD   | 2.32                     | 0.59              |
| 1:A:135:LEU:HD13  | 1:A:223:LYS:HG2   | 1.84                     | 0.59              |
| 1:A:11:ARG:HD2    | 4:A:401:2BF:O3P   | 2.02                     | 0.59              |
| 1:D:3176:VAL:O    | 1:D:3179:PRO:HD2  | 2.02                     | 0.59              |
| 1:A:245:ILE:HD12  | 1:A:246:PRO:HD2   | 1.84                     | 0.59              |
| 1:D:3069:VAL:HG13 | 1:D:3250:LEU:HB3  | 1.84                     | 0.59              |
| 1:A:10:PHE:CE1    | 1:A:255:SER:HA    | 2.38                     | 0.59              |
| 1:A:139:THR:HG21  | 1:A:223:LYS:HZ2   | 1.66                     | 0.59              |
| 1:A:56:ARG:HG2    | 1:A:57:TYR:CE2    | 2.37                     | 0.59              |
| 1:A:150:HIS:C     | 1:A:152:TYR:H     | 2.09                     | 0.59              |
| 1:C:2239:LYS:O    | 1:C:2243:GLN:HG3  | 2.02                     | 0.59              |
| 1:D:3070:TYR:HB2  | 1:D:3248:LYS:HE2  | 1.84                     | 0.59              |
| 1:D:3179:PRO:O    | 1:D:3183:GLU:HG2  | 2.02                     | 0.59              |
| 1:A:175:SER:O     | 1:A:180:PRO:HD3   | 2.03                     | 0.59              |
| 1:D:3142:GLU:O    | 1:D:3146:LYS:HD3  | 2.02                     | 0.59              |
| 1:D:3334:ASP:O    | 1:D:3338:GLU:HG3  | 2.03                     | 0.59              |
| 1:B:1239:ARG:HD2  | 1:B:1246:TYR:CE2  | 2.38                     | 0.59              |
| 1:C:2098:ILE:HG21 | 1:C:2104:LEU:CD2  | 2.32                     | 0.59              |
| 1:C:2100:ASN:ND2  | 1:C:2103:LEU:HB3  | 2.18                     | 0.59              |
| 1:C:2161:LEU:HD13 | 1:C:2193:TRP:CB   | 2.33                     | 0.59              |
| 1:C:2232:ASN:ND2  | 1:C:2331:ILE:HG21 | 2.18                     | 0.59              |
| 1:D:3167:GLN:O    | 1:D:3167:GLN:HG2  | 2.02                     | 0.59              |
| 1:D:3224:ARG:O    | 1:D:3332:PRO:HD3  | 2.02                     | 0.59              |
| 1:C:2048:LEU:O    | 1:C:2052:ILE:HG13 | 2.02                     | 0.59              |
| 1:C:2056:TYR:O    | 1:C:2059:PHE:N    | 2.36                     | 0.59              |
| 1:B:1014:ARG:HH22 | 1:B:1177:ASP:CG   | 2.10                     | 0.58              |
| 1:C:2214:TYR:HB2  | 1:C:2265:MET:HG3  | 1.85                     | 0.58              |
| 1:D:3340:MET:CE   | 1:D:3341:THR:HG22 | 2.33                     | 0.58              |
| 1:C:2169:LEU:HD21 | 1:C:2205:LEU:HB3  | 1.84                     | 0.58              |
| 1:A:170:LEU:HB3   | 1:A:210:SER:HB2   | 1.85                     | 0.58              |
| 1:B:1340:THR:HG23 | 1:B:1341:THR:N    | 2.19                     | 0.58              |
| 1:C:2071:ILE:HG13 | 1:C:2252:MET:HB2  | 1.83                     | 0.58              |
| 1:C:2089:ALA:O    | 1:C:2092:PRO:HD3  | 2.04                     | 0.58              |
| 1:C:2041:GLY:HA2  | 1:C:2044:GLN:OE1  | 2.03                     | 0.58              |
| 1:C:2151:TYR:CG   | 1:C:2205:LEU:HD21 | 2.38                     | 0.58              |
| 1:A:322:GLU:OE1   | 1:A:322:GLU:HA    | 2.03                     | 0.58              |
| 1:B:1186:ASN:ND2  | 6:B:1401:NDG:C1   | 2.67                     | 0.58              |
| 1:D:3127:ASN:HD22 | 1:D:3127:ASN:N    | 1.99                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3172:ILE:O    | 1:D:3176:VAL:HB   | 2.03                     | 0.58              |
| 1:A:11:ARG:HD3    | 1:A:258:ASP:HB3   | 1.86                     | 0.58              |
| 1:A:302:GLU:OE1   | 2:F:1:NAG:O1      | 2.21                     | 0.58              |
| 1:C:2072:ARG:HD3  | 1:C:2121:LEU:HD12 | 1.86                     | 0.58              |
| 1:C:2217:HIS:CD2  | 1:C:2218:LYS:HD3  | 2.38                     | 0.58              |
| 1:A:82:MET:HA     | 1:A:85:MET:HE3    | 1.85                     | 0.57              |
| 1:C:2048:LEU:HD13 | 1:C:2052:ILE:HD11 | 1.86                     | 0.57              |
| 1:D:3115:LEU:HD22 | 1:D:3122:TYR:CD1  | 2.39                     | 0.57              |
| 1:B:1163:LEU:HD21 | 1:B:1174:LYS:HD3  | 1.86                     | 0.57              |
| 1:C:2314:CYS:HB2  | 1:C:2326:LEU:CD1  | 2.34                     | 0.57              |
| 1:D:3072:ARG:O    | 1:D:3253:TYR:HA   | 2.04                     | 0.57              |
| 1:A:268:LEU:O     | 1:A:269:ASP:HB2   | 2.03                     | 0.57              |
| 1:C:2181:TYR:O    | 1:C:2185:VAL:HG23 | 2.04                     | 0.57              |
| 1:D:3004:PHE:CZ   | 1:D:3251:ILE:HD12 | 2.39                     | 0.57              |
| 1:D:3186:HIS:HA   | 7:D:3401:NAG:C8   | 2.35                     | 0.57              |
| 1:B:1009:PHE:CE2  | 1:B:1251:MET:HE3  | 2.39                     | 0.57              |
| 1:C:2056:TYR:O    | 1:C:2057:ARG:C    | 2.48                     | 0.57              |
| 1:C:2130:ARG:HH11 | 1:C:2221:GLU:CD   | 2.12                     | 0.57              |
| 1:C:2232:ASN:HD22 | 1:C:2331:ILE:HG21 | 1.70                     | 0.57              |
| 1:C:2310:MET:CE   | 1:C:2316:PRO:HD3  | 2.35                     | 0.57              |
| 1:D:3045:HIS:HD2  | 1:D:3086:ASN:ND2  | 2.02                     | 0.57              |
| 1:A:78:ASP:HB3    | 1:A:82:MET:HE3    | 1.85                     | 0.57              |
| 1:C:2161:LEU:HD13 | 1:C:2193:TRP:HB2  | 1.86                     | 0.57              |
| 1:D:3148:LEU:HD21 | 1:D:3167:GLN:HE21 | 1.69                     | 0.57              |
| 1:A:268:LEU:HD22  | 1:A:312:LEU:HD11  | 1.86                     | 0.57              |
| 1:C:2065:LYS:O    | 1:C:2068:GLN:N    | 2.38                     | 0.57              |
| 1:D:3047:GLU:C    | 1:D:3047:GLU:OE2  | 2.48                     | 0.57              |
| 1:A:127:ARG:CG    | 1:A:127:ARG:HH11  | 2.18                     | 0.57              |
| 1:D:3314:CYS:HB2  | 1:D:3326:LEU:CD1  | 2.34                     | 0.57              |
| 1:C:2166:GLY:O    | 1:C:2168:ASP:N    | 2.38                     | 0.57              |
| 1:C:2007:LEU:CD1  | 1:C:2052:ILE:HD13 | 2.35                     | 0.57              |
| 1:C:2053:ARG:NH1  | 1:C:2092:PRO:HG3  | 2.20                     | 0.57              |
| 1:C:2183:GLU:HB3  | 1:C:2190:LEU:HD21 | 1.87                     | 0.57              |
| 1:D:3169:LEU:HD11 | 1:D:3208:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:66:LYS:HD3    | 1:B:1032:GLN:NE2  | 2.10                     | 0.56              |
| 1:B:1010:ARG:O    | 1:B:1277:ALA:HA   | 2.04                     | 0.56              |
| 1:B:1189:LEU:HG   | 1:B:1190:PRO:HD2  | 1.87                     | 0.56              |
| 1:D:3065:LYS:O    | 1:D:3067:GLU:N    | 2.38                     | 0.56              |
| 1:D:3172:ILE:CB   | 8:D:3501:HOH:O    | 2.53                     | 0.56              |
| 1:A:120:GLN:HB3   | 5:A:402:1PE:H152  | 1.86                     | 0.56              |
| 1:A:132:PHE:O     | 1:A:133:GLN:C     | 2.48                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:181:LEU:CD2   | 1:A:191:LEU:HD22  | 2.33                     | 0.56              |
| 1:B:1243:ILE:HG22 | 1:B:1244:PRO:O    | 2.05                     | 0.56              |
| 1:C:2026:LYS:HE2  | 1:C:2026:LYS:HA   | 1.87                     | 0.56              |
| 1:A:68:GLU:H      | 1:A:68:GLU:CD     | 2.12                     | 0.56              |
| 8:A:501:HOH:O     | 2:E:1:NAG:H81     | 2.06                     | 0.56              |
| 1:A:277:PRO:HD2   | 1:A:280:SER:HB3   | 1.86                     | 0.56              |
| 1:A:334:GLN:NE2   | 1:A:334:GLN:HA    | 2.20                     | 0.56              |
| 1:C:2301:GLU:OE2  | 1:C:2304:HIS:HD2  | 1.88                     | 0.56              |
| 1:B:1080:LEU:O    | 1:B:1084:MET:HG3  | 2.06                     | 0.56              |
| 1:D:3157:THR:O    | 1:D:3161:LEU:HG   | 2.06                     | 0.56              |
| 1:D:3055:ARG:HG2  | 1:D:3056:TYR:CD2  | 2.41                     | 0.56              |
| 1:A:312:LEU:HD23  | 1:A:327:LEU:CD1   | 2.35                     | 0.55              |
| 1:B:1327:GLY:N    | 1:B:1328:PRO:HD2  | 2.21                     | 0.55              |
| 1:C:2274:LEU:HG   | 8:C:2501:HOH:O    | 2.06                     | 0.55              |
| 1:A:11:ARG:CD     | 1:A:258:ASP:HB3   | 2.36                     | 0.55              |
| 1:B:1146:ARG:O    | 1:B:1149:PRO:HD2  | 2.07                     | 0.55              |
| 1:B:1210:LEU:HD13 | 1:B:1215:ILE:HG12 | 1.88                     | 0.55              |
| 1:C:2310:MET:CE   | 1:C:2315:SER:HA   | 2.35                     | 0.55              |
| 1:B:1177:ASP:HB3  | 1:B:1178:PRO:HD3  | 1.89                     | 0.55              |
| 1:C:2010:ARG:HD2  | 1:C:2257:ASP:N    | 2.21                     | 0.55              |
| 1:C:2097:SER:HB3  | 1:C:2106:GLN:NE2  | 2.21                     | 0.55              |
| 1:D:3060:LEU:O    | 1:D:3062:GLU:N    | 2.40                     | 0.55              |
| 1:A:204:ARG:O     | 1:A:208:GLU:HG3   | 2.06                     | 0.55              |
| 1:C:2104:LEU:O    | 1:C:2105:TRP:HB3  | 2.05                     | 0.55              |
| 1:D:3230:LEU:HD23 | 1:D:3263:LEU:HB2  | 1.89                     | 0.55              |
| 1:C:2211:LEU:HD13 | 1:C:2211:LEU:O    | 2.07                     | 0.55              |
| 1:D:3002:LEU:HD23 | 1:D:3059:PHE:CG   | 2.41                     | 0.55              |
| 1:A:304:GLN:HG3   | 1:A:305:HIS:CE1   | 2.42                     | 0.55              |
| 1:B:1180:TYR:O    | 1:B:1184:VAL:HG23 | 2.07                     | 0.55              |
| 1:C:2288:GLU:CG   | 1:C:2289:LYS:N    | 2.69                     | 0.55              |
| 1:D:3340:MET:HE3  | 1:D:3340:MET:HA   | 1.88                     | 0.55              |
| 1:D:3178:ASP:HB3  | 1:D:3179:PRO:HD3  | 1.87                     | 0.54              |
| 1:B:1169:PHE:CD1  | 5:B:1404:1PE:H222 | 2.41                     | 0.54              |
| 1:C:2070:TYR:C    | 1:C:2071:ILE:HD12 | 2.33                     | 0.54              |
| 1:A:107:GLN:HG3   | 1:A:109:ILE:HD11  | 1.89                     | 0.54              |
| 1:A:113:THR:HG22  | 1:B:1112:THR:HG22 | 1.90                     | 0.54              |
| 1:A:139:THR:CG2   | 1:A:218:HIS:HB3   | 2.36                     | 0.54              |
| 1:C:2010:ARG:O    | 1:C:2278:ALA:HA   | 2.08                     | 0.54              |
| 1:A:213:SER:HB3   | 1:A:217:ILE:HD12  | 1.88                     | 0.54              |
| 1:D:3186:HIS:HA   | 7:D:3401:NAG:H81  | 1.88                     | 0.54              |
| 1:A:143:GLU:O     | 1:A:147:LYS:HB2   | 2.07                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:281:CYS:SG    | 1:A:283:LEU:HD22  | 2.48                     | 0.54              |
| 1:B:1010:ARG:O    | 1:B:1045:HIS:HE1  | 1.90                     | 0.54              |
| 1:D:3087:LEU:CB   | 1:D:3108:ILE:HD12 | 2.34                     | 0.54              |
| 1:B:1306:TYR:CZ   | 2:G:1:NAG:O1      | 2.60                     | 0.54              |
| 1:D:3167:GLN:HB2  | 8:D:3513:HOH:O    | 2.06                     | 0.54              |
| 1:A:152:TYR:O     | 1:A:155:PHE:N     | 2.40                     | 0.54              |
| 1:B:1306:TYR:CE1  | 2:G:1:NAG:O1      | 2.59                     | 0.54              |
| 1:D:3070:TYR:C    | 1:D:3071:ILE:HD12 | 2.33                     | 0.54              |
| 1:D:3287:PHE:CZ   | 1:D:3290:GLY:HA2  | 2.42                     | 0.54              |
| 1:B:1229:LEU:O    | 1:B:1232:GLU:HB3  | 2.08                     | 0.54              |
| 1:D:3151:TYR:O    | 1:D:3153:ASP:N    | 2.42                     | 0.54              |
| 1:D:3199:MET:O    | 1:D:3202:LEU:HB2  | 2.08                     | 0.54              |
| 1:A:233:ASN:HB2   | 1:A:332:ILE:HG23  | 1.90                     | 0.53              |
| 1:B:1295:MET:HE1  | 1:B:1310:LEU:HD13 | 1.89                     | 0.53              |
| 1:A:54:ARG:HG3    | 1:A:91:LEU:O      | 2.08                     | 0.53              |
| 1:C:2127:ASN:HD22 | 1:C:2127:ASN:H    | 1.56                     | 0.53              |
| 1:D:3020:PHE:CE2  | 1:D:3023:ASP:HB2  | 2.44                     | 0.53              |
| 1:B:1295:MET:HG3  | 8:B:1514:HOH:O    | 2.09                     | 0.53              |
| 1:A:245:ILE:HD12  | 1:A:246:PRO:N     | 2.23                     | 0.53              |
| 1:C:2065:LYS:HG2  | 1:C:2067:GLU:HG2  | 1.90                     | 0.53              |
| 1:C:2130:ARG:HG2  | 1:C:2225:LEU:HD11 | 1.90                     | 0.53              |
| 1:D:3065:LYS:O    | 1:D:3068:GLN:N    | 2.35                     | 0.53              |
| 1:D:3230:LEU:CD2  | 1:D:3263:LEU:HD22 | 2.38                     | 0.53              |
| 1:A:137:SER:O     | 1:A:140:LEU:HB2   | 2.08                     | 0.53              |
| 1:D:3128:CYS:HB2  | 1:D:3335:TRP:CZ2  | 2.42                     | 0.53              |
| 1:A:213:SER:HA    | 1:A:217:ILE:HD12  | 1.91                     | 0.53              |
| 1:B:1299:ASN:HD21 | 2:G:1:NAG:C2      | 2.21                     | 0.53              |
| 1:A:58:ARG:HG2    | 1:A:58:ARG:NH1    | 2.23                     | 0.53              |
| 1:C:2039:GLN:HA   | 1:C:2042:MET:HE3  | 1.90                     | 0.53              |
| 1:A:179:ASP:HB3   | 1:A:180:PRO:HD3   | 1.89                     | 0.53              |
| 1:B:1275:PRO:HG2  | 1:B:1299:ASN:HB2  | 1.90                     | 0.53              |
| 1:C:2235:LEU:C    | 1:C:2235:LEU:HD13 | 2.34                     | 0.53              |
| 1:C:2133:GLU:O    | 1:C:2137:GLU:HG3  | 2.08                     | 0.53              |
| 1:B:1298:ARG:NH1  | 1:B:1301:THR:HG22 | 2.23                     | 0.53              |
| 1:A:316:SER:HB2   | 1:A:317:PRO:CD    | 2.37                     | 0.52              |
| 1:D:3022:THR:HG22 | 1:D:3022:THR:O    | 2.07                     | 0.52              |
| 1:A:148:ARG:C     | 1:A:151:PRO:HD2   | 2.34                     | 0.52              |
| 1:A:274:LEU:HD12  | 2:F:1:NAG:H2      | 1.91                     | 0.52              |
| 1:D:3322:ARG:HH11 | 1:D:3322:ARG:CG   | 2.22                     | 0.52              |
| 1:A:50:GLY:O      | 1:A:53:ILE:HG23   | 2.09                     | 0.52              |
| 1:A:127:ARG:HH11  | 1:A:127:ARG:CB    | 2.22                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2010:ARG:O    | 1:C:2045:HIS:HE1  | 1.92                     | 0.52              |
| 1:C:2151:TYR:O    | 1:C:2155:ILE:HG13 | 2.09                     | 0.52              |
| 1:D:3045:HIS:ND1  | 1:D:3082:SER:HB3  | 2.24                     | 0.52              |
| 1:D:3060:LEU:O    | 1:D:3062:GLU:OE2  | 2.27                     | 0.52              |
| 1:A:6:VAL:HG12    | 1:A:7:THR:N       | 2.24                     | 0.52              |
| 1:B:1056:TYR:CB   | 1:B:1060:LEU:HD23 | 2.40                     | 0.52              |
| 1:B:1216:HIS:O    | 1:B:1221:LYS:HE3  | 2.10                     | 0.52              |
| 1:A:152:TYR:O     | 1:A:154:ASP:N     | 2.43                     | 0.52              |
| 1:B:1011:HIS:CE1  | 1:B:1078:ARG:HD2  | 2.45                     | 0.52              |
| 1:B:1112:THR:OG1  | 1:B:1113:VAL:N    | 2.43                     | 0.52              |
| 1:B:1210:LEU:HD13 | 1:B:1210:LEU:C    | 2.34                     | 0.52              |
| 1:C:2074:THR:O    | 1:C:2076:VAL:N    | 2.38                     | 0.52              |
| 1:C:2090:LEU:HD22 | 1:C:2091:PHE:CZ   | 2.45                     | 0.52              |
| 1:A:11:ARG:O      | 1:A:46:HIS:HE1    | 1.93                     | 0.52              |
| 1:D:3046:TYR:CD1  | 1:D:3089:ALA:HB2  | 2.44                     | 0.52              |
| 1:D:3193:TRP:O    | 1:D:3195:THR:HG23 | 2.10                     | 0.52              |
| 1:A:106:TRP:HB2   | 1:B:1103:LEU:HD11 | 1.92                     | 0.52              |
| 1:B:1007:LEU:HD13 | 1:B:1052:ILE:CD1  | 2.32                     | 0.52              |
| 1:C:2109:PRO:HA   | 1:D:3084:MET:HE1  | 1.92                     | 0.52              |
| 1:A:10:PHE:CE2    | 1:A:253:MET:HE2   | 2.43                     | 0.52              |
| 1:B:1138:LEU:N    | 1:B:1138:LEU:HD22 | 2.25                     | 0.52              |
| 1:B:1244:PRO:O    | 1:B:1246:TYR:N    | 2.43                     | 0.52              |
| 1:A:37:GLN:HE21   | 1:A:37:GLN:N      | 2.09                     | 0.51              |
| 1:D:3025:ILE:HD12 | 1:D:3025:ILE:N    | 2.21                     | 0.51              |
| 1:A:302:GLU:OE2   | 1:A:305:HIS:HD2   | 1.92                     | 0.51              |
| 1:C:2016:PRO:HG2  | 1:C:2034:PHE:CE2  | 2.46                     | 0.51              |
| 1:C:2169:LEU:CD2  | 1:C:2205:LEU:HB3  | 2.40                     | 0.51              |
| 1:B:1000:LYS:HB2  | 1:B:1287:GLU:OE1  | 2.10                     | 0.51              |
| 1:C:2098:ILE:HG22 | 1:C:2099:TRP:N    | 2.26                     | 0.51              |
| 1:D:3090:LEU:HD13 | 1:D:3091:PHE:CE1  | 2.45                     | 0.51              |
| 1:A:100:TRP:HA    | 8:A:524:HOH:O     | 2.10                     | 0.51              |
| 1:D:3068:GLN:HE21 | 1:D:3249:LYS:HE3  | 1.75                     | 0.51              |
| 1:C:2000:LYS:HG3  | 1:C:2286:TYR:HB3  | 1.93                     | 0.51              |
| 1:C:2056:TYR:HB3  | 1:C:2059:PHE:HB3  | 1.93                     | 0.51              |
| 1:C:2098:ILE:O    | 1:C:2099:TRP:CB   | 2.59                     | 0.51              |
| 1:D:3009:PHE:HE2  | 1:D:3252:MET:HE2  | 1.75                     | 0.51              |
| 1:D:3212:SER:HA   | 1:D:3216:ILE:HG13 | 1.91                     | 0.51              |
| 1:A:150:HIS:O     | 1:A:152:TYR:N     | 2.44                     | 0.51              |
| 2:H:1:NAG:H61     | 2:H:2:NAG:C2      | 2.37                     | 0.51              |
| 1:D:3007:LEU:HD12 | 1:D:3252:MET:HE3  | 1.93                     | 0.51              |
| 1:A:127:ARG:HE    | 5:A:403:1PE:H262  | 1.76                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1126:ARG:NH1  | 1:B:1126:ARG:HG2  | 2.26                     | 0.51              |
| 1:C:2061:ASN:HD22 | 1:C:2061:ASN:H    | 1.59                     | 0.51              |
| 1:A:28:GLU:HA     | 1:A:35:PHE:CE2    | 2.46                     | 0.50              |
| 1:B:1100:ASN:ND2  | 1:B:1103:LEU:HB3  | 2.25                     | 0.50              |
| 1:B:1128:CYS:O    | 1:B:1131:GLN:HG2  | 2.11                     | 0.50              |
| 1:B:1144:GLN:HA   | 1:B:1144:GLN:NE2  | 2.26                     | 0.50              |
| 1:D:3040:LEU:O    | 1:D:3043:GLU:HB2  | 2.11                     | 0.50              |
| 1:D:3163:GLY:O    | 1:D:3164:LEU:HD23 | 2.10                     | 0.50              |
| 1:A:49:LEU:HD13   | 1:A:87:ASN:ND2    | 2.23                     | 0.50              |
| 1:A:159:LEU:HD13  | 1:A:159:LEU:O     | 2.10                     | 0.50              |
| 1:A:287:TYR:O     | 1:A:293:TYR:HA    | 2.11                     | 0.50              |
| 1:C:2005:VAL:HG22 | 1:C:2250:LEU:CD1  | 2.41                     | 0.50              |
| 1:C:2266:ALA:O    | 1:C:2330:VAL:HG11 | 2.12                     | 0.50              |
| 1:D:3235:LEU:HD11 | 1:D:3324:ALA:HB2  | 1.93                     | 0.50              |
| 1:A:152:TYR:O     | 1:A:153:LYS:C     | 2.53                     | 0.50              |
| 1:B:1145:LYS:HA   | 1:B:1145:LYS:CE   | 2.21                     | 0.50              |
| 1:C:2126:ARG:HG3  | 5:C:2403:1PE:H122 | 1.94                     | 0.50              |
| 1:D:3056:TYR:HB3  | 1:D:3059:PHE:HB3  | 1.93                     | 0.50              |
| 1:D:3071:ILE:HG22 | 1:D:3110:VAL:HG13 | 1.93                     | 0.50              |
| 1:A:155:PHE:CE1   | 1:A:199:THR:HG22  | 2.45                     | 0.50              |
| 1:D:3181:TYR:O    | 1:D:3184:SER:HB3  | 2.11                     | 0.50              |
| 1:A:236:LEU:O     | 1:A:240:LYS:HG2   | 2.12                     | 0.50              |
| 1:B:1124:PRO:HD2  | 5:B:1404:1PE:H131 | 1.93                     | 0.50              |
| 1:B:1184:VAL:O    | 6:B:1401:NDG:C8   | 2.60                     | 0.50              |
| 1:C:2013:ASP:N    | 1:C:2044:GLN:OE1  | 2.37                     | 0.50              |
| 1:A:64:SER:HB2    | 1:A:95:GLU:CD     | 2.37                     | 0.50              |
| 1:B:1163:LEU:HD11 | 1:B:1174:LYS:HB3  | 1.94                     | 0.50              |
| 1:C:2017:ILE:HD11 | 4:C:2401:2BF:O1P  | 2.12                     | 0.50              |
| 1:A:40:GLN:HG2    | 1:B:1099:TRP:HB3  | 1.92                     | 0.49              |
| 1:B:1065:LYS:HB3  | 1:B:1067:GLU:CD   | 2.37                     | 0.49              |
| 1:C:2120:LEU:HD23 | 1:C:2120:LEU:C    | 2.37                     | 0.49              |
| 1:D:3098:ILE:HG23 | 1:D:3104:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:57:TYR:HB3    | 1:A:61:LEU:HD13   | 1.93                     | 0.49              |
| 1:B:1210:LEU:CD1  | 1:B:1215:ILE:HG12 | 2.43                     | 0.49              |
| 1:A:114:VAL:CG1   | 1:A:115:PRO:HD2   | 2.41                     | 0.49              |
| 1:B:1056:TYR:OH   | 1:B:1283:GLU:OE1  | 2.29                     | 0.49              |
| 1:D:3062:GLU:O    | 1:D:3064:TYR:N    | 2.45                     | 0.49              |
| 1:B:1060:LEU:N    | 1:B:1060:LEU:HD22 | 2.27                     | 0.49              |
| 1:D:3016:PRO:HG2  | 1:D:3034:PHE:CE2  | 2.46                     | 0.49              |
| 1:D:3322:ARG:HG2  | 1:D:3322:ARG:NH1  | 2.24                     | 0.49              |
| 1:A:6:VAL:CG1     | 1:A:7:THR:N       | 2.75                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:116:LEU:HD22  | 1:A:123:TYR:CE1   | 2.47                     | 0.49              |
| 1:A:301:ASN:C     | 1:A:302:GLU:HG3   | 2.37                     | 0.49              |
| 1:B:1002:LEU:HD13 | 1:B:1285:TYR:CE2  | 2.48                     | 0.49              |
| 1:C:2048:LEU:HD23 | 1:C:2299:ARG:NH2  | 2.28                     | 0.49              |
| 1:B:1244:PRO:O    | 1:B:1245:SER:C    | 2.55                     | 0.49              |
| 1:C:2096:VAL:HG22 | 1:C:2096:VAL:O    | 2.13                     | 0.49              |
| 1:A:109:ILE:HD12  | 1:A:109:ILE:N     | 2.27                     | 0.49              |
| 1:C:2071:ILE:HG12 | 1:C:2087:LEU:HD21 | 1.95                     | 0.49              |
| 1:B:1070:TYR:HB2  | 1:B:1247:LYS:HE2  | 1.95                     | 0.49              |
| 1:B:1165:GLY:C    | 1:B:1167:ASP:H    | 2.21                     | 0.49              |
| 1:C:2184:SER:O    | 1:C:2185:VAL:C    | 2.55                     | 0.49              |
| 1:C:2009:PHE:CE1  | 1:C:2254:SER:HA   | 2.47                     | 0.49              |
| 1:D:3149:HIS:C    | 1:D:3151:TYR:H    | 2.21                     | 0.49              |
| 1:D:3217:HIS:O    | 1:D:3222:LYS:HE3  | 2.13                     | 0.49              |
| 1:A:172:GLY:O     | 1:A:176:LYS:HB2   | 2.13                     | 0.49              |
| 1:B:1070:TYR:CE1  | 1:B:1111:HIS:CD2  | 3.01                     | 0.49              |
| 1:B:1163:LEU:HD11 | 1:B:1174:LYS:HD3  | 1.94                     | 0.49              |
| 1:B:1256:ASP:OD2  | 4:B:1402:2BF:H7   | 2.13                     | 0.49              |
| 1:A:124:LEU:HB3   | 1:A:125:PRO:HA    | 1.95                     | 0.48              |
| 1:B:1171:ILE:O    | 1:B:1175:VAL:HB   | 2.13                     | 0.48              |
| 1:B:1194:THR:O    | 1:B:1197:THR:N    | 2.46                     | 0.48              |
| 1:C:2022:THR:HG23 | 1:C:2162:SER:O    | 2.13                     | 0.48              |
| 1:C:2071:ILE:HD12 | 1:C:2071:ILE:N    | 2.28                     | 0.48              |
| 1:A:125:PRO:HD2   | 5:A:403:1PE:H131  | 1.95                     | 0.48              |
| 1:C:2061:ASN:H    | 1:C:2061:ASN:ND2  | 2.11                     | 0.48              |
| 1:B:1007:LEU:HD23 | 1:B:1281:LEU:HB3  | 1.95                     | 0.48              |
| 1:C:2083:ALA:O    | 1:C:2087:LEU:HG   | 2.13                     | 0.48              |
| 1:D:3257:ASP:OD2  | 1:D:3258:THR:N    | 2.46                     | 0.48              |
| 1:A:213:SER:CA    | 1:A:217:ILE:HD12  | 2.44                     | 0.48              |
| 1:D:3159:GLY:HA3  | 1:D:3164:LEU:O    | 2.14                     | 0.48              |
| 1:D:3289:LYS:O    | 1:D:3289:LYS:HG2  | 2.14                     | 0.48              |
| 1:A:165:LEU:HD11  | 1:A:176:LYS:HD2   | 1.95                     | 0.48              |
| 1:B:1281:LEU:N    | 1:B:1281:LEU:CD2  | 2.77                     | 0.48              |
| 1:D:3155:ILE:HG22 | 8:D:3513:HOH:O    | 2.14                     | 0.48              |
| 1:D:3286:TYR:O    | 1:D:3292:TYR:HA   | 2.14                     | 0.48              |
| 1:B:1016:PRO:HG2  | 1:B:1034:PHE:CE2  | 2.49                     | 0.48              |
| 1:B:1093:PRO:HB3  | 1:B:1106:GLN:HB3  | 1.95                     | 0.48              |
| 1:B:1157:LEU:HD23 | 1:B:1171:ILE:HD12 | 1.96                     | 0.48              |
| 1:C:2104:LEU:O    | 1:C:2105:TRP:CB   | 2.61                     | 0.48              |
| 1:B:1175:VAL:C    | 1:B:1178:PRO:HD2  | 2.38                     | 0.48              |
| 1:B:1238:LYS:HE3  | 8:B:1507:HOH:O    | 2.14                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2127:ASN:H    | 1:C:2127:ASN:ND2  | 2.11                     | 0.48              |
| 1:C:2128:CYS:SG   | 1:C:2225:LEU:HD13 | 2.53                     | 0.48              |
| 1:A:97:VAL:O      | 1:B:1039:GLN:NE2  | 2.47                     | 0.48              |
| 1:B:1036:GLN:HE22 | 1:B:1077:ASP:HB2  | 1.79                     | 0.48              |
| 1:D:3322:ARG:CG   | 1:D:3322:ARG:NH1  | 2.77                     | 0.48              |
| 1:A:19:ASP:OD2    | 1:A:176:LYS:HG2   | 2.14                     | 0.48              |
| 1:B:1019:THR:OG1  | 1:B:1020:PHE:N    | 2.46                     | 0.48              |
| 1:D:3148:LEU:HD11 | 1:D:3155:ILE:CD1  | 2.44                     | 0.48              |
| 1:C:2105:TRP:CZ2  | 1:C:2107:PRO:HB3  | 2.49                     | 0.47              |
| 1:D:3270:TYR:CE2  | 1:D:3272:GLY:HA2  | 2.48                     | 0.47              |
| 1:A:74:SER:CB     | 1:A:255:SER:HB3   | 2.42                     | 0.47              |
| 1:A:135:LEU:HD13  | 1:A:223:LYS:HG3   | 1.96                     | 0.47              |
| 1:B:1087:LEU:HD13 | 1:B:1108:ILE:CG2  | 2.44                     | 0.47              |
| 1:D:3123:LEU:N    | 1:D:3123:LEU:HD12 | 2.29                     | 0.47              |
| 1:A:64:SER:HB2    | 1:A:95:GLU:OE2    | 2.15                     | 0.47              |
| 1:C:2215:GLY:O    | 1:C:2216:ILE:HB   | 2.13                     | 0.47              |
| 1:D:3055:ARG:NH2  | 1:D:3284:GLU:OE1  | 2.45                     | 0.47              |
| 1:D:3115:LEU:HD22 | 1:D:3122:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:113:THR:OG1   | 1:A:114:VAL:N     | 2.47                     | 0.47              |
| 1:C:2334:ASP:O    | 1:C:2338:GLU:HG3  | 2.14                     | 0.47              |
| 1:D:3025:ILE:H    | 1:D:3025:ILE:CD1  | 2.23                     | 0.47              |
| 1:C:2018:ASP:CG   | 1:C:2019:THR:H    | 2.23                     | 0.47              |
| 1:D:3065:LYS:C    | 1:D:3067:GLU:N    | 2.72                     | 0.47              |
| 1:D:3090:LEU:HD22 | 1:D:3091:PHE:CE2  | 2.49                     | 0.47              |
| 1:D:3093:PRO:HB2  | 1:D:3098:ILE:HG12 | 1.95                     | 0.47              |
| 1:A:88:LEU:HD13   | 1:A:109:ILE:CG2   | 2.45                     | 0.47              |
| 1:B:1200:LYS:HE2  | 8:B:1527:HOH:O    | 2.14                     | 0.47              |
| 1:B:1239:ARG:HB3  | 1:B:1246:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:2310:MET:HE2  | 1:C:2314:CYS:O    | 2.14                     | 0.47              |
| 1:A:328:VAL:O     | 1:A:331:VAL:HG22  | 2.15                     | 0.47              |
| 1:B:1006:THR:HG22 | 1:B:1006:THR:O    | 2.15                     | 0.47              |
| 1:D:3048:LEU:HD13 | 1:D:3086:ASN:HD21 | 1.79                     | 0.47              |
| 1:D:3177:TYR:HB2  | 1:D:3202:LEU:HB3  | 1.95                     | 0.47              |
| 1:D:3337:THR:O    | 1:D:3340:MET:HB2  | 2.14                     | 0.47              |
| 1:A:301:ASN:O     | 1:A:302:GLU:HG3   | 2.14                     | 0.47              |
| 1:D:3193:TRP:O    | 1:D:3195:THR:N    | 2.40                     | 0.47              |
| 1:D:3232:ASN:HB2  | 1:D:3331:ILE:CG2  | 2.42                     | 0.47              |
| 1:D:3239:LYS:O    | 1:D:3242:THR:HG22 | 2.14                     | 0.47              |
| 1:A:115:PRO:HD3   | 1:B:1113:VAL:HG22 | 1.97                     | 0.47              |
| 1:A:150:HIS:HB3   | 1:A:151:PRO:CD    | 2.35                     | 0.47              |
| 1:C:2010:ARG:NH2  | 4:C:2401:2BF:O2P  | 2.46                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1126:ARG:HG2  | 1:B:1126:ARG:HH11 | 1.80                     | 0.46              |
| 1:B:1163:LEU:CD2  | 1:B:1174:LYS:HD3  | 2.45                     | 0.46              |
| 1:C:2061:ASN:N    | 1:C:2061:ASN:ND2  | 2.63                     | 0.46              |
| 1:C:2120:LEU:HD11 | 1:C:2233:GLU:HG2  | 1.96                     | 0.46              |
| 1:D:3071:ILE:HD12 | 1:D:3071:ILE:N    | 2.30                     | 0.46              |
| 1:D:3298:TYR:HB2  | 1:D:3309:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:24:ASP:OD1    | 1:A:26:ILE:N      | 2.47                     | 0.46              |
| 1:A:51:GLU:HG3    | 1:A:90:ALA:HB1    | 1.97                     | 0.46              |
| 1:A:312:LEU:O     | 1:A:313:PRO:C     | 2.56                     | 0.46              |
| 1:C:2145:GLN:HE21 | 1:C:2145:GLN:CA   | 2.11                     | 0.46              |
| 1:D:3071:ILE:CG2  | 1:D:3110:VAL:HG13 | 2.45                     | 0.46              |
| 1:C:2006:THR:O    | 1:C:2007:LEU:HD23 | 2.15                     | 0.46              |
| 1:C:2123:LEU:HD22 | 1:C:2259:THR:HA   | 1.97                     | 0.46              |
| 1:C:2224:ARG:HG3  | 1:C:2224:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:82:MET:HA     | 1:A:85:MET:CE     | 2.45                     | 0.46              |
| 1:C:2099:TRP:HH2  | 1:D:3046:TYR:CD1  | 2.33                     | 0.46              |
| 1:C:2288:GLU:OE2  | 1:C:2288:GLU:HA   | 2.16                     | 0.46              |
| 1:D:3045:HIS:HD2  | 1:D:3086:ASN:HD22 | 1.54                     | 0.46              |
| 1:A:245:ILE:HD12  | 1:A:246:PRO:CG    | 2.45                     | 0.46              |
| 1:D:3046:TYR:CE1  | 1:D:3089:ALA:HB2  | 2.49                     | 0.46              |
| 1:C:2076:VAL:O    | 1:C:2077:ASP:C    | 2.58                     | 0.46              |
| 1:D:3176:VAL:C    | 1:D:3179:PRO:HD2  | 2.40                     | 0.46              |
| 1:A:88:LEU:HD13   | 1:A:109:ILE:HB    | 1.98                     | 0.46              |
| 1:A:176:LYS:C     | 1:A:180:PRO:HG2   | 2.41                     | 0.46              |
| 1:A:200:MET:O     | 1:A:203:LEU:HB2   | 2.16                     | 0.46              |
| 1:A:246:PRO:HG2   | 1:A:247:SER:H     | 1.80                     | 0.46              |
| 1:B:1056:TYR:HB3  | 1:B:1060:LEU:CD2  | 2.44                     | 0.46              |
| 1:C:2124:PRO:HG3  | 1:C:2213:LEU:HD21 | 1.96                     | 0.46              |
| 1:C:2127:ASN:HD21 | 5:C:2402:1PE:H242 | 1.80                     | 0.46              |
| 1:D:3235:LEU:HD21 | 1:D:3324:ALA:HB1  | 1.98                     | 0.46              |
| 2:E:1:NAG:C6      | 2:E:2:NAG:H82     | 2.32                     | 0.46              |
| 1:A:121:LEU:HD21  | 1:A:234:GLU:HG2   | 1.97                     | 0.46              |
| 1:A:127:ARG:NH1   | 1:A:127:ARG:HG2   | 2.30                     | 0.46              |
| 1:A:178:TYR:CE1   | 1:A:204:ARG:HB2   | 2.51                     | 0.46              |
| 1:C:2000:LYS:HE2  | 1:C:2286:TYR:CE2  | 2.51                     | 0.46              |
| 1:C:2235:LEU:HD13 | 1:C:2235:LEU:O    | 2.15                     | 0.46              |
| 1:D:3020:PHE:CD2  | 1:D:3023:ASP:HB2  | 2.51                     | 0.46              |
| 1:D:3068:GLN:HE21 | 1:D:3249:LYS:CE   | 2.29                     | 0.46              |
| 1:D:3173:TRP:CD1  | 1:D:3206:SER:HG   | 2.34                     | 0.46              |
| 1:D:3190:LEU:HD12 | 1:D:3190:LEU:N    | 2.30                     | 0.46              |
| 1:A:241:ARG:HD2   | 1:A:248:TYR:OH    | 2.16                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1002:LEU:HD23 | 1:B:1059:PHE:CG   | 2.52                     | 0.46              |
| 1:C:2126:ARG:NH1  | 1:C:2132:GLN:OE1  | 2.47                     | 0.46              |
| 1:C:2270:TYR:CE2  | 1:C:2272:GLY:HA2  | 2.51                     | 0.46              |
| 1:D:3002:LEU:HD13 | 1:D:3286:TYR:CZ   | 2.51                     | 0.46              |
| 1:D:3190:LEU:HB3  | 1:D:3191:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:212:LEU:HD12  | 1:A:217:ILE:CG1   | 2.42                     | 0.45              |
| 1:A:308:TYR:CE2   | 2:F:1:NAG:H5      | 2.51                     | 0.45              |
| 1:C:2002:LEU:HD23 | 1:C:2059:PHE:CG   | 2.51                     | 0.45              |
| 1:C:2234:ILE:HG22 | 1:C:2238:MET:HE2  | 1.98                     | 0.45              |
| 1:D:3032:GLN:HB3  | 1:D:3036:GLN:CG   | 2.38                     | 0.45              |
| 1:D:3076:VAL:O    | 1:D:3080:LEU:HG   | 2.16                     | 0.45              |
| 1:B:1090:LEU:HD13 | 1:B:1091:PHE:CE1  | 2.51                     | 0.45              |
| 1:C:2055:ARG:NH2  | 1:C:2284:GLU:OE1  | 2.50                     | 0.45              |
| 1:C:2070:TYR:HB3  | 1:C:2251:ILE:HG12 | 1.98                     | 0.45              |
| 1:D:3149:HIS:O    | 1:D:3151:TYR:N    | 2.49                     | 0.45              |
| 1:C:2288:GLU:CG   | 1:C:2289:LYS:H    | 2.14                     | 0.45              |
| 1:C:2315:SER:HB2  | 1:C:2316:PRO:CD   | 2.47                     | 0.45              |
| 1:A:7:THR:HG21    | 1:A:235:ILE:HG12  | 1.98                     | 0.45              |
| 1:A:12:HIS:NE2    | 4:A:401:2BF:P     | 2.90                     | 0.45              |
| 1:D:3057:ARG:HG3  | 1:D:3058:LYS:N    | 2.32                     | 0.45              |
| 1:D:3060:LEU:HD11 | 1:D:3250:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:5:PHE:CZ      | 1:A:238:HIS:HB3   | 2.51                     | 0.45              |
| 1:A:204:ARG:NH1   | 1:A:208:GLU:OE1   | 2.49                     | 0.45              |
| 1:A:213:SER:CB    | 1:A:217:ILE:HD12  | 2.46                     | 0.45              |
| 1:A:245:ILE:HD11  | 1:A:247:SER:O     | 2.16                     | 0.45              |
| 1:B:1010:ARG:CD   | 1:B:1256:ASP:HB3  | 2.39                     | 0.45              |
| 1:C:2300:ASN:CG   | 2:H:1:NAG:HN2     | 2.24                     | 0.45              |
| 1:D:3129:PRO:O    | 1:D:3132:GLN:HB2  | 2.16                     | 0.45              |
| 1:C:2107:PRO:O    | 1:D:3081:MET:HG2  | 2.16                     | 0.45              |
| 1:D:3215:GLY:O    | 1:D:3222:LYS:NZ   | 2.46                     | 0.45              |
| 1:D:3264:GLN:HE21 | 1:D:3270:TYR:HA   | 1.81                     | 0.45              |
| 1:A:127:ARG:CG    | 1:A:127:ARG:NH1   | 2.76                     | 0.45              |
| 1:A:315:CYS:HB2   | 1:A:327:LEU:CD1   | 2.46                     | 0.45              |
| 1:B:1147:LEU:O    | 1:B:1148:HIS:C    | 2.60                     | 0.45              |
| 1:C:2242:THR:HB   | 1:C:2292:TYR:CE1  | 2.52                     | 0.45              |
| 1:D:3062:GLU:OE2  | 1:D:3068:GLN:NE2  | 2.43                     | 0.45              |
| 1:D:3094:GLU:H    | 1:D:3097:SER:HB2  | 1.82                     | 0.45              |
| 1:A:61:LEU:HD23   | 1:A:92:PHE:CE2    | 2.52                     | 0.45              |
| 1:A:71:TYR:HB2    | 1:A:249:LYS:HE2   | 1.99                     | 0.45              |
| 1:A:239:MET:O     | 1:A:243:THR:HG23  | 2.17                     | 0.45              |
| 1:B:1145:LYS:HE3  | 1:B:1145:LYS:CA   | 2.21                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2056:TYR:HB2  | 1:C:2060:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:2161:LEU:HD13 | 1:C:2193:TRP:CG   | 2.52                     | 0.45              |
| 1:D:3198:THR:O    | 1:D:3199:MET:C    | 2.59                     | 0.45              |
| 1:A:150:HIS:HA    | 1:A:153:LYS:HG3   | 1.99                     | 0.44              |
| 1:A:301:ASN:OD1   | 2:F:1:NAG:O1      | 2.35                     | 0.44              |
| 1:B:1186:ASN:HD21 | 6:B:1401:NDG:C2   | 2.29                     | 0.44              |
| 1:D:3175:LYS:O    | 1:D:3179:PRO:HG2  | 2.18                     | 0.44              |
| 1:A:107:GLN:HG3   | 1:A:109:ILE:CD1   | 2.48                     | 0.44              |
| 1:A:245:ILE:HD11  | 1:A:247:SER:C     | 2.42                     | 0.44              |
| 1:A:288:PHE:CE1   | 1:A:291:GLY:HA2   | 2.53                     | 0.44              |
| 1:D:3212:SER:HA   | 1:D:3216:ILE:CG1  | 2.46                     | 0.44              |
| 1:B:1223:ARG:NH2  | 1:B:1331:PRO:HA   | 2.32                     | 0.44              |
| 1:C:2013:ASP:OD1  | 1:C:2186:HIS:HE1  | 2.00                     | 0.44              |
| 1:C:2115:LEU:HD13 | 1:C:2122:TYR:CE1  | 2.52                     | 0.44              |
| 1:C:2337:THR:O    | 1:C:2339:CYS:N    | 2.50                     | 0.44              |
| 1:D:3154:PHE:CD1  | 1:D:3201:LYS:HD2  | 2.52                     | 0.44              |
| 1:D:3328:GLY:N    | 1:D:3329:PRO:HD2  | 2.33                     | 0.44              |
| 1:A:49:LEU:HA     | 1:A:300:ARG:HH22  | 1.81                     | 0.44              |
| 1:A:66:LYS:HG3    | 1:A:69:GLN:NE2    | 2.32                     | 0.44              |
| 1:B:1134:GLU:O    | 1:B:1138:LEU:HD23 | 2.17                     | 0.44              |
| 1:D:3064:TYR:C    | 1:D:3065:LYS:HG3  | 2.42                     | 0.44              |
| 1:D:3230:LEU:HD23 | 1:D:3263:LEU:HD22 | 1.99                     | 0.44              |
| 1:A:40:GLN:OE1    | 1:B:1097:SER:HA   | 2.18                     | 0.44              |
| 1:D:3340:MET:HE3  | 1:D:3341:THR:N    | 2.28                     | 0.44              |
| 1:A:53:ILE:CD1    | 1:A:57:TYR:CD1    | 3.01                     | 0.44              |
| 1:A:201:THR:O     | 1:A:205:GLU:HG3   | 2.18                     | 0.44              |
| 1:B:1023:ASP:HA   | 1:B:1024:PRO:HD3  | 1.82                     | 0.44              |
| 1:C:2093:PRO:HB2  | 1:C:2104:LEU:HB3  | 2.00                     | 0.44              |
| 1:D:3169:LEU:HD21 | 1:D:3205:LEU:HD22 | 1.99                     | 0.44              |
| 1:D:3311:LEU:O    | 1:D:3312:PRO:C    | 2.59                     | 0.44              |
| 1:A:72:ILE:N      | 1:A:72:ILE:HD12   | 2.33                     | 0.44              |
| 1:C:2061:ASN:O    | 1:C:2062:GLU:HG3  | 2.18                     | 0.44              |
| 1:A:49:LEU:HD22   | 1:A:53:ILE:HG22   | 2.00                     | 0.44              |
| 1:B:1214:GLY:HA3  | 1:B:1264:MET:HE1  | 2.00                     | 0.44              |
| 1:A:142:SER:O     | 1:A:146:GLN:HG2   | 2.18                     | 0.43              |
| 1:A:150:HIS:C     | 1:A:152:TYR:N     | 2.73                     | 0.43              |
| 1:C:2098:ILE:C    | 1:C:2099:TRP:CD1  | 2.96                     | 0.43              |
| 1:C:2303:GLN:HG3  | 1:C:2304:HIS:CD2  | 2.53                     | 0.43              |
| 1:B:1318:PRO:HG2  | 1:B:1321:ARG:CB   | 2.49                     | 0.43              |
| 1:C:2149:HIS:HB3  | 1:C:2150:PRO:CD   | 2.41                     | 0.43              |
| 1:D:3026:LYS:O    | 1:D:3027:GLU:C    | 2.60                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3154:PHE:CZ   | 1:D:3201:LYS:HB2  | 2.53                     | 0.43              |
| 1:D:3287:PHE:HA   | 1:D:3291:GLU:O    | 2.18                     | 0.43              |
| 1:A:127:ARG:HH11  | 1:A:127:ARG:HB3   | 1.83                     | 0.43              |
| 1:B:1321:ARG:NH1  | 1:B:1321:ARG:HG2  | 2.33                     | 0.43              |
| 1:D:3094:GLU:O    | 1:D:3094:GLU:HG3  | 2.18                     | 0.43              |
| 1:C:2190:LEU:HB3  | 1:C:2191:PRO:CD   | 2.40                     | 0.43              |
| 1:C:2276:PRO:HD2  | 1:C:2279:SER:HB3  | 2.00                     | 0.43              |
| 1:D:3065:LYS:C    | 1:D:3067:GLU:H    | 2.26                     | 0.43              |
| 1:A:18:ILE:HG22   | 1:A:18:ILE:O      | 2.17                     | 0.43              |
| 1:B:1075:ASP:HB2  | 1:B:1113:VAL:O    | 2.18                     | 0.43              |
| 1:B:1326:VAL:O    | 1:B:1329:VAL:HG22 | 2.16                     | 0.43              |
| 1:C:2224:ARG:HG3  | 1:C:2224:ARG:NH1  | 2.34                     | 0.43              |
| 1:D:3160:LYS:HD2  | 1:D:3160:LYS:HA   | 1.89                     | 0.43              |
| 1:D:3295:GLU:OE1  | 1:D:3297:TYR:OH   | 2.34                     | 0.43              |
| 1:A:177:VAL:O     | 1:A:180:PRO:HD2   | 2.19                     | 0.43              |
| 1:B:1230:VAL:HG11 | 1:B:1326:VAL:CG2  | 2.48                     | 0.43              |
| 1:C:2261:SER:O    | 1:C:2265:MET:HG2  | 2.19                     | 0.43              |
| 1:D:3006:THR:HG21 | 1:D:3234:ILE:HG12 | 2.00                     | 0.43              |
| 1:D:3062:GLU:HB2  | 1:D:3065:LYS:HD2  | 2.00                     | 0.43              |
| 1:D:3121:LEU:HD11 | 1:D:3253:TYR:HD2  | 1.83                     | 0.43              |
| 1:A:100:TRP:CE3   | 1:A:101:ASN:HB2   | 2.53                     | 0.43              |
| 1:A:124:LEU:HD12  | 1:A:260:THR:HA    | 2.01                     | 0.43              |
| 1:C:2169:LEU:HD23 | 1:C:2169:LEU:HA   | 1.82                     | 0.43              |
| 1:C:2257:ASP:HB2  | 1:C:2275:PRO:HD2  | 2.01                     | 0.43              |
| 1:D:3273:LEU:HD12 | 3:I:1:NAG:H2      | 2.01                     | 0.43              |
| 1:B:1060:LEU:C    | 1:B:1062:GLU:N    | 2.73                     | 0.43              |
| 1:B:1216:HIS:CE1  | 1:B:1217:LYS:HG3  | 2.53                     | 0.43              |
| 1:C:2126:ARG:NH1  | 1:C:2126:ARG:HG2  | 2.34                     | 0.43              |
| 1:D:3088:ALA:HA   | 1:D:3105:TRP:HE1  | 1.84                     | 0.43              |
| 1:D:3240:ARG:HB3  | 1:D:3247:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:17:PRO:HG2    | 1:A:35:PHE:CE2    | 2.53                     | 0.43              |
| 1:C:2130:ARG:HB3  | 1:C:2339:CYS:HA   | 2.01                     | 0.43              |
| 1:C:2154:PHE:O    | 1:C:2158:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:2188:PHE:O    | 1:C:2189:THR:C    | 2.62                     | 0.43              |
| 1:A:245:ILE:HD12  | 1:A:246:PRO:HG2   | 2.00                     | 0.43              |
| 1:D:3013:ASP:O    | 1:D:3037:LEU:HD12 | 2.19                     | 0.43              |
| 1:A:17:PRO:HB3    | 1:A:180:PRO:HA    | 2.01                     | 0.42              |
| 1:A:24:ASP:HA     | 1:A:25:PRO:HD3    | 1.93                     | 0.42              |
| 1:A:178:TYR:HD1   | 1:A:203:LEU:HB3   | 1.84                     | 0.42              |
| 1:A:218:HIS:CE1   | 1:A:219:LYS:HE3   | 2.54                     | 0.42              |
| 1:B:1060:LEU:O    | 1:B:1062:GLU:N    | 2.51                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1168:LEU:HD22 | 1:B:1204:LEU:HD22 | 2.01                     | 0.42              |
| 1:C:2168:ASP:OD2  | 1:C:2171:GLY:N    | 2.43                     | 0.42              |
| 1:C:2217:HIS:NE2  | 1:C:2218:LYS:HD3  | 2.33                     | 0.42              |
| 1:D:3269:VAL:HB   | 1:D:3309:LEU:HD22 | 1.99                     | 0.42              |
| 1:B:1038:THR:O    | 1:B:1042:MET:HG3  | 2.18                     | 0.42              |
| 1:B:1138:LEU:N    | 1:B:1138:LEU:CD2  | 2.82                     | 0.42              |
| 1:C:2086:ASN:ND2  | 1:C:2252:MET:CE   | 2.81                     | 0.42              |
| 1:D:3103:LEU:C    | 1:D:3103:LEU:HD23 | 2.44                     | 0.42              |
| 1:B:1115:LEU:HD22 | 1:B:1122:TYR:CD2  | 2.54                     | 0.42              |
| 1:B:1184:VAL:O    | 6:B:1401:NDG:H8C3 | 2.19                     | 0.42              |
| 1:B:1322:PHE:O    | 1:B:1326:VAL:HG12 | 2.19                     | 0.42              |
| 1:D:3045:HIS:CE1  | 1:D:3082:SER:HB3  | 2.54                     | 0.42              |
| 1:D:3319:PRO:HG2  | 1:D:3322:ARG:HB3  | 2.01                     | 0.42              |
| 1:B:1166:GLN:HE21 | 1:B:1166:GLN:HB2  | 1.67                     | 0.42              |
| 1:B:1184:VAL:O    | 6:B:1401:NDG:H8C1 | 2.19                     | 0.42              |
| 1:C:2013:ASP:HA   | 1:C:2277:TYR:CE1  | 2.55                     | 0.42              |
| 1:C:2051:TYR:CE2  | 1:C:2299:ARG:HD2  | 2.54                     | 0.42              |
| 1:D:3213:LEU:HD23 | 1:D:3214:TYR:CE1  | 2.54                     | 0.42              |
| 1:A:143:GLU:OE1   | 1:A:147:LYS:NZ    | 2.50                     | 0.42              |
| 1:B:1069:VAL:HG12 | 1:B:1070:TYR:N    | 2.35                     | 0.42              |
| 1:C:2327:VAL:O    | 1:C:2327:VAL:HG12 | 2.19                     | 0.42              |
| 1:D:3119:GLN:HA   | 1:D:3125:PHE:HE1  | 1.84                     | 0.42              |
| 1:D:3169:LEU:HD23 | 1:D:3169:LEU:HA   | 1.89                     | 0.42              |
| 1:A:311:MET:HG2   | 1:A:317:PRO:HD3   | 2.01                     | 0.42              |
| 1:B:1068:GLN:O    | 1:B:1247:LYS:HG3  | 2.20                     | 0.42              |
| 1:C:2027:GLU:HB2  | 1:C:2034:PHE:CE1  | 2.55                     | 0.42              |
| 1:C:2301:GLU:OE1  | 2:H:1:NAG:H83     | 2.19                     | 0.42              |
| 1:D:3208:LEU:O    | 1:D:3212:SER:HB3  | 2.20                     | 0.42              |
| 1:A:232:VAL:HG11  | 1:A:328:VAL:CG2   | 2.50                     | 0.42              |
| 1:A:323:ARG:HD2   | 1:A:323:ARG:HA    | 1.79                     | 0.42              |
| 1:B:1216:HIS:CE1  | 1:B:1217:LYS:HE3  | 2.54                     | 0.42              |
| 1:C:2168:ASP:O    | 1:C:2169:LEU:C    | 2.63                     | 0.42              |
| 1:D:3167:GLN:HA   | 8:D:3507:HOH:O    | 2.19                     | 0.42              |
| 1:B:1063:SER:O    | 1:B:1064:TYR:O    | 2.38                     | 0.42              |
| 1:B:1210:LEU:HD13 | 1:B:1210:LEU:O    | 2.20                     | 0.42              |
| 1:B:1321:ARG:HG2  | 1:B:1321:ARG:HH11 | 1.85                     | 0.42              |
| 1:C:2064:TYR:OH   | 1:C:2066:HIS:HB3  | 2.19                     | 0.42              |
| 1:C:2090:LEU:HD22 | 1:C:2091:PHE:CE1  | 2.54                     | 0.42              |
| 1:D:3230:LEU:HD21 | 1:D:3263:LEU:HD22 | 2.01                     | 0.42              |
| 7:D:3401:NAG:C7   | 7:D:3401:NAG:O1   | 2.56                     | 0.42              |
| 1:A:116:LEU:C     | 1:A:118:GLU:H     | 2.28                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:216:GLY:O     | 1:A:217:ILE:HB    | 2.19                     | 0.42              |
| 1:C:2148:LEU:O    | 1:C:2149:HIS:C    | 2.63                     | 0.42              |
| 1:D:3222:LYS:O    | 1:D:3223:SER:C    | 2.63                     | 0.42              |
| 1:B:1023:ASP:OD2  | 1:B:1182:GLU:OE2  | 2.37                     | 0.42              |
| 1:B:1150:TYR:O    | 1:B:1154:ILE:HG23 | 2.20                     | 0.42              |
| 1:B:1169:PHE:CE1  | 5:B:1404:1PE:H222 | 2.55                     | 0.42              |
| 1:D:3245:PRO:C    | 1:D:3247:TYR:H    | 2.28                     | 0.42              |
| 1:B:1089:ALA:O    | 1:B:1092:PRO:HD3  | 2.20                     | 0.41              |
| 1:C:2191:PRO:HB2  | 1:C:2193:TRP:NE1  | 2.35                     | 0.41              |
| 1:C:2319:PRO:HG2  | 1:C:2322:ARG:CB   | 2.48                     | 0.41              |
| 1:A:215:TYR:CE1   | 1:A:263:GLY:HA2   | 2.54                     | 0.41              |
| 1:C:2093:PRO:O    | 1:C:2094:GLU:HB3  | 2.20                     | 0.41              |
| 1:C:2126:ARG:CG   | 1:C:2126:ARG:HH11 | 2.33                     | 0.41              |
| 1:A:122:LEU:HD11  | 1:A:254:TYR:HD2   | 1.86                     | 0.41              |
| 1:A:313:PRO:HD3   | 8:A:525:HOH:O     | 2.18                     | 0.41              |
| 1:B:1071:ILE:HG12 | 1:B:1087:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:1229:LEU:HD23 | 1:B:1262:LEU:HB2  | 2.03                     | 0.41              |
| 1:D:3269:VAL:CG2  | 1:D:3309:LEU:HD13 | 2.50                     | 0.41              |
| 1:A:8:LEU:CD2     | 1:A:283:LEU:HB3   | 2.43                     | 0.41              |
| 1:A:122:LEU:O     | 1:A:124:LEU:N     | 2.53                     | 0.41              |
| 1:A:245:ILE:HG13  | 1:A:248:TYR:HB2   | 2.01                     | 0.41              |
| 1:C:2115:LEU:HD13 | 1:C:2122:TYR:CZ   | 2.55                     | 0.41              |
| 1:C:2154:PHE:CE1  | 1:C:2158:LEU:HD23 | 2.55                     | 0.41              |
| 1:C:2235:LEU:HD11 | 1:C:2239:LYS:HE3  | 2.01                     | 0.41              |
| 1:D:3064:TYR:OH   | 1:D:3066:HIS:HB3  | 2.19                     | 0.41              |
| 1:D:3093:PRO:O    | 1:D:3094:GLU:HB3  | 2.20                     | 0.41              |
| 1:A:315:CYS:HB2   | 1:A:327:LEU:HD11  | 2.03                     | 0.41              |
| 1:C:2307:TYR:HA   | 1:C:2308:PRO:HD3  | 1.85                     | 0.41              |
| 1:C:2307:TYR:CD1  | 2:H:1:NAG:O1      | 2.67                     | 0.41              |
| 1:A:176:LYS:O     | 1:A:180:PRO:HG2   | 2.20                     | 0.41              |
| 1:B:1176:TYR:CE1  | 1:B:1202:ARG:HB2  | 2.55                     | 0.41              |
| 1:B:1239:ARG:C    | 1:B:1241:THR:N    | 2.78                     | 0.41              |
| 1:C:2120:LEU:CD2  | 1:C:2121:LEU:HG   | 2.48                     | 0.41              |
| 1:C:2169:LEU:HD11 | 1:C:2208:LEU:CD2  | 2.50                     | 0.41              |
| 1:D:3151:TYR:O    | 1:D:3152:LYS:C    | 2.63                     | 0.41              |
| 1:C:2039:GLN:O    | 1:C:2042:MET:HB2  | 2.20                     | 0.41              |
| 1:D:3119:GLN:HB3  | 5:D:3403:1PE:OH4  | 2.21                     | 0.41              |
| 1:A:41:LEU:O      | 1:A:41:LEU:HD12   | 2.21                     | 0.41              |
| 1:A:61:LEU:C      | 1:A:63:GLU:H      | 2.28                     | 0.41              |
| 1:A:70:VAL:HG12   | 1:A:71:TYR:N      | 2.35                     | 0.41              |
| 1:A:116:LEU:HD22  | 1:A:123:TYR:CD1   | 2.55                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:2023:ASP:HA   | 1:C:2024:PRO:HD3  | 1.96                     | 0.41              |
| 1:D:3073:SER:OG   | 1:D:3080:LEU:HD23 | 2.21                     | 0.41              |
| 1:A:4:LYS:O       | 1:A:4:LYS:HD3     | 2.20                     | 0.41              |
| 1:B:1225:GLN:NE2  | 1:B:1225:GLN:HA   | 2.36                     | 0.41              |
| 1:B:1333:ASP:O    | 1:B:1337:GLU:HG3  | 2.21                     | 0.41              |
| 1:C:2013:ASP:H    | 1:C:2041:GLY:HA2  | 1.85                     | 0.41              |
| 1:C:2143:GLU:O    | 1:C:2147:ARG:HG3  | 2.20                     | 0.41              |
| 1:C:2177:TYR:CE1  | 1:C:2203:ARG:HB2  | 2.56                     | 0.41              |
| 1:D:3119:GLN:HA   | 1:D:3125:PHE:CE1  | 2.56                     | 0.41              |
| 1:D:3186:HIS:HA   | 7:D:3401:NAG:H83  | 2.03                     | 0.41              |
| 1:D:3282:LEU:N    | 1:D:3282:LEU:CD2  | 2.84                     | 0.41              |
| 1:A:15:ARG:HG3    | 1:A:15:ARG:HH11   | 1.86                     | 0.41              |
| 1:A:149:LEU:HD11  | 1:A:156:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:301:ASN:O     | 1:A:302:GLU:CG    | 2.68                     | 0.41              |
| 1:B:1055:ARG:HG2  | 1:B:1056:TYR:CE2  | 2.56                     | 0.41              |
| 1:C:2068:GLN:CG   | 1:C:2249:LYS:HG3  | 2.47                     | 0.41              |
| 1:C:2098:ILE:CG2  | 1:C:2099:TRP:H    | 2.29                     | 0.41              |
| 1:C:2099:TRP:CH2  | 1:D:3046:TYR:CD1  | 3.09                     | 0.41              |
| 1:A:11:ARG:HG3    | 1:A:257:HIS:HA    | 2.04                     | 0.40              |
| 1:A:19:ASP:CG     | 1:A:20:THR:H      | 2.30                     | 0.40              |
| 1:A:20:THR:OG1    | 1:A:21:PHE:N      | 2.55                     | 0.40              |
| 1:A:53:ILE:HD12   | 1:A:57:TYR:CD1    | 2.55                     | 0.40              |
| 1:A:54:ARG:CB     | 1:A:91:LEU:HD23   | 2.51                     | 0.40              |
| 1:B:1004:PHE:CZ   | 1:B:1236:HIS:HB3  | 2.56                     | 0.40              |
| 1:B:1126:ARG:HH21 | 5:B:1404:1PE:H121 | 1.85                     | 0.40              |
| 1:B:1175:VAL:O    | 1:B:1178:PRO:HD2  | 2.20                     | 0.40              |
| 1:C:2042:MET:O    | 1:C:2046:TYR:HB2  | 2.20                     | 0.40              |
| 1:C:2309:LEU:HD23 | 1:C:2309:LEU:HA   | 1.91                     | 0.40              |
| 1:D:3224:ARG:NH2  | 1:D:3332:PRO:HA   | 2.36                     | 0.40              |
| 1:A:77:VAL:O      | 1:A:78:ASP:C      | 2.64                     | 0.40              |
| 1:A:179:ASP:N     | 1:A:180:PRO:CD    | 2.84                     | 0.40              |
| 1:B:1048:LEU:HD22 | 1:B:1052:ILE:CD1  | 2.51                     | 0.40              |
| 1:D:3015:SER:HB2  | 1:D:3016:PRO:HD2  | 2.02                     | 0.40              |
| 1:D:3148:LEU:HD11 | 1:D:3155:ILE:HD11 | 2.03                     | 0.40              |
| 1:D:3244:ILE:HG22 | 1:D:3245:PRO:O    | 2.22                     | 0.40              |
| 2:H:1:NAG:C6      | 2:H:2:NAG:O5      | 2.69                     | 0.40              |
| 1:A:141:LYS:HD2   | 1:A:141:LYS:N     | 2.36                     | 0.40              |
| 1:B:1014:ARG:HG3  | 1:B:1014:ARG:HH11 | 1.85                     | 0.40              |
| 1:B:1069:VAL:CG1  | 1:B:1070:TYR:N    | 2.84                     | 0.40              |
| 1:C:2177:TYR:OH   | 1:C:2203:ARG:HD3  | 2.21                     | 0.40              |
| 1:D:3010:ARG:NH1  | 1:D:3275:PRO:O    | 2.55                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:8:LEU:HD12    | 1:A:253:MET:HG2  | 2.03                     | 0.40              |
| 1:A:149:LEU:HD11  | 1:A:156:ILE:CD1  | 2.52                     | 0.40              |
| 1:B:1005:VAL:HG21 | 1:B:1056:TYR:CZ  | 2.57                     | 0.40              |
| 1:B:1242:GLN:NE2  | 1:D:3189:THR:OG1 | 2.47                     | 0.40              |
| 1:C:2057:ARG:HA   | 1:C:2057:ARG:HD2 | 1.99                     | 0.40              |
| 1:C:2099:TRP:HB3  | 1:D:3039:GLN:HG3 | 2.02                     | 0.40              |
| 1:D:3255:ALA:HB1  | 1:D:3259:THR:OG1 | 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     | 340/354 (96%)   | 288 (85%)  | 39 (12%)  | 13 (4%)  | 2           | 10 |
| 1   | B     | 338/354 (96%)   | 284 (84%)  | 43 (13%)  | 11 (3%)  | 3           | 13 |
| 1   | C     | 340/354 (96%)   | 282 (83%)  | 41 (12%)  | 17 (5%)  | 1           | 6  |
| 1   | D     | 340/354 (96%)   | 287 (84%)  | 37 (11%)  | 16 (5%)  | 2           | 7  |
| All | All   | 1358/1416 (96%) | 1141 (84%) | 160 (12%) | 57 (4%)  | 2           | 9  |

All (57) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 62   | ASN  |
| 1   | A     | 65   | TYR  |
| 1   | B     | 1064 | TYR  |
| 1   | B     | 1245 | SER  |
| 1   | C     | 2099 | TRP  |
| 1   | C     | 2105 | TRP  |
| 1   | C     | 2167 | GLN  |
| 1   | D     | 3061 | ASN  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 3063 | SER  |
| 1   | D     | 3152 | LYS  |
| 1   | D     | 3167 | GLN  |
| 1   | A     | 123  | TYR  |
| 1   | A     | 153  | LYS  |
| 1   | B     | 1140 | SER  |
| 1   | B     | 1340 | THR  |
| 1   | C     | 2031 | PRO  |
| 1   | C     | 2033 | GLY  |
| 1   | C     | 2057 | ARG  |
| 1   | C     | 2066 | HIS  |
| 1   | C     | 2098 | ILE  |
| 1   | C     | 2149 | HIS  |
| 1   | C     | 2334 | ASP  |
| 1   | C     | 2338 | GLU  |
| 1   | D     | 3011 | HIS  |
| 1   | D     | 3066 | HIS  |
| 1   | D     | 3094 | GLU  |
| 1   | D     | 3102 | ILE  |
| 1   | D     | 3289 | LYS  |
| 1   | A     | 117  | SER  |
| 1   | A     | 151  | PRO  |
| 1   | A     | 246  | PRO  |
| 1   | A     | 335  | ASP  |
| 1   | B     | 1027 | GLU  |
| 1   | B     | 1061 | ASN  |
| 1   | C     | 2094 | GLU  |
| 1   | B     | 1148 | HIS  |
| 1   | C     | 2011 | HIS  |
| 1   | D     | 3064 | TYR  |
| 1   | D     | 3150 | PRO  |
| 1   | D     | 3153 | ASP  |
| 1   | A     | 64   | SER  |
| 1   | B     | 1063 | SER  |
| 1   | C     | 2075 | ASP  |
| 1   | C     | 2216 | ILE  |
| 1   | D     | 3028 | SER  |
| 1   | D     | 3166 | GLY  |
| 1   | A     | 269  | ASP  |
| 1   | B     | 1300 | GLU  |
| 1   | C     | 2021 | PRO  |
| 1   | D     | 3108 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 330  | PRO  |
| 1   | C     | 2102 | ILE  |
| 1   | A     | 228  | GLY  |
| 1   | B     | 1215 | ILE  |
| 1   | A     | 32   | PRO  |
| 1   | B     | 1031 | PRO  |
| 1   | D     | 3312 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 314/325 (97%)   | 292 (93%)  | 22 (7%)  | 14          | 40 |
| 1   | B     | 314/325 (97%)   | 297 (95%)  | 17 (5%)  | 20          | 51 |
| 1   | C     | 314/325 (97%)   | 291 (93%)  | 23 (7%)  | 13          | 38 |
| 1   | D     | 314/325 (97%)   | 295 (94%)  | 19 (6%)  | 17          | 46 |
| All | All   | 1256/1300 (97%) | 1175 (94%) | 81 (6%)  | 16          | 44 |

All (81) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LYS  |
| 1   | A     | 37  | GLN  |
| 1   | A     | 46  | HIS  |
| 1   | A     | 49  | LEU  |
| 1   | A     | 53  | ILE  |
| 1   | A     | 58  | ARG  |
| 1   | A     | 68  | GLU  |
| 1   | A     | 91  | LEU  |
| 1   | A     | 127 | ARG  |
| 1   | A     | 144 | GLU  |
| 1   | A     | 147 | LYS  |
| 1   | A     | 158 | THR  |
| 1   | A     | 197 | GLU  |
| 1   | A     | 212 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 214  | LEU  |
| 1   | A     | 231  | LEU  |
| 1   | A     | 240  | LYS  |
| 1   | A     | 245  | ILE  |
| 1   | A     | 283  | LEU  |
| 1   | A     | 312  | LEU  |
| 1   | A     | 315  | CYS  |
| 1   | A     | 317  | PRO  |
| 1   | B     | 1005 | VAL  |
| 1   | B     | 1006 | THR  |
| 1   | B     | 1027 | GLU  |
| 1   | B     | 1036 | GLN  |
| 1   | B     | 1045 | HIS  |
| 1   | B     | 1048 | LEU  |
| 1   | B     | 1078 | ARG  |
| 1   | B     | 1090 | LEU  |
| 1   | B     | 1127 | ASN  |
| 1   | B     | 1145 | LYS  |
| 1   | B     | 1166 | GLN  |
| 1   | B     | 1168 | LEU  |
| 1   | B     | 1189 | LEU  |
| 1   | B     | 1212 | LEU  |
| 1   | B     | 1241 | THR  |
| 1   | B     | 1281 | LEU  |
| 1   | B     | 1304 | GLU  |
| 1   | C     | 2000 | LYS  |
| 1   | C     | 2005 | VAL  |
| 1   | C     | 2036 | GLN  |
| 1   | C     | 2048 | LEU  |
| 1   | C     | 2061 | ASN  |
| 1   | C     | 2069 | VAL  |
| 1   | C     | 2072 | ARG  |
| 1   | C     | 2082 | SER  |
| 1   | C     | 2102 | ILE  |
| 1   | C     | 2105 | TRP  |
| 1   | C     | 2126 | ARG  |
| 1   | C     | 2129 | PRO  |
| 1   | C     | 2130 | ARG  |
| 1   | C     | 2135 | GLU  |
| 1   | C     | 2145 | GLN  |
| 1   | C     | 2158 | LEU  |
| 1   | C     | 2169 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2189 | THR  |
| 1   | C     | 2211 | LEU  |
| 1   | C     | 2213 | LEU  |
| 1   | C     | 2230 | LEU  |
| 1   | C     | 2250 | LEU  |
| 1   | C     | 2322 | ARG  |
| 1   | D     | 3003 | LYS  |
| 1   | D     | 3005 | VAL  |
| 1   | D     | 3006 | THR  |
| 1   | D     | 3042 | MET  |
| 1   | D     | 3045 | HIS  |
| 1   | D     | 3048 | LEU  |
| 1   | D     | 3062 | GLU  |
| 1   | D     | 3069 | VAL  |
| 1   | D     | 3090 | LEU  |
| 1   | D     | 3108 | ILE  |
| 1   | D     | 3127 | ASN  |
| 1   | D     | 3139 | LEU  |
| 1   | D     | 3153 | ASP  |
| 1   | D     | 3242 | THR  |
| 1   | D     | 3243 | GLN  |
| 1   | D     | 3268 | ASP  |
| 1   | D     | 3282 | LEU  |
| 1   | D     | 3289 | LYS  |
| 1   | D     | 3301 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 37   | GLN  |
| 1   | A     | 46   | HIS  |
| 1   | A     | 67   | HIS  |
| 1   | A     | 87   | ASN  |
| 1   | A     | 120  | GLN  |
| 1   | A     | 233  | ASN  |
| 1   | A     | 237  | ASN  |
| 1   | A     | 305  | HIS  |
| 1   | A     | 334  | GLN  |
| 1   | B     | 1032 | GLN  |
| 1   | B     | 1036 | GLN  |
| 1   | B     | 1045 | HIS  |
| 1   | B     | 1068 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1086 | ASN  |
| 1   | B     | 1119 | GLN  |
| 1   | B     | 1127 | ASN  |
| 1   | B     | 1131 | GLN  |
| 1   | B     | 1144 | GLN  |
| 1   | B     | 1166 | GLN  |
| 1   | B     | 1185 | HIS  |
| 1   | B     | 1186 | ASN  |
| 1   | B     | 1225 | GLN  |
| 1   | B     | 1231 | ASN  |
| 1   | B     | 1263 | GLN  |
| 1   | B     | 1280 | HIS  |
| 1   | C     | 2061 | ASN  |
| 1   | C     | 2086 | ASN  |
| 1   | C     | 2106 | GLN  |
| 1   | C     | 2127 | ASN  |
| 1   | C     | 2145 | GLN  |
| 1   | C     | 2149 | HIS  |
| 1   | C     | 2186 | HIS  |
| 1   | C     | 2232 | ASN  |
| 1   | C     | 2264 | GLN  |
| 1   | C     | 2304 | HIS  |
| 1   | C     | 2333 | GLN  |
| 1   | D     | 3039 | GLN  |
| 1   | D     | 3045 | HIS  |
| 1   | D     | 3061 | ASN  |
| 1   | D     | 3068 | GLN  |
| 1   | D     | 3086 | ASN  |
| 1   | D     | 3100 | ASN  |
| 1   | D     | 3106 | GLN  |
| 1   | D     | 3219 | GLN  |
| 1   | D     | 3226 | GLN  |
| 1   | D     | 3264 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

11 monosaccharides 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$ |
| 2   | NAG  | E     | 1   | 2,1  | 15,15,15     | 0.53 | 0           | 21,21,21    | 0.91 | 1 (4%)      |
| 2   | NAG  | E     | 2   | 2    | 15,15,15     | 0.43 | 0           | 21,21,21    | 0.52 | 0           |
| 2   | NAG  | F     | 1   | 2,1  | 15,15,15     | 0.42 | 0           | 21,21,21    | 0.69 | 0           |
| 2   | NAG  | F     | 2   | 2    | 15,15,15     | 0.45 | 0           | 21,21,21    | 1.07 | 2 (9%)      |
| 2   | NAG  | G     | 1   | 2    | 15,15,15     | 0.43 | 0           | 21,21,21    | 0.59 | 0           |
| 2   | NAG  | G     | 2   | 2    | 15,15,15     | 0.50 | 0           | 21,21,21    | 1.01 | 1 (4%)      |
| 2   | NAG  | H     | 1   | 2,1  | 15,15,15     | 0.74 | 0           | 21,21,21    | 1.04 | 1 (4%)      |
| 2   | NAG  | H     | 2   | 2    | 15,15,15     | 0.45 | 0           | 21,21,21    | 0.89 | 1 (4%)      |
| 3   | NAG  | I     | 1   | 3,1  | 15,15,15     | 0.54 | 0           | 21,21,21    | 0.58 | 0           |
| 3   | NAG  | I     | 2   | 3    | 15,15,15     | 0.47 | 0           | 21,21,21    | 1.05 | 1 (4%)      |
| 3   | MAN  | I     | 3   | 3    | 12,12,12     | 0.60 | 0           | 17,17,17    | 0.52 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | NAG  | E     | 1   | 2,1  | -       | 4/6/26/26 | 0/1/1/1 |
| 2   | NAG  | E     | 2   | 2    | 1/1/6/7 | 4/6/26/26 | 0/1/1/1 |
| 2   | NAG  | F     | 1   | 2,1  | 1/1/6/7 | 2/6/26/26 | 0/1/1/1 |
| 2   | NAG  | F     | 2   | 2    | -       | 2/6/26/26 | 0/1/1/1 |
| 2   | NAG  | G     | 1   | 2    | 1/1/6/7 | 2/6/26/26 | 0/1/1/1 |
| 2   | NAG  | G     | 2   | 2    | -       | 4/6/26/26 | 0/1/1/1 |
| 2   | NAG  | H     | 1   | 2,1  | 1/1/6/7 | 6/6/26/26 | 0/1/1/1 |
| 2   | NAG  | H     | 2   | 2    | 1/1/6/7 | 3/6/26/26 | 0/1/1/1 |
| 3   | NAG  | I     | 1   | 3,1  | 1/1/6/7 | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | I     | 2   | 3    | -       | 2/6/26/26 | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | MAN  | I     | 3   | 3    | -       | 2/2/22/22 | 0/1/1/1 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | F     | 2   | NAG  | O1-C1-C2 | -3.52 | 101.91      | 109.22   |
| 3   | I     | 2   | NAG  | O1-C1-C2 | -3.49 | 101.96      | 109.22   |
| 2   | H     | 1   | NAG  | C1-C2-C3 | -3.30 | 106.05      | 110.54   |
| 2   | G     | 2   | NAG  | O1-C1-C2 | -3.28 | 102.41      | 109.22   |
| 2   | E     | 1   | NAG  | O1-C1-C2 | -2.92 | 103.16      | 109.22   |
| 2   | H     | 2   | NAG  | O5-C1-C2 | 2.60  | 112.13      | 109.52   |
| 2   | F     | 2   | NAG  | C1-C2-C3 | -2.00 | 107.81      | 110.54   |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | E     | 2   | NAG  | C1   |
| 2   | F     | 1   | NAG  | C1   |
| 2   | G     | 1   | NAG  | C1   |
| 2   | H     | 1   | NAG  | C1   |
| 2   | H     | 2   | NAG  | C1   |
| 3   | I     | 1   | NAG  | C1   |

All (31) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | E     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | E     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | H     | 1   | NAG  | C1-C2-N2-C7 |
| 2   | H     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | H     | 2   | NAG  | C3-C2-N2-C7 |
| 2   | H     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | H     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 3   | MAN  | C4-C5-C6-O6 |
| 2   | H     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | H     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | F     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | G     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 3   | MAN  | O5-C5-C6-O6 |
| 2   | G     | 2   | NAG  | C4-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | H     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | E     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | F     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | E     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | I     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | E     | 2   | NAG  | C3-C2-N2-C7 |
| 2   | E     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | E     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | G     | 1   | NAG  | C4-C5-C6-O6 |
| 2   | G     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | G     | 2   | NAG  | C8-C7-N2-C2 |
| 2   | F     | 1   | NAG  | C8-C7-N2-C2 |
| 2   | F     | 1   | NAG  | O7-C7-N2-C2 |
| 2   | G     | 2   | NAG  | O7-C7-N2-C2 |
| 2   | E     | 2   | NAG  | C1-C2-N2-C7 |
| 2   | H     | 1   | NAG  | C3-C2-N2-C7 |

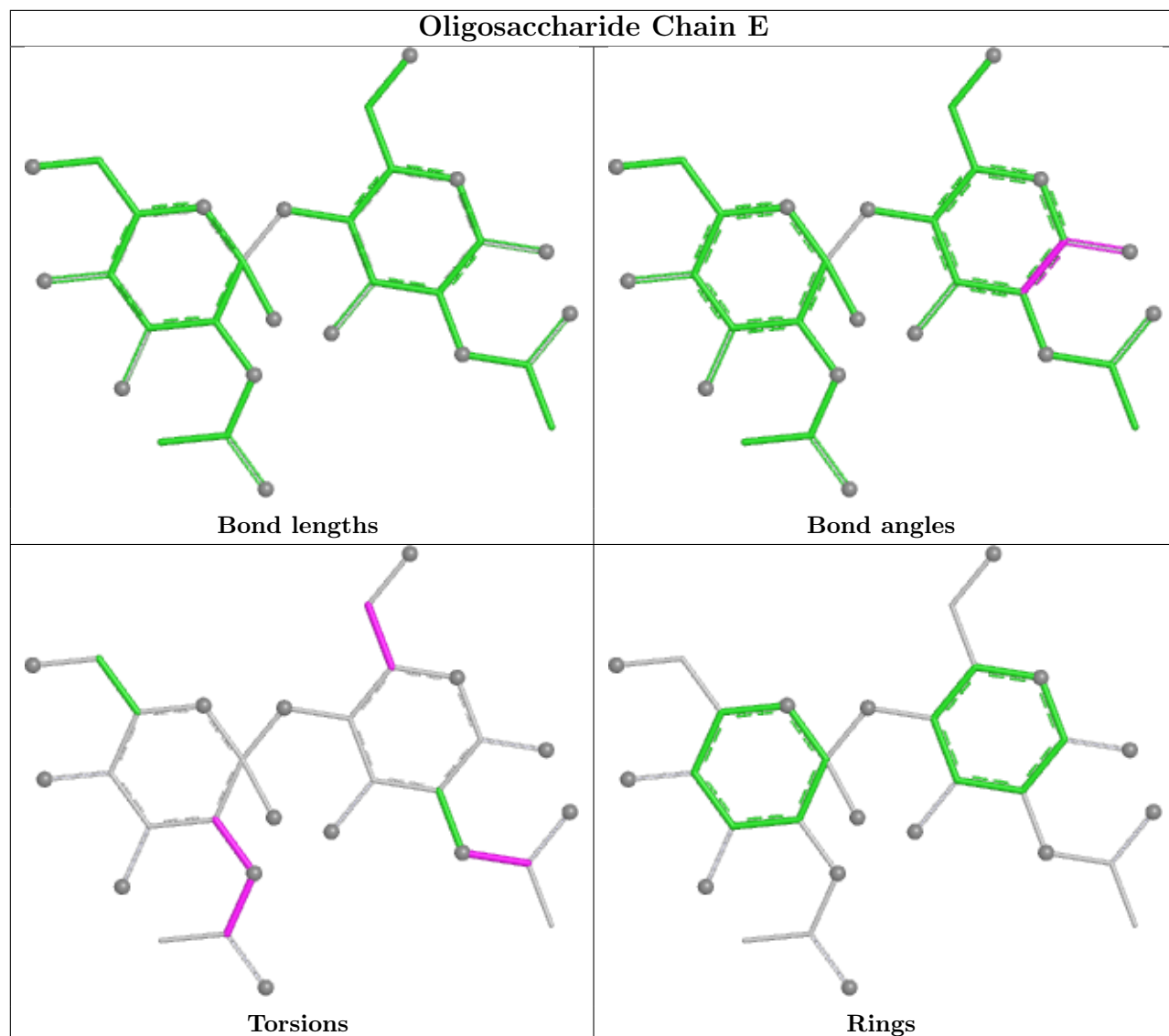
There are no ring outliers.

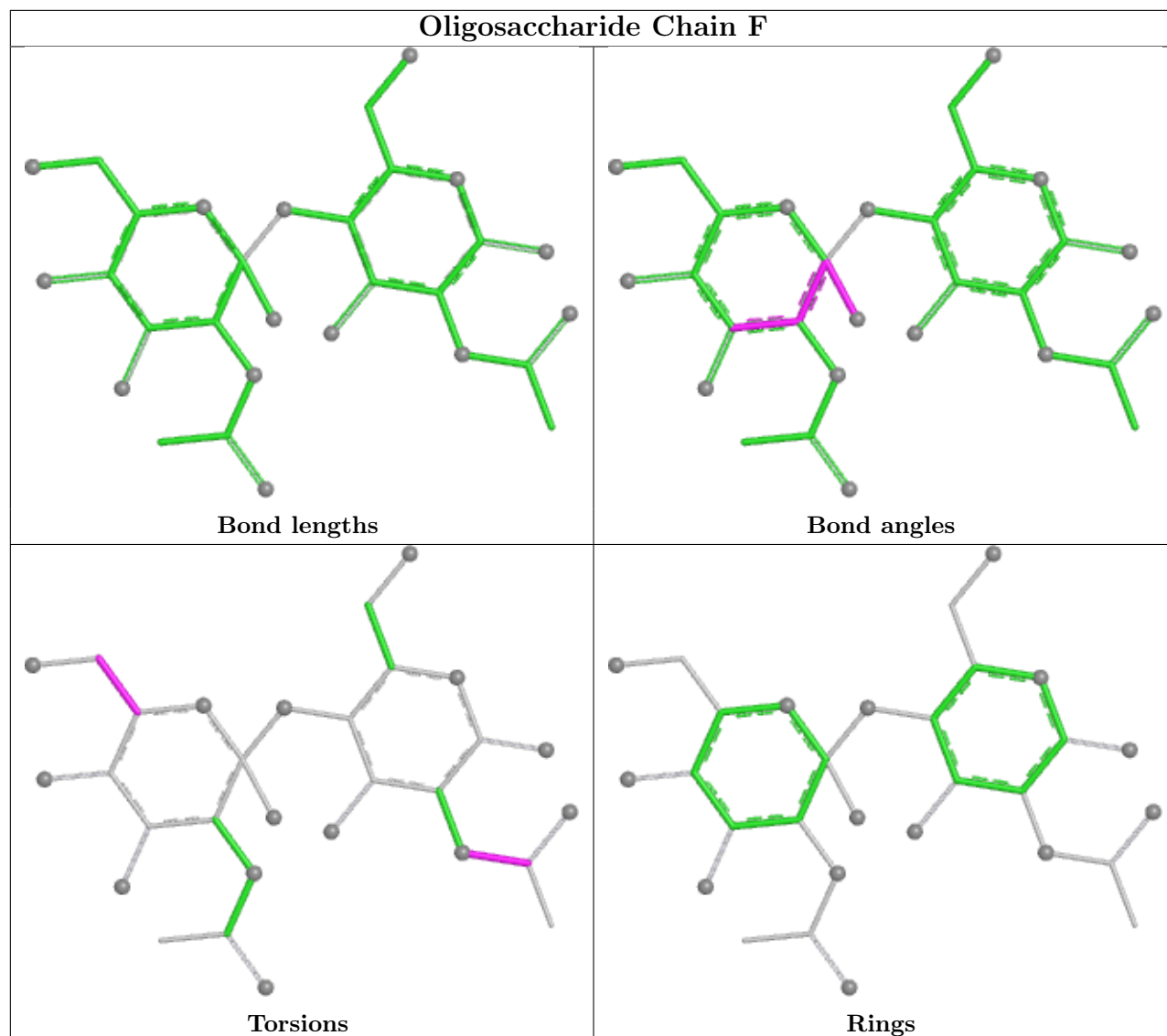
8 monomers are involved in 29 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | G     | 1   | NAG  | 9       | 0            |
| 2   | F     | 1   | NAG  | 4       | 0            |
| 3   | I     | 2   | NAG  | 3       | 0            |
| 2   | H     | 2   | NAG  | 4       | 0            |
| 3   | I     | 1   | NAG  | 4       | 0            |
| 2   | E     | 2   | NAG  | 2       | 0            |
| 2   | H     | 1   | NAG  | 7       | 0            |
| 2   | E     | 1   | NAG  | 4       | 0            |

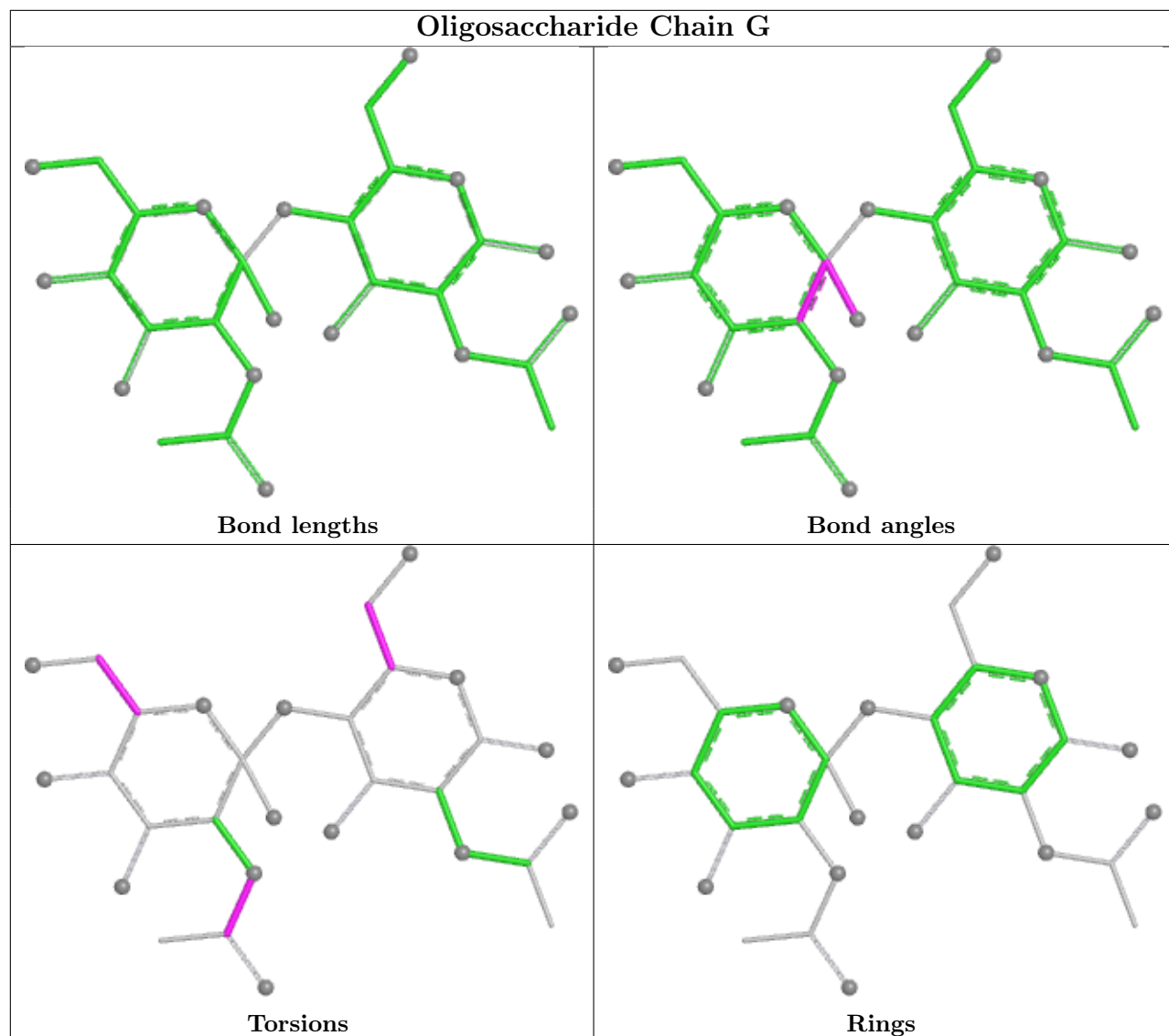
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

## Oligosaccharide Chain E

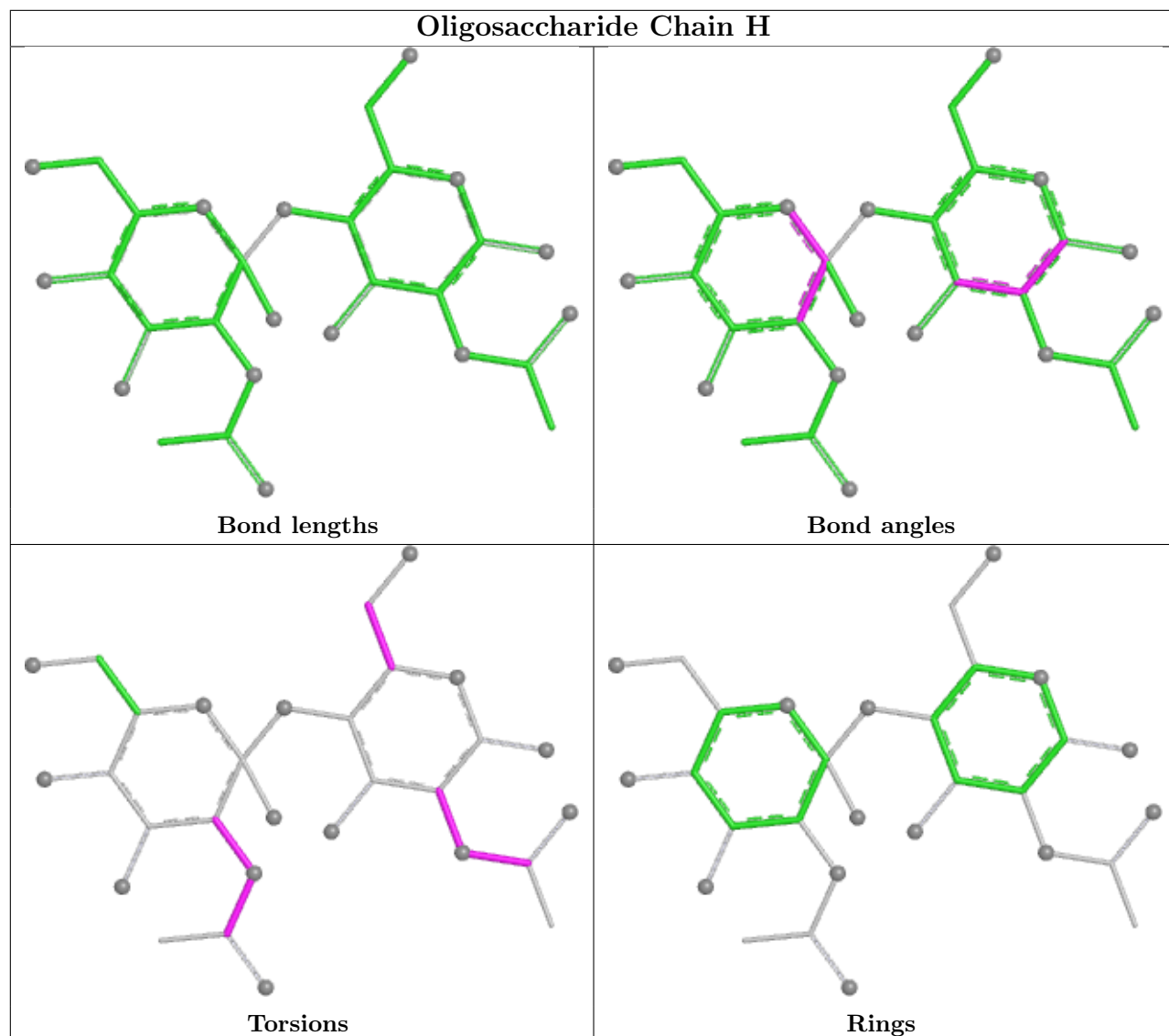


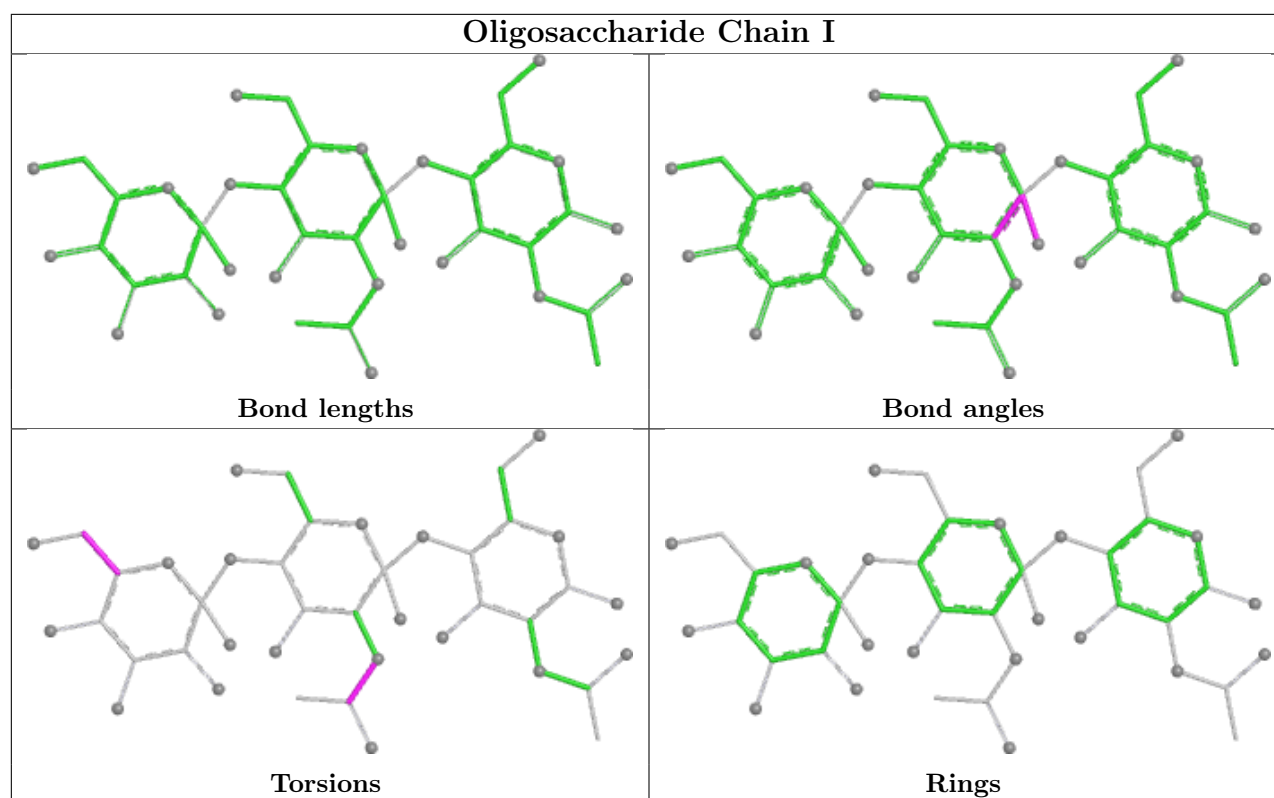


## Oligosaccharide Chain G



## Oligosaccharide Chain H





## 5.6 Ligand geometry [i](#)

14 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 |
| 5   | 1PE  | B     | 1404 | -    | 15,15,15     | 0.83 | 0        | 14,14,14    | 1.52 | 4 (28%)  |
| 5   | 1PE  | B     | 1403 | -    | 15,15,15     | 0.72 | 0        | 14,14,14    | 1.46 | 4 (28%)  |
| 6   | NDG  | B     | 1401 | -    | 15,15,15     | 0.31 | 0        | 21,21,21    | 0.65 | 0        |
| 5   | 1PE  | A     | 404  | -    | 15,15,15     | 0.95 | 0        | 14,14,14    | 1.51 | 4 (28%)  |
| 4   | 2BF  | C     | 2401 | -    | 20,20,20     | 4.20 | 15 (75%) | 24,27,27    | 1.38 | 4 (16%)  |
| 5   | 1PE  | C     | 2403 | -    | 15,15,15     | 0.88 | 0        | 14,14,14    | 1.51 | 4 (28%)  |
| 7   | NAG  | D     | 3401 | 1    | 15,15,15     | 0.43 | 0        | 21,21,21    | 0.62 | 0        |
| 5   | 1PE  | D     | 3403 | -    | 15,15,15     | 0.84 | 0        | 14,14,14    | 1.46 | 4 (28%)  |
| 4   | 2BF  | D     | 3402 | -    | 20,20,20     | 4.33 | 16 (80%) | 24,27,27    | 1.26 | 3 (12%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | 1PE  | C     | 2402 | -    | 15,15,15     | 0.86 | 0        | 14,14,14    | 1.52 | 4 (28%)  |
| 5   | 1PE  | A     | 403  | -    | 15,15,15     | 0.79 | 0        | 14,14,14    | 1.53 | 4 (28%)  |
| 5   | 1PE  | A     | 402  | -    | 15,15,15     | 0.90 | 0        | 14,14,14    | 1.50 | 4 (28%)  |
| 4   | 2BF  | B     | 1402 | -    | 20,20,20     | 4.15 | 15 (75%) | 24,27,27    | 1.35 | 3 (12%)  |
| 4   | 2BF  | A     | 401  | -    | 20,20,20     | 4.34 | 14 (70%) | 24,27,27    | 1.32 | 3 (12%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | 1PE  | B     | 1404 | -    | -       | 6/13/13/13 | -       |
| 5   | 1PE  | B     | 1403 | -    | -       | 5/13/13/13 | -       |
| 6   | NDG  | B     | 1401 | -    | -       | 4/6/26/26  | 0/1/1/1 |
| 5   | 1PE  | A     | 404  | -    | -       | 5/13/13/13 | -       |
| 4   | 2BF  | C     | 2401 | -    | -       | 1/15/15/15 | 0/2/2/2 |
| 5   | 1PE  | C     | 2403 | -    | -       | 8/13/13/13 | -       |
| 7   | NAG  | D     | 3401 | 1    | 1/1/6/7 | 5/6/26/26  | 0/1/1/1 |
| 5   | 1PE  | D     | 3403 | -    | -       | 3/13/13/13 | -       |
| 4   | 2BF  | D     | 3402 | -    | -       | 7/15/15/15 | 0/2/2/2 |
| 5   | 1PE  | C     | 2402 | -    | -       | 4/13/13/13 | -       |
| 5   | 1PE  | A     | 403  | -    | -       | 6/13/13/13 | -       |
| 5   | 1PE  | A     | 402  | -    | -       | 8/13/13/13 | -       |
| 4   | 2BF  | B     | 1402 | -    | -       | 7/15/15/15 | 0/2/2/2 |
| 4   | 2BF  | A     | 401  | -    | -       | 7/15/15/15 | 0/2/2/2 |

All (60) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | A     | 401  | 2BF  | C9-C8   | 9.14 | 1.56        | 1.38     |
| 4   | C     | 2401 | 2BF  | C9-C8   | 9.08 | 1.56        | 1.38     |
| 4   | D     | 3402 | 2BF  | C9-C8   | 8.98 | 1.56        | 1.38     |
| 4   | B     | 1402 | 2BF  | C9-C8   | 8.95 | 1.56        | 1.38     |
| 4   | A     | 401  | 2BF  | C12-C11 | 7.88 | 1.55        | 1.38     |
| 4   | B     | 1402 | 2BF  | C12-C11 | 7.73 | 1.55        | 1.38     |
| 4   | D     | 3402 | 2BF  | C12-C11 | 7.67 | 1.55        | 1.38     |
| 4   | A     | 401  | 2BF  | C3-C2   | 7.59 | 1.54        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | C     | 2401 | 2BF  | C12-C11 | 7.57 | 1.54        | 1.38     |
| 4   | D     | 3402 | 2BF  | C3-C2   | 7.26 | 1.54        | 1.38     |
| 4   | B     | 1402 | 2BF  | C3-C2   | 7.20 | 1.54        | 1.38     |
| 4   | D     | 3402 | 2BF  | P-O1P   | 7.06 | 1.61        | 1.49     |
| 4   | C     | 2401 | 2BF  | C3-C2   | 7.04 | 1.53        | 1.38     |
| 4   | A     | 401  | 2BF  | P-O1P   | 6.66 | 1.60        | 1.49     |
| 4   | C     | 2401 | 2BF  | P-O1P   | 6.18 | 1.60        | 1.49     |
| 4   | B     | 1402 | 2BF  | P-O1P   | 5.79 | 1.59        | 1.49     |
| 4   | D     | 3402 | 2BF  | P-O2P   | 4.79 | 1.62        | 1.54     |
| 4   | B     | 1402 | 2BF  | P-O2P   | 4.66 | 1.62        | 1.54     |
| 4   | A     | 401  | 2BF  | C6-C5   | 4.51 | 1.46        | 1.39     |
| 4   | D     | 3402 | 2BF  | C6-C5   | 4.51 | 1.46        | 1.39     |
| 4   | A     | 401  | 2BF  | P-O3P   | 4.47 | 1.61        | 1.54     |
| 4   | D     | 3402 | 2BF  | P-O3P   | 4.30 | 1.61        | 1.54     |
| 4   | A     | 401  | 2BF  | P-O2P   | 4.10 | 1.61        | 1.54     |
| 4   | C     | 2401 | 2BF  | P-O2P   | 4.10 | 1.61        | 1.54     |
| 4   | C     | 2401 | 2BF  | P-O3P   | 4.00 | 1.61        | 1.54     |
| 4   | C     | 2401 | 2BF  | C6-C5   | 3.90 | 1.45        | 1.39     |
| 4   | B     | 1402 | 2BF  | C6-C5   | 3.87 | 1.45        | 1.39     |
| 4   | A     | 401  | 2BF  | C4-C5   | 3.82 | 1.45        | 1.39     |
| 4   | B     | 1402 | 2BF  | C4-C5   | 3.71 | 1.45        | 1.39     |
| 4   | C     | 2401 | 2BF  | C4-C5   | 3.54 | 1.44        | 1.39     |
| 4   | D     | 3402 | 2BF  | C4-C5   | 3.50 | 1.44        | 1.39     |
| 4   | C     | 2401 | 2BF  | C13-C8  | 3.47 | 1.45        | 1.38     |
| 4   | B     | 1402 | 2BF  | P-O3P   | 3.46 | 1.60        | 1.54     |
| 4   | A     | 401  | 2BF  | C3-C4   | 3.34 | 1.44        | 1.38     |
| 4   | B     | 1402 | 2BF  | C3-C4   | 3.31 | 1.44        | 1.38     |
| 4   | A     | 401  | 2BF  | C1-C6   | 3.27 | 1.44        | 1.38     |
| 4   | C     | 2401 | 2BF  | C1-C6   | 3.19 | 1.44        | 1.38     |
| 4   | B     | 1402 | 2BF  | C1-C6   | 3.18 | 1.44        | 1.38     |
| 4   | C     | 2401 | 2BF  | C11-C10 | 3.15 | 1.45        | 1.38     |
| 4   | C     | 2401 | 2BF  | C3-C4   | 3.09 | 1.44        | 1.38     |
| 4   | D     | 3402 | 2BF  | C13-C8  | 3.01 | 1.44        | 1.38     |
| 4   | D     | 3402 | 2BF  | C1-C6   | 2.91 | 1.43        | 1.38     |
| 4   | D     | 3402 | 2BF  | C3-C4   | 2.78 | 1.43        | 1.38     |
| 4   | B     | 1402 | 2BF  | C13-C8  | 2.77 | 1.44        | 1.38     |
| 4   | B     | 1402 | 2BF  | C12-C13 | 2.76 | 1.43        | 1.38     |
| 4   | D     | 3402 | 2BF  | P-C7    | 2.74 | 1.88        | 1.84     |
| 4   | A     | 401  | 2BF  | C13-C8  | 2.73 | 1.44        | 1.38     |
| 4   | D     | 3402 | 2BF  | C11-C10 | 2.71 | 1.44        | 1.38     |
| 4   | D     | 3402 | 2BF  | C12-C13 | 2.64 | 1.43        | 1.38     |
| 4   | A     | 401  | 2BF  | C2-C1   | 2.64 | 1.44        | 1.38     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | C     | 2401 | 2BF  | C12-C13 | 2.63 | 1.43        | 1.38     |
| 4   | C     | 2401 | 2BF  | C2-C1   | 2.59 | 1.43        | 1.38     |
| 4   | A     | 401  | 2BF  | C11-C10 | 2.54 | 1.43        | 1.38     |
| 4   | B     | 1402 | 2BF  | C2-C1   | 2.53 | 1.43        | 1.38     |
| 4   | A     | 401  | 2BF  | C12-C13 | 2.50 | 1.43        | 1.38     |
| 4   | B     | 1402 | 2BF  | C11-C10 | 2.46 | 1.43        | 1.38     |
| 4   | D     | 3402 | 2BF  | C10-C9  | 2.27 | 1.42        | 1.38     |
| 4   | B     | 1402 | 2BF  | C10-C9  | 2.26 | 1.42        | 1.38     |
| 4   | D     | 3402 | 2BF  | C2-C1   | 2.25 | 1.43        | 1.38     |
| 4   | C     | 2401 | 2BF  | C10-C9  | 2.19 | 1.42        | 1.38     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | B     | 1402 | 2BF  | O1P-P-C7    | -4.26 | 104.03      | 110.89   |
| 4   | C     | 2401 | 2BF  | O1P-P-C7    | -3.93 | 104.56      | 110.89   |
| 4   | A     | 401  | 2BF  | O1P-P-C7    | -3.39 | 105.42      | 110.89   |
| 4   | D     | 3402 | 2BF  | C8-C19-N    | -2.88 | 105.73      | 112.66   |
| 5   | C     | 2403 | 1PE  | C25-OH5-C14 | 2.74  | 125.26      | 113.26   |
| 5   | D     | 3403 | 1PE  | C25-OH5-C14 | 2.65  | 124.88      | 113.26   |
| 5   | A     | 404  | 1PE  | C25-OH5-C14 | 2.65  | 124.84      | 113.26   |
| 5   | A     | 402  | 1PE  | C25-OH5-C14 | 2.64  | 124.82      | 113.26   |
| 5   | B     | 1403 | 1PE  | C25-OH5-C14 | 2.64  | 124.81      | 113.26   |
| 5   | A     | 403  | 1PE  | C25-OH5-C14 | 2.62  | 124.72      | 113.26   |
| 5   | B     | 1404 | 1PE  | C25-OH5-C14 | 2.62  | 124.71      | 113.26   |
| 5   | A     | 403  | 1PE  | OH6-C26-C16 | 2.61  | 121.62      | 110.11   |
| 5   | C     | 2402 | 1PE  | OH6-C26-C16 | 2.59  | 121.51      | 110.11   |
| 5   | C     | 2402 | 1PE  | C25-OH5-C14 | 2.53  | 124.32      | 113.26   |
| 5   | A     | 402  | 1PE  | OH4-C13-C23 | 2.53  | 121.88      | 110.35   |
| 4   | D     | 3402 | 2BF  | C6-C5-C7    | -2.52 | 117.89      | 120.76   |
| 5   | D     | 3403 | 1PE  | OH6-C26-C16 | 2.52  | 121.22      | 110.11   |
| 5   | C     | 2403 | 1PE  | OH6-C26-C16 | 2.52  | 121.21      | 110.11   |
| 4   | A     | 401  | 2BF  | C8-C19-N    | -2.50 | 106.64      | 112.66   |
| 4   | C     | 2401 | 2BF  | C8-C19-N    | -2.47 | 106.71      | 112.66   |
| 5   | B     | 1404 | 1PE  | OH6-C26-C16 | 2.46  | 120.96      | 110.11   |
| 5   | B     | 1404 | 1PE  | OH3-C22-C12 | 2.45  | 120.91      | 110.11   |
| 5   | B     | 1403 | 1PE  | OH6-C26-C16 | 2.42  | 120.79      | 110.11   |
| 5   | A     | 402  | 1PE  | OH6-C26-C16 | 2.42  | 120.78      | 110.11   |
| 4   | D     | 3402 | 2BF  | O1P-P-C7    | -2.42 | 106.99      | 110.89   |
| 5   | B     | 1404 | 1PE  | OH4-C13-C23 | 2.42  | 121.38      | 110.35   |
| 5   | A     | 402  | 1PE  | OH3-C22-C12 | 2.41  | 120.72      | 110.11   |
| 5   | C     | 2403 | 1PE  | OH3-C22-C12 | 2.41  | 120.72      | 110.11   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | A     | 404  | 1PE  | OH6-C26-C16 | 2.39  | 120.66      | 110.11   |
| 5   | C     | 2402 | 1PE  | OH4-C13-C23 | 2.37  | 121.16      | 110.35   |
| 5   | A     | 403  | 1PE  | OH3-C22-C12 | 2.37  | 120.54      | 110.11   |
| 5   | B     | 1403 | 1PE  | OH3-C22-C12 | 2.36  | 120.52      | 110.11   |
| 5   | C     | 2403 | 1PE  | OH4-C13-C23 | 2.34  | 121.00      | 110.35   |
| 4   | A     | 401  | 2BF  | C6-C5-C7    | -2.33 | 118.11      | 120.76   |
| 5   | A     | 404  | 1PE  | OH4-C13-C23 | 2.33  | 120.96      | 110.35   |
| 5   | C     | 2402 | 1PE  | OH3-C22-C12 | 2.30  | 120.27      | 110.11   |
| 5   | A     | 403  | 1PE  | OH4-C13-C23 | 2.30  | 120.84      | 110.35   |
| 5   | D     | 3403 | 1PE  | OH4-C13-C23 | 2.29  | 120.80      | 110.35   |
| 5   | B     | 1403 | 1PE  | OH4-C13-C23 | 2.28  | 120.74      | 110.35   |
| 5   | D     | 3403 | 1PE  | OH3-C22-C12 | 2.26  | 120.06      | 110.11   |
| 4   | B     | 1402 | 2BF  | C8-C19-N    | -2.22 | 107.30      | 112.66   |
| 5   | A     | 404  | 1PE  | OH3-C22-C12 | 2.19  | 119.75      | 110.11   |
| 4   | B     | 1402 | 2BF  | C6-C5-C7    | -2.14 | 118.33      | 120.76   |
| 4   | C     | 2401 | 2BF  | O3P-P-O1P   | -2.13 | 108.10      | 113.45   |
| 4   | C     | 2401 | 2BF  | C6-C5-C7    | -2.09 | 118.39      | 120.76   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 7   | D     | 3401 | NAG  | C1   |

All (76) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 401  | 2BF  | C5-C7-P-O1P |
| 4   | A     | 401  | 2BF  | C5-C7-P-O2P |
| 4   | A     | 401  | 2BF  | C5-C7-P-O3P |
| 4   | A     | 401  | 2BF  | N-C7-P-O1P  |
| 4   | A     | 401  | 2BF  | N-C7-P-O2P  |
| 4   | A     | 401  | 2BF  | N-C7-P-O3P  |
| 4   | B     | 1402 | 2BF  | C5-C7-P-O3P |
| 4   | B     | 1402 | 2BF  | N-C7-P-O1P  |
| 4   | B     | 1402 | 2BF  | N-C7-P-O2P  |
| 4   | B     | 1402 | 2BF  | N-C7-P-O3P  |
| 4   | D     | 3402 | 2BF  | C5-C7-P-O1P |
| 4   | D     | 3402 | 2BF  | C5-C7-P-O2P |
| 4   | D     | 3402 | 2BF  | C5-C7-P-O3P |
| 4   | D     | 3402 | 2BF  | N-C7-P-O1P  |
| 4   | D     | 3402 | 2BF  | N-C7-P-O2P  |
| 4   | D     | 3402 | 2BF  | N-C7-P-O3P  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | D     | 3401 | NAG  | C1-C2-N2-C7     |
| 7   | D     | 3401 | NAG  | C8-C7-N2-C2     |
| 7   | D     | 3401 | NAG  | O7-C7-N2-C2     |
| 7   | D     | 3401 | NAG  | O5-C5-C6-O6     |
| 5   | B     | 1404 | 1PE  | OH5-C14-C24-OH4 |
| 6   | B     | 1401 | NDG  | C8-C7-N2-C2     |
| 6   | B     | 1401 | NDG  | O7-C7-N2-C2     |
| 5   | B     | 1404 | 1PE  | OH4-C13-C23-OH3 |
| 5   | C     | 2403 | 1PE  | OH5-C14-C24-OH4 |
| 4   | A     | 401  | 2BF  | C8-C19-N-C7     |
| 4   | B     | 1402 | 2BF  | C8-C19-N-C7     |
| 4   | C     | 2401 | 2BF  | C8-C19-N-C7     |
| 5   | A     | 403  | 1PE  | OH6-C15-C25-OH5 |
| 5   | C     | 2403 | 1PE  | OH4-C13-C23-OH3 |
| 6   | B     | 1401 | NDG  | O5-C5-C6-O6     |
| 7   | D     | 3401 | NAG  | C4-C5-C6-O6     |
| 5   | C     | 2403 | 1PE  | OH6-C15-C25-OH5 |
| 4   | B     | 1402 | 2BF  | C5-C7-P-O1P     |
| 5   | B     | 1403 | 1PE  | OH5-C14-C24-OH4 |
| 5   | A     | 404  | 1PE  | OH5-C14-C24-OH4 |
| 5   | B     | 1403 | 1PE  | OH4-C13-C23-OH3 |
| 5   | A     | 402  | 1PE  | OH7-C16-C26-OH6 |
| 5   | B     | 1403 | 1PE  | OH7-C16-C26-OH6 |
| 5   | A     | 403  | 1PE  | OH7-C16-C26-OH6 |
| 5   | C     | 2403 | 1PE  | OH2-C12-C22-OH3 |
| 4   | D     | 3402 | 2BF  | C8-C19-N-C7     |
| 5   | A     | 402  | 1PE  | OH5-C14-C24-OH4 |
| 5   | C     | 2403 | 1PE  | OH7-C16-C26-OH6 |
| 5   | A     | 403  | 1PE  | OH5-C14-C24-OH4 |
| 6   | B     | 1401 | NDG  | C4-C5-C6-O6     |
| 5   | A     | 402  | 1PE  | OH2-C12-C22-OH3 |
| 5   | D     | 3403 | 1PE  | OH6-C15-C25-OH5 |
| 5   | A     | 402  | 1PE  | OH4-C13-C23-OH3 |
| 5   | C     | 2402 | 1PE  | OH4-C13-C23-OH3 |
| 5   | D     | 3403 | 1PE  | OH2-C12-C22-OH3 |
| 5   | A     | 404  | 1PE  | OH4-C13-C23-OH3 |
| 5   | B     | 1404 | 1PE  | C15-C25-OH5-C14 |
| 5   | C     | 2402 | 1PE  | OH2-C12-C22-OH3 |
| 5   | A     | 402  | 1PE  | C14-C24-OH4-C13 |
| 4   | B     | 1402 | 2BF  | C5-C7-P-O2P     |
| 5   | C     | 2403 | 1PE  | C13-C23-OH3-C22 |
| 5   | D     | 3403 | 1PE  | C13-C23-OH3-C22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 404  | 1PE  | C24-C14-OH5-C25 |
| 5   | A     | 404  | 1PE  | OH7-C16-C26-OH6 |
| 5   | C     | 2402 | 1PE  | C15-C25-OH5-C14 |
| 5   | C     | 2402 | 1PE  | C12-C22-OH3-C23 |
| 5   | B     | 1404 | 1PE  | C14-C24-OH4-C13 |
| 5   | A     | 402  | 1PE  | C12-C22-OH3-C23 |
| 5   | A     | 402  | 1PE  | OH6-C15-C25-OH5 |
| 5   | A     | 402  | 1PE  | C24-C14-OH5-C25 |
| 5   | B     | 1404 | 1PE  | C13-C23-OH3-C22 |
| 5   | B     | 1403 | 1PE  | OH2-C12-C22-OH3 |
| 5   | C     | 2403 | 1PE  | C24-C14-OH5-C25 |
| 5   | A     | 404  | 1PE  | OH2-C12-C22-OH3 |
| 5   | A     | 403  | 1PE  | C13-C23-OH3-C22 |
| 5   | B     | 1403 | 1PE  | OH6-C15-C25-OH5 |
| 5   | B     | 1404 | 1PE  | OH6-C15-C25-OH5 |
| 5   | A     | 403  | 1PE  | C15-C25-OH5-C14 |
| 5   | A     | 403  | 1PE  | OH4-C13-C23-OH3 |
| 5   | C     | 2403 | 1PE  | C14-C24-OH4-C13 |

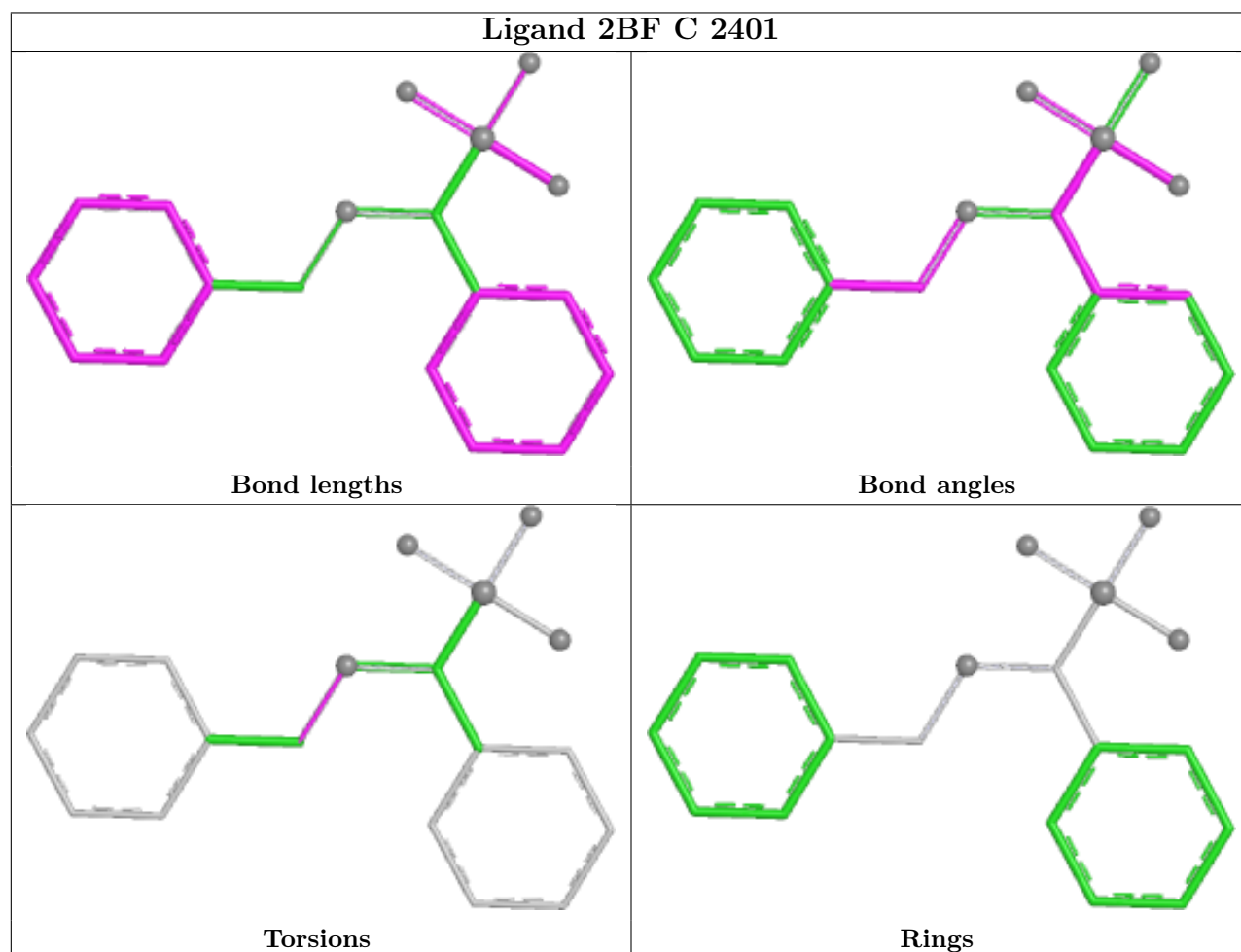
There are no ring outliers.

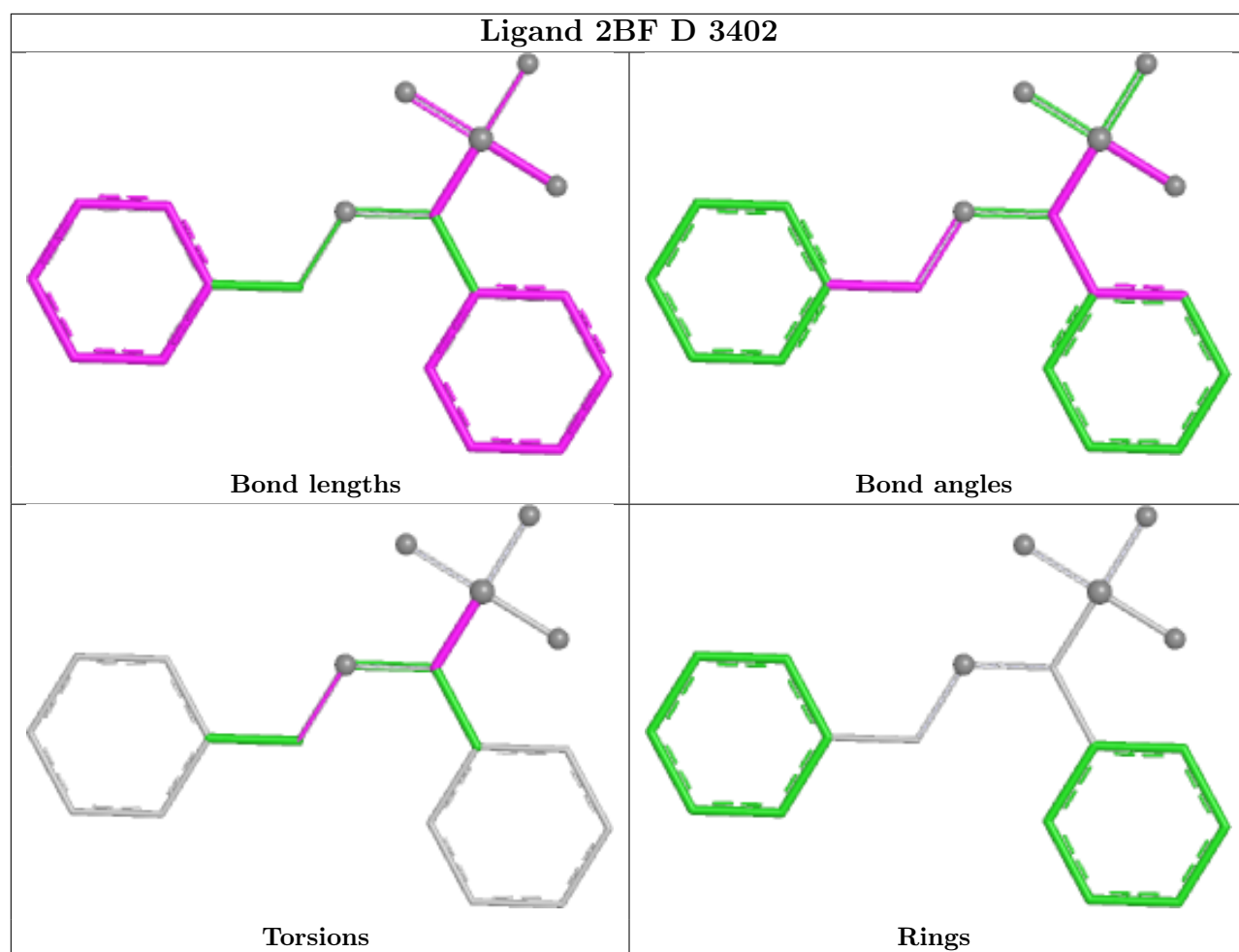
12 monomers are involved in 31 short contacts:

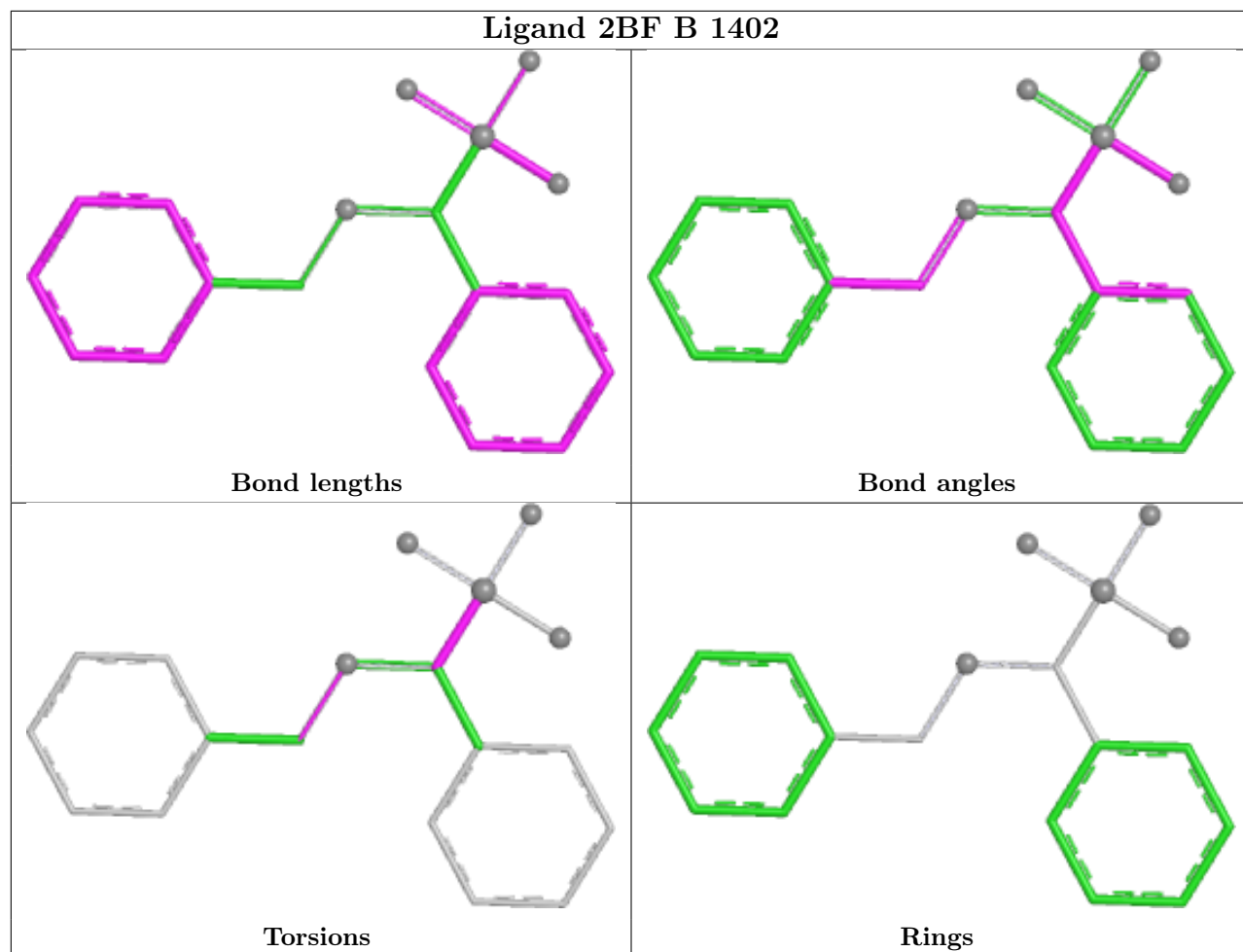
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | B     | 1404 | 1PE  | 4       | 0            |
| 5   | B     | 1403 | 1PE  | 1       | 0            |
| 6   | B     | 1401 | NDG  | 7       | 0            |
| 4   | C     | 2401 | 2BF  | 2       | 0            |
| 5   | C     | 2403 | 1PE  | 1       | 0            |
| 7   | D     | 3401 | NAG  | 6       | 0            |
| 5   | D     | 3403 | 1PE  | 1       | 0            |
| 5   | C     | 2402 | 1PE  | 1       | 0            |
| 5   | A     | 403  | 1PE  | 2       | 0            |
| 5   | A     | 402  | 1PE  | 1       | 0            |
| 4   | B     | 1402 | 2BF  | 2       | 0            |
| 4   | A     | 401  | 2BF  | 3       | 0            |

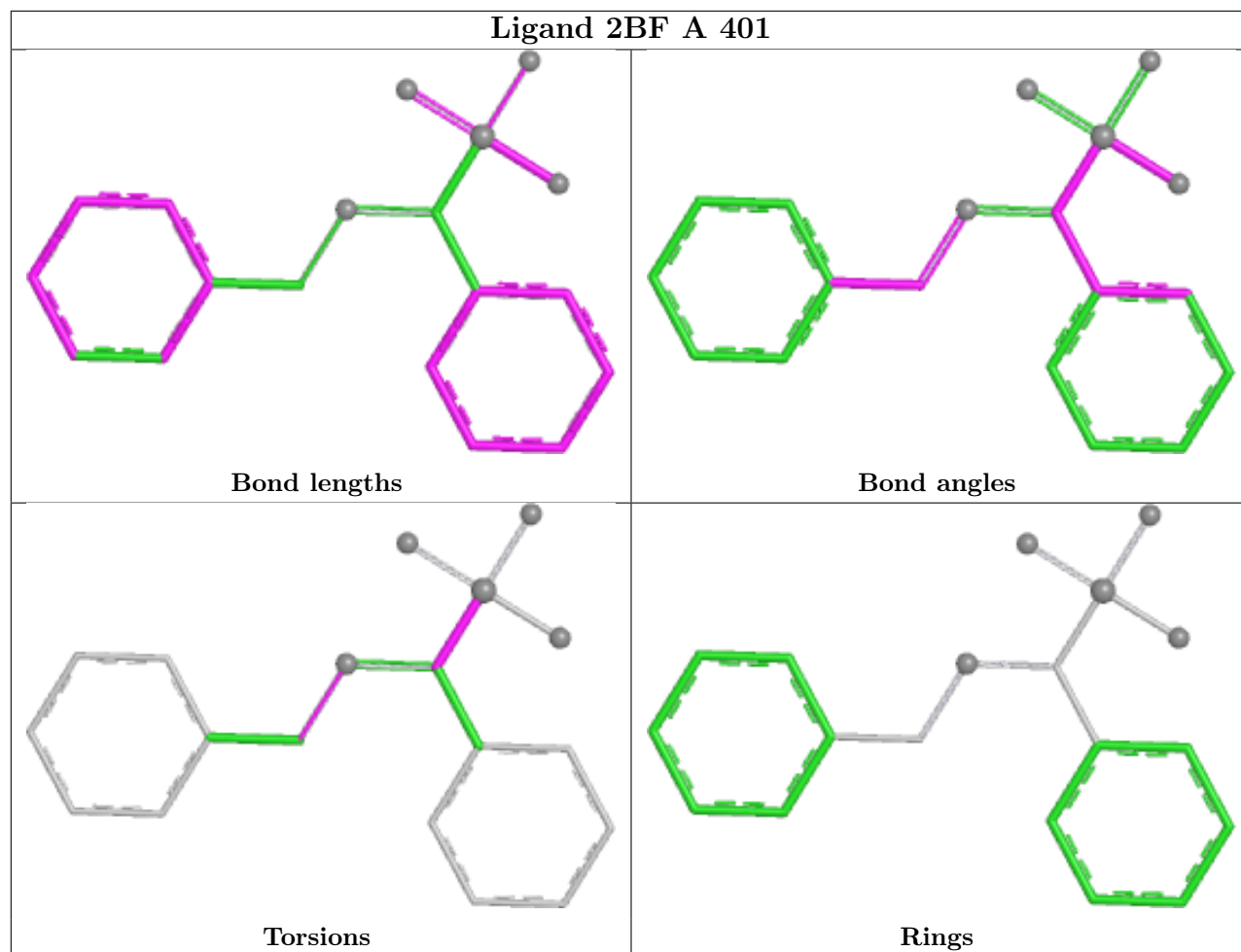
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.