



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 03:52 AM UTC

PDB ID : 3KQ4 / pdb\_00003kq4  
Title : Structure of Intrinsic Factor-Cobalamin bound to its receptor Cubilin  
Authors : Andersen, C.B.F.; Madsen, M.; Moestrup, S.K.; Andersen, G.R.  
Deposited on : 2009-11-17  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

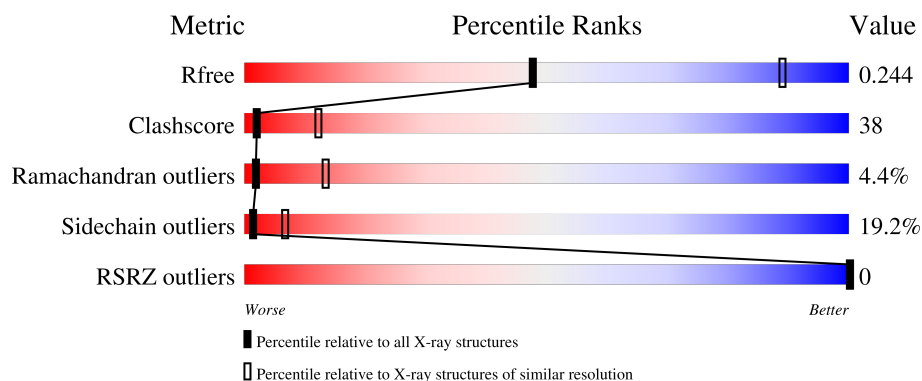
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



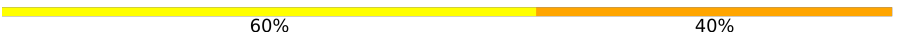
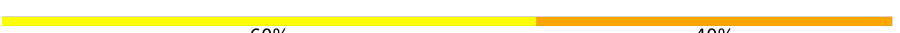
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1169 (3.32-3.28)                                      |
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers         | 180081                      | 1169 (3.32-3.28)                                      |

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

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 393    | <div> <div>49%</div> <div>36%</div> <div>12%</div> <div>..</div> </div> |
| 1   | C     | 393    | <div> <div>50%</div> <div>36%</div> <div>12%</div> <div>..</div> </div> |
| 1   | E     | 393    | <div> <div>50%</div> <div>36%</div> <div>11%</div> <div>..</div> </div> |
| 2   | B     | 457    | <div> <div>34%</div> <div>47%</div> <div>17%</div> <div>.</div> </div>  |
| 2   | D     | 457    | <div> <div>35%</div> <div>46%</div> <div>18%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | F     | 457    |  |
| 3   | G     | 5      |  |
| 3   | H     | 5      |  |
| 3   | J     | 5      |  |
| 3   | K     | 5      |  |
| 3   | M     | 5      |  |
| 3   | N     | 5      |  |
| 4   | I     | 2      |  |
| 4   | L     | 2      |  |
| 4   | O     | 2      |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5   | NAG  | A     | 2001 | X         | -        | X       | -                |
| 5   | NAG  | B     | 2001 | X         | -        | -       | -                |
| 5   | NAG  | B     | 2008 | X         | -        | -       | -                |
| 5   | NAG  | C     | 2001 | X         | -        | X       | -                |
| 5   | NAG  | D     | 2001 | X         | -        | -       | -                |
| 5   | NAG  | D     | 2008 | X         | -        | -       | -                |
| 5   | NAG  | E     | 2001 | X         | -        | X       | -                |
| 5   | NAG  | F     | 2001 | X         | -        | -       | -                |
| 5   | NAG  | F     | 2008 | X         | -        | -       | -                |
| 6   | B12  | A     | 2007 | X         | -        | X       | -                |
| 6   | B12  | C     | 2007 | X         | -        | X       | -                |
| 6   | B12  | E     | 2007 | X         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20793 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 Gastric intrinsic factor.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 385      | Total | C    | N   | O   | S  | 3       | 0       | 0     |
|     |       |          | 2950  | 1870 | 488 | 573 | 19 |         |         |       |
| 1   | C     | 385      | Total | C    | N   | O   | S  | 3       | 0       | 0     |
|     |       |          | 2950  | 1870 | 488 | 573 | 19 |         |         |       |
| 1   | E     | 385      | Total | C    | N   | O   | S  | 3       | 0       | 0     |
|     |       |          | 2950  | 1870 | 488 | 573 | 19 |         |         |       |

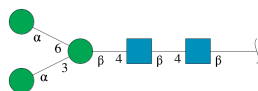
There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 91      | HIS      | GLN    | SEE REMARK 999 | UNP P27352 |
| C     | 91      | HIS      | GLN    | SEE REMARK 999 | UNP P27352 |
| E     | 91      | HIS      | GLN    | SEE REMARK 999 | UNP P27352 |

- Molecule 2 is a protein called Cubilin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 457      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3638  | 2311 | 598 | 709 | 20 |         |         |       |
| 2   | D     | 457      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3638  | 2311 | 598 | 709 | 20 |         |         |       |
| 2   | F     | 457      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3638  | 2311 | 598 | 709 | 20 |         |         |       |

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



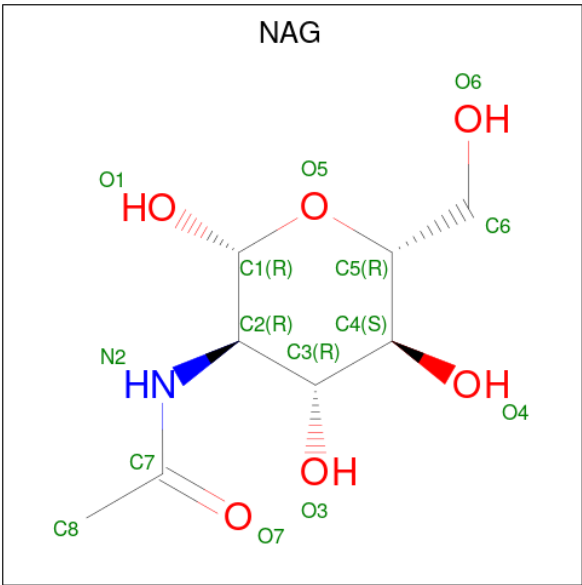
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 3   | G     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 3   | H     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 3   | J     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 3   | K     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 3   | M     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |
| 3   | N     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

- Molecule 4 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 |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4   | I     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 4   | L     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 4   | O     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



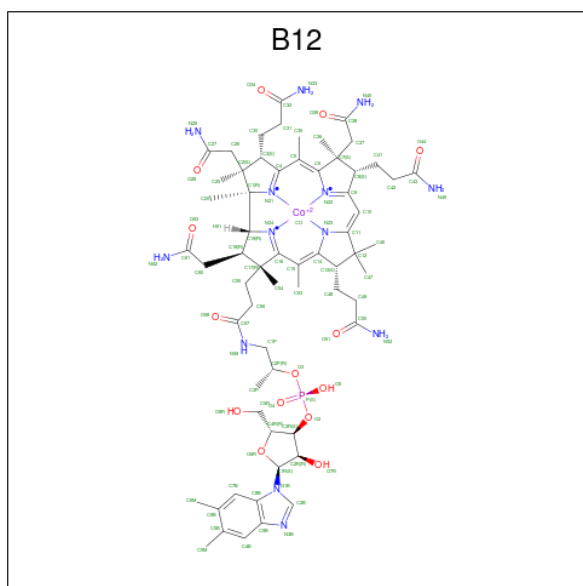
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



| Mol | Chain | Residues | Atoms |    |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|
| 6   | A     | 1        | Total | C  | Co | N  | O  | P | 0       | 0       |
|     |       |          | 91    | 62 | 1  | 13 | 14 | 1 |         |         |
| 6   | C     | 1        | Total | C  | Co | N  | O  | P | 0       | 0       |
|     |       |          | 91    | 62 | 1  | 13 | 14 | 1 |         |         |
| 6   | E     | 1        | Total | C  | Co | N  | O  | P | 0       | 0       |
|     |       |          | 91    | 62 | 1  | 13 | 14 | 1 |         |         |

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

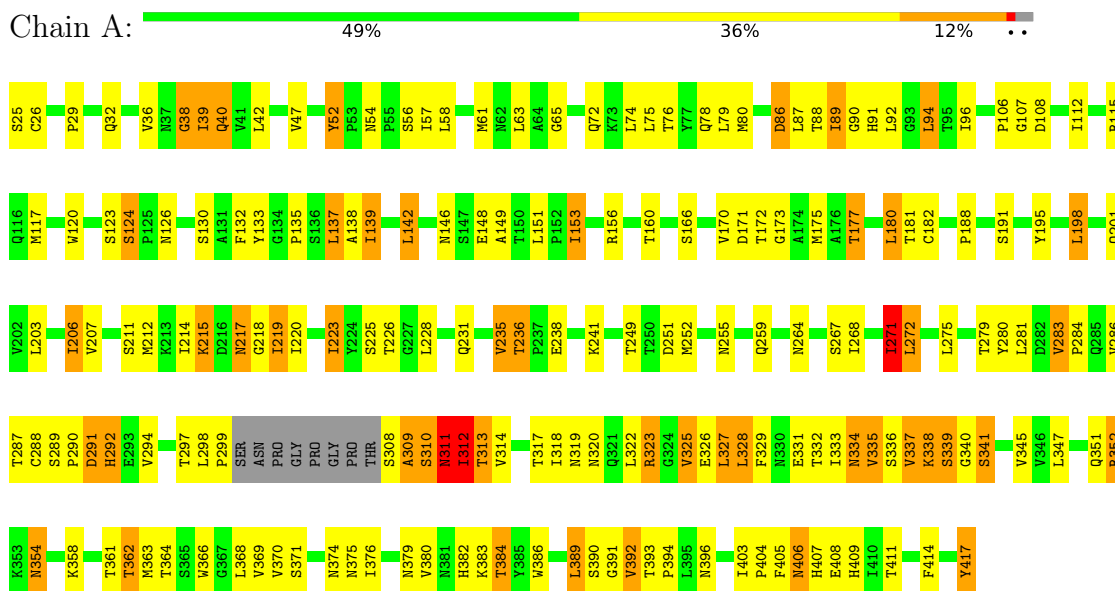
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 7   | B     | 4        | Total<br>4 | Ca<br>4 | 0       | 0       |
| 7   | D     | 4        | Total<br>4 | Ca<br>4 | 0       | 0       |
| 7   | F     | 4        | Total<br>4 | Ca<br>4 | 0       | 0       |



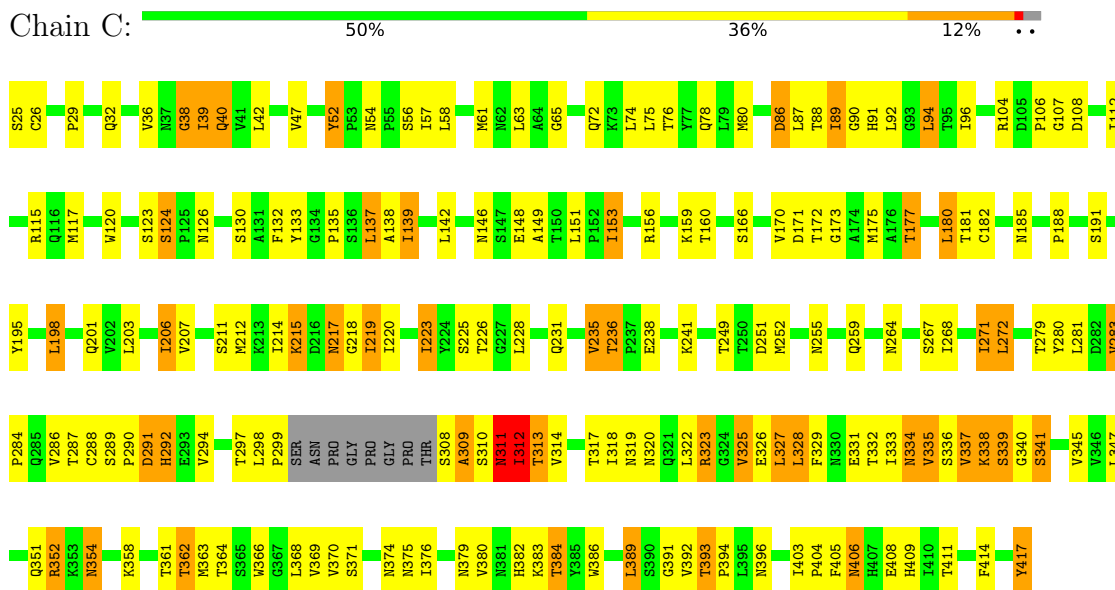
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

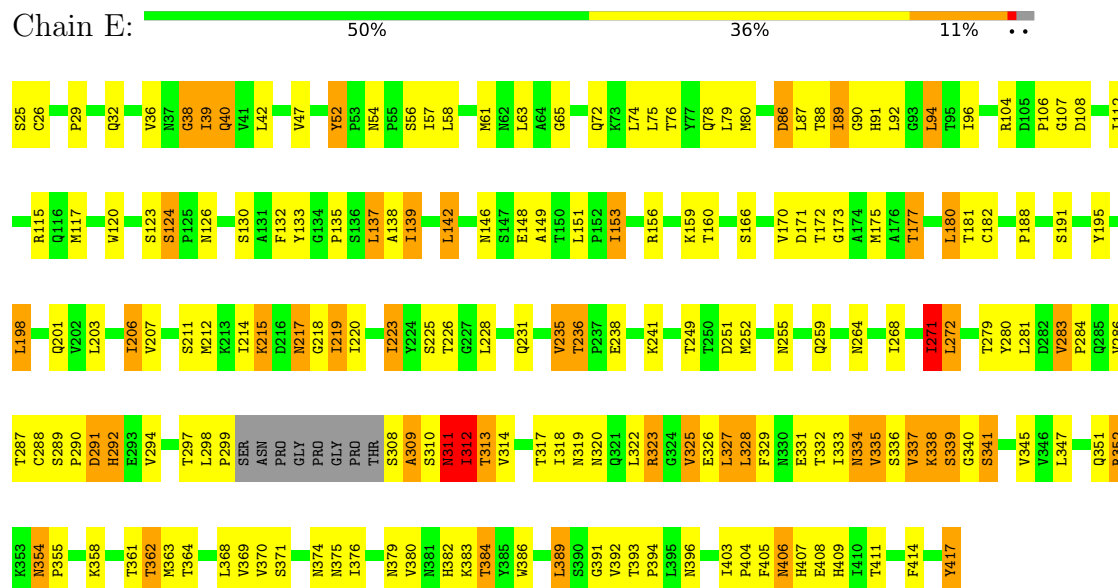
#### • Molecule 1: Gastric intrinsic factor



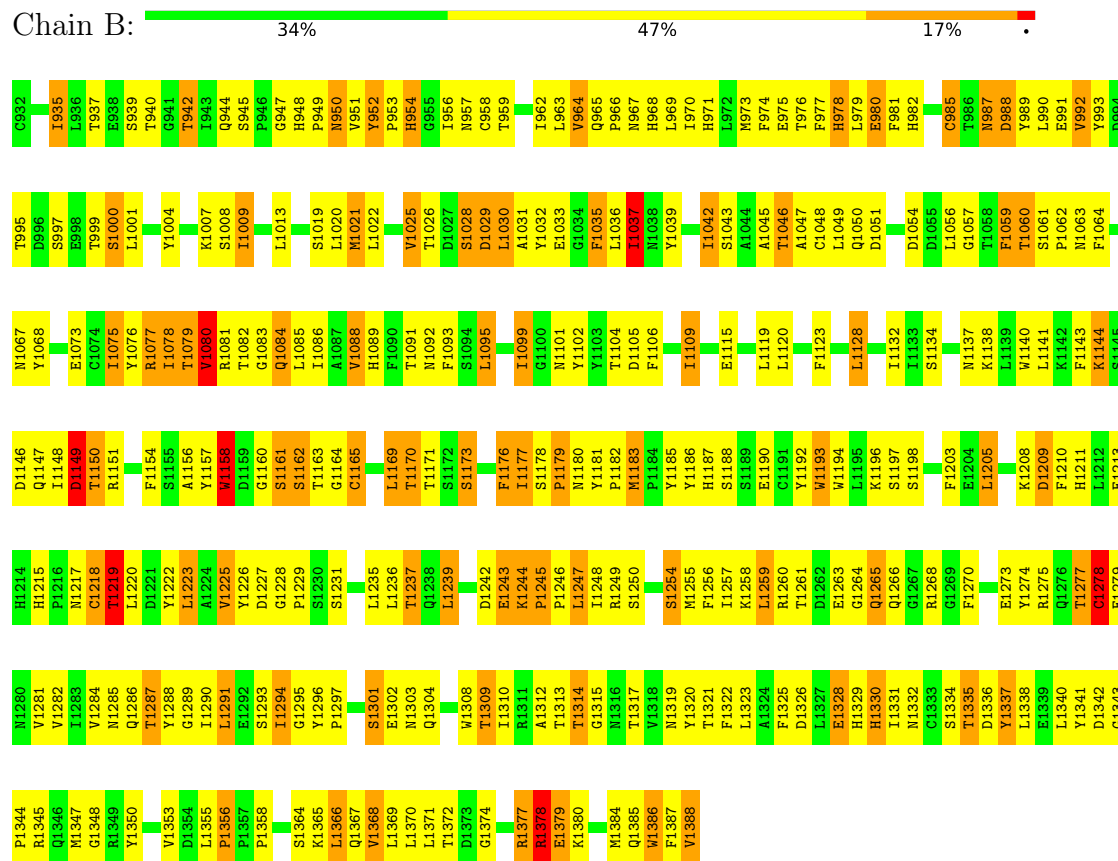
#### • Molecule 1: Gastric intrinsic factor



- Molecule 1: Gastric intrinsic factor

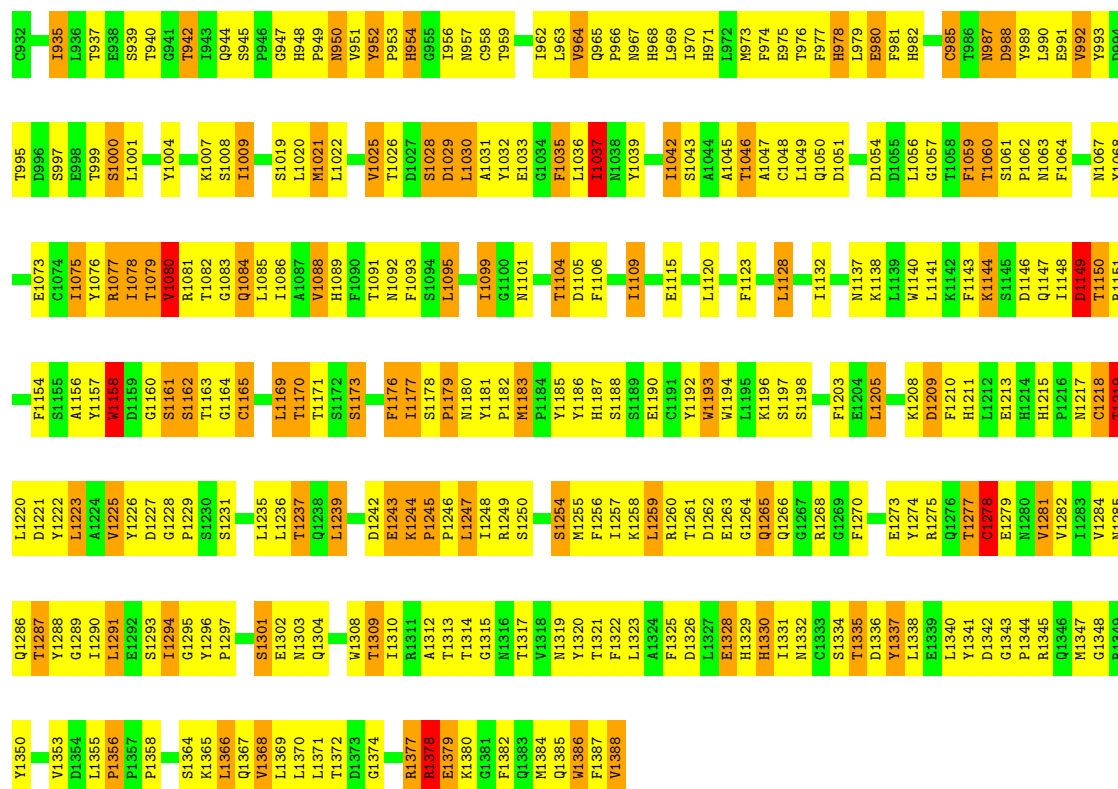


- Molecule 2: Cubilin



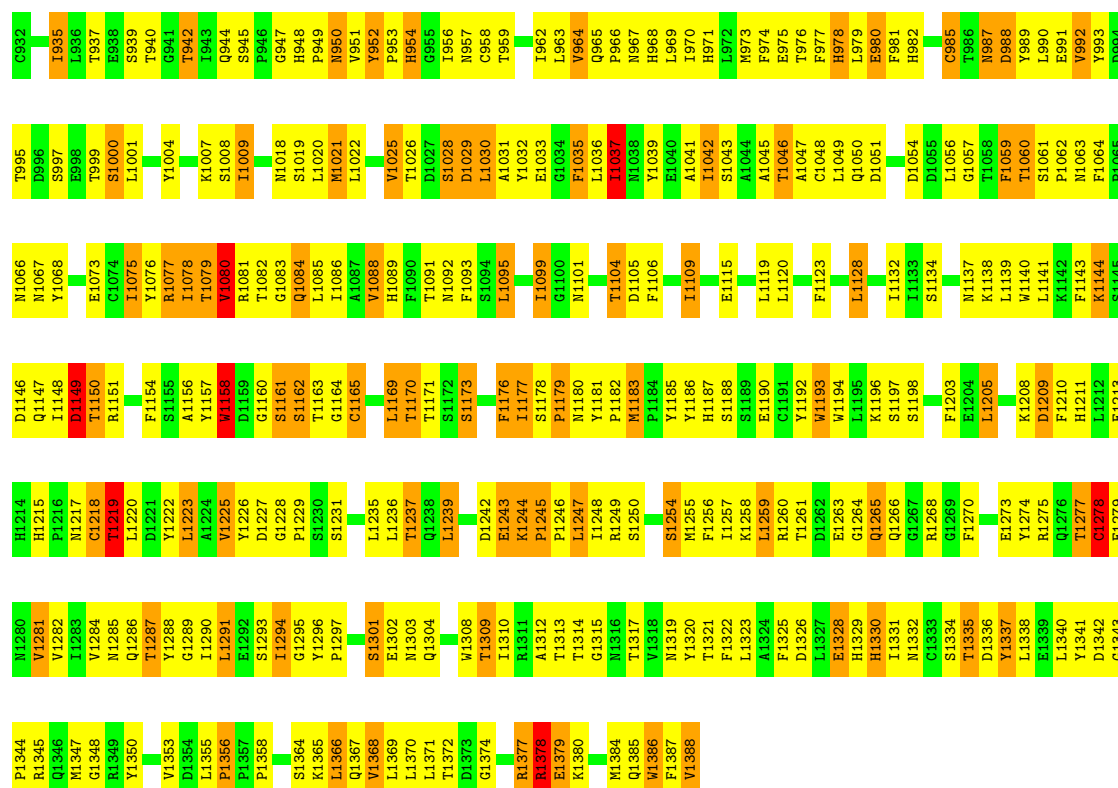
- Molecule 2: Cubilin





• Molecule 2: Cubilin

Chain F: 34% 47% 18%



● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  60% 40%

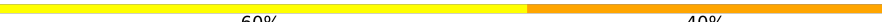


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  20% 80%



● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  60% 40%

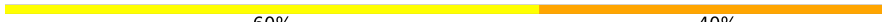


● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  20% 80%



● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  60% 40%



● Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  20% 80%



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

Chain I:  100%



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

Chain L:  100%



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

Chain O:  100%



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 117.68Å 204.18Å 410.02Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 47.85 – 3.30<br>47.85 – 3.30                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.0 (47.85-3.30)<br>96.6 (47.85-3.30)                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                                          | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                               | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.71 (at 3.33Å)                                                               | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine)                                                        | Depositor        |
| R, $R_{free}$                                                           | 0.211 , 0.242<br>0.207 , 0.244                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1102 reflections (1.52%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 93.9                                                                          | Xtriage          |
| Anisotropy                                                              | 0.035                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 82.1                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.428 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.437 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                                          | EDS              |
| Total number of atoms                                                   | 20793                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 104.0                                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, B12, MAN, CA

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     | 0.88         | 1/3007 (0.0%)  | 1.18        | 22/4090 (0.5%)   |
| 1   | C     | 0.88         | 1/3007 (0.0%)  | 1.19        | 22/4090 (0.5%)   |
| 1   | E     | 0.88         | 2/3007 (0.1%)  | 1.18        | 22/4090 (0.5%)   |
| 2   | B     | 0.68         | 0/3748         | 1.11        | 27/5110 (0.5%)   |
| 2   | D     | 0.68         | 0/3748         | 1.11        | 27/5110 (0.5%)   |
| 2   | F     | 0.68         | 0/3748         | 1.11        | 27/5110 (0.5%)   |
| All | All   | 0.78         | 4/20265 (0.0%) | 1.14        | 147/27600 (0.5%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 153 | ILE  | CA-CB | -5.15 | 1.48        | 1.54     |
| 1   | A     | 153 | ILE  | CA-CB | -5.13 | 1.48        | 1.54     |
| 1   | C     | 153 | ILE  | CA-CB | -5.10 | 1.48        | 1.54     |
| 1   | E     | 271 | ILE  | CA-CB | -5.09 | 1.48        | 1.54     |

All (147) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 271  | ILE  | CB-CA-C | -9.58 | 102.63      | 111.06   |
| 1   | C     | 271  | ILE  | CB-CA-C | -9.54 | 102.67      | 111.06   |
| 2   | B     | 1356 | PRO  | CA-C-N  | 9.08  | 126.29      | 119.66   |
| 2   | B     | 1356 | PRO  | C-N-CA  | 9.08  | 126.29      | 119.66   |
| 2   | F     | 1356 | PRO  | CA-C-N  | 9.08  | 126.29      | 119.66   |
| 2   | F     | 1356 | PRO  | C-N-CA  | 9.08  | 126.29      | 119.66   |
| 2   | D     | 1356 | PRO  | CA-C-N  | 9.07  | 126.28      | 119.66   |
| 2   | D     | 1356 | PRO  | C-N-CA  | 9.07  | 126.28      | 119.66   |
| 2   | B     | 952  | TYR  | CA-C-N  | 8.87  | 128.81      | 119.85   |
| 2   | B     | 952  | TYR  | C-N-CA  | 8.87  | 128.81      | 119.85   |
| 2   | D     | 952  | TYR  | CA-C-N  | 8.85  | 128.78      | 119.85   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 952  | TYR  | C-N-CA  | 8.85  | 128.78      | 119.85   |
| 2   | F     | 952  | TYR  | CA-C-N  | 8.85  | 128.78      | 119.85   |
| 2   | F     | 952  | TYR  | C-N-CA  | 8.85  | 128.78      | 119.85   |
| 1   | E     | 166  | SER  | CA-C-N  | 8.16  | 130.04      | 119.84   |
| 1   | E     | 166  | SER  | C-N-CA  | 8.16  | 130.04      | 119.84   |
| 1   | C     | 166  | SER  | CA-C-N  | 8.15  | 130.03      | 119.84   |
| 1   | C     | 166  | SER  | C-N-CA  | 8.15  | 130.03      | 119.84   |
| 1   | A     | 166  | SER  | CA-C-N  | 8.15  | 130.02      | 119.84   |
| 1   | A     | 166  | SER  | C-N-CA  | 8.15  | 130.02      | 119.84   |
| 2   | D     | 1084 | GLN  | N-CA-C  | 7.80  | 119.86      | 110.19   |
| 2   | F     | 1084 | GLN  | N-CA-C  | 7.79  | 119.85      | 110.19   |
| 2   | B     | 1084 | GLN  | N-CA-C  | 7.78  | 119.84      | 110.19   |
| 1   | E     | 271  | ILE  | CB-CA-C | -7.55 | 102.65      | 110.88   |
| 1   | C     | 26   | CYS  | N-CA-C  | -7.17 | 102.64      | 112.03   |
| 1   | A     | 26   | CYS  | N-CA-C  | -7.16 | 102.65      | 112.03   |
| 1   | E     | 26   | CYS  | N-CA-C  | -7.14 | 102.68      | 112.03   |
| 1   | C     | 311  | ASN  | CB-CA-C | 6.94  | 121.24      | 109.72   |
| 1   | A     | 329  | PHE  | N-CA-C  | -6.71 | 104.23      | 114.16   |
| 1   | E     | 329  | PHE  | N-CA-C  | -6.71 | 104.23      | 114.16   |
| 1   | C     | 329  | PHE  | N-CA-C  | -6.69 | 104.26      | 114.16   |
| 2   | B     | 1314 | THR  | CB-CA-C | -6.66 | 108.18      | 117.23   |
| 2   | F     | 1337 | TYR  | N-CA-C  | 6.65  | 117.36      | 108.38   |
| 2   | F     | 1244 | LYS  | CA-C-N  | 6.65  | 127.23      | 120.38   |
| 2   | F     | 1244 | LYS  | C-N-CA  | 6.65  | 127.23      | 120.38   |
| 2   | B     | 1337 | TYR  | N-CA-C  | 6.65  | 117.35      | 108.38   |
| 2   | D     | 1337 | TYR  | N-CA-C  | 6.64  | 117.34      | 108.38   |
| 1   | A     | 311  | ASN  | CB-CA-C | 6.58  | 120.65      | 109.72   |
| 1   | A     | 340  | GLY  | N-CA-C  | -6.53 | 106.78      | 115.40   |
| 1   | E     | 340  | GLY  | N-CA-C  | -6.53 | 106.78      | 115.40   |
| 1   | C     | 340  | GLY  | N-CA-C  | -6.52 | 106.79      | 115.40   |
| 2   | D     | 1244 | LYS  | CA-C-N  | 6.50  | 127.08      | 120.38   |
| 2   | D     | 1244 | LYS  | C-N-CA  | 6.50  | 127.08      | 120.38   |
| 1   | E     | 311  | ASN  | CB-CA-C | 6.38  | 120.31      | 109.72   |
| 1   | C     | 292  | HIS  | N-CA-C  | 6.34  | 118.90      | 110.53   |
| 1   | A     | 292  | HIS  | N-CA-C  | 6.33  | 118.88      | 110.53   |
| 1   | E     | 292  | HIS  | N-CA-C  | 6.32  | 118.87      | 110.53   |
| 2   | D     | 1281 | VAL  | CB-CA-C | -6.28 | 104.68      | 111.59   |
| 2   | F     | 1281 | VAL  | CB-CA-C | -6.27 | 104.69      | 111.59   |
| 2   | F     | 1059 | PHE  | N-CA-C  | 6.02  | 119.64      | 109.76   |
| 2   | D     | 1059 | PHE  | N-CA-C  | 6.00  | 119.61      | 109.76   |
| 2   | B     | 1059 | PHE  | N-CA-C  | 6.00  | 119.60      | 109.76   |
| 2   | D     | 1245 | PRO  | CA-C-N  | 5.91  | 128.23      | 120.25   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1245 | PRO  | C-N-CA  | 5.91  | 128.23      | 120.25   |
| 2   | F     | 1245 | PRO  | CA-C-N  | 5.91  | 128.23      | 120.25   |
| 2   | F     | 1245 | PRO  | C-N-CA  | 5.91  | 128.23      | 120.25   |
| 2   | B     | 1245 | PRO  | CA-C-N  | 5.88  | 128.18      | 120.25   |
| 2   | B     | 1245 | PRO  | C-N-CA  | 5.88  | 128.18      | 120.25   |
| 2   | D     | 1329 | HIS  | N-CA-C  | 5.85  | 118.94      | 109.40   |
| 2   | B     | 1329 | HIS  | N-CA-C  | 5.85  | 118.94      | 109.40   |
| 2   | F     | 1329 | HIS  | N-CA-C  | 5.84  | 118.91      | 109.40   |
| 1   | C     | 268  | ILE  | N-CA-C  | -5.75 | 105.12      | 110.53   |
| 2   | B     | 1244 | LYS  | CA-C-N  | 5.75  | 126.30      | 120.38   |
| 2   | B     | 1244 | LYS  | C-N-CA  | 5.75  | 126.30      | 120.38   |
| 2   | F     | 1028 | SER  | N-CA-C  | 5.70  | 117.36      | 111.03   |
| 1   | A     | 268  | ILE  | N-CA-C  | -5.70 | 105.17      | 110.53   |
| 2   | B     | 1028 | SER  | N-CA-C  | 5.68  | 117.34      | 111.03   |
| 2   | D     | 1028 | SER  | N-CA-C  | 5.68  | 117.34      | 111.03   |
| 1   | E     | 268  | ILE  | N-CA-C  | -5.68 | 105.19      | 110.53   |
| 2   | B     | 1104 | THR  | N-CA-C  | -5.66 | 100.48      | 109.59   |
| 2   | F     | 1104 | THR  | N-CA-C  | -5.65 | 100.50      | 109.59   |
| 2   | D     | 1104 | THR  | N-CA-C  | -5.64 | 100.51      | 109.59   |
| 2   | B     | 1386 | TRP  | N-CA-C  | 5.63  | 117.63      | 109.07   |
| 1   | C     | 396  | ASN  | N-CA-C  | 5.63  | 117.65      | 110.61   |
| 2   | D     | 1386 | TRP  | N-CA-C  | 5.63  | 117.62      | 109.07   |
| 1   | A     | 396  | ASN  | N-CA-C  | 5.62  | 117.64      | 110.61   |
| 1   | E     | 396  | ASN  | N-CA-C  | 5.62  | 117.63      | 110.61   |
| 2   | F     | 1386 | TRP  | N-CA-C  | 5.62  | 117.61      | 109.07   |
| 2   | D     | 1099 | ILE  | CB-CA-C | -5.61 | 105.24      | 111.35   |
| 1   | C     | 112  | ILE  | N-CA-C  | 5.61  | 116.25      | 110.36   |
| 2   | B     | 1099 | ILE  | CB-CA-C | -5.59 | 105.26      | 111.35   |
| 2   | F     | 1099 | ILE  | CB-CA-C | -5.58 | 105.27      | 111.35   |
| 1   | A     | 112  | ILE  | N-CA-C  | 5.57  | 116.21      | 110.36   |
| 1   | E     | 112  | ILE  | N-CA-C  | 5.52  | 116.15      | 110.36   |
| 1   | C     | 153  | ILE  | CB-CA-C | -5.50 | 104.94      | 111.97   |
| 1   | A     | 153  | ILE  | CB-CA-C | -5.48 | 104.96      | 111.97   |
| 2   | D     | 1228 | GLY  | CA-C-N  | 5.47  | 125.09      | 119.56   |
| 2   | D     | 1228 | GLY  | C-N-CA  | 5.47  | 125.09      | 119.56   |
| 1   | E     | 153  | ILE  | CB-CA-C | -5.47 | 104.97      | 111.97   |
| 2   | B     | 1228 | GLY  | CA-C-N  | 5.45  | 125.06      | 119.56   |
| 2   | B     | 1228 | GLY  | C-N-CA  | 5.45  | 125.06      | 119.56   |
| 2   | B     | 1273 | GLU  | N-CA-C  | -5.44 | 101.60      | 110.20   |
| 2   | F     | 1273 | GLU  | N-CA-C  | -5.44 | 101.60      | 110.20   |
| 2   | F     | 1228 | GLY  | CA-C-N  | 5.44  | 125.06      | 119.56   |
| 2   | F     | 1228 | GLY  | C-N-CA  | 5.44  | 125.06      | 119.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 323  | ARG  | N-CA-C  | 5.44  | 117.61      | 108.96   |
| 1   | C     | 323  | ARG  | N-CA-C  | 5.43  | 117.60      | 108.96   |
| 2   | D     | 1273 | GLU  | N-CA-C  | -5.43 | 101.62      | 110.20   |
| 1   | E     | 323  | ARG  | N-CA-C  | 5.42  | 117.59      | 108.96   |
| 1   | E     | 312  | ILE  | CB-CA-C | -5.41 | 103.64      | 112.03   |
| 1   | C     | 47   | VAL  | N-CA-C  | 5.41  | 116.15      | 107.98   |
| 1   | E     | 47   | VAL  | N-CA-C  | 5.41  | 116.15      | 107.98   |
| 1   | A     | 47   | VAL  | N-CA-C  | 5.40  | 116.14      | 107.98   |
| 1   | C     | 345  | VAL  | CB-CA-C | -5.40 | 104.85      | 112.14   |
| 1   | E     | 345  | VAL  | CB-CA-C | -5.38 | 104.88      | 112.14   |
| 2   | B     | 1384 | MET  | N-CA-C  | 5.38  | 117.43      | 108.99   |
| 1   | A     | 345  | VAL  | CB-CA-C | -5.37 | 104.89      | 112.14   |
| 2   | D     | 1384 | MET  | N-CA-C  | 5.36  | 117.40      | 108.99   |
| 2   | F     | 1384 | MET  | N-CA-C  | 5.35  | 117.38      | 108.99   |
| 1   | A     | 312  | ILE  | CB-CA-C | -5.34 | 103.76      | 112.03   |
| 1   | C     | 406  | ASN  | N-CA-C  | 5.32  | 118.56      | 111.75   |
| 1   | C     | 312  | ILE  | CB-CA-C | -5.31 | 103.80      | 112.03   |
| 1   | A     | 406  | ASN  | N-CA-C  | 5.30  | 118.54      | 111.75   |
| 1   | E     | 406  | ASN  | N-CA-C  | 5.29  | 118.52      | 111.75   |
| 2   | F     | 1158 | TRP  | N-CA-C  | 5.26  | 117.25      | 108.99   |
| 2   | B     | 1158 | TRP  | N-CA-C  | 5.25  | 117.23      | 108.99   |
| 2   | D     | 1158 | TRP  | N-CA-C  | 5.25  | 117.23      | 108.99   |
| 2   | D     | 1348 | GLY  | N-CA-C  | 5.24  | 118.06      | 111.09   |
| 2   | F     | 1348 | GLY  | N-CA-C  | 5.23  | 118.04      | 111.09   |
| 2   | B     | 1348 | GLY  | N-CA-C  | 5.22  | 118.04      | 111.09   |
| 1   | A     | 319  | ASN  | N-CA-C  | 5.21  | 116.91      | 108.41   |
| 1   | A     | 264  | ASN  | CA-C-N  | 5.21  | 124.87      | 119.56   |
| 1   | A     | 264  | ASN  | C-N-CA  | 5.21  | 124.87      | 119.56   |
| 1   | E     | 264  | ASN  | CA-C-N  | 5.21  | 124.87      | 119.56   |
| 1   | E     | 264  | ASN  | C-N-CA  | 5.21  | 124.87      | 119.56   |
| 1   | E     | 319  | ASN  | N-CA-C  | 5.21  | 116.89      | 108.41   |
| 1   | C     | 319  | ASN  | N-CA-C  | 5.20  | 116.88      | 108.41   |
| 1   | C     | 264  | ASN  | CA-C-N  | 5.17  | 124.83      | 119.56   |
| 1   | C     | 264  | ASN  | C-N-CA  | 5.17  | 124.83      | 119.56   |
| 2   | D     | 1278 | CYS  | CA-C-N  | -5.17 | 115.55      | 122.42   |
| 2   | D     | 1278 | CYS  | C-N-CA  | -5.17 | 115.55      | 122.42   |
| 2   | F     | 1278 | CYS  | CA-C-N  | -5.15 | 115.57      | 122.42   |
| 2   | F     | 1278 | CYS  | C-N-CA  | -5.15 | 115.57      | 122.42   |
| 2   | B     | 1278 | CYS  | CA-C-N  | -5.15 | 115.57      | 122.42   |
| 2   | B     | 1278 | CYS  | C-N-CA  | -5.15 | 115.57      | 122.42   |
| 2   | B     | 1177 | ILE  | N-CA-C  | 5.11  | 115.63      | 108.17   |
| 2   | F     | 1177 | ILE  | N-CA-C  | 5.11  | 115.63      | 108.17   |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1   | E     | 354  | ASN  | CA-C-N | 5.10 | 125.17      | 119.87   |
| 1   | E     | 354  | ASN  | C-N-CA | 5.10 | 125.17      | 119.87   |
| 2   | D     | 1177 | ILE  | N-CA-C | 5.09 | 115.61      | 108.17   |
| 1   | A     | 354  | ASN  | CA-C-N | 5.08 | 125.15      | 119.87   |
| 1   | A     | 354  | ASN  | C-N-CA | 5.08 | 125.15      | 119.87   |
| 2   | B     | 1109 | ILE  | N-CA-C | 5.06 | 115.14      | 107.80   |
| 2   | D     | 1109 | ILE  | N-CA-C | 5.06 | 115.14      | 107.80   |
| 2   | F     | 1109 | ILE  | N-CA-C | 5.06 | 115.14      | 107.80   |
| 1   | C     | 354  | ASN  | CA-C-N | 5.05 | 125.12      | 119.87   |
| 1   | C     | 354  | ASN  | C-N-CA | 5.05 | 125.12      | 119.87   |

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     | 2950  | 0        | 2961     | 165     | 0            |
| 1   | C     | 2950  | 0        | 2961     | 163     | 0            |
| 1   | E     | 2950  | 0        | 2961     | 167     | 0            |
| 2   | B     | 3638  | 0        | 3373     | 326     | 0            |
| 2   | D     | 3638  | 0        | 3373     | 321     | 0            |
| 2   | F     | 3638  | 0        | 3373     | 327     | 0            |
| 3   | G     | 61    | 0        | 52       | 3       | 0            |
| 3   | H     | 61    | 0        | 52       | 5       | 0            |
| 3   | J     | 61    | 0        | 52       | 3       | 0            |
| 3   | K     | 61    | 0        | 52       | 5       | 0            |
| 3   | M     | 61    | 0        | 52       | 4       | 0            |
| 3   | N     | 61    | 0        | 52       | 5       | 0            |
| 4   | I     | 28    | 0        | 25       | 2       | 0            |
| 4   | L     | 28    | 0        | 25       | 2       | 0            |
| 4   | O     | 28    | 0        | 25       | 2       | 0            |
| 5   | A     | 14    | 0        | 13       | 7       | 0            |
| 5   | B     | 84    | 0        | 78       | 7       | 0            |
| 5   | C     | 14    | 0        | 13       | 8       | 0            |
| 5   | D     | 84    | 0        | 78       | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | E     | 14    | 0        | 13       | 7       | 0            |
| 5   | F     | 84    | 0        | 78       | 8       | 0            |
| 6   | A     | 91    | 0        | 87       | 29      | 0            |
| 6   | C     | 91    | 0        | 87       | 26      | 0            |
| 6   | E     | 91    | 0        | 87       | 25      | 0            |
| 7   | B     | 4     | 0        | 0        | 0       | 0            |
| 7   | D     | 4     | 0        | 0        | 0       | 0            |
| 7   | F     | 4     | 0        | 0        | 0       | 0            |
| All | All   | 20793 | 0        | 19923    | 1548    | 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 38.

All (1548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:311:ASN:HB2   | 1:C:337:VAL:HA    | 1.19                     | 1.18              |
| 1:A:311:ASN:HB2   | 1:A:337:VAL:HA    | 1.19                     | 1.11              |
| 1:E:223:ILE:HD12  | 1:E:223:ILE:H     | 1.10                     | 1.10              |
| 1:E:311:ASN:HB2   | 1:E:337:VAL:HA    | 1.19                     | 1.08              |
| 1:A:223:ILE:HD12  | 1:A:223:ILE:H     | 1.10                     | 1.07              |
| 1:C:223:ILE:H     | 1:C:223:ILE:HD12  | 1.10                     | 1.06              |
| 2:F:1079:THR:HG23 | 2:F:1138:LYS:HG2  | 1.34                     | 1.06              |
| 2:B:1079:THR:HG23 | 2:B:1138:LYS:HG2  | 1.34                     | 1.05              |
| 2:D:1079:THR:HG23 | 2:D:1138:LYS:HG2  | 1.33                     | 1.03              |
| 1:E:352:ARG:HG3   | 1:E:352:ARG:HH11  | 1.24                     | 1.00              |
| 1:C:352:ARG:HH11  | 1:C:352:ARG:HG3   | 1.22                     | 1.00              |
| 6:A:2007:B12:H552 | 6:A:2007:B12:H531 | 1.44                     | 0.99              |
| 6:E:2007:B12:H552 | 6:E:2007:B12:H531 | 1.44                     | 0.99              |
| 2:B:1294:ILE:HD11 | 2:B:1301:SER:OG   | 1.62                     | 0.99              |
| 1:A:352:ARG:HG3   | 1:A:352:ARG:HH11  | 1.25                     | 0.98              |
| 6:C:2007:B12:H552 | 6:C:2007:B12:H531 | 1.44                     | 0.98              |
| 2:D:1294:ILE:HD11 | 2:D:1301:SER:OG   | 1.62                     | 0.97              |
| 2:F:1294:ILE:HD11 | 2:F:1301:SER:OG   | 1.62                     | 0.97              |
| 1:A:40:GLN:HG2    | 1:A:272:LEU:HD11  | 1.47                     | 0.97              |
| 1:E:40:GLN:HG2    | 1:E:272:LEU:HD11  | 1.47                     | 0.96              |
| 2:D:1057:GLY:HA2  | 2:D:1158:TRP:NE1  | 1.81                     | 0.95              |
| 1:C:40:GLN:HG2    | 1:C:272:LEU:HD11  | 1.47                     | 0.95              |
| 2:B:1057:GLY:HA2  | 2:B:1158:TRP:NE1  | 1.81                     | 0.95              |
| 6:E:2007:B12:H312 | 6:E:2007:B12:H353 | 1.50                     | 0.94              |
| 6:C:2007:B12:H312 | 6:C:2007:B12:H353 | 1.50                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:2007:B12:H312 | 6:A:2007:B12:H353 | 1.50                     | 0.93              |
| 2:F:1057:GLY:HA2  | 2:F:1158:TRP:NE1  | 1.81                     | 0.93              |
| 1:E:362:THR:HG22  | 1:E:371:SER:HB3   | 1.49                     | 0.93              |
| 1:C:362:THR:HG22  | 1:C:371:SER:HB3   | 1.50                     | 0.92              |
| 1:A:362:THR:HG22  | 1:A:371:SER:HB3   | 1.50                     | 0.92              |
| 2:B:1330:HIS:CE1  | 2:B:1332:ASN:H    | 1.88                     | 0.91              |
| 1:C:312:ILE:HG21  | 1:C:406:ASN:HA    | 1.51                     | 0.91              |
| 2:D:1330:HIS:CE1  | 2:D:1332:ASN:H    | 1.88                     | 0.91              |
| 1:A:312:ILE:HG21  | 1:A:406:ASN:HA    | 1.52                     | 0.90              |
| 1:E:312:ILE:HG21  | 1:E:406:ASN:HA    | 1.51                     | 0.90              |
| 2:F:1330:HIS:CE1  | 2:F:1332:ASN:H    | 1.89                     | 0.90              |
| 1:E:223:ILE:H     | 1:E:223:ILE:CD1   | 1.84                     | 0.90              |
| 1:A:223:ILE:H     | 1:A:223:ILE:CD1   | 1.84                     | 0.89              |
| 1:C:223:ILE:H     | 1:C:223:ILE:CD1   | 1.84                     | 0.88              |
| 2:B:1084:GLN:HG3  | 2:B:1163:THR:H    | 1.39                     | 0.88              |
| 2:F:1084:GLN:HG3  | 2:F:1163:THR:H    | 1.39                     | 0.87              |
| 2:D:1084:GLN:HG3  | 2:D:1163:THR:H    | 1.39                     | 0.87              |
| 1:A:337:VAL:HG22  | 5:A:2001:NAG:O7   | 1.76                     | 0.85              |
| 2:B:1319:ASN:HB2  | 2:B:1387:PHE:HD2  | 1.40                     | 0.85              |
| 2:D:1319:ASN:HB2  | 2:D:1387:PHE:HD2  | 1.42                     | 0.85              |
| 1:A:362:THR:CG2   | 1:A:371:SER:HB3   | 2.07                     | 0.84              |
| 1:E:156:ARG:O     | 1:E:160:THR:HG23  | 1.77                     | 0.84              |
| 2:F:1067:ASN:HB3  | 2:F:1150:THR:CG2  | 2.08                     | 0.84              |
| 2:F:1319:ASN:HB2  | 2:F:1387:PHE:HD2  | 1.41                     | 0.84              |
| 1:E:362:THR:CG2   | 1:E:371:SER:HB3   | 2.07                     | 0.84              |
| 2:F:1313:THR:HG22 | 5:F:2009:NAG:H82  | 1.59                     | 0.84              |
| 2:D:974:PHE:CE1   | 2:D:1037:ILE:HD12 | 2.13                     | 0.84              |
| 1:C:156:ARG:O     | 1:C:160:THR:HG23  | 1.78                     | 0.84              |
| 1:C:362:THR:CG2   | 1:C:371:SER:HB3   | 2.07                     | 0.83              |
| 1:E:317:THR:HG23  | 1:E:331:GLU:HG3   | 1.60                     | 0.83              |
| 2:F:974:PHE:CE1   | 2:F:1037:ILE:HD12 | 2.13                     | 0.83              |
| 2:B:974:PHE:CE1   | 2:B:1037:ILE:HD12 | 2.13                     | 0.83              |
| 2:D:1067:ASN:HB3  | 2:D:1150:THR:CG2  | 2.08                     | 0.83              |
| 2:D:1313:THR:HG22 | 5:D:2009:NAG:H82  | 1.59                     | 0.83              |
| 2:B:1067:ASN:HB3  | 2:B:1150:THR:CG2  | 2.08                     | 0.83              |
| 2:B:1313:THR:HG22 | 5:B:2009:NAG:H82  | 1.59                     | 0.83              |
| 2:F:1078:ILE:HD11 | 2:F:1086:ILE:HG12 | 1.60                     | 0.83              |
| 1:A:317:THR:HG23  | 1:A:331:GLU:HG3   | 1.59                     | 0.82              |
| 2:B:1078:ILE:HD11 | 2:B:1086:ILE:HG12 | 1.60                     | 0.82              |
| 2:D:1078:ILE:HD11 | 2:D:1086:ILE:HG12 | 1.60                     | 0.82              |
| 1:C:317:THR:HG23  | 1:C:331:GLU:HG3   | 1.60                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:223:ILE:HD12  | 1:E:223:ILE:N     | 1.94                     | 0.81              |
| 2:B:1342:ASP:HB2  | 2:B:1347:MET:HE2  | 1.61                     | 0.81              |
| 2:D:1342:ASP:HB2  | 2:D:1347:MET:HE2  | 1.61                     | 0.81              |
| 1:A:223:ILE:HD12  | 1:A:223:ILE:N     | 1.94                     | 0.81              |
| 2:F:1035:PHE:HD1  | 2:F:1035:PHE:O    | 1.63                     | 0.81              |
| 1:C:223:ILE:HD12  | 1:C:223:ILE:N     | 1.94                     | 0.81              |
| 2:F:1342:ASP:HB2  | 2:F:1347:MET:HE2  | 1.61                     | 0.81              |
| 2:F:1297:PRO:O    | 2:F:1380:LYS:HD3  | 1.82                     | 0.80              |
| 2:D:1035:PHE:HD1  | 2:D:1035:PHE:O    | 1.63                     | 0.80              |
| 2:D:1297:PRO:O    | 2:D:1380:LYS:HD3  | 1.82                     | 0.80              |
| 1:E:92:LEU:O      | 1:E:96:ILE:HG13   | 1.82                     | 0.80              |
| 2:F:1323:LEU:HD11 | 2:F:1385:GLN:HG3  | 1.64                     | 0.80              |
| 2:B:1035:PHE:HD1  | 2:B:1035:PHE:O    | 1.63                     | 0.80              |
| 2:B:1297:PRO:O    | 2:B:1380:LYS:HD3  | 1.82                     | 0.80              |
| 2:B:1323:LEU:HD11 | 2:B:1385:GLN:HG3  | 1.64                     | 0.80              |
| 2:D:1342:ASP:HB3  | 2:D:1345:ARG:HG2  | 1.62                     | 0.80              |
| 2:D:1323:LEU:HD11 | 2:D:1385:GLN:HG3  | 1.64                     | 0.80              |
| 1:A:177:THR:HG22  | 1:A:206:ILE:HG21  | 1.63                     | 0.80              |
| 1:E:337:VAL:HG22  | 5:E:2001:NAG:O7   | 1.81                     | 0.80              |
| 3:N:3:BMA:H61     | 3:N:5:MAN:H5      | 1.64                     | 0.79              |
| 1:A:92:LEU:O      | 1:A:96:ILE:HG13   | 1.82                     | 0.79              |
| 2:F:1342:ASP:HB3  | 2:F:1345:ARG:HG2  | 1.62                     | 0.79              |
| 2:B:1342:ASP:HB3  | 2:B:1345:ARG:HG2  | 1.62                     | 0.79              |
| 1:C:337:VAL:HG22  | 5:C:2001:NAG:O7   | 1.83                     | 0.79              |
| 6:C:2007:B12:H552 | 6:C:2007:B12:C53  | 2.12                     | 0.79              |
| 2:D:1378:ARG:HD2  | 2:D:1378:ARG:N    | 1.98                     | 0.78              |
| 2:F:1378:ARG:HD2  | 2:F:1378:ARG:N    | 1.97                     | 0.78              |
| 2:F:1187:HIS:HB3  | 2:F:1266:GLN:NE2  | 1.99                     | 0.78              |
| 3:H:3:BMA:H61     | 3:H:5:MAN:H5      | 1.64                     | 0.78              |
| 1:C:312:ILE:O     | 1:C:335:VAL:HA    | 1.82                     | 0.78              |
| 3:K:3:BMA:H61     | 3:K:5:MAN:H5      | 1.64                     | 0.78              |
| 2:B:1187:HIS:HB3  | 2:B:1266:GLN:NE2  | 1.99                     | 0.78              |
| 1:C:92:LEU:O      | 1:C:96:ILE:HG13   | 1.82                     | 0.78              |
| 1:E:312:ILE:O     | 1:E:335:VAL:HA    | 1.84                     | 0.78              |
| 1:C:177:THR:HG22  | 1:C:206:ILE:HG21  | 1.63                     | 0.78              |
| 2:D:1187:HIS:HB3  | 2:D:1266:GLN:NE2  | 1.99                     | 0.78              |
| 2:B:1078:ILE:HG13 | 2:B:1078:ILE:O    | 1.83                     | 0.77              |
| 1:A:312:ILE:O     | 1:A:335:VAL:HA    | 1.84                     | 0.77              |
| 1:E:177:THR:HG22  | 1:E:206:ILE:HG21  | 1.63                     | 0.77              |
| 2:D:1078:ILE:HG13 | 2:D:1078:ILE:O    | 1.83                     | 0.77              |
| 2:F:1078:ILE:O    | 2:F:1078:ILE:HG13 | 1.83                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:160:THR:HG21  | 2:F:1099:ILE:HG21 | 1.67                     | 0.77              |
| 6:E:2007:B12:H552 | 6:E:2007:B12:C53  | 2.12                     | 0.77              |
| 2:B:1378:ARG:HD2  | 2:B:1378:ARG:N    | 1.97                     | 0.77              |
| 6:E:2007:B12:H203 | 6:E:2007:B12:H302 | 1.66                     | 0.77              |
| 6:C:2007:B12:H203 | 6:C:2007:B12:H302 | 1.66                     | 0.76              |
| 2:F:1330:HIS:CG   | 2:F:1331:ILE:N    | 2.52                     | 0.76              |
| 1:A:156:ARG:O     | 1:A:160:THR:HG23  | 1.85                     | 0.76              |
| 2:D:1330:HIS:CG   | 2:D:1331:ILE:N    | 2.52                     | 0.76              |
| 2:F:1082:THR:HG23 | 2:F:1186:TYR:CD2  | 2.21                     | 0.76              |
| 2:B:1309:THR:HG23 | 2:B:1367:GLN:HG2  | 1.66                     | 0.76              |
| 2:F:1309:THR:HG23 | 2:F:1367:GLN:HG2  | 1.66                     | 0.76              |
| 3:G:3:BMA:H4      | 3:G:5:MAN:H2      | 1.66                     | 0.76              |
| 2:D:1309:THR:HG23 | 2:D:1367:GLN:HG2  | 1.66                     | 0.76              |
| 2:F:1330:HIS:CG   | 2:F:1331:ILE:H    | 2.04                     | 0.76              |
| 3:J:3:BMA:H4      | 3:J:5:MAN:H2      | 1.66                     | 0.76              |
| 1:A:160:THR:CG2   | 2:B:1099:ILE:HG21 | 2.15                     | 0.76              |
| 2:B:1035:PHE:O    | 2:B:1035:PHE:CD1  | 2.38                     | 0.76              |
| 2:B:1082:THR:HG23 | 2:B:1186:TYR:CD2  | 2.21                     | 0.76              |
| 2:F:1035:PHE:O    | 2:F:1035:PHE:CD1  | 2.38                     | 0.76              |
| 3:M:3:BMA:H4      | 3:M:5:MAN:H2      | 1.66                     | 0.76              |
| 2:D:1335:THR:HG23 | 2:D:1336:ASP:H    | 1.51                     | 0.76              |
| 1:C:160:THR:CG2   | 2:D:1099:ILE:HG21 | 2.16                     | 0.75              |
| 6:A:2007:B12:H302 | 6:A:2007:B12:H203 | 1.66                     | 0.75              |
| 2:B:1330:HIS:CG   | 2:B:1331:ILE:N    | 2.52                     | 0.75              |
| 1:C:160:THR:HG21  | 2:D:1099:ILE:HG21 | 1.66                     | 0.75              |
| 1:C:352:ARG:HG3   | 1:C:352:ARG:NH1   | 1.93                     | 0.75              |
| 1:E:160:THR:CG2   | 2:F:1099:ILE:HG21 | 2.16                     | 0.75              |
| 6:A:2007:B12:H552 | 6:A:2007:B12:C53  | 2.12                     | 0.75              |
| 2:B:1330:HIS:CG   | 2:B:1331:ILE:H    | 2.03                     | 0.75              |
| 1:C:61:MET:HE2    | 1:C:72:GLN:HB2    | 1.69                     | 0.75              |
| 2:B:1304:GLN:H    | 2:B:1372:THR:HG23 | 1.52                     | 0.75              |
| 2:D:1082:THR:HG23 | 2:D:1186:TYR:CD2  | 2.21                     | 0.75              |
| 4:L:1:NAG:O3      | 4:L:2:NAG:H2      | 1.87                     | 0.75              |
| 2:B:1194:TRP:HE1  | 2:B:1254:SER:HB3  | 1.52                     | 0.75              |
| 2:B:1335:THR:HG23 | 2:B:1336:ASP:H    | 1.51                     | 0.75              |
| 2:F:1335:THR:HG23 | 2:F:1336:ASP:H    | 1.51                     | 0.75              |
| 4:O:1:NAG:O3      | 4:O:2:NAG:H2      | 1.87                     | 0.75              |
| 2:D:1222:TYR:CE2  | 2:D:1260:ARG:HB3  | 2.21                     | 0.74              |
| 6:E:2007:B12:H362 | 6:E:2007:B12:H351 | 1.69                     | 0.74              |
| 1:A:61:MET:HE2    | 1:A:72:GLN:HB2    | 1.69                     | 0.74              |
| 2:B:1222:TYR:CE2  | 2:B:1260:ARG:HB3  | 2.21                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1222:TYR:CE2  | 2:F:1260:ARG:HB3  | 2.21                     | 0.74              |
| 2:D:1035:PHE:O    | 2:D:1035:PHE:CD1  | 2.38                     | 0.74              |
| 2:F:1194:TRP:HE1  | 2:F:1254:SER:HB3  | 1.51                     | 0.74              |
| 1:E:61:MET:HE2    | 1:E:72:GLN:HB2    | 1.69                     | 0.74              |
| 2:F:1304:GLN:H    | 2:F:1372:THR:HG23 | 1.52                     | 0.74              |
| 1:A:160:THR:HG21  | 2:B:1099:ILE:HG21 | 1.69                     | 0.74              |
| 4:I:1:NAG:O3      | 4:I:2:NAG:H2      | 1.87                     | 0.74              |
| 1:E:352:ARG:HG3   | 1:E:352:ARG:NH1   | 1.95                     | 0.74              |
| 1:E:389:LEU:HB3   | 1:E:394:PRO:HA    | 1.70                     | 0.74              |
| 2:D:1304:GLN:H    | 2:D:1372:THR:HG23 | 1.52                     | 0.73              |
| 2:D:1194:TRP:HE1  | 2:D:1254:SER:HB3  | 1.51                     | 0.73              |
| 1:A:389:LEU:HB3   | 1:A:394:PRO:HA    | 1.70                     | 0.73              |
| 2:B:999:THR:HG22  | 2:B:1000:SER:H    | 1.53                     | 0.73              |
| 2:D:1181:TYR:CD1  | 2:D:1182:PRO:HA   | 2.24                     | 0.73              |
| 6:A:2007:B12:H362 | 6:A:2007:B12:H351 | 1.69                     | 0.73              |
| 1:E:297:THR:HG22  | 1:E:299:PRO:HD3   | 1.71                     | 0.73              |
| 1:A:311:ASN:HB2   | 1:A:337:VAL:CA    | 2.11                     | 0.72              |
| 6:C:2007:B12:H362 | 6:C:2007:B12:H351 | 1.69                     | 0.72              |
| 3:H:3:BMA:H61     | 3:H:5:MAN:C5      | 2.18                     | 0.72              |
| 6:C:2007:B12:N22  | 6:C:2007:B12:H4B  | 2.04                     | 0.72              |
| 2:D:999:THR:HG22  | 2:D:1000:SER:H    | 1.53                     | 0.72              |
| 2:F:1181:TYR:CD1  | 2:F:1182:PRO:HA   | 2.24                     | 0.72              |
| 6:A:2007:B12:H4B  | 6:A:2007:B12:N22  | 2.04                     | 0.72              |
| 2:D:1330:HIS:CG   | 2:D:1331:ILE:H    | 2.03                     | 0.72              |
| 2:F:954:HIS:H     | 2:F:954:HIS:CD2   | 2.06                     | 0.72              |
| 2:F:999:THR:HG22  | 2:F:1000:SER:H    | 1.53                     | 0.72              |
| 2:F:944:GLN:OE1   | 2:F:944:GLN:HA    | 1.90                     | 0.72              |
| 1:A:352:ARG:HG3   | 1:A:352:ARG:NH1   | 1.96                     | 0.72              |
| 2:B:1181:TYR:CD1  | 2:B:1182:PRO:HA   | 2.24                     | 0.72              |
| 1:A:297:THR:HG22  | 1:A:299:PRO:HD3   | 1.71                     | 0.72              |
| 6:E:2007:B12:N22  | 6:E:2007:B12:H4B  | 2.04                     | 0.72              |
| 2:D:1185:TYR:CE1  | 2:D:1266:GLN:HG3  | 2.25                     | 0.72              |
| 1:C:389:LEU:HB3   | 1:C:394:PRO:HA    | 1.70                     | 0.72              |
| 2:B:944:GLN:HA    | 2:B:944:GLN:OE1   | 1.90                     | 0.71              |
| 2:B:954:HIS:CD2   | 2:B:954:HIS:H     | 2.06                     | 0.71              |
| 2:D:954:HIS:CD2   | 2:D:954:HIS:H     | 2.06                     | 0.71              |
| 2:D:1243:GLU:OE1  | 2:D:1243:GLU:HA   | 1.90                     | 0.71              |
| 3:N:3:BMA:H61     | 3:N:5:MAN:C5      | 2.18                     | 0.71              |
| 2:B:1243:GLU:OE1  | 2:B:1243:GLU:HA   | 1.90                     | 0.71              |
| 2:D:944:GLN:HA    | 2:D:944:GLN:OE1   | 1.90                     | 0.71              |
| 2:B:1185:TYR:CE1  | 2:B:1266:GLN:HG3  | 2.25                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:953:PRO:HB2   | 2:F:956:ILE:HD11  | 1.73                     | 0.71              |
| 2:B:1182:PRO:HB3  | 2:B:1268:ARG:HH21 | 1.56                     | 0.71              |
| 1:C:297:THR:HG22  | 1:C:299:PRO:HD3   | 1.71                     | 0.71              |
| 2:F:1182:PRO:HB3  | 2:F:1268:ARG:HH21 | 1.56                     | 0.71              |
| 2:D:1182:PRO:HB3  | 2:D:1268:ARG:HH21 | 1.56                     | 0.71              |
| 2:B:978:HIS:HB2   | 2:B:1033:GLU:OE2  | 1.90                     | 0.71              |
| 2:B:1308:TRP:HB2  | 2:B:1368:VAL:CG2  | 2.21                     | 0.71              |
| 2:D:1308:TRP:HB2  | 2:D:1368:VAL:CG2  | 2.21                     | 0.71              |
| 2:B:953:PRO:HB2   | 2:B:956:ILE:HD11  | 1.73                     | 0.70              |
| 2:D:1319:ASN:HB2  | 2:D:1387:PHE:CD2  | 2.26                     | 0.70              |
| 2:B:1188:SER:HA   | 2:B:1261:THR:O    | 1.92                     | 0.70              |
| 2:F:978:HIS:HB2   | 2:F:1033:GLU:OE2  | 1.91                     | 0.70              |
| 2:F:1188:SER:HA   | 2:F:1261:THR:O    | 1.92                     | 0.70              |
| 2:D:978:HIS:HB2   | 2:D:1033:GLU:OE2  | 1.91                     | 0.70              |
| 2:F:1277:THR:HG22 | 2:F:1279:GLU:H    | 1.56                     | 0.70              |
| 2:F:1308:TRP:HB2  | 2:F:1368:VAL:CG2  | 2.21                     | 0.70              |
| 2:F:1319:ASN:HB2  | 2:F:1387:PHE:CD2  | 2.25                     | 0.70              |
| 2:B:1366:LEU:HD22 | 2:B:1366:LEU:C    | 2.17                     | 0.70              |
| 2:D:1057:GLY:HA2  | 2:D:1158:TRP:HE1  | 1.56                     | 0.70              |
| 2:D:953:PRO:HB2   | 2:D:956:ILE:HD11  | 1.73                     | 0.70              |
| 1:E:87:LEU:HD22   | 1:E:91:HIS:HB3    | 1.73                     | 0.70              |
| 2:F:1185:TYR:CE1  | 2:F:1266:GLN:HG3  | 2.25                     | 0.70              |
| 2:F:1277:THR:HG22 | 2:F:1278:CYS:H    | 1.56                     | 0.70              |
| 2:B:1277:THR:HG22 | 2:B:1279:GLU:H    | 1.56                     | 0.70              |
| 1:A:313:THR:HA    | 1:A:334:ASN:O     | 1.92                     | 0.69              |
| 2:B:1277:THR:HG22 | 2:B:1278:CYS:H    | 1.56                     | 0.69              |
| 2:D:1277:THR:HG22 | 2:D:1278:CYS:H    | 1.56                     | 0.69              |
| 1:E:311:ASN:HB2   | 1:E:337:VAL:CA    | 2.12                     | 0.69              |
| 2:F:1243:GLU:HA   | 2:F:1243:GLU:OE1  | 1.90                     | 0.69              |
| 2:D:1366:LEU:C    | 2:D:1366:LEU:HD22 | 2.17                     | 0.69              |
| 3:K:3:BMA:H61     | 3:K:5:MAN:C5      | 2.18                     | 0.69              |
| 2:D:1188:SER:HA   | 2:D:1261:THR:O    | 1.92                     | 0.69              |
| 1:E:313:THR:HA    | 1:E:334:ASN:O     | 1.92                     | 0.69              |
| 2:D:1277:THR:HG22 | 2:D:1279:GLU:H    | 1.56                     | 0.69              |
| 1:A:87:LEU:HD22   | 1:A:91:HIS:HB3    | 1.73                     | 0.69              |
| 2:F:951:VAL:HB    | 2:F:1032:TYR:O    | 1.92                     | 0.69              |
| 2:F:1366:LEU:C    | 2:F:1366:LEU:HD22 | 2.17                     | 0.69              |
| 1:A:173:GLY:O     | 1:A:177:THR:HG23  | 1.93                     | 0.69              |
| 6:C:2007:B12:H4B  | 6:C:2007:B12:C6   | 2.23                     | 0.69              |
| 1:C:173:GLY:O     | 1:C:177:THR:HG23  | 1.93                     | 0.69              |
| 2:F:1057:GLY:HA2  | 2:F:1158:TRP:HE1  | 1.56                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1177:ILE:HG23 | 2:F:1181:TYR:HB3  | 1.75                     | 0.68              |
| 6:A:2007:B12:H4B  | 6:A:2007:B12:C6   | 2.23                     | 0.68              |
| 1:C:87:LEU:HD22   | 1:C:91:HIS:HB3    | 1.73                     | 0.68              |
| 2:F:1304:GLN:HB2  | 2:F:1372:THR:HG22 | 1.75                     | 0.68              |
| 2:F:1183:MET:HE2  | 2:F:1183:MET:N    | 2.09                     | 0.68              |
| 2:B:951:VAL:HB    | 2:B:1032:TYR:O    | 1.92                     | 0.68              |
| 2:B:1177:ILE:HG23 | 2:B:1181:TYR:HB3  | 1.75                     | 0.68              |
| 2:F:1057:GLY:HA3  | 2:F:1157:TYR:HA   | 1.75                     | 0.68              |
| 2:B:1057:GLY:HA2  | 2:B:1158:TRP:HE1  | 1.56                     | 0.68              |
| 1:C:313:THR:HA    | 1:C:334:ASN:O     | 1.92                     | 0.68              |
| 2:D:1304:GLN:HB2  | 2:D:1372:THR:HG22 | 1.75                     | 0.68              |
| 2:D:935:ILE:HG13  | 2:D:935:ILE:O     | 1.94                     | 0.68              |
| 6:E:2007:B12:H4B  | 6:E:2007:B12:C6   | 2.23                     | 0.68              |
| 1:E:173:GLY:O     | 1:E:177:THR:HG23  | 1.93                     | 0.68              |
| 2:B:1319:ASN:HB2  | 2:B:1387:PHE:CD2  | 2.26                     | 0.68              |
| 2:D:1183:MET:N    | 2:D:1183:MET:HE2  | 2.08                     | 0.67              |
| 1:C:311:ASN:HB2   | 1:C:337:VAL:CA    | 2.13                     | 0.67              |
| 2:B:1057:GLY:HA3  | 2:B:1157:TYR:HA   | 1.75                     | 0.67              |
| 1:C:156:ARG:HG3   | 2:D:1099:ILE:HD12 | 1.77                     | 0.67              |
| 2:D:951:VAL:HB    | 2:D:1032:TYR:O    | 1.93                     | 0.67              |
| 2:D:1177:ILE:HG23 | 2:D:1181:TYR:HB3  | 1.75                     | 0.67              |
| 1:E:156:ARG:HG3   | 2:F:1099:ILE:HD12 | 1.77                     | 0.67              |
| 2:B:935:ILE:O     | 2:B:935:ILE:HG13  | 1.94                     | 0.67              |
| 2:B:1183:MET:N    | 2:B:1183:MET:HE2  | 2.08                     | 0.67              |
| 2:D:1060:THR:CG2  | 2:D:1064:PHE:HB3  | 2.24                     | 0.67              |
| 2:D:1057:GLY:HA3  | 2:D:1157:TYR:HA   | 1.75                     | 0.67              |
| 2:F:1213:GLU:OE2  | 2:F:1265:GLN:HB3  | 1.95                     | 0.67              |
| 2:F:1060:THR:CG2  | 2:F:1064:PHE:HB3  | 2.24                     | 0.67              |
| 2:F:1084:GLN:HG3  | 2:F:1162:SER:N    | 2.10                     | 0.67              |
| 2:B:1084:GLN:HG3  | 2:B:1162:SER:N    | 2.10                     | 0.67              |
| 2:D:1213:GLU:OE2  | 2:D:1265:GLN:HB3  | 1.95                     | 0.67              |
| 2:B:1213:GLU:OE2  | 2:B:1265:GLN:HB3  | 1.95                     | 0.66              |
| 1:E:211:SER:HA    | 1:E:214:ILE:HD12  | 1.77                     | 0.66              |
| 2:F:935:ILE:HG13  | 2:F:935:ILE:O     | 1.94                     | 0.66              |
| 2:F:1008:SER:HB3  | 2:F:1182:PRO:O    | 1.95                     | 0.66              |
| 2:D:999:THR:HG22  | 2:D:1000:SER:N    | 2.11                     | 0.66              |
| 2:B:1060:THR:CG2  | 2:B:1064:PHE:HB3  | 2.24                     | 0.66              |
| 2:B:1304:GLN:HB2  | 2:B:1372:THR:HG22 | 1.75                     | 0.66              |
| 1:A:156:ARG:HG3   | 2:B:1099:ILE:HD12 | 1.77                     | 0.66              |
| 2:D:1084:GLN:HG3  | 2:D:1162:SER:N    | 2.10                     | 0.66              |
| 1:A:211:SER:HA    | 1:A:214:ILE:HD12  | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1109:ILE:HG12 | 2:F:1141:LEU:HD22 | 1.78                     | 0.66              |
| 2:B:999:THR:HG22  | 2:B:1000:SER:N    | 2.11                     | 0.66              |
| 2:B:1109:ILE:HG12 | 2:B:1141:LEU:HD22 | 1.78                     | 0.65              |
| 2:D:1109:ILE:HG12 | 2:D:1141:LEU:HD22 | 1.78                     | 0.65              |
| 2:D:1008:SER:HB3  | 2:D:1182:PRO:O    | 1.95                     | 0.65              |
| 1:E:318:ILE:HG13  | 1:E:318:ILE:O     | 1.97                     | 0.65              |
| 2:B:1089:HIS:O    | 2:B:1156:ALA:HB1  | 1.97                     | 0.65              |
| 2:D:1109:ILE:HG23 | 2:D:1141:LEU:HD21 | 1.78                     | 0.65              |
| 2:D:1341:TYR:HB2  | 2:D:1367:GLN:HB2  | 1.79                     | 0.65              |
| 2:B:1008:SER:HB3  | 2:B:1182:PRO:O    | 1.95                     | 0.65              |
| 2:F:999:THR:HG22  | 2:F:1000:SER:N    | 2.11                     | 0.65              |
| 2:F:1259:LEU:HD23 | 2:F:1259:LEU:O    | 1.97                     | 0.65              |
| 2:B:1341:TYR:HB2  | 2:B:1367:GLN:HB2  | 1.79                     | 0.65              |
| 2:D:1182:PRO:HB3  | 2:D:1268:ARG:NH2  | 2.12                     | 0.65              |
| 2:F:1084:GLN:HG2  | 2:F:1161:SER:HA   | 1.79                     | 0.65              |
| 2:F:1089:HIS:O    | 2:F:1156:ALA:HB1  | 1.97                     | 0.65              |
| 1:A:318:ILE:O     | 1:A:318:ILE:HG13  | 1.97                     | 0.65              |
| 2:B:1109:ILE:HG23 | 2:B:1141:LEU:HD21 | 1.78                     | 0.65              |
| 1:C:318:ILE:HG13  | 1:C:318:ILE:O     | 1.97                     | 0.65              |
| 1:C:211:SER:HA    | 1:C:214:ILE:HD12  | 1.77                     | 0.65              |
| 2:D:1308:TRP:HB2  | 2:D:1368:VAL:HG23 | 1.79                     | 0.65              |
| 2:D:956:ILE:HG22  | 2:D:958:CYS:H     | 1.62                     | 0.64              |
| 2:D:1089:HIS:O    | 2:D:1156:ALA:HB1  | 1.97                     | 0.64              |
| 2:F:1294:ILE:HD11 | 2:F:1301:SER:HG   | 1.61                     | 0.64              |
| 2:F:1308:TRP:HB2  | 2:F:1368:VAL:HG23 | 1.79                     | 0.64              |
| 2:B:956:ILE:HG22  | 2:B:958:CYS:H     | 1.62                     | 0.64              |
| 2:B:1182:PRO:HB3  | 2:B:1268:ARG:NH2  | 2.12                     | 0.64              |
| 1:C:312:ILE:HG22  | 1:C:313:THR:H     | 1.63                     | 0.64              |
| 2:B:1049:LEU:CD2  | 2:B:1075:ILE:HB   | 2.28                     | 0.64              |
| 2:B:1308:TRP:HB2  | 2:B:1368:VAL:HG23 | 1.79                     | 0.64              |
| 2:D:993:TYR:HB3   | 2:D:1021:MET:HB2  | 1.79                     | 0.64              |
| 6:A:2007:B12:N22  | 6:A:2007:B12:C4B  | 2.60                     | 0.64              |
| 2:F:1049:LEU:CD2  | 2:F:1075:ILE:HB   | 2.28                     | 0.64              |
| 2:F:1341:TYR:HB2  | 2:F:1367:GLN:HB2  | 1.79                     | 0.64              |
| 1:E:203:LEU:O     | 1:E:207:VAL:HG23  | 1.98                     | 0.64              |
| 6:E:2007:B12:N22  | 6:E:2007:B12:C4B  | 2.60                     | 0.64              |
| 1:A:317:THR:HG1   | 1:A:409:HIS:HE2   | 1.45                     | 0.64              |
| 1:C:203:LEU:O     | 1:C:207:VAL:HG23  | 1.98                     | 0.64              |
| 2:B:1285:ASN:HD21 | 5:B:2009:NAG:H61  | 1.63                     | 0.63              |
| 2:D:1049:LEU:CD2  | 2:D:1075:ILE:HB   | 2.28                     | 0.63              |
| 2:D:1259:LEU:HD23 | 2:D:1259:LEU:O    | 1.97                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1285:ASN:HD21 | 5:D:2009:NAG:H61  | 1.63                     | 0.63              |
| 2:F:1109:ILE:HG23 | 2:F:1141:LEU:HD21 | 1.78                     | 0.63              |
| 6:C:2007:B12:N22  | 6:C:2007:B12:C4B  | 2.60                     | 0.63              |
| 2:D:1084:GLN:HG2  | 2:D:1161:SER:HA   | 1.79                     | 0.63              |
| 2:F:956:ILE:HG22  | 2:F:958:CYS:H     | 1.62                     | 0.63              |
| 2:B:1259:LEU:HD23 | 2:B:1259:LEU:O    | 1.97                     | 0.63              |
| 2:D:1296:TYR:CG   | 2:D:1297:PRO:HA   | 2.34                     | 0.63              |
| 2:F:1060:THR:HG23 | 2:F:1064:PHE:HB3  | 1.79                     | 0.63              |
| 2:B:1049:LEU:HD23 | 2:B:1075:ILE:HB   | 1.81                     | 0.63              |
| 2:B:1296:TYR:CG   | 2:B:1297:PRO:HA   | 2.34                     | 0.63              |
| 1:E:389:LEU:HD23  | 1:E:389:LEU:H     | 1.62                     | 0.63              |
| 2:F:1296:TYR:CG   | 2:F:1297:PRO:HA   | 2.34                     | 0.63              |
| 2:B:1287:THR:O    | 2:B:1388:VAL:HG23 | 1.99                     | 0.63              |
| 1:C:389:LEU:H     | 1:C:389:LEU:HD23  | 1.62                     | 0.63              |
| 2:D:1287:THR:O    | 2:D:1388:VAL:HG23 | 1.99                     | 0.63              |
| 1:A:389:LEU:H     | 1:A:389:LEU:HD23  | 1.62                     | 0.63              |
| 2:F:1287:THR:O    | 2:F:1388:VAL:HG23 | 1.99                     | 0.63              |
| 2:F:993:TYR:HB3   | 2:F:1021:MET:HB2  | 1.79                     | 0.63              |
| 2:F:1182:PRO:HB3  | 2:F:1268:ARG:NH2  | 2.12                     | 0.63              |
| 1:A:203:LEU:O     | 1:A:207:VAL:HG23  | 1.98                     | 0.63              |
| 2:B:1060:THR:HG23 | 2:B:1064:PHE:HB3  | 1.79                     | 0.63              |
| 1:E:312:ILE:HG22  | 1:E:313:THR:H     | 1.64                     | 0.63              |
| 1:A:312:ILE:HG22  | 1:A:313:THR:H     | 1.63                     | 0.62              |
| 2:D:1060:THR:HG23 | 2:D:1064:PHE:HB3  | 1.79                     | 0.62              |
| 2:B:1084:GLN:HG2  | 2:B:1161:SER:HA   | 1.79                     | 0.62              |
| 2:B:993:TYR:HB3   | 2:B:1021:MET:HB2  | 1.79                     | 0.62              |
| 1:C:219:ILE:CG1   | 1:C:252:MET:HE2   | 2.30                     | 0.62              |
| 2:F:978:HIS:HB2   | 2:F:1033:GLU:CD   | 2.24                     | 0.62              |
| 2:F:1049:LEU:HD23 | 2:F:1075:ILE:HB   | 1.81                     | 0.62              |
| 2:B:1076:TYR:HB2  | 2:B:1141:LEU:HB2  | 1.82                     | 0.62              |
| 1:A:308:SER:O     | 1:A:309:ALA:HB2   | 2.00                     | 0.62              |
| 1:C:317:THR:HG1   | 1:C:409:HIS:HE2   | 1.46                     | 0.62              |
| 2:D:978:HIS:HB2   | 2:D:1033:GLU:CD   | 2.24                     | 0.62              |
| 1:A:219:ILE:CG1   | 1:A:252:MET:HE2   | 2.30                     | 0.62              |
| 2:D:1067:ASN:HA   | 2:D:1151:ARG:O    | 1.99                     | 0.62              |
| 2:D:1076:TYR:HB2  | 2:D:1141:LEU:HB2  | 1.82                     | 0.62              |
| 1:E:317:THR:HG1   | 1:E:409:HIS:HE2   | 1.48                     | 0.62              |
| 1:E:337:VAL:HG13  | 5:E:2001:NAG:H2   | 1.81                     | 0.62              |
| 2:D:1049:LEU:HD23 | 2:D:1075:ILE:HB   | 1.81                     | 0.62              |
| 2:B:1106:PHE:CZ   | 2:B:1144:LYS:HB2  | 2.35                     | 0.62              |
| 2:D:1277:THR:HG22 | 2:D:1278:CYS:N    | 2.15                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1325:PHE:HB2  | 2:D:1355:LEU:HD12 | 1.82                     | 0.62              |
| 2:F:966:PRO:O     | 2:F:967:ASN:CG    | 2.43                     | 0.62              |
| 2:F:1340:LEU:CD2  | 2:F:1368:VAL:HG12 | 2.30                     | 0.62              |
| 2:F:1285:ASN:HD21 | 5:F:2009:NAG:H61  | 1.63                     | 0.61              |
| 2:B:1067:ASN:HA   | 2:B:1151:ARG:O    | 1.99                     | 0.61              |
| 2:D:1106:PHE:CZ   | 2:D:1144:LYS:HB2  | 2.35                     | 0.61              |
| 2:D:1340:LEU:CD2  | 2:D:1368:VAL:HG12 | 2.30                     | 0.61              |
| 2:F:1067:ASN:HA   | 2:F:1151:ARG:O    | 1.99                     | 0.61              |
| 2:B:978:HIS:HB2   | 2:B:1033:GLU:CD   | 2.24                     | 0.61              |
| 2:B:1325:PHE:HB2  | 2:B:1355:LEU:HD12 | 1.82                     | 0.61              |
| 2:B:1340:LEU:CD2  | 2:B:1368:VAL:HG12 | 2.30                     | 0.61              |
| 2:F:1076:TYR:HB2  | 2:F:1141:LEU:HB2  | 1.82                     | 0.61              |
| 2:F:1106:PHE:CZ   | 2:F:1144:LYS:HB2  | 2.35                     | 0.61              |
| 1:A:337:VAL:HG13  | 5:A:2001:NAG:H2   | 1.83                     | 0.61              |
| 2:B:1277:THR:HG22 | 2:B:1278:CYS:N    | 2.15                     | 0.61              |
| 1:E:76:THR:O      | 1:E:80:MET:HG3    | 2.01                     | 0.61              |
| 1:E:219:ILE:CG1   | 1:E:252:MET:HE2   | 2.30                     | 0.61              |
| 6:E:2007:B12:H262 | 6:E:2007:B12:H601 | 1.82                     | 0.61              |
| 2:D:966:PRO:O     | 2:D:967:ASN:CG    | 2.44                     | 0.61              |
| 1:C:308:SER:O     | 1:C:309:ALA:HB2   | 2.00                     | 0.61              |
| 2:B:1320:TYR:OH   | 2:B:1366:LEU:HD23 | 2.00                     | 0.61              |
| 2:F:1277:THR:HG22 | 2:F:1278:CYS:N    | 2.15                     | 0.61              |
| 2:D:978:HIS:O     | 2:D:979:LEU:HD23  | 2.01                     | 0.61              |
| 2:F:1325:PHE:HB2  | 2:F:1355:LEU:HD12 | 1.82                     | 0.61              |
| 2:B:1079:THR:HG23 | 2:B:1138:LYS:CG   | 2.23                     | 0.60              |
| 1:E:308:SER:O     | 1:E:309:ALA:HB2   | 2.00                     | 0.60              |
| 2:F:1320:TYR:OH   | 2:F:1366:LEU:HD23 | 2.02                     | 0.60              |
| 2:F:1225:VAL:CG1  | 2:F:1236:LEU:HB2  | 2.32                     | 0.60              |
| 1:A:76:THR:O      | 1:A:80:MET:HG3    | 2.01                     | 0.60              |
| 6:A:2007:B12:H601 | 6:A:2007:B12:H262 | 1.82                     | 0.60              |
| 2:B:1225:VAL:CG1  | 2:B:1236:LEU:HB2  | 2.32                     | 0.60              |
| 6:C:2007:B12:H262 | 6:C:2007:B12:H601 | 1.82                     | 0.60              |
| 2:D:1320:TYR:OH   | 2:D:1366:LEU:HD23 | 2.02                     | 0.60              |
| 2:D:954:HIS:CD2   | 2:D:954:HIS:N     | 2.70                     | 0.60              |
| 2:B:1182:PRO:CB   | 2:B:1268:ARG:HH21 | 2.15                     | 0.60              |
| 1:C:76:THR:O      | 1:C:80:MET:HG3    | 2.01                     | 0.60              |
| 1:C:290:PRO:O     | 1:C:291:ASP:HB2   | 2.01                     | 0.60              |
| 1:E:379:ASN:H     | 1:E:384:THR:HG22  | 1.67                     | 0.60              |
| 6:E:2007:B12:H531 | 6:E:2007:B12:C55  | 2.23                     | 0.60              |
| 2:B:1294:ILE:HD11 | 2:B:1301:SER:HG   | 1.65                     | 0.60              |
| 2:D:1182:PRO:CB   | 2:D:1268:ARG:HH21 | 2.15                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:966:PRO:O     | 2:B:967:ASN:CG    | 2.45                     | 0.59              |
| 2:B:971:HIS:HB2   | 2:B:1042:ILE:HD12 | 1.83                     | 0.59              |
| 6:C:2007:B12:H531 | 6:C:2007:B12:C55  | 2.23                     | 0.59              |
| 2:D:971:HIS:HB2   | 2:D:1042:ILE:HD12 | 1.84                     | 0.59              |
| 2:F:978:HIS:O     | 2:F:979:LEU:HD23  | 2.02                     | 0.59              |
| 1:A:379:ASN:H     | 1:A:384:THR:HG22  | 1.67                     | 0.59              |
| 2:B:954:HIS:CD2   | 2:B:954:HIS:N     | 2.70                     | 0.59              |
| 1:C:339:SER:C     | 1:C:341:SER:H     | 2.10                     | 0.59              |
| 1:E:320:ASN:HB3   | 1:E:328:LEU:HG    | 1.83                     | 0.59              |
| 2:B:978:HIS:O     | 2:B:979:LEU:HD23  | 2.02                     | 0.59              |
| 2:D:1225:VAL:CG1  | 2:D:1236:LEU:HB2  | 2.32                     | 0.59              |
| 2:F:1182:PRO:CB   | 2:F:1268:ARG:HH21 | 2.15                     | 0.59              |
| 1:C:405:PHE:CZ    | 1:C:408:GLU:HG3   | 2.37                     | 0.59              |
| 1:C:379:ASN:H     | 1:C:384:THR:HG22  | 1.67                     | 0.59              |
| 2:D:1079:THR:HG23 | 2:D:1138:LYS:CG   | 2.23                     | 0.59              |
| 1:E:339:SER:C     | 1:E:341:SER:H     | 2.10                     | 0.59              |
| 1:E:405:PHE:CZ    | 1:E:408:GLU:HG3   | 2.37                     | 0.59              |
| 1:A:337:VAL:CG2   | 5:A:2001:NAG:O7   | 2.49                     | 0.59              |
| 1:E:290:PRO:O     | 1:E:291:ASP:HB2   | 2.01                     | 0.59              |
| 2:F:971:HIS:HB2   | 2:F:1042:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:290:PRO:O     | 1:A:291:ASP:HB2   | 2.01                     | 0.59              |
| 2:F:954:HIS:CD2   | 2:F:954:HIS:N     | 2.70                     | 0.59              |
| 1:C:320:ASN:HB3   | 1:C:328:LEU:HG    | 1.83                     | 0.59              |
| 1:A:320:ASN:HB3   | 1:A:328:LEU:HG    | 1.83                     | 0.59              |
| 2:B:990:LEU:HD12  | 2:B:1035:PHE:CE2  | 2.39                     | 0.58              |
| 1:E:218:GLY:O     | 1:E:249:THR:HG23  | 2.03                     | 0.58              |
| 1:A:405:PHE:CZ    | 1:A:408:GLU:HG3   | 2.37                     | 0.58              |
| 2:F:948:HIS:CG    | 2:F:949:PRO:HA    | 2.39                     | 0.58              |
| 2:F:1148:ILE:HG22 | 2:F:1149:ASP:N    | 2.18                     | 0.58              |
| 1:A:339:SER:C     | 1:A:341:SER:H     | 2.10                     | 0.58              |
| 2:B:948:HIS:CG    | 2:B:949:PRO:HA    | 2.39                     | 0.58              |
| 2:B:1296:TYR:CD2  | 2:B:1297:PRO:HA   | 2.39                     | 0.58              |
| 2:D:948:HIS:CG    | 2:D:949:PRO:HA    | 2.39                     | 0.58              |
| 2:D:1296:TYR:CD2  | 2:D:1297:PRO:HA   | 2.39                     | 0.58              |
| 2:F:942:THR:CG2   | 2:F:1036:LEU:HD11 | 2.33                     | 0.58              |
| 2:B:942:THR:CG2   | 2:B:1036:LEU:HD11 | 2.33                     | 0.58              |
| 1:E:389:LEU:HD23  | 1:E:389:LEU:N     | 2.19                     | 0.58              |
| 2:B:1148:ILE:HG22 | 2:B:1149:ASP:N    | 2.18                     | 0.57              |
| 2:B:1158:TRP:N    | 2:B:1158:TRP:CD1  | 2.72                     | 0.57              |
| 1:C:219:ILE:HG12  | 1:C:252:MET:HE2   | 1.86                     | 0.57              |
| 2:D:942:THR:CG2   | 2:D:1036:LEU:HD11 | 2.33                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1148:ILE:HG22 | 2:D:1149:ASP:N    | 2.18                     | 0.57              |
| 2:D:1330:HIS:CE1  | 2:D:1332:ASN:N    | 2.67                     | 0.57              |
| 2:F:1084:GLN:CG   | 2:F:1163:THR:H    | 2.15                     | 0.57              |
| 1:A:389:LEU:HD23  | 1:A:389:LEU:N     | 2.19                     | 0.57              |
| 6:A:2007:B12:H351 | 6:A:2007:B12:H372 | 1.85                     | 0.57              |
| 2:B:1084:GLN:CG   | 2:B:1163:THR:H    | 2.15                     | 0.57              |
| 1:C:389:LEU:HD23  | 1:C:389:LEU:N     | 2.19                     | 0.57              |
| 2:D:989:TYR:CD1   | 2:D:989:TYR:C     | 2.83                     | 0.57              |
| 6:E:2007:B12:H351 | 6:E:2007:B12:H372 | 1.85                     | 0.57              |
| 2:F:990:LEU:HD12  | 2:F:1035:PHE:CE2  | 2.39                     | 0.57              |
| 2:F:1158:TRP:CD1  | 2:F:1158:TRP:N    | 2.72                     | 0.57              |
| 1:A:58:LEU:HB2    | 1:A:75:LEU:CD2    | 2.35                     | 0.57              |
| 1:A:218:GLY:O     | 1:A:249:THR:HG23  | 2.03                     | 0.57              |
| 2:D:990:LEU:HD12  | 2:D:1035:PHE:CE2  | 2.39                     | 0.57              |
| 2:D:1158:TRP:CD1  | 2:D:1158:TRP:N    | 2.72                     | 0.57              |
| 1:A:219:ILE:HG12  | 1:A:252:MET:HE2   | 1.86                     | 0.57              |
| 6:A:2007:B12:H531 | 6:A:2007:B12:C55  | 2.23                     | 0.57              |
| 2:B:993:TYR:CD1   | 2:B:1000:SER:HB2  | 2.40                     | 0.57              |
| 1:C:58:LEU:HB2    | 1:C:75:LEU:CD2    | 2.35                     | 0.57              |
| 2:F:1296:TYR:CD2  | 2:F:1297:PRO:HA   | 2.39                     | 0.57              |
| 2:B:989:TYR:CD1   | 2:B:989:TYR:C     | 2.83                     | 0.57              |
| 1:C:218:GLY:O     | 1:C:249:THR:HG23  | 2.03                     | 0.57              |
| 6:C:2007:B12:H351 | 6:C:2007:B12:H372 | 1.85                     | 0.57              |
| 1:A:337:VAL:HG22  | 5:A:2001:NAG:C7   | 2.35                     | 0.57              |
| 1:C:117:MET:HB3   | 1:C:153:ILE:HD13  | 1.87                     | 0.57              |
| 2:D:993:TYR:CD1   | 2:D:1000:SER:HB2  | 2.40                     | 0.57              |
| 2:D:1057:GLY:HA2  | 2:D:1158:TRP:CD1  | 2.40                     | 0.57              |
| 2:F:1353:VAL:HG22 | 2:F:1353:VAL:O    | 2.05                     | 0.57              |
| 2:B:1057:GLY:HA2  | 2:B:1158:TRP:CD1  | 2.40                     | 0.57              |
| 2:D:1210:PHE:HD2  | 2:D:1211:HIS:N    | 2.03                     | 0.57              |
| 2:D:1350:TYR:CE1  | 2:D:1356:PRO:HB3  | 2.40                     | 0.57              |
| 2:F:1350:TYR:CE1  | 2:F:1356:PRO:HB3  | 2.40                     | 0.57              |
| 2:B:1350:TYR:CE1  | 2:B:1356:PRO:HB3  | 2.40                     | 0.56              |
| 1:E:214:ILE:HG13  | 1:E:220:ILE:HG23  | 1.87                     | 0.56              |
| 2:F:990:LEU:HD23  | 2:F:991:GLU:N     | 2.20                     | 0.56              |
| 1:A:94:LEU:HD22   | 1:A:137:LEU:HG    | 1.87                     | 0.56              |
| 1:A:173:GLY:O     | 1:A:177:THR:CG2   | 2.53                     | 0.56              |
| 2:B:1330:HIS:CE1  | 2:B:1332:ASN:N    | 2.68                     | 0.56              |
| 2:D:1342:ASP:CB   | 2:D:1347:MET:HE2  | 2.34                     | 0.56              |
| 1:E:29:PRO:HB2    | 1:E:32:GLN:CG     | 2.35                     | 0.56              |
| 2:F:989:TYR:CD1   | 2:F:989:TYR:C     | 2.83                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:993:TYR:CD1   | 2:F:1000:SER:HB2  | 2.40                     | 0.56              |
| 1:A:117:MET:HE2   | 1:A:138:ALA:HB3   | 1.87                     | 0.56              |
| 6:C:2007:B12:O28  | 6:C:2007:B12:H3   | 2.06                     | 0.56              |
| 2:D:1235:LEU:HD11 | 2:D:1237:THR:O    | 2.06                     | 0.56              |
| 1:E:219:ILE:HG12  | 1:E:252:MET:HE2   | 1.86                     | 0.56              |
| 2:F:1342:ASP:CB   | 2:F:1347:MET:HE2  | 2.33                     | 0.56              |
| 1:A:117:MET:HB3   | 1:A:153:ILE:HD13  | 1.87                     | 0.56              |
| 1:C:311:ASN:HA    | 1:C:338:LYS:H     | 1.70                     | 0.56              |
| 2:D:1084:GLN:CG   | 2:D:1163:THR:H    | 2.15                     | 0.56              |
| 1:E:58:LEU:HB2    | 1:E:75:LEU:CD2    | 2.35                     | 0.56              |
| 2:B:1009:ILE:HG23 | 2:B:1009:ILE:O    | 2.06                     | 0.56              |
| 2:B:1342:ASP:CB   | 2:B:1347:MET:HE2  | 2.33                     | 0.56              |
| 2:B:1353:VAL:HG22 | 2:B:1353:VAL:O    | 2.05                     | 0.56              |
| 1:E:173:GLY:O     | 1:E:177:THR:CG2   | 2.53                     | 0.56              |
| 2:F:1035:PHE:CD1  | 2:F:1035:PHE:C    | 2.83                     | 0.56              |
| 2:B:1035:PHE:CD1  | 2:B:1035:PHE:C    | 2.83                     | 0.56              |
| 1:C:173:GLY:O     | 1:C:177:THR:CG2   | 2.53                     | 0.56              |
| 2:D:1247:LEU:C    | 2:D:1247:LEU:HD12 | 2.31                     | 0.56              |
| 2:F:1084:GLN:HG3  | 2:F:1162:SER:H    | 1.70                     | 0.56              |
| 1:C:29:PRO:HB2    | 1:C:32:GLN:CG     | 2.35                     | 0.56              |
| 2:D:1210:PHE:CD2  | 2:D:1211:HIS:N    | 2.74                     | 0.56              |
| 2:F:1057:GLY:HA2  | 2:F:1158:TRP:CD1  | 2.40                     | 0.56              |
| 2:F:1210:PHE:HD2  | 2:F:1211:HIS:N    | 2.03                     | 0.56              |
| 1:A:214:ILE:HG13  | 1:A:220:ILE:HG23  | 1.87                     | 0.56              |
| 2:B:990:LEU:HD23  | 2:B:991:GLU:N     | 2.20                     | 0.56              |
| 1:C:362:THR:CG2   | 1:C:371:SER:CB    | 2.83                     | 0.56              |
| 2:D:990:LEU:HD23  | 2:D:991:GLU:N     | 2.20                     | 0.56              |
| 2:F:956:ILE:HG22  | 2:F:957:ASN:N     | 2.21                     | 0.56              |
| 2:F:1281:VAL:HG21 | 2:F:1308:TRP:CD1  | 2.41                     | 0.56              |
| 2:B:956:ILE:HG22  | 2:B:957:ASN:N     | 2.21                     | 0.56              |
| 6:C:2007:B12:H362 | 6:C:2007:B12:C35  | 2.36                     | 0.56              |
| 2:D:956:ILE:HG22  | 2:D:957:ASN:N     | 2.21                     | 0.56              |
| 1:E:311:ASN:HA    | 1:E:338:LYS:H     | 1.70                     | 0.56              |
| 2:F:1223:LEU:HD23 | 2:F:1259:LEU:HB2  | 1.88                     | 0.56              |
| 2:B:1210:PHE:CD2  | 2:B:1211:HIS:N    | 2.74                     | 0.56              |
| 2:B:1247:LEU:C    | 2:B:1247:LEU:HD12 | 2.31                     | 0.56              |
| 1:E:94:LEU:HD22   | 1:E:137:LEU:HG    | 1.87                     | 0.56              |
| 1:E:117:MET:HB3   | 1:E:153:ILE:HD13  | 1.87                     | 0.56              |
| 6:A:2007:B12:O28  | 6:A:2007:B12:H3   | 2.05                     | 0.55              |
| 2:D:1029:ASP:C    | 2:D:1030:LEU:HG   | 2.30                     | 0.55              |
| 2:D:1294:ILE:HD11 | 2:D:1301:SER:HG   | 1.65                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1247:LEU:C    | 2:F:1247:LEU:HD12 | 2.31                     | 0.55              |
| 1:A:417:TYR:N     | 1:A:417:TYR:CD2   | 2.74                     | 0.55              |
| 2:B:1222:TYR:HE2  | 2:B:1260:ARG:HD3  | 1.72                     | 0.55              |
| 2:B:1281:VAL:HG21 | 2:B:1308:TRP:CD1  | 2.41                     | 0.55              |
| 2:D:1353:VAL:HG22 | 2:D:1353:VAL:O    | 2.05                     | 0.55              |
| 1:E:215:LYS:C     | 1:E:217:ASN:H     | 2.14                     | 0.55              |
| 6:E:2007:B12:H362 | 6:E:2007:B12:C35  | 2.36                     | 0.55              |
| 2:F:1029:ASP:C    | 2:F:1030:LEU:HG   | 2.30                     | 0.55              |
| 2:F:1210:PHE:CD2  | 2:F:1211:HIS:N    | 2.74                     | 0.55              |
| 2:F:1366:LEU:O    | 2:F:1366:LEU:HD13 | 2.07                     | 0.55              |
| 1:A:29:PRO:HB2    | 1:A:32:GLN:CG     | 2.35                     | 0.55              |
| 2:D:1281:VAL:HG21 | 2:D:1308:TRP:CD1  | 2.41                     | 0.55              |
| 1:E:117:MET:HE2   | 1:E:138:ALA:HB3   | 1.87                     | 0.55              |
| 1:A:215:LYS:C     | 1:A:217:ASN:H     | 2.14                     | 0.55              |
| 2:B:949:PRO:O     | 2:B:950:ASN:HB3   | 2.07                     | 0.55              |
| 2:D:949:PRO:O     | 2:D:950:ASN:HB3   | 2.07                     | 0.55              |
| 2:D:1222:TYR:HE2  | 2:D:1260:ARG:HD3  | 1.72                     | 0.55              |
| 2:B:1029:ASP:C    | 2:B:1030:LEU:HG   | 2.30                     | 0.55              |
| 2:B:1235:LEU:HD11 | 2:B:1237:THR:O    | 2.06                     | 0.55              |
| 1:C:94:LEU:HD22   | 1:C:137:LEU:HG    | 1.87                     | 0.55              |
| 1:C:215:LYS:C     | 1:C:217:ASN:H     | 2.14                     | 0.55              |
| 2:D:1035:PHE:CD1  | 2:D:1035:PHE:C    | 2.83                     | 0.55              |
| 2:D:1249:ARG:HG3  | 2:D:1250:SER:O    | 2.07                     | 0.55              |
| 1:A:40:GLN:CG     | 1:A:272:LEU:HD11  | 2.30                     | 0.55              |
| 2:B:942:THR:HG21  | 2:B:1036:LEU:HD11 | 1.89                     | 0.55              |
| 1:C:117:MET:HE2   | 1:C:138:ALA:HB3   | 1.88                     | 0.55              |
| 1:C:214:ILE:HG13  | 1:C:220:ILE:HG23  | 1.87                     | 0.55              |
| 2:D:1009:ILE:HG23 | 2:D:1009:ILE:O    | 2.06                     | 0.55              |
| 2:D:1080:VAL:HG23 | 2:D:1137:ASN:HB2  | 1.89                     | 0.55              |
| 1:C:417:TYR:N     | 1:C:417:TYR:CD2   | 2.74                     | 0.55              |
| 1:E:337:VAL:HG22  | 5:E:2001:NAG:C7   | 2.37                     | 0.55              |
| 6:A:2007:B12:H362 | 6:A:2007:B12:C35  | 2.36                     | 0.55              |
| 2:B:1223:LEU:HD23 | 2:B:1259:LEU:HB2  | 1.88                     | 0.55              |
| 2:F:1009:ILE:O    | 2:F:1009:ILE:HG23 | 2.06                     | 0.55              |
| 2:F:1036:LEU:HD12 | 2:F:1037:ILE:H    | 1.72                     | 0.55              |
| 2:F:1177:ILE:HD12 | 2:F:1181:TYR:CD2  | 2.42                     | 0.55              |
| 1:A:311:ASN:HA    | 1:A:338:LYS:H     | 1.71                     | 0.55              |
| 2:B:1036:LEU:HD12 | 2:B:1037:ILE:H    | 1.72                     | 0.55              |
| 1:C:325:VAL:HG23  | 1:C:325:VAL:O     | 2.06                     | 0.55              |
| 2:D:1366:LEU:HD13 | 2:D:1366:LEU:O    | 2.06                     | 0.55              |
| 1:E:417:TYR:CD2   | 1:E:417:TYR:N     | 2.74                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1080:VAL:HG23 | 2:F:1137:ASN:HB2  | 1.89                     | 0.55              |
| 1:A:106:PRO:O     | 1:A:108:ASP:N     | 2.40                     | 0.55              |
| 2:B:1177:ILE:HD12 | 2:B:1181:TYR:CD2  | 2.42                     | 0.55              |
| 6:E:2007:B12:O28  | 6:E:2007:B12:H3   | 2.06                     | 0.55              |
| 2:F:949:PRO:O     | 2:F:950:ASN:HB3   | 2.07                     | 0.55              |
| 2:B:1210:PHE:HD2  | 2:B:1211:HIS:N    | 2.03                     | 0.54              |
| 1:C:337:VAL:HG22  | 5:C:2001:NAG:C7   | 2.36                     | 0.54              |
| 2:B:1366:LEU:HD13 | 2:B:1366:LEU:O    | 2.07                     | 0.54              |
| 2:B:1387:PHE:O    | 2:B:1388:VAL:HG22 | 2.07                     | 0.54              |
| 2:D:1036:LEU:HD12 | 2:D:1037:ILE:H    | 1.72                     | 0.54              |
| 2:F:1387:PHE:O    | 2:F:1388:VAL:HG22 | 2.07                     | 0.54              |
| 2:B:1170:THR:HG23 | 2:B:1170:THR:O    | 2.07                     | 0.54              |
| 5:C:2001:NAG:C3   | 5:C:2001:NAG:H83  | 2.38                     | 0.54              |
| 2:D:1084:GLN:HG3  | 2:D:1162:SER:H    | 1.70                     | 0.54              |
| 1:E:106:PRO:O     | 1:E:108:ASP:N     | 2.40                     | 0.54              |
| 6:A:2007:B12:N22  | 6:A:2007:B12:C9B  | 2.71                     | 0.54              |
| 6:C:2007:B12:N22  | 6:C:2007:B12:C9B  | 2.71                     | 0.54              |
| 1:E:325:VAL:HG23  | 1:E:325:VAL:O     | 2.06                     | 0.54              |
| 2:D:1170:THR:HG23 | 2:D:1170:THR:O    | 2.07                     | 0.54              |
| 1:E:182:CYS:HB2   | 1:E:281:LEU:HD21  | 1.90                     | 0.54              |
| 2:F:942:THR:HG21  | 2:F:1036:LEU:HD11 | 1.89                     | 0.54              |
| 2:B:1084:GLN:HG3  | 2:B:1162:SER:H    | 1.70                     | 0.54              |
| 1:C:182:CYS:HB2   | 1:C:281:LEU:HD21  | 1.89                     | 0.54              |
| 6:C:2007:B12:H8   | 6:C:2007:B12:O39  | 2.07                     | 0.54              |
| 2:D:942:THR:HG21  | 2:D:1036:LEU:HD11 | 1.89                     | 0.54              |
| 2:D:1387:PHE:O    | 2:D:1388:VAL:HG22 | 2.07                     | 0.54              |
| 2:F:951:VAL:HB    | 2:F:1032:TYR:C    | 2.33                     | 0.54              |
| 2:F:1235:LEU:HD11 | 2:F:1237:THR:O    | 2.06                     | 0.54              |
| 2:F:1249:ARG:HG3  | 2:F:1250:SER:O    | 2.07                     | 0.54              |
| 1:A:325:VAL:O     | 1:A:325:VAL:HG23  | 2.06                     | 0.54              |
| 2:B:1192:TYR:CE1  | 2:B:1258:LYS:HG3  | 2.43                     | 0.54              |
| 1:C:106:PRO:O     | 1:C:108:ASP:N     | 2.40                     | 0.54              |
| 2:D:1223:LEU:HD23 | 2:D:1259:LEU:HB2  | 1.88                     | 0.54              |
| 2:D:1377:ARG:O    | 2:D:1378:ARG:HB2  | 2.08                     | 0.54              |
| 6:E:2007:B12:N22  | 6:E:2007:B12:C9B  | 2.71                     | 0.54              |
| 2:F:1222:TYR:HE2  | 2:F:1260:ARG:HD3  | 1.72                     | 0.54              |
| 2:B:1377:ARG:O    | 2:B:1378:ARG:HB2  | 2.08                     | 0.54              |
| 1:C:337:VAL:HG13  | 5:C:2001:NAG:H2   | 1.90                     | 0.54              |
| 2:D:999:THR:CG2   | 2:D:1000:SER:H    | 2.21                     | 0.54              |
| 2:F:1170:THR:O    | 2:F:1170:THR:HG23 | 2.07                     | 0.54              |
| 1:A:182:CYS:HB2   | 1:A:281:LEU:HD21  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:386:TRP:CH2   | 1:A:414:PHE:HB2  | 2.43                     | 0.54              |
| 2:B:1080:VAL:HG23 | 2:B:1137:ASN:HB2 | 1.89                     | 0.54              |
| 2:B:1285:ASN:O    | 2:B:1286:GLN:HG3 | 2.08                     | 0.54              |
| 2:B:1309:THR:HG23 | 2:B:1367:GLN:CG  | 2.38                     | 0.54              |
| 2:D:951:VAL:HB    | 2:D:1032:TYR:C   | 2.33                     | 0.54              |
| 2:D:1109:ILE:HG23 | 2:D:1141:LEU:CD2 | 2.37                     | 0.54              |
| 2:D:1177:ILE:HD12 | 2:D:1181:TYR:CD2 | 2.42                     | 0.54              |
| 2:B:951:VAL:HB    | 2:B:1032:TYR:C   | 2.33                     | 0.53              |
| 2:B:1249:ARG:HG3  | 2:B:1250:SER:O   | 2.07                     | 0.53              |
| 2:D:1192:TYR:CE1  | 2:D:1258:LYS:HG3 | 2.43                     | 0.53              |
| 1:E:386:TRP:CH2   | 1:E:414:PHE:HB2  | 2.43                     | 0.53              |
| 1:E:40:GLN:CG     | 1:E:272:LEU:HD11 | 2.30                     | 0.53              |
| 2:F:1109:ILE:HG23 | 2:F:1141:LEU:CD2 | 2.37                     | 0.53              |
| 6:A:2007:B12:O39  | 6:A:2007:B12:H8  | 2.07                     | 0.53              |
| 1:C:386:TRP:CH2   | 1:C:414:PHE:HB2  | 2.43                     | 0.53              |
| 2:F:948:HIS:CD2   | 2:F:949:PRO:HA   | 2.44                     | 0.53              |
| 2:F:1219:THR:HG23 | 2:F:1219:THR:O   | 2.07                     | 0.53              |
| 2:F:1285:ASN:O    | 2:F:1286:GLN:HG3 | 2.08                     | 0.53              |
| 1:A:65:GLY:HA3    | 1:A:292:HIS:CE1  | 2.44                     | 0.53              |
| 2:D:962:ILE:HG23  | 2:D:1020:LEU:HB2 | 1.91                     | 0.53              |
| 2:D:1285:ASN:O    | 2:D:1286:GLN:HG3 | 2.08                     | 0.53              |
| 1:E:362:THR:CG2   | 1:E:371:SER:CB   | 2.83                     | 0.53              |
| 2:F:1377:ARG:O    | 2:F:1378:ARG:HB2 | 2.08                     | 0.53              |
| 2:B:1219:THR:HG23 | 2:B:1219:THR:O   | 2.07                     | 0.53              |
| 1:C:326:GLU:O     | 1:C:326:GLU:HG2  | 2.09                     | 0.53              |
| 1:E:65:GLY:HA3    | 1:E:292:HIS:CE1  | 2.44                     | 0.53              |
| 6:E:2007:B12:H8   | 6:E:2007:B12:O39 | 2.07                     | 0.53              |
| 2:F:967:ASN:ND2   | 2:F:968:HIS:ND1  | 2.57                     | 0.53              |
| 2:B:962:ILE:HG23  | 2:B:1020:LEU:HB2 | 1.91                     | 0.53              |
| 2:B:999:THR:CG2   | 2:B:1000:SER:H   | 2.21                     | 0.53              |
| 2:D:1225:VAL:HG13 | 2:D:1236:LEU:HB2 | 1.89                     | 0.53              |
| 2:F:962:ILE:HG23  | 2:F:1020:LEU:HB2 | 1.91                     | 0.53              |
| 2:F:1073:GLU:HB2  | 2:F:1144:LYS:HD3 | 1.90                     | 0.53              |
| 2:B:948:HIS:CD2   | 2:B:949:PRO:HA   | 2.44                     | 0.53              |
| 2:B:1109:ILE:HG23 | 2:B:1141:LEU:CD2 | 2.37                     | 0.53              |
| 1:C:40:GLN:CG     | 1:C:272:LEU:HD11 | 2.30                     | 0.53              |
| 1:C:65:GLY:HA3    | 1:C:292:HIS:CE1  | 2.44                     | 0.53              |
| 2:D:948:HIS:CD2   | 2:D:949:PRO:HA   | 2.44                     | 0.53              |
| 2:F:1330:HIS:CE1  | 2:F:1332:ASN:N   | 2.68                     | 0.53              |
| 2:D:993:TYR:HD1   | 2:D:1000:SER:HB2 | 1.74                     | 0.53              |
| 2:D:1197:SER:OG   | 2:D:1198:SER:N   | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1244:LYS:HG2  | 2:D:1244:LYS:O    | 2.08                     | 0.53              |
| 1:A:175:MET:HE1   | 1:A:280:TYR:HE2   | 1.74                     | 0.52              |
| 2:B:1181:TYR:CG   | 2:B:1182:PRO:HA   | 2.44                     | 0.52              |
| 2:B:1197:SER:OG   | 2:B:1198:SER:N    | 2.42                     | 0.52              |
| 1:C:146:ASN:ND2   | 1:C:149:ALA:HB2   | 2.24                     | 0.52              |
| 1:C:337:VAL:CG2   | 5:C:2001:NAG:O7   | 2.55                     | 0.52              |
| 2:D:1219:THR:HG23 | 2:D:1219:THR:O    | 2.07                     | 0.52              |
| 1:E:175:MET:HE1   | 1:E:280:TYR:HE2   | 1.74                     | 0.52              |
| 1:E:326:GLU:O     | 1:E:326:GLU:HG2   | 2.09                     | 0.52              |
| 2:F:1035:PHE:HD1  | 2:F:1035:PHE:C    | 2.17                     | 0.52              |
| 2:F:1192:TYR:CE1  | 2:F:1258:LYS:HG3  | 2.43                     | 0.52              |
| 2:F:1225:VAL:HG13 | 2:F:1236:LEU:HB2  | 1.90                     | 0.52              |
| 2:F:1181:TYR:CG   | 2:F:1182:PRO:HA   | 2.44                     | 0.52              |
| 2:F:1256:PHE:O    | 2:F:1257:ILE:HG13 | 2.10                     | 0.52              |
| 2:B:1209:ASP:OD2  | 2:B:1268:ARG:NH1  | 2.43                     | 0.52              |
| 2:D:1073:GLU:HB2  | 2:D:1144:LYS:HD3  | 1.90                     | 0.52              |
| 2:F:1209:ASP:OD2  | 2:F:1268:ARG:NH1  | 2.43                     | 0.52              |
| 2:F:1309:THR:HG23 | 2:F:1367:GLN:CG   | 2.38                     | 0.52              |
| 2:B:967:ASN:ND2   | 2:B:968:HIS:ND1   | 2.57                     | 0.52              |
| 2:B:993:TYR:HD1   | 2:B:1000:SER:HB2  | 1.75                     | 0.52              |
| 1:C:354:ASN:C     | 1:C:354:ASN:OD1   | 2.53                     | 0.52              |
| 1:A:354:ASN:C     | 1:A:354:ASN:OD1   | 2.53                     | 0.52              |
| 2:B:1225:VAL:HG13 | 2:B:1236:LEU:HB2  | 1.90                     | 0.52              |
| 2:D:967:ASN:ND2   | 2:D:968:HIS:ND1   | 2.57                     | 0.52              |
| 2:D:1181:TYR:CG   | 2:D:1182:PRO:HA   | 2.44                     | 0.52              |
| 2:D:1035:PHE:HD1  | 2:D:1035:PHE:C    | 2.17                     | 0.52              |
| 2:D:1177:ILE:CG2  | 2:D:1181:TYR:HB3  | 2.40                     | 0.52              |
| 1:E:146:ASN:ND2   | 1:E:149:ALA:HB2   | 2.24                     | 0.52              |
| 1:E:337:VAL:CG2   | 5:E:2001:NAG:O7   | 2.55                     | 0.52              |
| 2:B:1328:GLU:HG3  | 2:B:1336:ASP:OD2  | 2.10                     | 0.52              |
| 2:D:1209:ASP:OD2  | 2:D:1268:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:146:ASN:ND2   | 1:A:149:ALA:HB2   | 2.24                     | 0.52              |
| 2:B:1256:PHE:O    | 2:B:1257:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:362:THR:CG2   | 1:A:371:SER:CB    | 2.83                     | 0.52              |
| 2:B:1073:GLU:HB2  | 2:B:1144:LYS:HD3  | 1.90                     | 0.52              |
| 5:C:2001:NAG:H83  | 5:C:2001:NAG:O3   | 2.09                     | 0.52              |
| 2:F:1310:ILE:HD13 | 2:F:1386:TRP:CD2  | 2.45                     | 0.52              |
| 1:C:120:TRP:O     | 1:C:156:ARG:NH1   | 2.43                     | 0.51              |
| 2:D:1092:ASN:OD1  | 3:K:1:NAG:N2      | 2.43                     | 0.51              |
| 1:E:354:ASN:OD1   | 1:E:354:ASN:C     | 2.53                     | 0.51              |
| 2:D:1328:GLU:HG3  | 2:D:1336:ASP:OD2  | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:326:GLU:HG2   | 1:A:326:GLU:O     | 2.09                     | 0.51              |
| 2:B:1092:ASN:OD1  | 3:H:1:NAG:N2      | 2.43                     | 0.51              |
| 1:C:175:MET:HE1   | 1:C:280:TYR:HE2   | 1.74                     | 0.51              |
| 2:F:1328:GLU:HG3  | 2:F:1336:ASP:OD2  | 2.10                     | 0.51              |
| 2:B:1045:ALA:C    | 2:B:1047:ALA:H    | 2.19                     | 0.51              |
| 2:B:1177:ILE:CG2  | 2:B:1181:TYR:HB3  | 2.40                     | 0.51              |
| 2:F:988:ASP:O     | 2:F:989:TYR:HB3   | 2.11                     | 0.51              |
| 1:C:219:ILE:HG13  | 1:C:252:MET:HE2   | 1.92                     | 0.51              |
| 2:F:1244:LYS:O    | 2:F:1244:LYS:HG2  | 2.09                     | 0.51              |
| 1:A:120:TRP:O     | 1:A:156:ARG:NH1   | 2.43                     | 0.51              |
| 1:E:36:VAL:O      | 1:E:39:ILE:HG12   | 2.11                     | 0.51              |
| 1:E:120:TRP:O     | 1:E:156:ARG:NH1   | 2.43                     | 0.51              |
| 2:F:1045:ALA:C    | 2:F:1047:ALA:H    | 2.19                     | 0.51              |
| 2:F:1092:ASN:OD1  | 3:N:1:NAG:N2      | 2.43                     | 0.51              |
| 2:B:1161:SER:O    | 2:B:1162:SER:HB2  | 2.11                     | 0.51              |
| 2:D:1256:PHE:O    | 2:D:1257:ILE:HG13 | 2.10                     | 0.51              |
| 2:F:993:TYR:HD1   | 2:F:1000:SER:HB2  | 1.74                     | 0.51              |
| 2:F:999:THR:CG2   | 2:F:1000:SER:H    | 2.21                     | 0.51              |
| 1:A:219:ILE:HG13  | 1:A:252:MET:HE2   | 1.92                     | 0.51              |
| 2:B:1035:PHE:HD1  | 2:B:1035:PHE:C    | 2.17                     | 0.51              |
| 2:B:1310:ILE:HD13 | 2:B:1386:TRP:CD2  | 2.45                     | 0.51              |
| 2:D:1208:LYS:O    | 2:D:1209:ASP:HB2  | 2.11                     | 0.51              |
| 1:E:312:ILE:HG22  | 1:E:313:THR:N     | 2.26                     | 0.51              |
| 6:E:2007:B12:O39  | 6:E:2007:B12:C8   | 2.59                     | 0.51              |
| 2:F:1161:SER:O    | 2:F:1162:SER:HB2  | 2.11                     | 0.51              |
| 1:C:133:TYR:HE1   | 6:C:2007:B12:H1P1 | 1.75                     | 0.51              |
| 1:C:207:VAL:CG2   | 1:C:236:THR:HG21  | 2.41                     | 0.51              |
| 2:D:1161:SER:O    | 2:D:1162:SER:HB2  | 2.11                     | 0.51              |
| 1:A:133:TYR:HE1   | 6:A:2007:B12:H1P1 | 1.75                     | 0.51              |
| 1:A:207:VAL:CG2   | 1:A:236:THR:HG21  | 2.41                     | 0.51              |
| 1:A:405:PHE:CD1   | 1:A:408:GLU:HB2   | 2.46                     | 0.51              |
| 1:C:29:PRO:HB2    | 1:C:32:GLN:HG3    | 1.93                     | 0.51              |
| 2:F:1162:SER:C    | 2:F:1164:GLY:H    | 2.18                     | 0.51              |
| 2:F:1177:ILE:CG2  | 2:F:1181:TYR:HB3  | 2.40                     | 0.51              |
| 2:B:1029:ASP:OD1  | 2:B:1029:ASP:N    | 2.42                     | 0.50              |
| 1:C:312:ILE:HG21  | 1:C:406:ASN:CA    | 2.35                     | 0.50              |
| 2:D:1088:VAL:HG13 | 2:D:1132:ILE:HB   | 1.93                     | 0.50              |
| 2:B:1192:TYR:HE1  | 2:B:1258:LYS:CD   | 2.24                     | 0.50              |
| 2:B:1332:ASN:ND2  | 5:B:2013:NAG:C6   | 2.74                     | 0.50              |
| 1:C:405:PHE:CD1   | 1:C:408:GLU:HB2   | 2.46                     | 0.50              |
| 2:D:1192:TYR:HE1  | 2:D:1258:LYS:CD   | 2.24                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:36:VAL:O      | 1:A:39:ILE:HG12   | 2.11                     | 0.50              |
| 1:A:310:SER:CB    | 2:F:1150:THR:HB   | 2.41                     | 0.50              |
| 2:B:988:ASP:O     | 2:B:989:TYR:HB3   | 2.11                     | 0.50              |
| 2:D:1045:ALA:C    | 2:D:1047:ALA:H    | 2.19                     | 0.50              |
| 1:E:90:GLY:HA3    | 6:E:2007:B12:H3P3 | 1.93                     | 0.50              |
| 1:A:312:ILE:HG21  | 1:A:406:ASN:CA    | 2.35                     | 0.50              |
| 2:B:1331:ILE:O    | 2:B:1331:ILE:HG22 | 2.12                     | 0.50              |
| 2:D:1218:CYS:O    | 2:D:1219:THR:CB   | 2.59                     | 0.50              |
| 2:B:971:HIS:O     | 2:B:1039:TYR:HA   | 2.12                     | 0.50              |
| 1:C:36:VAL:O      | 1:C:39:ILE:HG12   | 2.11                     | 0.50              |
| 1:C:90:GLY:HA3    | 6:C:2007:B12:H3P3 | 1.93                     | 0.50              |
| 2:D:1296:TYR:CD2  | 2:D:1297:PRO:CA   | 2.95                     | 0.50              |
| 1:E:405:PHE:CD1   | 1:E:408:GLU:HB2   | 2.46                     | 0.50              |
| 2:F:956:ILE:HG22  | 2:F:957:ASN:H     | 1.77                     | 0.50              |
| 2:B:1338:LEU:C    | 2:B:1338:LEU:HD23 | 2.37                     | 0.50              |
| 1:C:374:ASN:O     | 1:C:375:ASN:HB2   | 2.11                     | 0.50              |
| 2:D:1310:ILE:HD13 | 2:D:1386:TRP:CD2  | 2.45                     | 0.50              |
| 2:D:1338:LEU:C    | 2:D:1338:LEU:HD23 | 2.37                     | 0.50              |
| 1:E:133:TYR:HE1   | 6:E:2007:B12:H1P1 | 1.76                     | 0.50              |
| 1:E:207:VAL:CG2   | 1:E:236:THR:HG21  | 2.41                     | 0.50              |
| 1:E:374:ASN:O     | 1:E:375:ASN:HB2   | 2.11                     | 0.50              |
| 2:F:980:GLU:OE1   | 2:F:1030:LEU:HB2  | 2.12                     | 0.50              |
| 2:F:1281:VAL:CG2  | 2:F:1308:TRP:CD1  | 2.95                     | 0.50              |
| 1:A:374:ASN:O     | 1:A:375:ASN:HB2   | 2.11                     | 0.50              |
| 2:B:1162:SER:C    | 2:B:1164:GLY:H    | 2.19                     | 0.50              |
| 2:B:1337:TYR:O    | 2:B:1370:LEU:HD12 | 2.11                     | 0.50              |
| 6:C:2007:B12:O39  | 6:C:2007:B12:C8   | 2.59                     | 0.50              |
| 1:E:219:ILE:HG13  | 1:E:252:MET:HE2   | 1.92                     | 0.50              |
| 2:F:1037:ILE:HG12 | 2:F:1037:ILE:O    | 2.11                     | 0.50              |
| 2:B:980:GLU:OE1   | 2:B:1030:LEU:HB2  | 2.12                     | 0.50              |
| 2:B:1037:ILE:O    | 2:B:1037:ILE:HG12 | 2.11                     | 0.50              |
| 1:C:89:ILE:HG23   | 1:C:138:ALA:HB2   | 1.93                     | 0.50              |
| 1:E:309:ALA:HB1   | 1:E:338:LYS:HG3   | 1.94                     | 0.50              |
| 2:F:1192:TYR:HE1  | 2:F:1258:LYS:CD   | 2.24                     | 0.50              |
| 2:F:1237:THR:CG2  | 2:F:1239:LEU:HD13 | 2.42                     | 0.50              |
| 2:D:988:ASP:O     | 2:D:989:TYR:HB3   | 2.11                     | 0.50              |
| 2:D:1162:SER:C    | 2:D:1164:GLY:H    | 2.19                     | 0.50              |
| 2:D:1237:THR:CG2  | 2:D:1239:LEU:HD13 | 2.42                     | 0.50              |
| 2:D:1331:ILE:O    | 2:D:1331:ILE:HG22 | 2.12                     | 0.50              |
| 1:E:89:ILE:HG23   | 1:E:138:ALA:HB2   | 1.93                     | 0.50              |
| 2:F:968:HIS:O     | 2:F:969:LEU:HD12  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1338:LEU:C    | 2:F:1338:LEU:HD23 | 2.37                     | 0.50              |
| 2:B:1332:ASN:ND2  | 5:B:2013:NAG:H62  | 2.27                     | 0.49              |
| 1:C:88:THR:O      | 1:C:91:HIS:HB2    | 2.12                     | 0.49              |
| 1:C:124:SER:HB2   | 1:C:126:ASN:OD1   | 2.12                     | 0.49              |
| 2:D:971:HIS:O     | 2:D:1039:TYR:HA   | 2.12                     | 0.49              |
| 2:D:1037:ILE:HG12 | 2:D:1037:ILE:O    | 2.11                     | 0.49              |
| 2:D:1281:VAL:HG21 | 2:D:1308:TRP:HD1  | 1.77                     | 0.49              |
| 1:E:29:PRO:HB2    | 1:E:32:GLN:HG3    | 1.92                     | 0.49              |
| 2:F:1222:TYR:N    | 2:F:1222:TYR:CD2  | 2.80                     | 0.49              |
| 2:B:968:HIS:O     | 2:B:969:LEU:HD12  | 2.12                     | 0.49              |
| 2:B:1088:VAL:HG13 | 2:B:1132:ILE:HB   | 1.93                     | 0.49              |
| 2:B:1093:PHE:CD2  | 2:B:1093:PHE:C    | 2.91                     | 0.49              |
| 2:B:1296:TYR:CD2  | 2:B:1297:PRO:CA   | 2.95                     | 0.49              |
| 2:D:956:ILE:HG22  | 2:D:957:ASN:H     | 1.77                     | 0.49              |
| 1:E:124:SER:HB2   | 1:E:126:ASN:OD1   | 2.12                     | 0.49              |
| 1:A:29:PRO:HB2    | 1:A:32:GLN:HG3    | 1.92                     | 0.49              |
| 1:A:89:ILE:HG23   | 1:A:138:ALA:HB2   | 1.93                     | 0.49              |
| 1:A:124:SER:HB2   | 1:A:126:ASN:OD1   | 2.12                     | 0.49              |
| 2:D:1093:PHE:C    | 2:D:1093:PHE:CD2  | 2.90                     | 0.49              |
| 2:D:1302:GLU:O    | 2:D:1303:ASN:HB2  | 2.11                     | 0.49              |
| 2:B:1222:TYR:CD2  | 2:B:1222:TYR:N    | 2.80                     | 0.49              |
| 2:B:1237:THR:CG2  | 2:B:1239:LEU:HD13 | 2.42                     | 0.49              |
| 2:D:1332:ASN:ND2  | 5:D:2013:NAG:C6   | 2.76                     | 0.49              |
| 2:F:1029:ASP:OD1  | 2:F:1029:ASP:N    | 2.43                     | 0.49              |
| 2:F:1079:THR:HG23 | 2:F:1138:LYS:CG   | 2.23                     | 0.49              |
| 2:F:1332:ASN:ND2  | 5:F:2013:NAG:C6   | 2.75                     | 0.49              |
| 2:F:1332:ASN:ND2  | 5:F:2013:NAG:H62  | 2.28                     | 0.49              |
| 1:A:88:THR:O      | 1:A:91:HIS:HB2    | 2.12                     | 0.49              |
| 2:B:1218:CYS:O    | 2:B:1219:THR:CB   | 2.59                     | 0.49              |
| 2:B:1302:GLU:O    | 2:B:1303:ASN:HB2  | 2.12                     | 0.49              |
| 2:D:968:HIS:O     | 2:D:969:LEU:HD12  | 2.12                     | 0.49              |
| 1:E:283:VAL:HG12  | 1:E:284:PRO:HD3   | 1.94                     | 0.49              |
| 2:F:1337:TYR:O    | 2:F:1370:LEU:HD12 | 2.11                     | 0.49              |
| 1:A:90:GLY:HA3    | 6:A:2007:B12:H3P3 | 1.93                     | 0.49              |
| 1:A:309:ALA:HB1   | 1:A:338:LYS:HG3   | 1.94                     | 0.49              |
| 2:D:1337:TYR:O    | 2:D:1370:LEU:HD12 | 2.11                     | 0.49              |
| 1:E:88:THR:O      | 1:E:91:HIS:HB2    | 2.12                     | 0.49              |
| 2:F:1218:CYS:O    | 2:F:1219:THR:CB   | 2.59                     | 0.49              |
| 1:C:351:GLN:OE1   | 1:C:358:LYS:HG3   | 2.13                     | 0.49              |
| 2:D:1281:VAL:CG2  | 2:D:1308:TRP:CD1  | 2.95                     | 0.49              |
| 2:D:1309:THR:HG23 | 2:D:1367:GLN:CG   | 2.38                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:971:HIS:O     | 2:F:1039:TYR:HA   | 2.12                     | 0.49              |
| 2:F:1296:TYR:CD2  | 2:F:1297:PRO:CA   | 2.95                     | 0.49              |
| 2:B:1281:VAL:CG2  | 2:B:1308:TRP:CD1  | 2.95                     | 0.49              |
| 2:F:1008:SER:HB2  | 2:F:1183:MET:SD   | 2.53                     | 0.49              |
| 2:F:1237:THR:HG22 | 2:F:1239:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:351:GLN:OE1   | 1:A:358:LYS:HG3   | 2.13                     | 0.49              |
| 6:C:2007:B12:H302 | 6:C:2007:B12:H253 | 1.54                     | 0.49              |
| 2:F:1088:VAL:HG13 | 2:F:1132:ILE:HB   | 1.93                     | 0.49              |
| 2:F:1093:PHE:C    | 2:F:1093:PHE:CD2  | 2.90                     | 0.49              |
| 2:F:1281:VAL:HG21 | 2:F:1308:TRP:HD1  | 1.77                     | 0.49              |
| 2:B:1176:PHE:HD2  | 2:B:1193:TRP:CE3  | 2.31                     | 0.49              |
| 2:B:1185:TYR:CZ   | 2:B:1266:GLN:HA   | 2.48                     | 0.49              |
| 2:D:980:GLU:OE1   | 2:D:1030:LEU:HB2  | 2.12                     | 0.49              |
| 2:D:1008:SER:HB2  | 2:D:1183:MET:SD   | 2.53                     | 0.49              |
| 2:B:1008:SER:HB2  | 2:B:1183:MET:SD   | 2.53                     | 0.48              |
| 6:C:2007:B12:H312 | 6:C:2007:B12:C35  | 2.34                     | 0.48              |
| 2:D:1185:TYR:CZ   | 2:D:1266:GLN:HA   | 2.48                     | 0.48              |
| 1:E:351:GLN:OE1   | 1:E:358:LYS:HG3   | 2.12                     | 0.48              |
| 2:F:1304:GLN:HB2  | 2:F:1372:THR:CG2  | 2.43                     | 0.48              |
| 2:B:1281:VAL:HG21 | 2:B:1308:TRP:HD1  | 1.77                     | 0.48              |
| 1:C:148:GLU:HG3   | 1:C:188:PRO:CG    | 2.43                     | 0.48              |
| 1:C:228:LEU:O     | 1:C:231:GLN:HB2   | 2.13                     | 0.48              |
| 2:D:1237:THR:HG22 | 2:D:1239:LEU:HD13 | 1.94                     | 0.48              |
| 1:E:312:ILE:HG21  | 1:E:406:ASN:CA    | 2.35                     | 0.48              |
| 2:F:1004:TYR:CG   | 2:F:1009:ILE:HD12 | 2.48                     | 0.48              |
| 2:F:1185:TYR:CZ   | 2:F:1266:GLN:HA   | 2.48                     | 0.48              |
| 2:F:1302:GLU:O    | 2:F:1303:ASN:HB2  | 2.12                     | 0.48              |
| 1:A:283:VAL:HG12  | 1:A:284:PRO:HD3   | 1.94                     | 0.48              |
| 2:D:1093:PHE:HB3  | 2:D:1128:LEU:HD23 | 1.95                     | 0.48              |
| 2:D:1192:TYR:HE1  | 2:D:1258:LYS:HG3  | 1.78                     | 0.48              |
| 1:E:148:GLU:HG3   | 1:E:188:PRO:CG    | 2.43                     | 0.48              |
| 2:F:1192:TYR:HE1  | 2:F:1258:LYS:HG3  | 1.78                     | 0.48              |
| 2:B:1004:TYR:CG   | 2:B:1009:ILE:HD12 | 2.48                     | 0.48              |
| 2:B:1237:THR:HG22 | 2:B:1239:LEU:HD13 | 1.94                     | 0.48              |
| 2:B:1304:GLN:HB2  | 2:B:1372:THR:CG2  | 2.43                     | 0.48              |
| 1:C:133:TYR:CE1   | 6:C:2007:B12:H1P1 | 2.48                     | 0.48              |
| 2:D:1222:TYR:N    | 2:D:1222:TYR:CD2  | 2.80                     | 0.48              |
| 6:A:2007:B12:O39  | 6:A:2007:B12:C8   | 2.59                     | 0.48              |
| 2:B:1093:PHE:HB3  | 2:B:1128:LEU:HD23 | 1.96                     | 0.48              |
| 1:C:312:ILE:HG22  | 1:C:313:THR:N     | 2.27                     | 0.48              |
| 2:D:1337:TYR:OH   | 2:D:1371:LEU:HD22 | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:133:TYR:CE1   | 6:E:2007:B12:H1P1 | 2.49                     | 0.48              |
| 2:F:1067:ASN:HB3  | 2:F:1150:THR:HG21 | 1.91                     | 0.48              |
| 2:F:1093:PHE:HB3  | 2:F:1128:LEU:HD23 | 1.96                     | 0.48              |
| 2:F:1197:SER:OG   | 2:F:1198:SER:N    | 2.42                     | 0.48              |
| 2:B:956:ILE:HG22  | 2:B:957:ASN:H     | 1.77                     | 0.48              |
| 1:C:309:ALA:HB1   | 1:C:338:LYS:HG3   | 1.94                     | 0.48              |
| 1:E:255:ASN:O     | 1:E:259:GLN:HG2   | 2.13                     | 0.48              |
| 2:F:1176:PHE:HD2  | 2:F:1193:TRP:CE3  | 2.31                     | 0.48              |
| 2:F:1218:CYS:O    | 2:F:1219:THR:HB   | 2.13                     | 0.48              |
| 2:F:1331:ILE:HG22 | 2:F:1331:ILE:O    | 2.12                     | 0.48              |
| 2:F:1337:TYR:OH   | 2:F:1371:LEU:HD22 | 2.14                     | 0.48              |
| 2:B:1337:TYR:OH   | 2:B:1371:LEU:HD22 | 2.14                     | 0.48              |
| 1:C:255:ASN:O     | 1:C:259:GLN:HG2   | 2.13                     | 0.48              |
| 1:C:283:VAL:HG12  | 1:C:284:PRO:HD3   | 1.94                     | 0.48              |
| 3:H:2:NAG:O3      | 3:H:5:MAN:H3      | 2.14                     | 0.48              |
| 1:A:148:GLU:HG3   | 1:A:188:PRO:CG    | 2.43                     | 0.48              |
| 2:D:1004:TYR:CG   | 2:D:1009:ILE:HD12 | 2.48                     | 0.48              |
| 2:D:1218:CYS:O    | 2:D:1219:THR:HB   | 2.13                     | 0.48              |
| 2:F:981:PHE:CD1   | 2:F:982:HIS:N     | 2.82                     | 0.48              |
| 2:F:1004:TYR:CD1  | 2:F:1009:ILE:HD12 | 2.49                     | 0.48              |
| 2:F:1310:ILE:HB   | 2:F:1366:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:133:TYR:CE1   | 6:A:2007:B12:H1P1 | 2.48                     | 0.48              |
| 1:A:255:ASN:O     | 1:A:259:GLN:HG2   | 2.13                     | 0.48              |
| 2:D:947:GLY:HA3   | 2:D:951:VAL:O     | 2.14                     | 0.48              |
| 2:D:1387:PHE:C    | 2:D:1388:VAL:CG2  | 2.87                     | 0.48              |
| 2:F:1387:PHE:C    | 2:F:1388:VAL:CG2  | 2.87                     | 0.48              |
| 1:A:228:LEU:O     | 1:A:231:GLN:HB2   | 2.13                     | 0.48              |
| 2:B:1218:CYS:O    | 2:B:1219:THR:HB   | 2.13                     | 0.48              |
| 2:D:1304:GLN:HB2  | 2:D:1372:THR:CG2  | 2.43                     | 0.48              |
| 2:D:1310:ILE:HB   | 2:D:1366:LEU:HD12 | 1.96                     | 0.48              |
| 1:E:362:THR:HG22  | 1:E:371:SER:CB    | 2.35                     | 0.48              |
| 3:G:3:BMA:H4      | 3:G:5:MAN:C2      | 2.41                     | 0.48              |
| 2:B:1067:ASN:HB3  | 2:B:1150:THR:HG21 | 1.91                     | 0.47              |
| 2:B:1109:ILE:HD12 | 2:B:1123:PHE:CE2  | 2.49                     | 0.47              |
| 2:B:1193:TRP:N    | 2:B:1193:TRP:CD1  | 2.82                     | 0.47              |
| 2:D:1304:GLN:H    | 2:D:1372:THR:CG2  | 2.24                     | 0.47              |
| 3:K:2:NAG:O3      | 3:K:5:MAN:H3      | 2.14                     | 0.47              |
| 2:B:1004:TYR:CD1  | 2:B:1009:ILE:HD12 | 2.49                     | 0.47              |
| 2:B:1187:HIS:HB3  | 2:B:1266:GLN:HE22 | 1.78                     | 0.47              |
| 1:E:175:MET:HE1   | 1:E:280:TYR:CE2   | 2.49                     | 0.47              |
| 1:E:336:SER:O     | 1:E:337:VAL:C     | 2.58                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1092:ASN:OD1  | 3:N:1:NAG:C2      | 2.61                     | 0.47              |
| 2:F:1187:HIS:CB   | 2:F:1266:GLN:NE2  | 2.75                     | 0.47              |
| 2:F:1193:TRP:CD1  | 2:F:1193:TRP:N    | 2.82                     | 0.47              |
| 2:B:1192:TYR:HE1  | 2:B:1258:LYS:HG3  | 1.78                     | 0.47              |
| 2:B:1387:PHE:C    | 2:B:1388:VAL:CG2  | 2.87                     | 0.47              |
| 2:D:1004:TYR:CD1  | 2:D:1009:ILE:HD12 | 2.49                     | 0.47              |
| 1:E:228:LEU:O     | 1:E:231:GLN:HB2   | 2.13                     | 0.47              |
| 2:B:947:GLY:HA3   | 2:B:951:VAL:O     | 2.14                     | 0.47              |
| 2:B:1092:ASN:OD1  | 3:H:1:NAG:C2      | 2.61                     | 0.47              |
| 2:B:1179:PRO:C    | 2:B:1181:TYR:H    | 2.22                     | 0.47              |
| 2:B:1294:ILE:HG13 | 2:B:1295:GLY:H    | 1.79                     | 0.47              |
| 2:B:1310:ILE:HB   | 2:B:1366:LEU:HD12 | 1.96                     | 0.47              |
| 2:D:1294:ILE:HG13 | 2:D:1295:GLY:H    | 1.79                     | 0.47              |
| 1:E:389:LEU:N     | 1:E:389:LEU:CD2   | 2.76                     | 0.47              |
| 2:F:1179:PRO:C    | 2:F:1181:TYR:H    | 2.22                     | 0.47              |
| 2:F:1379:GLU:H    | 2:F:1379:GLU:CD   | 2.23                     | 0.47              |
| 1:A:312:ILE:HG22  | 1:A:313:THR:N     | 2.27                     | 0.47              |
| 1:A:389:LEU:N     | 1:A:389:LEU:CD2   | 2.76                     | 0.47              |
| 2:B:1128:LEU:HD23 | 2:B:1128:LEU:HA   | 1.65                     | 0.47              |
| 2:B:1314:THR:HG22 | 2:B:1315:GLY:N    | 2.29                     | 0.47              |
| 1:C:389:LEU:N     | 1:C:389:LEU:CD2   | 2.76                     | 0.47              |
| 2:D:981:PHE:CD1   | 2:D:982:HIS:N     | 2.82                     | 0.47              |
| 2:D:1176:PHE:HD2  | 2:D:1193:TRP:CE3  | 2.31                     | 0.47              |
| 2:D:1225:VAL:HG23 | 2:D:1257:ILE:HG12 | 1.96                     | 0.47              |
| 2:B:981:PHE:CD1   | 2:B:982:HIS:N     | 2.82                     | 0.47              |
| 1:C:336:SER:O     | 1:C:337:VAL:C     | 2.58                     | 0.47              |
| 2:D:1179:PRO:C    | 2:D:1181:TYR:H    | 2.22                     | 0.47              |
| 2:D:1193:TRP:CD1  | 2:D:1193:TRP:N    | 2.82                     | 0.47              |
| 1:E:287:THR:HG22  | 1:E:288:CYS:N     | 2.29                     | 0.47              |
| 1:E:337:VAL:C     | 1:E:338:LYS:O     | 2.57                     | 0.47              |
| 2:F:1294:ILE:HG13 | 2:F:1295:GLY:H    | 1.79                     | 0.47              |
| 1:A:175:MET:HE1   | 1:A:280:TYR:CE2   | 2.49                     | 0.47              |
| 2:B:1225:VAL:HG23 | 2:B:1257:ILE:HG12 | 1.96                     | 0.47              |
| 2:B:1379:GLU:CD   | 2:B:1379:GLU:H    | 2.23                     | 0.47              |
| 1:C:320:ASN:O     | 1:C:327:LEU:HB2   | 2.15                     | 0.47              |
| 2:D:1109:ILE:HD12 | 2:D:1123:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:135:PRO:O     | 1:E:139:ILE:HG13  | 2.14                     | 0.47              |
| 2:F:947:GLY:HA3   | 2:F:951:VAL:O     | 2.14                     | 0.47              |
| 2:F:1060:THR:HG21 | 2:F:1064:PHE:HB3  | 1.96                     | 0.47              |
| 2:F:1314:THR:HG22 | 2:F:1315:GLY:N    | 2.29                     | 0.47              |
| 1:A:320:ASN:O     | 1:A:327:LEU:HB2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:175:MET:HE1   | 1:C:280:TYR:CE2   | 2.49                     | 0.47              |
| 1:C:287:THR:HG22  | 1:C:288:CYS:N     | 2.29                     | 0.47              |
| 2:D:1060:THR:HG21 | 2:D:1064:PHE:HB3  | 1.96                     | 0.47              |
| 3:N:2:NAG:O3      | 3:N:5:MAN:H3      | 2.14                     | 0.47              |
| 1:A:318:ILE:O     | 1:A:318:ILE:CG1   | 2.63                     | 0.47              |
| 2:B:1140:TRP:O    | 2:B:1141:LEU:HD23 | 2.15                     | 0.47              |
| 2:B:1208:LYS:O    | 2:B:1209:ASP:HB2  | 2.13                     | 0.47              |
| 1:C:318:ILE:O     | 1:C:318:ILE:CG1   | 2.63                     | 0.47              |
| 2:D:1067:ASN:ND2  | 2:D:1150:THR:HG22 | 2.29                     | 0.47              |
| 2:D:1068:TYR:CD1  | 2:D:1068:TYR:C    | 2.93                     | 0.47              |
| 2:D:1140:TRP:O    | 2:D:1141:LEU:HD23 | 2.15                     | 0.47              |
| 2:D:1229:PRO:HG3  | 2:D:1254:SER:OG   | 2.15                     | 0.47              |
| 1:A:336:SER:O     | 1:A:337:VAL:C     | 2.58                     | 0.47              |
| 1:C:117:MET:HE2   | 1:C:138:ALA:CB    | 2.45                     | 0.47              |
| 1:C:135:PRO:O     | 1:C:139:ILE:HG13  | 2.14                     | 0.47              |
| 1:E:117:MET:HE2   | 1:E:138:ALA:CB    | 2.45                     | 0.47              |
| 1:A:279:THR:C     | 1:A:281:LEU:H     | 2.23                     | 0.46              |
| 6:A:2007:B12:H312 | 6:A:2007:B12:C35  | 2.34                     | 0.46              |
| 1:C:279:THR:C     | 1:C:281:LEU:H     | 2.23                     | 0.46              |
| 1:E:308:SER:O     | 1:E:309:ALA:CB    | 2.64                     | 0.46              |
| 2:F:1068:TYR:CD1  | 2:F:1068:TYR:C    | 2.93                     | 0.46              |
| 2:F:1140:TRP:O    | 2:F:1141:LEU:HD23 | 2.15                     | 0.46              |
| 1:A:135:PRO:O     | 1:A:139:ILE:HG13  | 2.14                     | 0.46              |
| 1:C:36:VAL:C      | 1:C:38:GLY:N      | 2.73                     | 0.46              |
| 2:D:1314:THR:HG22 | 2:D:1315:GLY:N    | 2.29                     | 0.46              |
| 2:D:1332:ASN:ND2  | 5:D:2013:NAG:H62  | 2.30                     | 0.46              |
| 1:E:318:ILE:O     | 1:E:318:ILE:CG1   | 2.63                     | 0.46              |
| 2:F:974:PHE:O     | 2:F:975:GLU:C     | 2.57                     | 0.46              |
| 3:M:3:BMA:H4      | 3:M:5:MAN:C2      | 2.41                     | 0.46              |
| 2:D:974:PHE:O     | 2:D:975:GLU:C     | 2.57                     | 0.46              |
| 1:E:354:ASN:HA    | 1:E:355:PRO:HD3   | 1.71                     | 0.46              |
| 2:F:1061:SER:HB3  | 2:F:1154:PHE:CD2  | 2.51                     | 0.46              |
| 2:F:1109:ILE:HD12 | 2:F:1123:PHE:CE2  | 2.49                     | 0.46              |
| 1:A:117:MET:HE2   | 1:A:138:ALA:CB    | 2.45                     | 0.46              |
| 2:D:1215:HIS:HB2  | 2:D:1220:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:283:VAL:O     | 1:E:286:VAL:HG23  | 2.16                     | 0.46              |
| 1:E:320:ASN:O     | 1:E:327:LEU:HB2   | 2.15                     | 0.46              |
| 2:F:1225:VAL:HG23 | 2:F:1257:ILE:HG12 | 1.96                     | 0.46              |
| 4:L:1:NAG:H2      | 4:L:1:NAG:H82     | 1.65                     | 0.46              |
| 1:A:283:VAL:O     | 1:A:286:VAL:HG23  | 2.16                     | 0.46              |
| 1:A:287:THR:HG22  | 1:A:288:CYS:N     | 2.29                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:974:PHE:O     | 2:B:975:GLU:C     | 2.57                     | 0.46              |
| 2:B:982:HIS:CD2   | 2:B:987:ASN:HB2   | 2.51                     | 0.46              |
| 2:B:1061:SER:HB3  | 2:B:1154:PHE:CD2  | 2.51                     | 0.46              |
| 2:B:1217:ASN:HB2  | 5:B:2008:NAG:H61  | 1.98                     | 0.46              |
| 1:E:228:LEU:HD23  | 1:E:228:LEU:HA    | 1.66                     | 0.46              |
| 1:E:279:THR:C     | 1:E:281:LEU:H     | 2.23                     | 0.46              |
| 2:F:1084:GLN:HG2  | 2:F:1161:SER:CA   | 2.46                     | 0.46              |
| 2:D:1081:ARG:NH2  | 2:D:1084:GLN:HE22 | 2.14                     | 0.46              |
| 2:F:952:TYR:HA    | 2:F:953:PRO:HD3   | 1.78                     | 0.46              |
| 2:B:1067:ASN:ND2  | 2:B:1150:THR:HG22 | 2.29                     | 0.46              |
| 2:B:1068:TYR:C    | 2:B:1068:TYR:CD1  | 2.93                     | 0.46              |
| 2:B:1176:PHE:N    | 2:B:1176:PHE:CD1  | 2.84                     | 0.46              |
| 2:B:1187:HIS:CB   | 2:B:1266:GLN:NE2  | 2.75                     | 0.46              |
| 2:B:1243:GLU:O    | 2:B:1245:PRO:HD3  | 2.16                     | 0.46              |
| 1:C:308:SER:O     | 1:C:309:ALA:CB    | 2.64                     | 0.46              |
| 1:C:339:SER:C     | 1:C:341:SER:N     | 2.74                     | 0.46              |
| 2:F:982:HIS:CD2   | 2:F:987:ASN:HB2   | 2.51                     | 0.46              |
| 2:F:1067:ASN:ND2  | 2:F:1150:THR:HG22 | 2.30                     | 0.46              |
| 2:F:1215:HIS:HB2  | 2:F:1220:LEU:CD1  | 2.45                     | 0.46              |
| 2:F:1229:PRO:HG3  | 2:F:1254:SER:OG   | 2.15                     | 0.46              |
| 1:A:403:ILE:HA    | 1:A:404:PRO:HD3   | 1.70                     | 0.46              |
| 2:B:1215:HIS:HB2  | 2:B:1220:LEU:CD1  | 2.45                     | 0.46              |
| 2:B:1229:PRO:HG3  | 2:B:1254:SER:OG   | 2.15                     | 0.46              |
| 1:C:198:LEU:HD22  | 1:C:198:LEU:C     | 2.41                     | 0.46              |
| 1:C:281:LEU:HD23  | 1:C:281:LEU:HA    | 1.80                     | 0.46              |
| 2:D:1187:HIS:HB3  | 2:D:1266:GLN:HE22 | 1.78                     | 0.46              |
| 6:E:2007:B12:H312 | 6:E:2007:B12:C35  | 2.35                     | 0.46              |
| 2:F:1178:SER:HB3  | 2:F:1270:PHE:CE2  | 2.51                     | 0.46              |
| 2:F:1205:LEU:HB2  | 2:F:1248:ILE:HB   | 1.98                     | 0.46              |
| 3:M:3:BMA:C4      | 3:M:5:MAN:H2      | 2.42                     | 0.46              |
| 2:B:1081:ARG:NH2  | 2:B:1084:GLN:HE22 | 2.14                     | 0.46              |
| 1:C:198:LEU:C     | 1:C:198:LEU:CD2   | 2.89                     | 0.46              |
| 1:C:283:VAL:O     | 1:C:286:VAL:HG23  | 2.16                     | 0.46              |
| 2:D:1061:SER:HB3  | 2:D:1154:PHE:CD2  | 2.51                     | 0.46              |
| 2:D:1092:ASN:OD1  | 3:K:1:NAG:C2      | 2.61                     | 0.46              |
| 2:D:1176:PHE:CD1  | 2:D:1176:PHE:N    | 2.84                     | 0.46              |
| 6:E:2007:B12:H302 | 6:E:2007:B12:H253 | 1.54                     | 0.46              |
| 2:B:1178:SER:HB3  | 2:B:1270:PHE:CE2  | 2.51                     | 0.45              |
| 1:C:180:LEU:HD12  | 1:C:180:LEU:HA    | 1.49                     | 0.45              |
| 1:C:279:THR:C     | 1:C:281:LEU:N     | 2.72                     | 0.45              |
| 2:D:1205:LEU:HB2  | 2:D:1248:ILE:HB   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1379:GLU:H    | 2:D:1379:GLU:CD   | 2.22                     | 0.45              |
| 2:F:1208:LYS:O    | 2:F:1209:ASP:HB2  | 2.14                     | 0.45              |
| 1:A:36:VAL:C      | 1:A:38:GLY:N      | 2.73                     | 0.45              |
| 1:A:308:SER:O     | 1:A:309:ALA:CB    | 2.64                     | 0.45              |
| 2:B:1084:GLN:HG2  | 2:B:1161:SER:CA   | 2.46                     | 0.45              |
| 1:C:215:LYS:C     | 1:C:217:ASN:N     | 2.73                     | 0.45              |
| 2:D:982:HIS:CD2   | 2:D:987:ASN:HB2   | 2.51                     | 0.45              |
| 1:E:36:VAL:C      | 1:E:38:GLY:N      | 2.73                     | 0.45              |
| 1:E:86:ASP:N      | 1:E:86:ASP:OD1    | 2.49                     | 0.45              |
| 1:E:198:LEU:C     | 1:E:198:LEU:HD22  | 2.41                     | 0.45              |
| 4:O:1:NAG:H82     | 4:O:1:NAG:H2      | 1.65                     | 0.45              |
| 2:B:1056:LEU:O    | 2:B:1158:TRP:CZ2  | 2.70                     | 0.45              |
| 2:D:948:HIS:HA    | 2:D:949:PRO:C     | 2.41                     | 0.45              |
| 2:D:1243:GLU:O    | 2:D:1245:PRO:HD3  | 2.16                     | 0.45              |
| 2:B:999:THR:CG2   | 2:B:1000:SER:N    | 2.78                     | 0.45              |
| 1:E:180:LEU:HA    | 1:E:180:LEU:HD12  | 1.49                     | 0.45              |
| 2:F:1081:ARG:NH2  | 2:F:1084:GLN:HE22 | 2.14                     | 0.45              |
| 2:F:1243:GLU:O    | 2:F:1245:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:170:VAL:O     | 1:A:171:ASP:C     | 2.59                     | 0.45              |
| 1:A:215:LYS:C     | 1:A:217:ASN:N     | 2.73                     | 0.45              |
| 1:A:335:VAL:CG2   | 5:A:2001:NAG:H5   | 2.46                     | 0.45              |
| 1:A:335:VAL:HG23  | 5:A:2001:NAG:H5   | 1.99                     | 0.45              |
| 2:B:947:GLY:O     | 2:B:948:HIS:C     | 2.60                     | 0.45              |
| 2:B:982:HIS:HB3   | 2:B:985:CYS:HA    | 1.98                     | 0.45              |
| 2:B:1196:LYS:HA   | 2:B:1203:PHE:HE1  | 1.82                     | 0.45              |
| 2:D:1056:LEU:O    | 2:D:1158:TRP:CZ2  | 2.70                     | 0.45              |
| 2:D:1067:ASN:HB3  | 2:D:1150:THR:HG21 | 1.91                     | 0.45              |
| 2:D:1260:ARG:HG2  | 2:D:1261:THR:N    | 2.31                     | 0.45              |
| 5:E:2001:NAG:C3   | 5:E:2001:NAG:H83  | 2.46                     | 0.45              |
| 2:F:1196:LYS:HA   | 2:F:1203:PHE:HE1  | 1.82                     | 0.45              |
| 2:B:952:TYR:HE1   | 2:B:988:ASP:OD2   | 2.00                     | 0.45              |
| 2:B:1060:THR:HG21 | 2:B:1064:PHE:HB3  | 1.96                     | 0.45              |
| 2:B:1169:LEU:HD12 | 2:B:1169:LEU:H    | 1.82                     | 0.45              |
| 2:B:1196:LYS:HA   | 2:B:1203:PHE:CE1  | 2.52                     | 0.45              |
| 2:B:1304:GLN:H    | 2:B:1372:THR:CG2  | 2.24                     | 0.45              |
| 2:D:1245:PRO:HA   | 2:D:1246:PRO:HD3  | 1.67                     | 0.45              |
| 1:E:363:MET:C     | 1:E:364:THR:CG2   | 2.90                     | 0.45              |
| 1:A:198:LEU:C     | 1:A:198:LEU:CD2   | 2.89                     | 0.45              |
| 1:A:362:THR:HG22  | 1:A:371:SER:CB    | 2.35                     | 0.45              |
| 2:B:1317:THR:O    | 2:B:1388:VAL:HA   | 2.17                     | 0.45              |
| 2:F:1169:LEU:HD12 | 2:F:1169:LEU:H    | 1.82                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:3:BMA:H4      | 3:J:5:MAN:C2     | 2.41                     | 0.45              |
| 1:A:94:LEU:HD13   | 1:A:94:LEU:HA    | 1.78                     | 0.45              |
| 1:A:198:LEU:C     | 1:A:198:LEU:HD22 | 2.41                     | 0.45              |
| 1:A:201:GLN:HE22  | 2:B:1147:GLN:HG2 | 1.82                     | 0.45              |
| 1:C:337:VAL:C     | 1:C:338:LYS:O    | 2.57                     | 0.45              |
| 1:C:363:MET:C     | 1:C:364:THR:CG2  | 2.90                     | 0.45              |
| 2:F:992:VAL:HG13  | 2:F:1001:LEU:HB2 | 1.98                     | 0.45              |
| 2:F:999:THR:CG2   | 2:F:1000:SER:N   | 2.78                     | 0.45              |
| 2:F:1196:LYS:HA   | 2:F:1203:PHE:CE1 | 2.52                     | 0.45              |
| 2:F:1217:ASN:HB2  | 5:F:2008:NAG:H61 | 1.98                     | 0.45              |
| 2:F:1304:GLN:H    | 2:F:1372:THR:CG2 | 2.24                     | 0.45              |
| 3:G:3:BMA:C4      | 3:G:5:MAN:H2     | 2.42                     | 0.45              |
| 1:A:281:LEU:HA    | 1:A:281:LEU:HD23 | 1.80                     | 0.45              |
| 1:A:310:SER:HB2   | 2:F:1150:THR:HB  | 1.98                     | 0.45              |
| 1:A:338:LYS:C     | 1:A:339:SER:O    | 2.58                     | 0.45              |
| 2:B:1205:LEU:HB2  | 2:B:1248:ILE:HB  | 1.98                     | 0.45              |
| 2:D:1196:LYS:HA   | 2:D:1203:PHE:CE1 | 2.52                     | 0.45              |
| 2:D:1350:TYR:CD1  | 2:D:1356:PRO:HB3 | 2.52                     | 0.45              |
| 1:E:58:LEU:HB2    | 1:E:75:LEU:HD23  | 1.98                     | 0.45              |
| 2:F:1245:PRO:HA   | 2:F:1246:PRO:HD3 | 1.67                     | 0.45              |
| 1:A:146:ASN:ND2   | 1:A:149:ALA:CB   | 2.80                     | 0.45              |
| 2:B:1013:LEU:HD23 | 2:B:1013:LEU:HA  | 1.81                     | 0.45              |
| 1:C:58:LEU:HB2    | 1:C:75:LEU:HD23  | 1.99                     | 0.45              |
| 2:D:1084:GLN:HG2  | 2:D:1161:SER:CA  | 2.46                     | 0.45              |
| 2:F:1260:ARG:HG2  | 2:F:1261:THR:N   | 2.31                     | 0.45              |
| 1:A:58:LEU:HB2    | 1:A:75:LEU:HD23  | 1.98                     | 0.44              |
| 1:A:86:ASP:N      | 1:A:86:ASP:OD1   | 2.49                     | 0.44              |
| 1:A:89:ILE:HG22   | 1:A:90:GLY:N     | 2.32                     | 0.44              |
| 2:B:948:HIS:HA    | 2:B:949:PRO:C    | 2.41                     | 0.44              |
| 2:D:1338:LEU:HA   | 2:D:1369:LEU:O   | 2.17                     | 0.44              |
| 1:E:146:ASN:ND2   | 1:E:149:ALA:CB   | 2.80                     | 0.44              |
| 1:E:170:VAL:O     | 1:E:171:ASP:C    | 2.59                     | 0.44              |
| 1:E:201:GLN:HE22  | 2:F:1147:GLN:HG2 | 1.82                     | 0.44              |
| 1:E:215:LYS:C     | 1:E:217:ASN:N    | 2.73                     | 0.44              |
| 1:E:279:THR:C     | 1:E:281:LEU:N    | 2.72                     | 0.44              |
| 2:F:1056:LEU:O    | 2:F:1158:TRP:CZ2 | 2.70                     | 0.44              |
| 2:B:1043:SER:O    | 2:B:1047:ALA:HB2 | 2.17                     | 0.44              |
| 1:C:29:PRO:HB2    | 1:C:32:GLN:HG2   | 1.99                     | 0.44              |
| 1:C:146:ASN:ND2   | 1:C:149:ALA:CB   | 2.81                     | 0.44              |
| 1:C:201:GLN:HE22  | 2:D:1147:GLN:HG2 | 1.82                     | 0.44              |
| 2:D:982:HIS:HB3   | 2:D:985:CYS:HA   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:992:VAL:HG13  | 2:D:1001:LEU:HB2  | 1.99                     | 0.44              |
| 2:D:1095:LEU:HD21 | 2:D:1143:PHE:HE1  | 1.82                     | 0.44              |
| 2:D:1178:SER:HB3  | 2:D:1270:PHE:CE2  | 2.51                     | 0.44              |
| 2:D:1235:LEU:HD11 | 2:D:1237:THR:C    | 2.42                     | 0.44              |
| 2:D:1317:THR:O    | 2:D:1388:VAL:HA   | 2.17                     | 0.44              |
| 1:E:198:LEU:C     | 1:E:198:LEU:CD2   | 2.89                     | 0.44              |
| 1:E:339:SER:C     | 1:E:341:SER:N     | 2.74                     | 0.44              |
| 2:F:948:HIS:HA    | 2:F:949:PRO:C     | 2.41                     | 0.44              |
| 2:F:952:TYR:HE1   | 2:F:988:ASP:OD2   | 1.99                     | 0.44              |
| 2:F:982:HIS:HB3   | 2:F:985:CYS:HA    | 1.99                     | 0.44              |
| 2:F:1317:THR:O    | 2:F:1388:VAL:HA   | 2.17                     | 0.44              |
| 1:A:180:LEU:HA    | 1:A:180:LEU:HD12  | 1.49                     | 0.44              |
| 6:A:2007:B12:H302 | 6:A:2007:B12:H253 | 1.54                     | 0.44              |
| 1:C:298:LEU:N     | 1:C:299:PRO:HD3   | 2.32                     | 0.44              |
| 2:D:1043:SER:O    | 2:D:1047:ALA:HB2  | 2.17                     | 0.44              |
| 2:D:1169:LEU:HD12 | 2:D:1169:LEU:H    | 1.82                     | 0.44              |
| 2:D:1217:ASN:HB2  | 5:D:2008:NAG:H61  | 1.98                     | 0.44              |
| 1:E:281:LEU:HA    | 1:E:281:LEU:HD23  | 1.80                     | 0.44              |
| 1:E:338:LYS:C     | 1:E:339:SER:O     | 2.58                     | 0.44              |
| 2:F:1051:ASP:CG   | 2:F:1077:ARG:HD2  | 2.43                     | 0.44              |
| 2:F:1176:PHE:CD1  | 2:F:1176:PHE:N    | 2.84                     | 0.44              |
| 1:A:369:VAL:HG13  | 6:A:2007:B12:O44  | 2.17                     | 0.44              |
| 2:B:1146:ASP:HB2  | 2:B:1147:GLN:OE1  | 2.17                     | 0.44              |
| 1:C:89:ILE:HG22   | 1:C:90:GLY:N      | 2.32                     | 0.44              |
| 1:C:369:VAL:HG13  | 6:C:2007:B12:O44  | 2.17                     | 0.44              |
| 2:D:1146:ASP:HB2  | 2:D:1147:GLN:OE1  | 2.17                     | 0.44              |
| 2:F:1067:ASN:HB3  | 2:F:1150:THR:HG22 | 1.98                     | 0.44              |
| 3:J:3:BMA:C4      | 3:J:5:MAN:H2      | 2.42                     | 0.44              |
| 1:A:337:VAL:C     | 1:A:338:LYS:O     | 2.57                     | 0.44              |
| 6:A:2007:B12:H562 | 6:A:2007:B12:H18  | 1.87                     | 0.44              |
| 2:B:1051:ASP:CG   | 2:B:1077:ARG:HD2  | 2.43                     | 0.44              |
| 2:B:1235:LEU:HD11 | 2:B:1237:THR:C    | 2.42                     | 0.44              |
| 1:C:338:LYS:C     | 1:C:339:SER:O     | 2.58                     | 0.44              |
| 1:C:403:ILE:HA    | 1:C:404:PRO:HD3   | 1.70                     | 0.44              |
| 1:E:142:LEU:HD12  | 1:E:142:LEU:HA    | 1.82                     | 0.44              |
| 1:E:369:VAL:HG13  | 6:E:2007:B12:O44  | 2.17                     | 0.44              |
| 1:E:379:ASN:ND2   | 1:E:382:HIS:ND1   | 2.66                     | 0.44              |
| 2:F:1338:LEU:HA   | 2:F:1369:LEU:O    | 2.17                     | 0.44              |
| 1:A:252:MET:SD    | 1:A:252:MET:C     | 3.01                     | 0.44              |
| 2:B:992:VAL:HG13  | 2:B:1001:LEU:HB2  | 1.99                     | 0.44              |
| 2:B:1260:ARG:HG2  | 2:B:1261:THR:N    | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:952:TYR:HE1   | 2:D:988:ASP:OD2   | 2.00                     | 0.44              |
| 2:D:1196:LYS:HA   | 2:D:1203:PHE:HE1  | 1.82                     | 0.44              |
| 2:D:1291:LEU:HA   | 2:D:1291:LEU:HD23 | 1.64                     | 0.44              |
| 1:E:54:ASN:HB3    | 1:E:57:ILE:HD12   | 2.00                     | 0.44              |
| 2:F:1043:SER:O    | 2:F:1047:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:390:SER:O     | 1:A:392:VAL:N     | 2.47                     | 0.44              |
| 2:B:978:HIS:CE1   | 2:B:1007:LYS:NZ   | 2.85                     | 0.44              |
| 2:B:1243:GLU:OE1  | 2:B:1243:GLU:CA   | 2.65                     | 0.44              |
| 2:B:1338:LEU:HA   | 2:B:1369:LEU:O    | 2.17                     | 0.44              |
| 1:C:86:ASP:OD1    | 1:C:86:ASP:N      | 2.49                     | 0.44              |
| 1:A:298:LEU:N     | 1:A:299:PRO:HD3   | 2.32                     | 0.44              |
| 1:A:363:MET:C     | 1:A:364:THR:CG2   | 2.90                     | 0.44              |
| 1:C:151:LEU:HD22  | 1:C:195:TYR:CD2   | 2.53                     | 0.44              |
| 1:C:379:ASN:ND2   | 1:C:382:HIS:ND1   | 2.66                     | 0.44              |
| 2:D:1190:GLU:HG2  | 2:D:1260:ARG:HB2  | 2.00                     | 0.44              |
| 1:E:151:LEU:HD22  | 1:E:195:TYR:CD2   | 2.53                     | 0.44              |
| 2:F:989:TYR:CZ    | 2:F:1025:VAL:HG12 | 2.53                     | 0.44              |
| 2:B:1190:GLU:HG2  | 2:B:1260:ARG:HB2  | 2.00                     | 0.44              |
| 2:B:1291:LEU:HD23 | 2:B:1291:LEU:HA   | 1.64                     | 0.44              |
| 2:D:947:GLY:O     | 2:D:948:HIS:C     | 2.60                     | 0.44              |
| 2:D:989:TYR:CZ    | 2:D:1025:VAL:HG12 | 2.53                     | 0.44              |
| 1:E:90:GLY:O      | 1:E:91:HIS:C      | 2.61                     | 0.44              |
| 2:F:1146:ASP:HB2  | 2:F:1147:GLN:OE1  | 2.17                     | 0.44              |
| 1:A:90:GLY:O      | 1:A:91:HIS:C      | 2.61                     | 0.43              |
| 2:B:1119:LEU:HD12 | 2:B:1119:LEU:HA   | 1.78                     | 0.43              |
| 2:D:967:ASN:ND2   | 2:D:968:HIS:CE1   | 2.87                     | 0.43              |
| 1:E:252:MET:SD    | 1:E:252:MET:C     | 3.01                     | 0.43              |
| 1:E:405:PHE:CE1   | 1:E:408:GLU:HB2   | 2.53                     | 0.43              |
| 2:F:1190:GLU:HG2  | 2:F:1260:ARG:HB2  | 2.00                     | 0.43              |
| 2:F:1235:LEU:HD11 | 2:F:1237:THR:C    | 2.42                     | 0.43              |
| 2:F:1289:GLY:O    | 2:F:1290:ILE:HD13 | 2.18                     | 0.43              |
| 2:F:1350:TYR:CD1  | 2:F:1356:PRO:HB3  | 2.52                     | 0.43              |
| 2:B:1022:LEU:HD23 | 2:B:1022:LEU:HA   | 1.66                     | 0.43              |
| 2:B:1322:PHE:C    | 2:B:1323:LEU:HD12 | 2.43                     | 0.43              |
| 2:F:1176:PHE:CD2  | 2:F:1193:TRP:CE3  | 3.07                     | 0.43              |
| 2:F:1322:PHE:C    | 2:F:1323:LEU:HD12 | 2.43                     | 0.43              |
| 1:A:279:THR:C     | 1:A:281:LEU:N     | 2.72                     | 0.43              |
| 2:B:1046:THR:O    | 2:B:1046:THR:HG22 | 2.18                     | 0.43              |
| 2:B:1086:ILE:H    | 2:B:1134:SER:HG   | 1.66                     | 0.43              |
| 1:C:90:GLY:O      | 1:C:91:HIS:C      | 2.61                     | 0.43              |
| 2:D:1187:HIS:CB   | 2:D:1266:GLN:NE2  | 2.75                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:298:LEU:N     | 1:E:299:PRO:HD3   | 2.32                     | 0.43              |
| 2:F:1022:LEU:HD23 | 2:F:1022:LEU:HA   | 1.66                     | 0.43              |
| 2:F:1089:HIS:HB2  | 2:F:1157:TYR:CZ   | 2.53                     | 0.43              |
| 2:F:1178:SER:HB3  | 2:F:1270:PHE:CD2  | 2.53                     | 0.43              |
| 1:A:29:PRO:HB2    | 1:A:32:GLN:HG2    | 2.00                     | 0.43              |
| 1:A:379:ASN:ND2   | 1:A:382:HIS:ND1   | 2.66                     | 0.43              |
| 6:A:2007:B12:H411 | 6:A:2007:B12:H363 | 1.48                     | 0.43              |
| 2:B:989:TYR:CZ    | 2:B:1025:VAL:HG12 | 2.53                     | 0.43              |
| 1:C:405:PHE:CE1   | 1:C:408:GLU:HB2   | 2.53                     | 0.43              |
| 6:C:2007:B12:N29  | 6:C:2007:B12:H251 | 2.32                     | 0.43              |
| 2:D:1046:THR:HG22 | 2:D:1046:THR:O    | 2.18                     | 0.43              |
| 2:D:1128:LEU:HD23 | 2:D:1128:LEU:HA   | 1.65                     | 0.43              |
| 1:E:352:ARG:NH1   | 1:E:352:ARG:CG    | 2.72                     | 0.43              |
| 6:A:2007:B12:N29  | 6:A:2007:B12:H251 | 2.32                     | 0.43              |
| 2:B:1095:LEU:HD21 | 2:B:1143:PHE:HE1  | 1.83                     | 0.43              |
| 2:B:1176:PHE:CD2  | 2:B:1193:TRP:CE3  | 3.07                     | 0.43              |
| 1:C:177:THR:CG2   | 1:C:206:ILE:HG21  | 2.42                     | 0.43              |
| 1:C:317:THR:HB    | 1:C:411:THR:HG23  | 2.01                     | 0.43              |
| 2:D:1051:ASP:CG   | 2:D:1077:ARG:HD2  | 2.43                     | 0.43              |
| 2:D:1171:THR:C    | 2:D:1173:SER:H    | 2.27                     | 0.43              |
| 2:F:1178:SER:O    | 2:F:1179:PRO:C    | 2.61                     | 0.43              |
| 1:A:317:THR:HB    | 1:A:411:THR:HG23  | 2.01                     | 0.43              |
| 2:B:942:THR:HG22  | 2:B:1036:LEU:HD11 | 1.99                     | 0.43              |
| 2:B:967:ASN:ND2   | 2:B:968:HIS:CE1   | 2.87                     | 0.43              |
| 2:B:1171:THR:C    | 2:B:1173:SER:H    | 2.27                     | 0.43              |
| 2:B:1289:GLY:O    | 2:B:1290:ILE:HD13 | 2.18                     | 0.43              |
| 1:C:252:MET:SD    | 1:C:252:MET:C     | 3.01                     | 0.43              |
| 2:D:948:HIS:HA    | 2:D:950:ASN:N     | 2.34                     | 0.43              |
| 2:D:1219:THR:O    | 2:D:1219:THR:CG2  | 2.66                     | 0.43              |
| 1:E:89:ILE:HG22   | 1:E:90:GLY:N      | 2.32                     | 0.43              |
| 1:E:369:VAL:HG12  | 1:E:370:VAL:N     | 2.34                     | 0.43              |
| 2:F:942:THR:HG22  | 2:F:1036:LEU:HD11 | 1.99                     | 0.43              |
| 2:F:948:HIS:HA    | 2:F:950:ASN:N     | 2.34                     | 0.43              |
| 2:F:1084:GLN:N    | 2:F:1084:GLN:OE1  | 2.51                     | 0.43              |
| 2:F:1177:ILE:HG23 | 2:F:1181:TYR:CB   | 2.47                     | 0.43              |
| 1:A:54:ASN:HB3    | 1:A:57:ILE:HD12   | 2.00                     | 0.43              |
| 1:A:228:LEU:HD23  | 1:A:228:LEU:HA    | 1.66                     | 0.43              |
| 6:A:2007:B12:H533 | 6:A:2007:B12:C48  | 2.49                     | 0.43              |
| 2:B:948:HIS:HA    | 2:B:950:ASN:N     | 2.34                     | 0.43              |
| 2:B:1350:TYR:CD1  | 2:B:1356:PRO:HB3  | 2.53                     | 0.43              |
| 2:D:988:ASP:OD2   | 2:D:1026:THR:HB   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:1061:SER:HB3  | 2:D:1154:PHE:H    | 1.84                     | 0.43              |
| 2:D:1322:PHE:C    | 2:D:1323:LEU:HD12 | 2.43                     | 0.43              |
| 2:F:954:HIS:H     | 2:F:954:HIS:HD2   | 1.59                     | 0.43              |
| 2:F:967:ASN:ND2   | 2:F:968:HIS:CE1   | 2.86                     | 0.43              |
| 2:F:1046:THR:HG22 | 2:F:1046:THR:O    | 2.18                     | 0.43              |
| 1:A:405:PHE:CE1   | 1:A:408:GLU:HB2   | 2.53                     | 0.43              |
| 2:B:1089:HIS:HB2  | 2:B:1157:TYR:CZ   | 2.53                     | 0.43              |
| 2:B:1248:ILE:O    | 2:B:1248:ILE:HG22 | 2.19                     | 0.43              |
| 2:D:1289:GLY:O    | 2:D:1290:ILE:HD13 | 2.19                     | 0.43              |
| 1:E:271:ILE:O     | 1:E:272:LEU:C     | 2.62                     | 0.43              |
| 2:F:947:GLY:O     | 2:F:948:HIS:C     | 2.60                     | 0.43              |
| 2:F:988:ASP:OD2   | 2:F:1026:THR:HB   | 2.19                     | 0.43              |
| 2:F:1031:ALA:C    | 2:F:1032:TYR:CG   | 2.97                     | 0.43              |
| 2:F:1312:ALA:O    | 2:F:1364:SER:HB2  | 2.19                     | 0.43              |
| 2:F:1313:THR:HG22 | 5:F:2009:NAG:C8   | 2.41                     | 0.43              |
| 4:I:1:NAG:H2      | 4:I:1:NAG:H82     | 1.65                     | 0.43              |
| 1:A:151:LEU:HD22  | 1:A:195:TYR:CD2   | 2.53                     | 0.43              |
| 2:B:952:TYR:HA    | 2:B:953:PRO:HD3   | 1.78                     | 0.43              |
| 2:B:964:VAL:CG2   | 2:B:965:GLN:N     | 2.82                     | 0.43              |
| 2:B:1312:ALA:O    | 2:B:1364:SER:HB2  | 2.19                     | 0.43              |
| 1:C:130:SER:HA    | 1:C:172:THR:OG1   | 2.19                     | 0.43              |
| 1:C:170:VAL:O     | 1:C:171:ASP:C     | 2.59                     | 0.43              |
| 2:D:1057:GLY:HA3  | 2:D:1157:TYR:CA   | 2.48                     | 0.43              |
| 2:D:1178:SER:O    | 2:D:1179:PRO:C    | 2.61                     | 0.43              |
| 2:D:1302:GLU:HB3  | 2:D:1374:GLY:HA2  | 2.01                     | 0.43              |
| 1:E:29:PRO:HB2    | 1:E:32:GLN:HG2    | 1.99                     | 0.43              |
| 2:F:1139:LEU:HD23 | 2:F:1139:LEU:HA   | 1.87                     | 0.43              |
| 2:B:1178:SER:HB3  | 2:B:1270:PHE:CD2  | 2.53                     | 0.43              |
| 2:B:1178:SER:O    | 2:B:1179:PRO:C    | 2.61                     | 0.43              |
| 2:B:1366:LEU:C    | 2:B:1366:LEU:CD2  | 2.90                     | 0.43              |
| 1:C:54:ASN:HB3    | 1:C:57:ILE:HD12   | 2.00                     | 0.43              |
| 1:C:389:LEU:CB    | 1:C:394:PRO:HA    | 2.45                     | 0.43              |
| 2:D:978:HIS:CE1   | 2:D:1007:LYS:NZ   | 2.87                     | 0.43              |
| 2:D:1089:HIS:HB2  | 2:D:1157:TYR:CZ   | 2.53                     | 0.43              |
| 2:D:1243:GLU:OE1  | 2:D:1243:GLU:CA   | 2.65                     | 0.43              |
| 2:D:1248:ILE:O    | 2:D:1248:ILE:HG22 | 2.19                     | 0.43              |
| 2:D:1304:GLN:HG3  | 2:D:1372:THR:HG21 | 2.01                     | 0.43              |
| 2:D:1355:LEU:HA   | 2:D:1356:PRO:HD3  | 1.92                     | 0.43              |
| 6:E:2007:B12:N29  | 6:E:2007:B12:H251 | 2.32                     | 0.43              |
| 2:F:978:HIS:CE1   | 2:F:1007:LYS:NZ   | 2.86                     | 0.43              |
| 2:F:1171:THR:C    | 2:F:1173:SER:H    | 2.27                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1302:GLU:HB3  | 2:F:1374:GLY:HA2  | 2.01                     | 0.43              |
| 1:A:130:SER:HA    | 1:A:172:THR:OG1   | 2.19                     | 0.42              |
| 2:B:1031:ALA:C    | 2:B:1032:TYR:CG   | 2.97                     | 0.42              |
| 2:B:1320:TYR:OH   | 2:B:1366:LEU:CD2  | 2.66                     | 0.42              |
| 2:D:1178:SER:HB3  | 2:D:1270:PHE:CD2  | 2.53                     | 0.42              |
| 2:D:1190:GLU:CG   | 2:D:1260:ARG:HG3  | 2.49                     | 0.42              |
| 1:E:297:THR:HG22  | 1:E:299:PRO:CD    | 2.46                     | 0.42              |
| 2:F:1331:ILE:HG22 | 2:F:1334:SER:OG   | 2.19                     | 0.42              |
| 2:B:1084:GLN:OE1  | 2:B:1084:GLN:N    | 2.51                     | 0.42              |
| 2:B:1205:LEU:CD2  | 2:B:1255:MET:SD   | 3.07                     | 0.42              |
| 2:B:1330:HIS:CD2  | 2:B:1331:ILE:H    | 2.35                     | 0.42              |
| 1:C:58:LEU:HB2    | 1:C:75:LEU:HD21   | 2.01                     | 0.42              |
| 1:C:172:THR:O     | 1:C:173:GLY:C     | 2.62                     | 0.42              |
| 1:C:374:ASN:O     | 1:C:375:ASN:CB    | 2.67                     | 0.42              |
| 1:C:393:THR:HA    | 1:C:394:PRO:HD3   | 1.91                     | 0.42              |
| 2:D:942:THR:HG22  | 2:D:1036:LEU:HD11 | 1.99                     | 0.42              |
| 2:D:1084:GLN:OE1  | 2:D:1084:GLN:N    | 2.51                     | 0.42              |
| 2:D:1120:LEU:HD23 | 2:D:1120:LEU:HA   | 1.90                     | 0.42              |
| 2:D:1205:LEU:CD2  | 2:D:1255:MET:SD   | 3.07                     | 0.42              |
| 2:F:964:VAL:CG2   | 2:F:965:GLN:N     | 2.82                     | 0.42              |
| 2:F:1057:GLY:HA3  | 2:F:1157:TYR:CA   | 2.48                     | 0.42              |
| 2:F:1330:HIS:ND1  | 2:F:1332:ASN:N    | 2.55                     | 0.42              |
| 2:B:1343:GLY:HA3  | 2:B:1344:PRO:HD3  | 1.88                     | 0.42              |
| 2:D:1161:SER:O    | 2:D:1162:SER:CB   | 2.67                     | 0.42              |
| 1:E:374:ASN:O     | 1:E:375:ASN:CB    | 2.67                     | 0.42              |
| 2:F:1084:GLN:HG2  | 2:F:1160:GLY:O    | 2.19                     | 0.42              |
| 2:F:1161:SER:O    | 2:F:1162:SER:CB   | 2.67                     | 0.42              |
| 2:B:978:HIS:HB3   | 2:B:1032:TYR:HB2  | 2.01                     | 0.42              |
| 2:B:988:ASP:OD2   | 2:B:1026:THR:HB   | 2.19                     | 0.42              |
| 2:B:1061:SER:HB3  | 2:B:1154:PHE:H    | 1.84                     | 0.42              |
| 2:B:1162:SER:C    | 2:B:1164:GLY:N    | 2.78                     | 0.42              |
| 1:C:369:VAL:HG12  | 1:C:370:VAL:N     | 2.34                     | 0.42              |
| 2:D:980:GLU:OE2   | 2:D:987:ASN:ND2   | 2.52                     | 0.42              |
| 2:D:1084:GLN:HG2  | 2:D:1160:GLY:O    | 2.19                     | 0.42              |
| 2:D:1176:PHE:CD2  | 2:D:1193:TRP:CE3  | 3.07                     | 0.42              |
| 2:D:1387:PHE:O    | 2:D:1388:VAL:CG2  | 2.68                     | 0.42              |
| 1:E:317:THR:HB    | 1:E:411:THR:HG23  | 2.01                     | 0.42              |
| 6:E:2007:B12:H533 | 6:E:2007:B12:C48  | 2.49                     | 0.42              |
| 2:F:1190:GLU:CG   | 2:F:1260:ARG:HG3  | 2.50                     | 0.42              |
| 2:F:1330:HIS:CD2  | 2:F:1331:ILE:H    | 2.36                     | 0.42              |
| 1:A:369:VAL:HG12  | 1:A:370:VAL:N     | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:335:VAL:CG2   | 5:C:2001:NAG:H5   | 2.50                     | 0.42              |
| 2:D:1031:ALA:C    | 2:D:1032:TYR:CG   | 2.97                     | 0.42              |
| 2:D:1162:SER:C    | 2:D:1164:GLY:N    | 2.78                     | 0.42              |
| 2:D:1335:THR:HG23 | 2:D:1336:ASP:N    | 2.29                     | 0.42              |
| 2:F:1205:LEU:CD2  | 2:F:1255:MET:SD   | 3.07                     | 0.42              |
| 2:F:1248:ILE:O    | 2:F:1248:ILE:HG22 | 2.19                     | 0.42              |
| 2:F:1320:TYR:OH   | 2:F:1366:LEU:CD2  | 2.68                     | 0.42              |
| 2:F:1340:LEU:HD23 | 2:F:1340:LEU:HA   | 1.82                     | 0.42              |
| 2:F:1387:PHE:O    | 2:F:1388:VAL:CG2  | 2.68                     | 0.42              |
| 1:A:294:VAL:HG23  | 1:A:294:VAL:O     | 2.20                     | 0.42              |
| 5:A:2001:NAG:C3   | 5:A:2001:NAG:H83  | 2.50                     | 0.42              |
| 2:B:980:GLU:OE2   | 2:B:987:ASN:ND2   | 2.52                     | 0.42              |
| 2:B:1304:GLN:HG3  | 2:B:1372:THR:HG21 | 2.01                     | 0.42              |
| 1:C:74:LEU:O      | 1:C:78:GLN:HG3    | 2.20                     | 0.42              |
| 1:C:386:TRP:CZ3   | 1:C:414:PHE:HB2   | 2.55                     | 0.42              |
| 6:C:2007:B12:H533 | 6:C:2007:B12:C48  | 2.49                     | 0.42              |
| 2:F:1162:SER:C    | 2:F:1164:GLY:N    | 2.78                     | 0.42              |
| 2:B:1190:GLU:CG   | 2:B:1260:ARG:HG3  | 2.50                     | 0.42              |
| 2:B:1291:LEU:HD11 | 2:B:1368:VAL:HG21 | 2.01                     | 0.42              |
| 2:B:1331:ILE:HG22 | 2:B:1334:SER:OG   | 2.19                     | 0.42              |
| 2:B:1355:LEU:HA   | 2:B:1356:PRO:HD3  | 1.92                     | 0.42              |
| 1:C:87:LEU:HA     | 1:C:91:HIS:CD2    | 2.55                     | 0.42              |
| 1:C:219:ILE:HG12  | 1:C:252:MET:CE    | 2.50                     | 0.42              |
| 1:C:228:LEU:HD23  | 1:C:228:LEU:HA    | 1.66                     | 0.42              |
| 2:D:1330:HIS:CD2  | 2:D:1331:ILE:H    | 2.35                     | 0.42              |
| 2:D:1331:ILE:HG22 | 2:D:1334:SER:OG   | 2.19                     | 0.42              |
| 1:E:130:SER:HA    | 1:E:172:THR:OG1   | 2.19                     | 0.42              |
| 1:E:294:VAL:HG23  | 1:E:294:VAL:O     | 2.20                     | 0.42              |
| 2:F:980:GLU:OE2   | 2:F:987:ASN:ND2   | 2.52                     | 0.42              |
| 2:F:1064:PHE:CD2  | 2:F:1064:PHE:C    | 2.98                     | 0.42              |
| 2:F:1095:LEU:HD21 | 2:F:1143:PHE:HE1  | 1.82                     | 0.42              |
| 1:A:389:LEU:CB    | 1:A:394:PRO:HA    | 2.45                     | 0.42              |
| 2:B:1064:PHE:CD2  | 2:B:1064:PHE:C    | 2.98                     | 0.42              |
| 2:B:1161:SER:O    | 2:B:1162:SER:CB   | 2.67                     | 0.42              |
| 1:C:181:THR:HG21  | 1:C:235:VAL:HG13  | 2.02                     | 0.42              |
| 1:C:362:THR:HG22  | 1:C:371:SER:CB    | 2.35                     | 0.42              |
| 6:C:2007:B12:H533 | 6:C:2007:B12:H482 | 2.02                     | 0.42              |
| 2:D:1205:LEU:HD23 | 2:D:1255:MET:SD   | 2.60                     | 0.42              |
| 2:F:1085:LEU:HD21 | 2:F:1165:CYS:HA   | 2.01                     | 0.42              |
| 2:F:1291:LEU:HD23 | 2:F:1291:LEU:HA   | 1.64                     | 0.42              |
| 2:F:1294:ILE:O    | 2:F:1295:GLY:C    | 2.62                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1205:LEU:HD23 | 2:B:1255:MET:SD   | 2.60                     | 0.42              |
| 2:B:1302:GLU:HB3  | 2:B:1374:GLY:HA2  | 2.01                     | 0.42              |
| 2:D:1060:THR:HG23 | 2:D:1064:PHE:CB   | 2.46                     | 0.42              |
| 2:D:1085:LEU:HD21 | 2:D:1165:CYS:HA   | 2.01                     | 0.42              |
| 1:E:52:TYR:CD1    | 1:E:52:TYR:C      | 2.98                     | 0.42              |
| 2:F:975:GLU:HG3   | 2:F:1036:LEU:HD23 | 2.02                     | 0.42              |
| 2:F:1060:THR:HG23 | 2:F:1064:PHE:CB   | 2.46                     | 0.42              |
| 2:F:1119:LEU:HD12 | 2:F:1119:LEU:HA   | 1.79                     | 0.42              |
| 2:F:1187:HIS:HB3  | 2:F:1266:GLN:HE22 | 1.78                     | 0.42              |
| 2:F:1226:TYR:CE1  | 2:F:1235:LEU:HB2  | 2.55                     | 0.42              |
| 2:F:1293:SER:O    | 2:F:1294:ILE:C    | 2.62                     | 0.42              |
| 1:A:74:LEU:O      | 1:A:78:GLN:HG3    | 2.20                     | 0.42              |
| 1:A:203:LEU:HD22  | 1:A:236:THR:HG22  | 2.02                     | 0.42              |
| 6:A:2007:B12:H533 | 6:A:2007:B12:H482 | 2.02                     | 0.42              |
| 1:C:185:ASN:HB3   | 1:E:287:THR:HG23  | 2.02                     | 0.42              |
| 2:D:964:VAL:CG2   | 2:D:965:GLN:N     | 2.82                     | 0.42              |
| 1:E:386:TRP:CZ3   | 1:E:414:PHE:HB2   | 2.55                     | 0.42              |
| 1:E:389:LEU:CB    | 1:E:394:PRO:HA    | 2.45                     | 0.42              |
| 2:F:1061:SER:HB3  | 2:F:1154:PHE:H    | 1.84                     | 0.42              |
| 2:F:1171:THR:C    | 2:F:1173:SER:N    | 2.78                     | 0.42              |
| 2:F:1217:ASN:HB2  | 5:F:2008:NAG:C6   | 2.50                     | 0.42              |
| 2:F:1304:GLN:HG3  | 2:F:1372:THR:HG21 | 2.01                     | 0.42              |
| 1:A:148:GLU:HG3   | 1:A:188:PRO:HG2   | 2.02                     | 0.41              |
| 1:A:275:LEU:HD23  | 1:A:275:LEU:HA    | 1.88                     | 0.41              |
| 2:B:1084:GLN:HG2  | 2:B:1160:GLY:O    | 2.20                     | 0.41              |
| 2:B:1217:ASN:HB2  | 5:B:2008:NAG:C6   | 2.50                     | 0.41              |
| 2:B:1294:ILE:O    | 2:B:1295:GLY:C    | 2.62                     | 0.41              |
| 1:C:148:GLU:HG3   | 1:C:188:PRO:HG2   | 2.02                     | 0.41              |
| 2:D:1217:ASN:HB2  | 5:D:2008:NAG:C6   | 2.50                     | 0.41              |
| 2:D:1226:TYR:CE1  | 2:D:1235:LEU:HB2  | 2.55                     | 0.41              |
| 2:D:1312:ALA:O    | 2:D:1364:SER:HB2  | 2.19                     | 0.41              |
| 1:E:335:VAL:CG2   | 5:E:2001:NAG:H5   | 2.50                     | 0.41              |
| 2:F:1205:LEU:HD23 | 2:F:1255:MET:SD   | 2.60                     | 0.41              |
| 1:A:271:ILE:O     | 1:A:272:LEU:C     | 2.62                     | 0.41              |
| 2:B:1387:PHE:O    | 2:B:1388:VAL:CG2  | 2.68                     | 0.41              |
| 1:C:89:ILE:HD13   | 1:C:89:ILE:HG21   | 1.66                     | 0.41              |
| 2:D:978:HIS:HB3   | 2:D:1032:TYR:HB2  | 2.02                     | 0.41              |
| 2:D:1150:THR:C    | 2:D:1151:ARG:HG2  | 2.46                     | 0.41              |
| 1:E:203:LEU:HD22  | 1:E:236:THR:HG22  | 2.02                     | 0.41              |
| 2:F:1062:PRO:O    | 2:F:1063:ASN:HB2  | 2.21                     | 0.41              |
| 2:F:1246:PRO:O    | 2:F:1247:LEU:C    | 2.63                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:1314:THR:HG22 | 2:F:1315:GLY:H    | 1.84                     | 0.41              |
| 1:A:363:MET:HG3   | 1:A:364:THR:N     | 2.36                     | 0.41              |
| 1:A:374:ASN:O     | 1:A:375:ASN:CB    | 2.67                     | 0.41              |
| 2:B:1293:SER:O    | 2:B:1294:ILE:C    | 2.62                     | 0.41              |
| 1:C:65:GLY:CA     | 1:C:292:HIS:CE1   | 3.03                     | 0.41              |
| 2:D:1064:PHE:CD2  | 2:D:1064:PHE:C    | 2.98                     | 0.41              |
| 2:D:1177:ILE:HG22 | 2:D:1178:SER:O    | 2.21                     | 0.41              |
| 1:E:132:PHE:C     | 1:E:135:PRO:HD2   | 2.46                     | 0.41              |
| 1:E:172:THR:O     | 1:E:173:GLY:C     | 2.62                     | 0.41              |
| 1:A:58:LEU:HB2    | 1:A:75:LEU:HD21   | 2.01                     | 0.41              |
| 1:A:132:PHE:C     | 1:A:135:PRO:HD2   | 2.46                     | 0.41              |
| 2:B:950:ASN:HA    | 2:B:951:VAL:HA    | 1.76                     | 0.41              |
| 2:B:1177:ILE:HG22 | 2:B:1178:SER:O    | 2.21                     | 0.41              |
| 2:B:1220:LEU:H    | 2:B:1220:LEU:HG   | 1.67                     | 0.41              |
| 1:C:294:VAL:O     | 1:C:294:VAL:HG23  | 2.20                     | 0.41              |
| 1:C:335:VAL:HG23  | 5:C:2001:NAG:H5   | 2.02                     | 0.41              |
| 2:D:1062:PRO:O    | 2:D:1063:ASN:HB2  | 2.20                     | 0.41              |
| 2:D:1067:ASN:HB3  | 2:D:1150:THR:HG22 | 1.98                     | 0.41              |
| 2:D:1220:LEU:O    | 2:D:1260:ARG:NH1  | 2.54                     | 0.41              |
| 2:D:1314:THR:HG22 | 2:D:1315:GLY:H    | 1.85                     | 0.41              |
| 2:D:1330:HIS:ND1  | 2:D:1332:ASN:N    | 2.55                     | 0.41              |
| 2:D:1382:PHE:CD1  | 2:D:1382:PHE:C    | 2.98                     | 0.41              |
| 1:E:146:ASN:OD1   | 1:E:146:ASN:C     | 2.64                     | 0.41              |
| 1:E:177:THR:CG2   | 1:E:206:ILE:HG21  | 2.42                     | 0.41              |
| 2:F:952:TYR:CE1   | 2:F:988:ASP:OD2   | 2.73                     | 0.41              |
| 2:F:1120:LEU:HD13 | 2:F:1132:ILE:CG2  | 2.51                     | 0.41              |
| 2:F:1192:TYR:HE1  | 2:F:1258:LYS:CG   | 2.33                     | 0.41              |
| 3:M:3:BMA:H61     | 3:M:5:MAN:H2      | 1.78                     | 0.41              |
| 1:A:123:SER:O     | 2:B:1101:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:219:ILE:HG12  | 1:A:252:MET:CE    | 2.50                     | 0.41              |
| 1:A:386:TRP:CZ3   | 1:A:414:PHE:HB2   | 2.55                     | 0.41              |
| 2:D:963:LEU:HD12  | 2:D:964:VAL:N     | 2.35                     | 0.41              |
| 2:D:1083:GLY:C    | 2:D:1163:THR:HA   | 2.45                     | 0.41              |
| 2:D:1291:LEU:HD11 | 2:D:1368:VAL:HG21 | 2.01                     | 0.41              |
| 2:D:1343:GLY:HA3  | 2:D:1344:PRO:HD3  | 1.88                     | 0.41              |
| 2:F:1086:ILE:H    | 2:F:1134:SER:HG   | 1.67                     | 0.41              |
| 2:F:1220:LEU:O    | 2:F:1260:ARG:NH1  | 2.54                     | 0.41              |
| 2:F:1291:LEU:HD11 | 2:F:1368:VAL:HG21 | 2.01                     | 0.41              |
| 2:F:1343:GLY:HA3  | 2:F:1344:PRO:HD3  | 1.88                     | 0.41              |
| 1:A:52:TYR:CD1    | 1:A:52:TYR:C      | 2.98                     | 0.41              |
| 1:A:87:LEU:HA     | 1:A:91:HIS:CD2    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:297:THR:HG22  | 1:A:299:PRO:CD    | 2.47                     | 0.41              |
| 2:B:1120:LEU:HD13 | 2:B:1132:ILE:CG2  | 2.51                     | 0.41              |
| 2:B:1148:ILE:CG2  | 2:B:1149:ASP:N    | 2.83                     | 0.41              |
| 2:B:1177:ILE:HD13 | 2:B:1177:ILE:HA   | 1.85                     | 0.41              |
| 1:C:94:LEU:HD13   | 1:C:94:LEU:HA     | 1.78                     | 0.41              |
| 2:D:952:TYR:CE1   | 2:D:988:ASP:OD2   | 2.73                     | 0.41              |
| 2:D:989:TYR:CZ    | 2:D:1025:VAL:CG1  | 3.04                     | 0.41              |
| 1:E:331:GLU:OE1   | 1:E:331:GLU:N     | 2.52                     | 0.41              |
| 2:F:1083:GLY:C    | 2:F:1163:THR:HA   | 2.45                     | 0.41              |
| 2:F:1148:ILE:CG2  | 2:F:1149:ASP:N    | 2.83                     | 0.41              |
| 5:F:2001:NAG:O3   | 5:F:2001:NAG:C7   | 2.69                     | 0.41              |
| 1:A:181:THR:HG21  | 1:A:235:VAL:HG13  | 2.02                     | 0.41              |
| 1:A:289:SER:N     | 1:A:290:PRO:HD3   | 2.36                     | 0.41              |
| 2:B:1083:GLY:C    | 2:B:1163:THR:HA   | 2.45                     | 0.41              |
| 2:B:1192:TYR:HE1  | 2:B:1258:LYS:CG   | 2.33                     | 0.41              |
| 2:B:1335:THR:HG23 | 2:B:1336:ASP:N    | 2.29                     | 0.41              |
| 1:E:181:THR:HG21  | 1:E:235:VAL:HG13  | 2.02                     | 0.41              |
| 1:E:363:MET:HG3   | 1:E:364:THR:N     | 2.35                     | 0.41              |
| 2:F:978:HIS:HB3   | 2:F:1032:TYR:HB2  | 2.03                     | 0.41              |
| 2:F:1177:ILE:HG22 | 2:F:1178:SER:O    | 2.21                     | 0.41              |
| 1:A:58:LEU:HD23   | 1:A:79:LEU:HD12   | 2.03                     | 0.41              |
| 1:A:146:ASN:OD1   | 1:A:146:ASN:C     | 2.64                     | 0.41              |
| 1:A:406:ASN:OD1   | 1:A:407:HIS:N     | 2.54                     | 0.41              |
| 2:B:954:HIS:ND1   | 2:B:1028:SER:O    | 2.54                     | 0.41              |
| 2:B:1060:THR:HG23 | 2:B:1064:PHE:CB   | 2.46                     | 0.41              |
| 2:B:1085:LEU:HD21 | 2:B:1165:CYS:HA   | 2.01                     | 0.41              |
| 2:B:1226:TYR:CE1  | 2:B:1235:LEU:HB2  | 2.55                     | 0.41              |
| 1:C:203:LEU:HD22  | 1:C:236:THR:HG22  | 2.02                     | 0.41              |
| 2:D:1120:LEU:HD13 | 2:D:1132:ILE:CG2  | 2.51                     | 0.41              |
| 2:D:1148:ILE:CG2  | 2:D:1149:ASP:N    | 2.83                     | 0.41              |
| 2:D:1293:SER:O    | 2:D:1294:ILE:C    | 2.62                     | 0.41              |
| 2:D:1294:ILE:O    | 2:D:1295:GLY:C    | 2.62                     | 0.41              |
| 1:E:74:LEU:O      | 1:E:78:GLN:HG3    | 2.20                     | 0.41              |
| 1:E:80:MET:HE1    | 1:E:104:ARG:HH11  | 1.86                     | 0.41              |
| 1:E:87:LEU:HA     | 1:E:91:HIS:CD2    | 2.55                     | 0.41              |
| 1:E:148:GLU:HG3   | 1:E:188:PRO:HG2   | 2.02                     | 0.41              |
| 1:E:159:LYS:HD3   | 2:F:1104:THR:HG22 | 2.02                     | 0.41              |
| 2:F:954:HIS:ND1   | 2:F:1028:SER:O    | 2.54                     | 0.41              |
| 2:F:964:VAL:O     | 2:F:1018:ASN:HB2  | 2.21                     | 0.41              |
| 1:A:267:SER:HB3   | 1:A:366:TRP:CH2   | 2.56                     | 0.41              |
| 1:A:331:GLU:OE1   | 1:A:331:GLU:N     | 2.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:954:HIS:H     | 2:B:954:HIS:HD2   | 1.59                     | 0.41              |
| 2:B:963:LEU:HD12  | 2:B:964:VAL:N     | 2.35                     | 0.41              |
| 2:B:975:GLU:HG3   | 2:B:1036:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:989:TYR:CZ    | 2:B:1025:VAL:CG1  | 3.04                     | 0.41              |
| 2:B:1062:PRO:O    | 2:B:1063:ASN:HB2  | 2.20                     | 0.41              |
| 2:B:1093:PHE:C    | 2:B:1093:PHE:HD2  | 2.29                     | 0.41              |
| 2:B:1177:ILE:HG23 | 2:B:1181:TYR:CB   | 2.48                     | 0.41              |
| 2:B:1213:GLU:CD   | 2:B:1265:GLN:HB3  | 2.46                     | 0.41              |
| 2:B:1288:TYR:N    | 2:B:1288:TYR:CD2  | 2.89                     | 0.41              |
| 1:C:52:TYR:CD1    | 1:C:52:TYR:C      | 2.98                     | 0.41              |
| 1:C:123:SER:O     | 2:D:1101:ASN:HB2  | 2.20                     | 0.41              |
| 1:C:317:THR:CG2   | 1:C:331:GLU:HG3   | 2.42                     | 0.41              |
| 2:D:954:HIS:ND1   | 2:D:1028:SER:O    | 2.54                     | 0.41              |
| 2:D:962:ILE:O     | 2:D:1019:SER:HA   | 2.21                     | 0.41              |
| 2:D:1093:PHE:C    | 2:D:1093:PHE:HD2  | 2.29                     | 0.41              |
| 2:D:1288:TYR:N    | 2:D:1288:TYR:CD2  | 2.89                     | 0.41              |
| 1:E:58:LEU:HB2    | 1:E:75:LEU:HD21   | 2.01                     | 0.41              |
| 1:E:403:ILE:HA    | 1:E:404:PRO:HD3   | 1.70                     | 0.41              |
| 6:E:2007:B12:H533 | 6:E:2007:B12:H482 | 2.02                     | 0.41              |
| 2:F:1128:LEU:HD23 | 2:F:1128:LEU:HA   | 1.65                     | 0.41              |
| 2:F:1213:GLU:CD   | 2:F:1265:GLN:HB3  | 2.46                     | 0.41              |
| 1:A:406:ASN:ND2   | 2:F:1066:ASN:HA   | 2.36                     | 0.41              |
| 6:A:2007:B12:H302 | 6:A:2007:B12:C20  | 2.45                     | 0.41              |
| 2:B:1051:ASP:OD1  | 2:B:1077:ARG:HD2  | 2.21                     | 0.41              |
| 2:B:1089:HIS:HB2  | 2:B:1157:TYR:CE2  | 2.56                     | 0.41              |
| 1:C:289:SER:N     | 1:C:290:PRO:HD3   | 2.36                     | 0.41              |
| 2:D:1051:ASP:OD1  | 2:D:1077:ARG:HD2  | 2.21                     | 0.41              |
| 2:D:1089:HIS:HB2  | 2:D:1157:TYR:CE2  | 2.56                     | 0.41              |
| 1:E:58:LEU:HD23   | 1:E:79:LEU:HD12   | 2.03                     | 0.41              |
| 1:E:89:ILE:HD11   | 1:E:117:MET:SD    | 2.61                     | 0.41              |
| 1:E:289:SER:N     | 1:E:290:PRO:HD3   | 2.36                     | 0.41              |
| 1:E:406:ASN:OD1   | 1:E:407:HIS:N     | 2.54                     | 0.41              |
| 1:A:65:GLY:CA     | 1:A:292:HIS:CE1   | 3.03                     | 0.40              |
| 2:B:962:ILE:O     | 2:B:1019:SER:HA   | 2.21                     | 0.40              |
| 2:B:1171:THR:C    | 2:B:1173:SER:N    | 2.78                     | 0.40              |
| 2:B:1220:LEU:O    | 2:B:1260:ARG:NH1  | 2.54                     | 0.40              |
| 2:B:1246:PRO:O    | 2:B:1247:LEU:C    | 2.62                     | 0.40              |
| 1:C:331:GLU:OE1   | 1:C:331:GLU:N     | 2.52                     | 0.40              |
| 6:C:2007:B12:H562 | 6:C:2007:B12:H18  | 1.87                     | 0.40              |
| 1:E:65:GLY:CA     | 1:E:292:HIS:CE1   | 3.03                     | 0.40              |
| 2:F:963:LEU:HD12  | 2:F:964:VAL:N     | 2.35                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:964:VAL:HG21  | 2:F:1041:ALA:HB2  | 2.03                     | 0.40              |
| 2:B:1084:GLN:HG3  | 2:B:1163:THR:N    | 2.21                     | 0.40              |
| 2:B:1150:THR:C    | 2:B:1151:ARG:HG2  | 2.46                     | 0.40              |
| 2:B:1274:TYR:O    | 2:B:1274:TYR:CG   | 2.74                     | 0.40              |
| 2:B:1330:HIS:ND1  | 2:B:1332:ASN:N    | 2.55                     | 0.40              |
| 1:C:132:PHE:C     | 1:C:135:PRO:HD2   | 2.46                     | 0.40              |
| 1:C:146:ASN:OD1   | 1:C:146:ASN:C     | 2.64                     | 0.40              |
| 1:C:159:LYS:HD3   | 2:D:1104:THR:HG22 | 2.02                     | 0.40              |
| 1:C:214:ILE:HG12  | 1:C:220:ILE:HG12  | 2.03                     | 0.40              |
| 1:C:363:MET:HG3   | 1:C:364:THR:N     | 2.36                     | 0.40              |
| 2:D:993:TYR:HB3   | 2:D:1021:MET:CB   | 2.51                     | 0.40              |
| 2:D:1177:ILE:HG23 | 2:D:1181:TYR:CB   | 2.47                     | 0.40              |
| 2:D:1320:TYR:OH   | 2:D:1366:LEU:CD2  | 2.68                     | 0.40              |
| 1:E:123:SER:O     | 2:F:1101:ASN:HB2  | 2.20                     | 0.40              |
| 1:E:219:ILE:HG12  | 1:E:252:MET:CE    | 2.50                     | 0.40              |
| 1:E:334:ASN:OD1   | 1:E:334:ASN:N     | 2.54                     | 0.40              |
| 2:F:1093:PHE:C    | 2:F:1093:PHE:HD2  | 2.29                     | 0.40              |
| 2:F:1274:TYR:O    | 2:F:1274:TYR:CG   | 2.73                     | 0.40              |
| 2:F:1331:ILE:O    | 2:F:1334:SER:OG   | 2.38                     | 0.40              |
| 1:A:89:ILE:HD11   | 1:A:117:MET:SD    | 2.61                     | 0.40              |
| 1:A:142:LEU:HD12  | 1:A:142:LEU:HA    | 1.82                     | 0.40              |
| 1:A:214:ILE:HG12  | 1:A:220:ILE:HG12  | 2.04                     | 0.40              |
| 2:B:952:TYR:CE1   | 2:B:988:ASP:OD2   | 2.73                     | 0.40              |
| 2:D:1274:TYR:O    | 2:D:1274:TYR:CG   | 2.74                     | 0.40              |
| 5:D:2001:NAG:O3   | 5:D:2001:NAG:C7   | 2.69                     | 0.40              |
| 2:F:966:PRO:C     | 2:F:968:HIS:N     | 2.78                     | 0.40              |
| 2:F:1051:ASP:OD1  | 2:F:1077:ARG:HD2  | 2.21                     | 0.40              |
| 2:B:1244:LYS:O    | 2:B:1244:LYS:HG2  | 2.22                     | 0.40              |
| 2:B:1314:THR:HG22 | 2:B:1315:GLY:H    | 1.84                     | 0.40              |
| 5:B:2001:NAG:O3   | 5:B:2001:NAG:C7   | 2.69                     | 0.40              |
| 1:C:267:SER:HB3   | 1:C:366:TRP:CH2   | 2.56                     | 0.40              |
| 2:D:975:GLU:HG3   | 2:D:1036:LEU:HD23 | 2.02                     | 0.40              |
| 2:D:1022:LEU:HA   | 2:D:1022:LEU:HD23 | 1.66                     | 0.40              |
| 2:D:1192:TYR:HE1  | 2:D:1258:LYS:CG   | 2.33                     | 0.40              |
| 1:E:214:ILE:HG12  | 1:E:220:ILE:HG12  | 2.03                     | 0.40              |
| 1:E:335:VAL:HG23  | 5:E:2001:NAG:H5   | 2.03                     | 0.40              |
| 2:F:962:ILE:O     | 2:F:1019:SER:HA   | 2.21                     | 0.40              |
| 6:A:2007:B12:H481 | 6:A:2007:B12:H473 | 1.14                     | 0.40              |
| 2:B:1099:ILE:O    | 2:B:1102:TYR:HB2  | 2.22                     | 0.40              |
| 2:B:1297:PRO:O    | 2:B:1380:LYS:CD   | 2.63                     | 0.40              |
| 1:C:80:MET:HE1    | 1:C:104:ARG:HH11  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:950:ASN:HA   | 2:D:951:VAL:HA   | 1.76                     | 0.40              |
| 2:D:966:PRO:C    | 2:D:968:HIS:N    | 2.78                     | 0.40              |
| 2:D:1221:ASP:OD2 | 2:D:1262:ASP:OD1 | 2.40                     | 0.40              |
| 2:D:1235:LEU:O   | 2:D:1235:LEU:HG  | 2.22                     | 0.40              |
| 2:F:1089:HIS:HB2 | 2:F:1157:TYR:CE2 | 2.56                     | 0.40              |
| 2:F:1288:TYR:N   | 2:F:1288:TYR:CD2 | 2.89                     | 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     | 381/393 (97%)   | 334 (88%)  | 37 (10%)  | 10 (3%)  | 4           | 23 |
| 1   | C     | 381/393 (97%)   | 334 (88%)  | 37 (10%)  | 10 (3%)  | 4           | 23 |
| 1   | E     | 381/393 (97%)   | 334 (88%)  | 37 (10%)  | 10 (3%)  | 4           | 23 |
| 2   | B     | 455/457 (100%)  | 376 (83%)  | 52 (11%)  | 27 (6%)  | 1           | 9  |
| 2   | D     | 455/457 (100%)  | 376 (83%)  | 52 (11%)  | 27 (6%)  | 1           | 9  |
| 2   | F     | 455/457 (100%)  | 376 (83%)  | 52 (11%)  | 27 (6%)  | 1           | 9  |
| All | All   | 2508/2550 (98%) | 2130 (85%) | 267 (11%) | 111 (4%) | 2           | 13 |

All (111) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 107  | GLY  |
| 1   | A     | 309  | ALA  |
| 2   | B     | 1105 | ASP  |
| 2   | B     | 1162 | SER  |
| 2   | B     | 1219 | THR  |
| 1   | C     | 107  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 309  | ALA  |
| 2   | D     | 1105 | ASP  |
| 2   | D     | 1162 | SER  |
| 2   | D     | 1219 | THR  |
| 1   | E     | 107  | GLY  |
| 1   | E     | 309  | ALA  |
| 2   | F     | 1105 | ASP  |
| 2   | F     | 1162 | SER  |
| 2   | F     | 1219 | THR  |
| 1   | A     | 291  | ASP  |
| 2   | B     | 950  | ASN  |
| 2   | B     | 987  | ASN  |
| 2   | B     | 1046 | THR  |
| 2   | B     | 1169 | LEU  |
| 2   | B     | 1179 | PRO  |
| 2   | B     | 1218 | CYS  |
| 2   | B     | 1227 | ASP  |
| 2   | B     | 1265 | GLN  |
| 2   | B     | 1294 | ILE  |
| 1   | C     | 291  | ASP  |
| 2   | D     | 950  | ASN  |
| 2   | D     | 987  | ASN  |
| 2   | D     | 1046 | THR  |
| 2   | D     | 1169 | LEU  |
| 2   | D     | 1179 | PRO  |
| 2   | D     | 1209 | ASP  |
| 2   | D     | 1218 | CYS  |
| 2   | D     | 1227 | ASP  |
| 2   | D     | 1265 | GLN  |
| 2   | D     | 1294 | ILE  |
| 1   | E     | 291  | ASP  |
| 2   | F     | 950  | ASN  |
| 2   | F     | 987  | ASN  |
| 2   | F     | 1046 | THR  |
| 2   | F     | 1169 | LEU  |
| 2   | F     | 1179 | PRO  |
| 2   | F     | 1218 | CYS  |
| 2   | F     | 1227 | ASP  |
| 2   | F     | 1265 | GLN  |
| 2   | F     | 1294 | ILE  |
| 1   | A     | 241  | LYS  |
| 1   | A     | 338  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1054 | ASP  |
| 2   | B     | 1209 | ASP  |
| 2   | B     | 1328 | GLU  |
| 2   | B     | 1378 | ARG  |
| 1   | C     | 241  | LYS  |
| 1   | C     | 338  | LYS  |
| 2   | D     | 1054 | ASP  |
| 2   | D     | 1328 | GLU  |
| 2   | D     | 1378 | ARG  |
| 1   | E     | 338  | LYS  |
| 2   | F     | 1054 | ASP  |
| 2   | F     | 1209 | ASP  |
| 2   | F     | 1328 | GLU  |
| 2   | F     | 1378 | ARG  |
| 1   | A     | 217  | ASN  |
| 1   | A     | 339  | SER  |
| 2   | B     | 1030 | LEU  |
| 2   | B     | 1180 | ASN  |
| 2   | B     | 1330 | HIS  |
| 1   | C     | 217  | ASN  |
| 1   | C     | 339  | SER  |
| 2   | D     | 1030 | LEU  |
| 2   | D     | 1180 | ASN  |
| 2   | D     | 1330 | HIS  |
| 1   | E     | 217  | ASN  |
| 1   | E     | 241  | LYS  |
| 1   | E     | 339  | SER  |
| 2   | F     | 1030 | LEU  |
| 2   | F     | 1180 | ASN  |
| 2   | F     | 1330 | HIS  |
| 2   | B     | 977  | PHE  |
| 2   | B     | 1009 | ILE  |
| 2   | B     | 1037 | ILE  |
| 2   | D     | 977  | PHE  |
| 2   | D     | 1009 | ILE  |
| 2   | D     | 1037 | ILE  |
| 2   | F     | 977  | PHE  |
| 2   | F     | 1009 | ILE  |
| 2   | F     | 1037 | ILE  |
| 2   | B     | 1149 | ASP  |
| 2   | B     | 1326 | ASP  |
| 2   | D     | 1149 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 1326 | ASP  |
| 2   | F     | 1149 | ASP  |
| 2   | F     | 1326 | ASP  |
| 1   | A     | 38   | GLY  |
| 2   | B     | 1080 | VAL  |
| 2   | B     | 1358 | PRO  |
| 1   | C     | 38   | GLY  |
| 2   | D     | 1080 | VAL  |
| 2   | D     | 1358 | PRO  |
| 1   | E     | 38   | GLY  |
| 2   | F     | 1080 | VAL  |
| 2   | F     | 1358 | PRO  |
| 1   | C     | 391  | GLY  |
| 1   | A     | 391  | GLY  |
| 1   | E     | 391  | GLY  |
| 1   | A     | 392  | VAL  |
| 2   | B     | 1264 | GLY  |
| 1   | C     | 392  | VAL  |
| 2   | D     | 1264 | GLY  |
| 1   | E     | 392  | VAL  |
| 2   | F     | 1264 | GLY  |

### 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     | 337/343 (98%)   | 276 (82%)  | 61 (18%)  | 2           | 8 |
| 1   | C     | 337/343 (98%)   | 276 (82%)  | 61 (18%)  | 2           | 8 |
| 1   | E     | 337/343 (98%)   | 276 (82%)  | 61 (18%)  | 2           | 8 |
| 2   | B     | 406/406 (100%)  | 324 (80%)  | 82 (20%)  | 1           | 6 |
| 2   | D     | 406/406 (100%)  | 324 (80%)  | 82 (20%)  | 1           | 6 |
| 2   | F     | 406/406 (100%)  | 324 (80%)  | 82 (20%)  | 1           | 6 |
| All | All   | 2229/2247 (99%) | 1800 (81%) | 429 (19%) | 1           | 7 |

All (429) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | SER  |
| 1   | A     | 39  | ILE  |
| 1   | A     | 40  | GLN  |
| 1   | A     | 42  | LEU  |
| 1   | A     | 52  | TYR  |
| 1   | A     | 56  | SER  |
| 1   | A     | 63  | LEU  |
| 1   | A     | 86  | ASP  |
| 1   | A     | 89  | ILE  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 115 | ARG  |
| 1   | A     | 124 | SER  |
| 1   | A     | 137 | LEU  |
| 1   | A     | 139 | ILE  |
| 1   | A     | 142 | LEU  |
| 1   | A     | 177 | THR  |
| 1   | A     | 180 | LEU  |
| 1   | A     | 191 | SER  |
| 1   | A     | 198 | LEU  |
| 1   | A     | 206 | ILE  |
| 1   | A     | 212 | MET  |
| 1   | A     | 215 | LYS  |
| 1   | A     | 219 | ILE  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 225 | SER  |
| 1   | A     | 226 | THR  |
| 1   | A     | 235 | VAL  |
| 1   | A     | 236 | THR  |
| 1   | A     | 238 | GLU  |
| 1   | A     | 251 | ASP  |
| 1   | A     | 271 | ILE  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 283 | VAL  |
| 1   | A     | 310 | SER  |
| 1   | A     | 311 | ASN  |
| 1   | A     | 312 | ILE  |
| 1   | A     | 313 | THR  |
| 1   | A     | 314 | VAL  |
| 1   | A     | 322 | LEU  |
| 1   | A     | 323 | ARG  |
| 1   | A     | 325 | VAL  |
| 1   | A     | 327 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 328  | LEU  |
| 1   | A     | 332  | THR  |
| 1   | A     | 333  | ILE  |
| 1   | A     | 334  | ASN  |
| 1   | A     | 335  | VAL  |
| 1   | A     | 337  | VAL  |
| 1   | A     | 341  | SER  |
| 1   | A     | 347  | LEU  |
| 1   | A     | 352  | ARG  |
| 1   | A     | 361  | THR  |
| 1   | A     | 362  | THR  |
| 1   | A     | 368  | LEU  |
| 1   | A     | 376  | ILE  |
| 1   | A     | 380  | VAL  |
| 1   | A     | 383  | LYS  |
| 1   | A     | 384  | THR  |
| 1   | A     | 389  | LEU  |
| 1   | A     | 393  | THR  |
| 1   | A     | 417  | TYR  |
| 2   | B     | 935  | ILE  |
| 2   | B     | 937  | THR  |
| 2   | B     | 939  | SER  |
| 2   | B     | 940  | THR  |
| 2   | B     | 942  | THR  |
| 2   | B     | 945  | SER  |
| 2   | B     | 954  | HIS  |
| 2   | B     | 959  | THR  |
| 2   | B     | 964  | VAL  |
| 2   | B     | 970  | ILE  |
| 2   | B     | 973  | MET  |
| 2   | B     | 976  | THR  |
| 2   | B     | 978  | HIS  |
| 2   | B     | 980  | GLU  |
| 2   | B     | 985  | CYS  |
| 2   | B     | 988  | ASP  |
| 2   | B     | 992  | VAL  |
| 2   | B     | 995  | THR  |
| 2   | B     | 997  | SER  |
| 2   | B     | 1000 | SER  |
| 2   | B     | 1021 | MET  |
| 2   | B     | 1025 | VAL  |
| 2   | B     | 1029 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1035 | PHE  |
| 2   | B     | 1037 | ILE  |
| 2   | B     | 1042 | ILE  |
| 2   | B     | 1048 | CYS  |
| 2   | B     | 1050 | GLN  |
| 2   | B     | 1059 | PHE  |
| 2   | B     | 1060 | THR  |
| 2   | B     | 1075 | ILE  |
| 2   | B     | 1077 | ARG  |
| 2   | B     | 1078 | ILE  |
| 2   | B     | 1079 | THR  |
| 2   | B     | 1080 | VAL  |
| 2   | B     | 1088 | VAL  |
| 2   | B     | 1091 | THR  |
| 2   | B     | 1095 | LEU  |
| 2   | B     | 1115 | GLU  |
| 2   | B     | 1128 | LEU  |
| 2   | B     | 1144 | LYS  |
| 2   | B     | 1149 | ASP  |
| 2   | B     | 1150 | THR  |
| 2   | B     | 1158 | TRP  |
| 2   | B     | 1161 | SER  |
| 2   | B     | 1165 | CYS  |
| 2   | B     | 1170 | THR  |
| 2   | B     | 1173 | SER  |
| 2   | B     | 1176 | PHE  |
| 2   | B     | 1183 | MET  |
| 2   | B     | 1193 | TRP  |
| 2   | B     | 1205 | LEU  |
| 2   | B     | 1219 | THR  |
| 2   | B     | 1223 | LEU  |
| 2   | B     | 1225 | VAL  |
| 2   | B     | 1231 | SER  |
| 2   | B     | 1237 | THR  |
| 2   | B     | 1239 | LEU  |
| 2   | B     | 1242 | ASP  |
| 2   | B     | 1243 | GLU  |
| 2   | B     | 1247 | LEU  |
| 2   | B     | 1254 | SER  |
| 2   | B     | 1259 | LEU  |
| 2   | B     | 1263 | GLU  |
| 2   | B     | 1275 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1277 | THR  |
| 2   | B     | 1278 | CYS  |
| 2   | B     | 1282 | VAL  |
| 2   | B     | 1284 | VAL  |
| 2   | B     | 1287 | THR  |
| 2   | B     | 1291 | LEU  |
| 2   | B     | 1301 | SER  |
| 2   | B     | 1309 | THR  |
| 2   | B     | 1321 | THR  |
| 2   | B     | 1335 | THR  |
| 2   | B     | 1365 | LYS  |
| 2   | B     | 1366 | LEU  |
| 2   | B     | 1368 | VAL  |
| 2   | B     | 1377 | ARG  |
| 2   | B     | 1378 | ARG  |
| 2   | B     | 1379 | GLU  |
| 2   | B     | 1388 | VAL  |
| 1   | C     | 25   | SER  |
| 1   | C     | 39   | ILE  |
| 1   | C     | 40   | GLN  |
| 1   | C     | 42   | LEU  |
| 1   | C     | 52   | TYR  |
| 1   | C     | 56   | SER  |
| 1   | C     | 63   | LEU  |
| 1   | C     | 86   | ASP  |
| 1   | C     | 89   | ILE  |
| 1   | C     | 94   | LEU  |
| 1   | C     | 115  | ARG  |
| 1   | C     | 124  | SER  |
| 1   | C     | 137  | LEU  |
| 1   | C     | 139  | ILE  |
| 1   | C     | 142  | LEU  |
| 1   | C     | 177  | THR  |
| 1   | C     | 180  | LEU  |
| 1   | C     | 191  | SER  |
| 1   | C     | 198  | LEU  |
| 1   | C     | 206  | ILE  |
| 1   | C     | 212  | MET  |
| 1   | C     | 215  | LYS  |
| 1   | C     | 219  | ILE  |
| 1   | C     | 223  | ILE  |
| 1   | C     | 225  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 226 | THR  |
| 1   | C     | 235 | VAL  |
| 1   | C     | 236 | THR  |
| 1   | C     | 238 | GLU  |
| 1   | C     | 251 | ASP  |
| 1   | C     | 271 | ILE  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 283 | VAL  |
| 1   | C     | 310 | SER  |
| 1   | C     | 311 | ASN  |
| 1   | C     | 312 | ILE  |
| 1   | C     | 313 | THR  |
| 1   | C     | 314 | VAL  |
| 1   | C     | 322 | LEU  |
| 1   | C     | 323 | ARG  |
| 1   | C     | 325 | VAL  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 328 | LEU  |
| 1   | C     | 332 | THR  |
| 1   | C     | 333 | ILE  |
| 1   | C     | 334 | ASN  |
| 1   | C     | 335 | VAL  |
| 1   | C     | 337 | VAL  |
| 1   | C     | 341 | SER  |
| 1   | C     | 347 | LEU  |
| 1   | C     | 352 | ARG  |
| 1   | C     | 361 | THR  |
| 1   | C     | 362 | THR  |
| 1   | C     | 368 | LEU  |
| 1   | C     | 376 | ILE  |
| 1   | C     | 380 | VAL  |
| 1   | C     | 383 | LYS  |
| 1   | C     | 384 | THR  |
| 1   | C     | 389 | LEU  |
| 1   | C     | 393 | THR  |
| 1   | C     | 417 | TYR  |
| 2   | D     | 935 | ILE  |
| 2   | D     | 937 | THR  |
| 2   | D     | 939 | SER  |
| 2   | D     | 940 | THR  |
| 2   | D     | 942 | THR  |
| 2   | D     | 945 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 954  | HIS  |
| 2   | D     | 959  | THR  |
| 2   | D     | 964  | VAL  |
| 2   | D     | 970  | ILE  |
| 2   | D     | 973  | MET  |
| 2   | D     | 976  | THR  |
| 2   | D     | 978  | HIS  |
| 2   | D     | 980  | GLU  |
| 2   | D     | 985  | CYS  |
| 2   | D     | 988  | ASP  |
| 2   | D     | 992  | VAL  |
| 2   | D     | 995  | THR  |
| 2   | D     | 997  | SER  |
| 2   | D     | 1000 | SER  |
| 2   | D     | 1021 | MET  |
| 2   | D     | 1025 | VAL  |
| 2   | D     | 1029 | ASP  |
| 2   | D     | 1035 | PHE  |
| 2   | D     | 1037 | ILE  |
| 2   | D     | 1042 | ILE  |
| 2   | D     | 1048 | CYS  |
| 2   | D     | 1050 | GLN  |
| 2   | D     | 1059 | PHE  |
| 2   | D     | 1060 | THR  |
| 2   | D     | 1075 | ILE  |
| 2   | D     | 1077 | ARG  |
| 2   | D     | 1078 | ILE  |
| 2   | D     | 1079 | THR  |
| 2   | D     | 1080 | VAL  |
| 2   | D     | 1088 | VAL  |
| 2   | D     | 1091 | THR  |
| 2   | D     | 1095 | LEU  |
| 2   | D     | 1115 | GLU  |
| 2   | D     | 1128 | LEU  |
| 2   | D     | 1144 | LYS  |
| 2   | D     | 1149 | ASP  |
| 2   | D     | 1150 | THR  |
| 2   | D     | 1158 | TRP  |
| 2   | D     | 1161 | SER  |
| 2   | D     | 1165 | CYS  |
| 2   | D     | 1170 | THR  |
| 2   | D     | 1173 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 1176 | PHE  |
| 2   | D     | 1183 | MET  |
| 2   | D     | 1193 | TRP  |
| 2   | D     | 1205 | LEU  |
| 2   | D     | 1219 | THR  |
| 2   | D     | 1223 | LEU  |
| 2   | D     | 1225 | VAL  |
| 2   | D     | 1231 | SER  |
| 2   | D     | 1237 | THR  |
| 2   | D     | 1239 | LEU  |
| 2   | D     | 1242 | ASP  |
| 2   | D     | 1243 | GLU  |
| 2   | D     | 1247 | LEU  |
| 2   | D     | 1254 | SER  |
| 2   | D     | 1259 | LEU  |
| 2   | D     | 1263 | GLU  |
| 2   | D     | 1275 | ARG  |
| 2   | D     | 1277 | THR  |
| 2   | D     | 1278 | CYS  |
| 2   | D     | 1282 | VAL  |
| 2   | D     | 1284 | VAL  |
| 2   | D     | 1287 | THR  |
| 2   | D     | 1291 | LEU  |
| 2   | D     | 1301 | SER  |
| 2   | D     | 1309 | THR  |
| 2   | D     | 1321 | THR  |
| 2   | D     | 1335 | THR  |
| 2   | D     | 1365 | LYS  |
| 2   | D     | 1366 | LEU  |
| 2   | D     | 1368 | VAL  |
| 2   | D     | 1377 | ARG  |
| 2   | D     | 1378 | ARG  |
| 2   | D     | 1379 | GLU  |
| 2   | D     | 1388 | VAL  |
| 1   | E     | 25   | SER  |
| 1   | E     | 39   | ILE  |
| 1   | E     | 40   | GLN  |
| 1   | E     | 42   | LEU  |
| 1   | E     | 52   | TYR  |
| 1   | E     | 56   | SER  |
| 1   | E     | 63   | LEU  |
| 1   | E     | 86   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 89  | ILE  |
| 1   | E     | 94  | LEU  |
| 1   | E     | 115 | ARG  |
| 1   | E     | 124 | SER  |
| 1   | E     | 137 | LEU  |
| 1   | E     | 139 | ILE  |
| 1   | E     | 142 | LEU  |
| 1   | E     | 177 | THR  |
| 1   | E     | 180 | LEU  |
| 1   | E     | 191 | SER  |
| 1   | E     | 198 | LEU  |
| 1   | E     | 206 | ILE  |
| 1   | E     | 212 | MET  |
| 1   | E     | 215 | LYS  |
| 1   | E     | 219 | ILE  |
| 1   | E     | 223 | ILE  |
| 1   | E     | 225 | SER  |
| 1   | E     | 226 | THR  |
| 1   | E     | 235 | VAL  |
| 1   | E     | 236 | THR  |
| 1   | E     | 238 | GLU  |
| 1   | E     | 251 | ASP  |
| 1   | E     | 271 | ILE  |
| 1   | E     | 272 | LEU  |
| 1   | E     | 283 | VAL  |
| 1   | E     | 310 | SER  |
| 1   | E     | 311 | ASN  |
| 1   | E     | 312 | ILE  |
| 1   | E     | 313 | THR  |
| 1   | E     | 314 | VAL  |
| 1   | E     | 322 | LEU  |
| 1   | E     | 323 | ARG  |
| 1   | E     | 325 | VAL  |
| 1   | E     | 327 | LEU  |
| 1   | E     | 328 | LEU  |
| 1   | E     | 332 | THR  |
| 1   | E     | 333 | ILE  |
| 1   | E     | 334 | ASN  |
| 1   | E     | 335 | VAL  |
| 1   | E     | 337 | VAL  |
| 1   | E     | 341 | SER  |
| 1   | E     | 347 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 352  | ARG  |
| 1   | E     | 361  | THR  |
| 1   | E     | 362  | THR  |
| 1   | E     | 368  | LEU  |
| 1   | E     | 376  | ILE  |
| 1   | E     | 380  | VAL  |
| 1   | E     | 383  | LYS  |
| 1   | E     | 384  | THR  |
| 1   | E     | 389  | LEU  |
| 1   | E     | 393  | THR  |
| 1   | E     | 417  | TYR  |
| 2   | F     | 935  | ILE  |
| 2   | F     | 937  | THR  |
| 2   | F     | 939  | SER  |
| 2   | F     | 940  | THR  |
| 2   | F     | 942  | THR  |
| 2   | F     | 945  | SER  |
| 2   | F     | 954  | HIS  |
| 2   | F     | 959  | THR  |
| 2   | F     | 964  | VAL  |
| 2   | F     | 970  | ILE  |
| 2   | F     | 973  | MET  |
| 2   | F     | 976  | THR  |
| 2   | F     | 978  | HIS  |
| 2   | F     | 980  | GLU  |
| 2   | F     | 985  | CYS  |
| 2   | F     | 988  | ASP  |
| 2   | F     | 992  | VAL  |
| 2   | F     | 995  | THR  |
| 2   | F     | 997  | SER  |
| 2   | F     | 1000 | SER  |
| 2   | F     | 1021 | MET  |
| 2   | F     | 1025 | VAL  |
| 2   | F     | 1029 | ASP  |
| 2   | F     | 1035 | PHE  |
| 2   | F     | 1037 | ILE  |
| 2   | F     | 1042 | ILE  |
| 2   | F     | 1048 | CYS  |
| 2   | F     | 1050 | GLN  |
| 2   | F     | 1059 | PHE  |
| 2   | F     | 1060 | THR  |
| 2   | F     | 1075 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | F     | 1077 | ARG  |
| 2   | F     | 1078 | ILE  |
| 2   | F     | 1079 | THR  |
| 2   | F     | 1080 | VAL  |
| 2   | F     | 1088 | VAL  |
| 2   | F     | 1091 | THR  |
| 2   | F     | 1095 | LEU  |
| 2   | F     | 1115 | GLU  |
| 2   | F     | 1128 | LEU  |
| 2   | F     | 1144 | LYS  |
| 2   | F     | 1149 | ASP  |
| 2   | F     | 1150 | THR  |
| 2   | F     | 1158 | TRP  |
| 2   | F     | 1161 | SER  |
| 2   | F     | 1165 | CYS  |
| 2   | F     | 1170 | THR  |
| 2   | F     | 1173 | SER  |
| 2   | F     | 1176 | PHE  |
| 2   | F     | 1183 | MET  |
| 2   | F     | 1193 | TRP  |
| 2   | F     | 1205 | LEU  |
| 2   | F     | 1219 | THR  |
| 2   | F     | 1223 | LEU  |
| 2   | F     | 1225 | VAL  |
| 2   | F     | 1231 | SER  |
| 2   | F     | 1237 | THR  |
| 2   | F     | 1239 | LEU  |
| 2   | F     | 1242 | ASP  |
| 2   | F     | 1243 | GLU  |
| 2   | F     | 1247 | LEU  |
| 2   | F     | 1254 | SER  |
| 2   | F     | 1259 | LEU  |
| 2   | F     | 1263 | GLU  |
| 2   | F     | 1275 | ARG  |
| 2   | F     | 1277 | THR  |
| 2   | F     | 1278 | CYS  |
| 2   | F     | 1282 | VAL  |
| 2   | F     | 1284 | VAL  |
| 2   | F     | 1287 | THR  |
| 2   | F     | 1291 | LEU  |
| 2   | F     | 1301 | SER  |
| 2   | F     | 1309 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | F     | 1321 | THR  |
| 2   | F     | 1335 | THR  |
| 2   | F     | 1365 | LYS  |
| 2   | F     | 1366 | LEU  |
| 2   | F     | 1368 | VAL  |
| 2   | F     | 1377 | ARG  |
| 2   | F     | 1378 | ARG  |
| 2   | F     | 1379 | GLU  |
| 2   | F     | 1388 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 32   | GLN  |
| 1   | A     | 72   | GLN  |
| 1   | A     | 85   | ASN  |
| 1   | A     | 144  | GLN  |
| 1   | A     | 295  | GLN  |
| 2   | B     | 954  | HIS  |
| 2   | B     | 961  | HIS  |
| 2   | B     | 967  | ASN  |
| 2   | B     | 978  | HIS  |
| 2   | B     | 1050 | GLN  |
| 2   | B     | 1070 | ASN  |
| 2   | B     | 1187 | HIS  |
| 2   | B     | 1265 | GLN  |
| 2   | B     | 1266 | GLN  |
| 2   | B     | 1280 | ASN  |
| 1   | C     | 32   | GLN  |
| 1   | C     | 72   | GLN  |
| 1   | C     | 85   | ASN  |
| 1   | C     | 144  | GLN  |
| 1   | C     | 292  | HIS  |
| 1   | C     | 295  | GLN  |
| 2   | D     | 954  | HIS  |
| 2   | D     | 961  | HIS  |
| 2   | D     | 967  | ASN  |
| 2   | D     | 978  | HIS  |
| 2   | D     | 1050 | GLN  |
| 2   | D     | 1070 | ASN  |
| 2   | D     | 1187 | HIS  |
| 2   | D     | 1265 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | D     | 1266 | GLN  |
| 2   | D     | 1280 | ASN  |
| 1   | E     | 32   | GLN  |
| 1   | E     | 72   | GLN  |
| 1   | E     | 85   | ASN  |
| 1   | E     | 144  | GLN  |
| 1   | E     | 292  | HIS  |
| 1   | E     | 295  | GLN  |
| 2   | F     | 954  | HIS  |
| 2   | F     | 961  | HIS  |
| 2   | F     | 967  | ASN  |
| 2   | F     | 978  | HIS  |
| 2   | F     | 982  | HIS  |
| 2   | F     | 1050 | GLN  |
| 2   | F     | 1070 | ASN  |
| 2   | F     | 1187 | HIS  |
| 2   | F     | 1265 | GLN  |
| 2   | F     | 1266 | GLN  |
| 2   | F     | 1280 | ASN  |
| 2   | F     | 1346 | 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 ⓘ

36 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 |
| 3   | NAG  | G     | 1   | 3,1  | 14,14,15     | 0.78 | 0        | 17,19,21    | 2.58 | 5 (29%)  |
| 3   | NAG  | G     | 2   | 3    | 14,14,15     | 1.03 | 1 (7%)   | 17,19,21    | 2.73 | 10 (58%) |
| 3   | BMA  | G     | 3   | 3    | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 3   | MAN  | G     | 4   | 3    | 11,11,12     | 1.26 | 2 (18%)  | 15,15,17    | 2.12 | 7 (46%)  |
| 3   | MAN  | G     | 5   | 3    | 11,11,12     | 1.28 | 2 (18%)  | 15,15,17    | 2.03 | 6 (40%)  |
| 3   | NAG  | H     | 1   | 2,3  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 3.28 | 9 (52%)  |
| 3   | NAG  | H     | 2   | 3    | 14,14,15     | 0.36 | 0        | 17,19,21    | 1.26 | 2 (11%)  |
| 3   | BMA  | H     | 3   | 3    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.05 | 4 (26%)  |
| 3   | MAN  | H     | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 2.98 | 11 (73%) |
| 3   | MAN  | H     | 5   | 3    | 11,11,12     | 1.13 | 1 (9%)   | 15,15,17    | 1.82 | 4 (26%)  |
| 4   | NAG  | I     | 1   | 4,2  | 14,14,15     | 0.55 | 0        | 17,19,21    | 2.16 | 3 (17%)  |
| 4   | NAG  | I     | 2   | 4    | 14,14,15     | 0.98 | 1 (7%)   | 17,19,21    | 1.69 | 3 (17%)  |
| 3   | NAG  | J     | 1   | 3,1  | 14,14,15     | 0.79 | 0        | 17,19,21    | 2.58 | 5 (29%)  |
| 3   | NAG  | J     | 2   | 3    | 14,14,15     | 1.04 | 1 (7%)   | 17,19,21    | 2.73 | 10 (58%) |
| 3   | BMA  | J     | 3   | 3    | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 3   | MAN  | J     | 4   | 3    | 11,11,12     | 1.26 | 2 (18%)  | 15,15,17    | 2.12 | 7 (46%)  |
| 3   | MAN  | J     | 5   | 3    | 11,11,12     | 1.28 | 2 (18%)  | 15,15,17    | 2.02 | 6 (40%)  |
| 3   | NAG  | K     | 1   | 2,3  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 3.28 | 9 (52%)  |
| 3   | NAG  | K     | 2   | 3    | 14,14,15     | 0.36 | 0        | 17,19,21    | 1.25 | 2 (11%)  |
| 3   | BMA  | K     | 3   | 3    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.05 | 4 (26%)  |
| 3   | MAN  | K     | 4   | 3    | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 2.97 | 11 (73%) |
| 3   | MAN  | K     | 5   | 3    | 11,11,12     | 1.13 | 1 (9%)   | 15,15,17    | 1.82 | 4 (26%)  |
| 4   | NAG  | L     | 1   | 4,2  | 14,14,15     | 0.55 | 0        | 17,19,21    | 2.16 | 3 (17%)  |
| 4   | NAG  | L     | 2   | 4    | 14,14,15     | 0.98 | 1 (7%)   | 17,19,21    | 1.69 | 3 (17%)  |
| 3   | NAG  | M     | 1   | 3,1  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 2.58 | 5 (29%)  |
| 3   | NAG  | M     | 2   | 3    | 14,14,15     | 1.02 | 1 (7%)   | 17,19,21    | 2.73 | 10 (58%) |
| 3   | BMA  | M     | 3   | 3    | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 3   | MAN  | M     | 4   | 3    | 11,11,12     | 1.26 | 2 (18%)  | 15,15,17    | 2.12 | 7 (46%)  |
| 3   | MAN  | M     | 5   | 3    | 11,11,12     | 1.27 | 2 (18%)  | 15,15,17    | 2.03 | 6 (40%)  |
| 3   | NAG  | N     | 1   | 2,3  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 3.28 | 9 (52%)  |
| 3   | NAG  | N     | 2   | 3    | 14,14,15     | 0.36 | 0        | 17,19,21    | 1.26 | 2 (11%)  |
| 3   | BMA  | N     | 3   | 3    | 11,11,12     | 0.60 | 0        | 15,15,17    | 2.06 | 4 (26%)  |
| 3   | MAN  | N     | 4   | 3    | 11,11,12     | 1.21 | 2 (18%)  | 15,15,17    | 2.97 | 11 (73%) |
| 3   | MAN  | N     | 5   | 3    | 11,11,12     | 1.13 | 1 (9%)   | 15,15,17    | 1.82 | 4 (26%)  |
| 4   | NAG  | O     | 1   | 4,2  | 14,14,15     | 0.56 | 0        | 17,19,21    | 2.16 | 3 (17%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | O     | 2   | 4    | 14,14,15     | 0.98 | 1 (7%)   | 17,19,21    | 1.69 | 3 (17%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | G     | 1   | 3,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | G     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | G     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | G     | 5   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | H     | 1   | 2,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | H     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | H     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | H     | 4   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | MAN  | H     | 5   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | NAG  | I     | 1   | 4,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 1   | 3,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | J     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | J     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | J     | 5   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | K     | 1   | 2,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | K     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | K     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | K     | 4   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | MAN  | K     | 5   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | NAG  | L     | 1   | 4,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | L     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 1   | 3,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | M     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | M     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | M     | 5   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | N     | 1   | 2,3  | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | N     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | N     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | N     | 4   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | MAN  | N     | 5   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | NAG  | O     | 1   | 4,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | O     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | J     | 2   | NAG  | C1-C2 | 3.11 | 1.56        | 1.52     |
| 3   | G     | 2   | NAG  | C1-C2 | 3.10 | 1.56        | 1.52     |
| 3   | M     | 2   | NAG  | C1-C2 | 3.06 | 1.56        | 1.52     |
| 3   | J     | 5   | MAN  | C1-C2 | 2.87 | 1.59        | 1.52     |
| 3   | G     | 5   | MAN  | C1-C2 | 2.86 | 1.59        | 1.52     |
| 3   | M     | 5   | MAN  | C1-C2 | 2.84 | 1.59        | 1.52     |
| 3   | M     | 4   | MAN  | O5-C1 | 2.53 | 1.47        | 1.43     |
| 3   | J     | 4   | MAN  | O5-C1 | 2.52 | 1.47        | 1.43     |
| 3   | G     | 4   | MAN  | O5-C1 | 2.51 | 1.47        | 1.43     |
| 3   | G     | 4   | MAN  | C1-C2 | 2.43 | 1.58        | 1.52     |
| 3   | M     | 4   | MAN  | C1-C2 | 2.43 | 1.58        | 1.52     |
| 3   | J     | 4   | MAN  | C1-C2 | 2.43 | 1.58        | 1.52     |
| 3   | N     | 4   | MAN  | O5-C1 | 2.30 | 1.47        | 1.43     |
| 4   | L     | 2   | NAG  | C1-C2 | 2.30 | 1.55        | 1.52     |
| 3   | H     | 4   | MAN  | O5-C1 | 2.28 | 1.47        | 1.43     |
| 4   | I     | 2   | NAG  | C1-C2 | 2.27 | 1.55        | 1.52     |
| 3   | K     | 4   | MAN  | O5-C1 | 2.26 | 1.47        | 1.43     |
| 4   | O     | 2   | NAG  | C1-C2 | 2.23 | 1.55        | 1.52     |
| 3   | M     | 5   | MAN  | O5-C1 | 2.10 | 1.47        | 1.43     |
| 3   | J     | 5   | MAN  | O5-C1 | 2.09 | 1.47        | 1.43     |
| 3   | G     | 5   | MAN  | O5-C1 | 2.09 | 1.47        | 1.43     |
| 3   | N     | 5   | MAN  | C1-C2 | 2.09 | 1.57        | 1.52     |
| 3   | H     | 5   | MAN  | C1-C2 | 2.08 | 1.57        | 1.52     |
| 3   | H     | 1   | NAG  | C1-C2 | 2.08 | 1.55        | 1.52     |
| 3   | K     | 1   | NAG  | C1-C2 | 2.07 | 1.55        | 1.52     |
| 3   | K     | 5   | MAN  | C1-C2 | 2.07 | 1.57        | 1.52     |
| 3   | N     | 1   | NAG  | C1-C2 | 2.06 | 1.55        | 1.52     |
| 3   | K     | 4   | MAN  | C1-C2 | 2.06 | 1.57        | 1.52     |
| 3   | N     | 4   | MAN  | C1-C2 | 2.06 | 1.57        | 1.52     |
| 3   | H     | 4   | MAN  | C1-C2 | 2.05 | 1.57        | 1.52     |
| 3   | M     | 1   | NAG  | C3-C2 | 2.01 | 1.56        | 1.52     |

All (198) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | K     | 1   | NAG  | C1-O5-C5 | 8.70  | 123.84      | 112.19   |
| 3   | H     | 1   | NAG  | C1-O5-C5 | 8.69  | 123.83      | 112.19   |
| 3   | N     | 1   | NAG  | C1-O5-C5 | 8.68  | 123.83      | 112.19   |
| 3   | J     | 1   | NAG  | C1-O5-C5 | 7.06  | 121.65      | 112.19   |
| 3   | G     | 1   | NAG  | C1-O5-C5 | 7.06  | 121.65      | 112.19   |
| 3   | M     | 1   | NAG  | C1-O5-C5 | 7.04  | 121.62      | 112.19   |
| 3   | H     | 4   | MAN  | C1-O5-C5 | 6.96  | 121.51      | 112.19   |
| 3   | N     | 4   | MAN  | C1-O5-C5 | 6.94  | 121.49      | 112.19   |
| 3   | K     | 4   | MAN  | C1-O5-C5 | 6.94  | 121.49      | 112.19   |
| 4   | L     | 1   | NAG  | O5-C1-C2 | -5.48 | 102.81      | 111.29   |
| 4   | O     | 1   | NAG  | O5-C1-C2 | -5.48 | 102.81      | 111.29   |
| 4   | I     | 1   | NAG  | O5-C1-C2 | -5.47 | 102.83      | 111.29   |
| 3   | N     | 3   | BMA  | C1-C2-C3 | 5.46  | 117.60      | 109.64   |
| 3   | K     | 3   | BMA  | C1-C2-C3 | 5.44  | 117.56      | 109.64   |
| 3   | H     | 3   | BMA  | C1-C2-C3 | 5.43  | 117.55      | 109.64   |
| 3   | J     | 2   | NAG  | C2-N2-C7 | 5.29  | 129.99      | 122.90   |
| 3   | G     | 2   | NAG  | C2-N2-C7 | 5.28  | 129.98      | 122.90   |
| 3   | M     | 2   | NAG  | C2-N2-C7 | 5.24  | 129.92      | 122.90   |
| 4   | L     | 1   | NAG  | C2-N2-C7 | -5.19 | 115.94      | 122.90   |
| 4   | O     | 1   | NAG  | C2-N2-C7 | -5.17 | 115.97      | 122.90   |
| 4   | I     | 1   | NAG  | C2-N2-C7 | -5.16 | 115.98      | 122.90   |
| 3   | J     | 2   | NAG  | O5-C1-C2 | -4.73 | 103.97      | 111.29   |
| 3   | G     | 2   | NAG  | O5-C1-C2 | -4.71 | 104.00      | 111.29   |
| 3   | M     | 2   | NAG  | O5-C1-C2 | -4.71 | 104.00      | 111.29   |
| 4   | I     | 2   | NAG  | C4-C3-C2 | 4.41  | 117.48      | 111.02   |
| 4   | L     | 2   | NAG  | C4-C3-C2 | 4.41  | 117.48      | 111.02   |
| 4   | O     | 2   | NAG  | C4-C3-C2 | 4.39  | 117.45      | 111.02   |
| 3   | H     | 5   | MAN  | C1-O5-C5 | 4.28  | 117.92      | 112.19   |
| 3   | N     | 5   | MAN  | C1-O5-C5 | 4.26  | 117.90      | 112.19   |
| 3   | K     | 5   | MAN  | C1-O5-C5 | 4.26  | 117.89      | 112.19   |
| 3   | M     | 2   | NAG  | C1-C2-N2 | 4.21  | 117.06      | 110.43   |
| 3   | H     | 1   | NAG  | C3-C4-C5 | 4.19  | 117.83      | 110.23   |
| 3   | G     | 2   | NAG  | C1-C2-N2 | 4.19  | 117.03      | 110.43   |
| 3   | N     | 1   | NAG  | C3-C4-C5 | 4.18  | 117.82      | 110.23   |
| 3   | K     | 1   | NAG  | C3-C4-C5 | 4.18  | 117.80      | 110.23   |
| 3   | J     | 2   | NAG  | C1-C2-N2 | 4.18  | 117.01      | 110.43   |
| 3   | M     | 4   | MAN  | C1-O5-C5 | 4.15  | 117.75      | 112.19   |
| 3   | M     | 1   | NAG  | O5-C5-C6 | -4.13 | 99.62       | 107.66   |
| 3   | G     | 4   | MAN  | C1-O5-C5 | 4.13  | 117.72      | 112.19   |
| 3   | G     | 1   | NAG  | O5-C5-C6 | -4.11 | 99.66       | 107.66   |
| 3   | J     | 1   | NAG  | O5-C5-C6 | -4.11 | 99.66       | 107.66   |
| 3   | J     | 4   | MAN  | C1-O5-C5 | 4.11  | 117.69      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | K     | 1   | NAG  | C2-N2-C7 | 4.07  | 128.35      | 122.90   |
| 3   | H     | 1   | NAG  | C2-N2-C7 | 4.05  | 128.33      | 122.90   |
| 3   | N     | 1   | NAG  | C2-N2-C7 | 4.02  | 128.29      | 122.90   |
| 3   | H     | 4   | MAN  | O5-C5-C6 | 3.88  | 115.22      | 107.66   |
| 3   | N     | 4   | MAN  | O5-C5-C6 | 3.87  | 115.19      | 107.66   |
| 3   | K     | 4   | MAN  | O5-C5-C6 | 3.87  | 115.19      | 107.66   |
| 3   | K     | 1   | NAG  | O4-C4-C3 | -3.85 | 101.30      | 110.38   |
| 3   | H     | 1   | NAG  | O4-C4-C3 | -3.84 | 101.31      | 110.38   |
| 3   | N     | 1   | NAG  | O4-C4-C3 | -3.84 | 101.32      | 110.38   |
| 3   | H     | 1   | NAG  | C4-C3-C2 | 3.81  | 116.59      | 111.02   |
| 3   | K     | 1   | NAG  | C4-C3-C2 | 3.80  | 116.59      | 111.02   |
| 3   | N     | 1   | NAG  | C4-C3-C2 | 3.80  | 116.59      | 111.02   |
| 3   | H     | 4   | MAN  | C2-C3-C4 | -3.75 | 104.27      | 110.86   |
| 3   | K     | 4   | MAN  | C2-C3-C4 | -3.74 | 104.28      | 110.86   |
| 3   | N     | 4   | MAN  | C2-C3-C4 | -3.73 | 104.29      | 110.86   |
| 3   | G     | 1   | NAG  | O4-C4-C3 | 3.63  | 118.94      | 110.38   |
| 3   | J     | 1   | NAG  | O4-C4-C3 | 3.62  | 118.92      | 110.38   |
| 3   | M     | 1   | NAG  | O4-C4-C3 | 3.61  | 118.89      | 110.38   |
| 3   | G     | 3   | BMA  | C1-O5-C5 | -3.49 | 107.51      | 112.19   |
| 3   | J     | 3   | BMA  | C1-O5-C5 | -3.48 | 107.52      | 112.19   |
| 3   | M     | 3   | BMA  | C1-O5-C5 | -3.48 | 107.52      | 112.19   |
| 3   | G     | 5   | MAN  | O2-C2-C1 | 3.43  | 117.08      | 109.22   |
| 3   | M     | 5   | MAN  | O2-C2-C1 | 3.43  | 117.08      | 109.22   |
| 3   | J     | 5   | MAN  | O2-C2-C1 | 3.43  | 117.08      | 109.22   |
| 3   | J     | 2   | NAG  | O5-C5-C4 | 3.38  | 119.04      | 110.83   |
| 3   | G     | 2   | NAG  | O5-C5-C4 | 3.38  | 119.04      | 110.83   |
| 3   | M     | 2   | NAG  | O5-C5-C4 | 3.37  | 119.03      | 110.83   |
| 3   | M     | 5   | MAN  | C1-O5-C5 | 3.36  | 116.69      | 112.19   |
| 3   | J     | 5   | MAN  | C1-O5-C5 | 3.34  | 116.66      | 112.19   |
| 3   | G     | 5   | MAN  | C1-O5-C5 | 3.34  | 116.66      | 112.19   |
| 3   | H     | 3   | BMA  | O5-C5-C6 | 3.28  | 114.05      | 107.66   |
| 3   | K     | 3   | BMA  | O5-C5-C6 | 3.28  | 114.05      | 107.66   |
| 3   | N     | 3   | BMA  | O5-C5-C6 | 3.28  | 114.04      | 107.66   |
| 4   | L     | 2   | NAG  | C2-N2-C7 | 3.27  | 127.28      | 122.90   |
| 4   | O     | 2   | NAG  | C2-N2-C7 | 3.25  | 127.26      | 122.90   |
| 4   | I     | 2   | NAG  | C2-N2-C7 | 3.25  | 127.25      | 122.90   |
| 3   | M     | 1   | NAG  | O5-C5-C4 | 3.24  | 118.70      | 110.83   |
| 3   | J     | 1   | NAG  | O5-C5-C4 | 3.24  | 118.70      | 110.83   |
| 3   | G     | 1   | NAG  | O5-C5-C4 | 3.23  | 118.70      | 110.83   |
| 3   | N     | 2   | NAG  | C1-C2-N2 | -3.21 | 105.38      | 110.43   |
| 3   | H     | 2   | NAG  | C1-C2-N2 | -3.20 | 105.39      | 110.43   |
| 3   | K     | 4   | MAN  | O3-C3-C2 | 3.20  | 116.58      | 110.05   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | H     | 4   | MAN  | O3-C3-C2 | 3.19  | 116.57      | 110.05   |
| 3   | K     | 2   | NAG  | C1-C2-N2 | -3.19 | 105.41      | 110.43   |
| 3   | N     | 4   | MAN  | O3-C3-C2 | 3.19  | 116.56      | 110.05   |
| 3   | J     | 2   | NAG  | O3-C3-C2 | 2.97  | 115.56      | 109.40   |
| 3   | M     | 2   | NAG  | O3-C3-C2 | 2.95  | 115.54      | 109.40   |
| 3   | G     | 2   | NAG  | O3-C3-C2 | 2.95  | 115.53      | 109.40   |
| 3   | M     | 4   | MAN  | O5-C5-C6 | 2.91  | 113.33      | 107.66   |
| 3   | G     | 4   | MAN  | O5-C5-C6 | 2.90  | 113.31      | 107.66   |
| 3   | J     | 4   | MAN  | O5-C5-C6 | 2.89  | 113.29      | 107.66   |
| 3   | H     | 1   | NAG  | O7-C7-N2 | 2.77  | 126.87      | 121.98   |
| 3   | N     | 1   | NAG  | O7-C7-N2 | 2.77  | 126.87      | 121.98   |
| 3   | K     | 1   | NAG  | O7-C7-N2 | 2.75  | 126.83      | 121.98   |
| 3   | G     | 4   | MAN  | O3-C3-C2 | 2.72  | 115.60      | 110.05   |
| 3   | J     | 4   | MAN  | O3-C3-C2 | 2.71  | 115.59      | 110.05   |
| 3   | M     | 4   | MAN  | O3-C3-C2 | 2.71  | 115.59      | 110.05   |
| 3   | K     | 1   | NAG  | C6-C5-C4 | -2.68 | 106.44      | 113.02   |
| 3   | H     | 1   | NAG  | C6-C5-C4 | -2.67 | 106.46      | 113.02   |
| 3   | N     | 1   | NAG  | C6-C5-C4 | -2.67 | 106.47      | 113.02   |
| 3   | N     | 4   | MAN  | O2-C2-C3 | 2.63  | 115.59      | 110.15   |
| 3   | M     | 5   | MAN  | C2-C3-C4 | -2.63 | 106.24      | 110.86   |
| 3   | N     | 4   | MAN  | O2-C2-C1 | 2.62  | 115.23      | 109.22   |
| 3   | K     | 4   | MAN  | O2-C2-C1 | 2.62  | 115.23      | 109.22   |
| 3   | H     | 4   | MAN  | O2-C2-C1 | 2.62  | 115.22      | 109.22   |
| 3   | G     | 5   | MAN  | C2-C3-C4 | -2.62 | 106.26      | 110.86   |
| 3   | J     | 5   | MAN  | C2-C3-C4 | -2.62 | 106.26      | 110.86   |
| 3   | H     | 4   | MAN  | O2-C2-C3 | 2.61  | 115.55      | 110.15   |
| 3   | K     | 4   | MAN  | O2-C2-C3 | 2.60  | 115.53      | 110.15   |
| 4   | O     | 1   | NAG  | O5-C5-C4 | 2.54  | 117.00      | 110.83   |
| 4   | I     | 1   | NAG  | O5-C5-C4 | 2.53  | 116.98      | 110.83   |
| 4   | L     | 1   | NAG  | O5-C5-C4 | 2.53  | 116.98      | 110.83   |
| 3   | H     | 5   | MAN  | O2-C2-C1 | 2.50  | 114.95      | 109.22   |
| 3   | K     | 5   | MAN  | O2-C2-C1 | 2.50  | 114.94      | 109.22   |
| 3   | N     | 5   | MAN  | O2-C2-C1 | 2.49  | 114.93      | 109.22   |
| 3   | M     | 5   | MAN  | O3-C3-C2 | 2.48  | 115.11      | 110.05   |
| 3   | G     | 5   | MAN  | O3-C3-C2 | 2.47  | 115.10      | 110.05   |
| 3   | J     | 5   | MAN  | O3-C3-C2 | 2.47  | 115.09      | 110.05   |
| 3   | H     | 2   | NAG  | O4-C4-C5 | 2.45  | 115.36      | 109.32   |
| 3   | N     | 2   | NAG  | O4-C4-C5 | 2.45  | 115.35      | 109.32   |
| 3   | K     | 2   | NAG  | O4-C4-C5 | 2.44  | 115.34      | 109.32   |
| 3   | J     | 5   | MAN  | O4-C4-C5 | 2.43  | 115.31      | 109.32   |
| 3   | K     | 3   | BMA  | O2-C2-C3 | -2.43 | 105.13      | 110.15   |
| 3   | G     | 5   | MAN  | O4-C4-C5 | 2.43  | 115.30      | 109.32   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | N     | 3   | BMA  | O2-C2-C3 | -2.42 | 105.14      | 110.15   |
| 3   | H     | 3   | BMA  | O2-C2-C3 | -2.41 | 105.15      | 110.15   |
| 3   | M     | 2   | NAG  | C3-C4-C5 | 2.41  | 114.61      | 110.23   |
| 3   | M     | 5   | MAN  | O4-C4-C5 | 2.41  | 115.27      | 109.32   |
| 3   | G     | 2   | NAG  | O3-C3-C4 | -2.41 | 104.69      | 110.38   |
| 3   | J     | 2   | NAG  | O7-C7-C8 | -2.41 | 117.77      | 122.05   |
| 3   | J     | 2   | NAG  | O3-C3-C4 | -2.41 | 104.70      | 110.38   |
| 3   | G     | 2   | NAG  | O7-C7-C8 | -2.40 | 117.77      | 122.05   |
| 3   | M     | 2   | NAG  | O3-C3-C4 | -2.40 | 104.73      | 110.38   |
| 3   | J     | 2   | NAG  | C3-C4-C5 | 2.39  | 114.57      | 110.23   |
| 3   | M     | 2   | NAG  | O7-C7-C8 | -2.39 | 117.80      | 122.05   |
| 3   | G     | 2   | NAG  | C3-C4-C5 | 2.39  | 114.56      | 110.23   |
| 3   | M     | 4   | MAN  | O4-C4-C5 | 2.36  | 115.14      | 109.32   |
| 3   | M     | 4   | MAN  | O4-C4-C3 | 2.36  | 115.93      | 110.38   |
| 3   | G     | 4   | MAN  | O4-C4-C5 | 2.35  | 115.12      | 109.32   |
| 3   | J     | 4   | MAN  | O4-C4-C3 | 2.35  | 115.91      | 110.38   |
| 3   | G     | 4   | MAN  | O4-C4-C3 | 2.34  | 115.90      | 110.38   |
| 3   | J     | 4   | MAN  | O4-C4-C5 | 2.34  | 115.08      | 109.32   |
| 3   | M     | 5   | MAN  | O5-C5-C6 | 2.29  | 112.12      | 107.66   |
| 3   | G     | 5   | MAN  | O5-C5-C6 | 2.29  | 112.12      | 107.66   |
| 3   | N     | 1   | NAG  | C1-C2-N2 | 2.29  | 114.04      | 110.43   |
| 3   | H     | 1   | NAG  | C1-C2-N2 | 2.29  | 114.04      | 110.43   |
| 3   | J     | 5   | MAN  | O5-C5-C6 | 2.28  | 112.11      | 107.66   |
| 3   | H     | 4   | MAN  | O3-C3-C4 | 2.28  | 115.75      | 110.38   |
| 3   | K     | 4   | MAN  | O3-C3-C4 | 2.28  | 115.75      | 110.38   |
| 3   | M     | 1   | NAG  | C3-C4-C5 | -2.27 | 106.11      | 110.23   |
| 3   | H     | 5   | MAN  | O5-C5-C6 | 2.27  | 112.09      | 107.66   |
| 3   | G     | 1   | NAG  | C3-C4-C5 | -2.27 | 106.11      | 110.23   |
| 3   | J     | 1   | NAG  | C3-C4-C5 | -2.27 | 106.11      | 110.23   |
| 3   | N     | 5   | MAN  | O5-C5-C6 | 2.27  | 112.08      | 107.66   |
| 3   | K     | 5   | MAN  | O5-C5-C6 | 2.26  | 112.07      | 107.66   |
| 3   | N     | 4   | MAN  | O3-C3-C4 | 2.26  | 115.70      | 110.38   |
| 3   | K     | 1   | NAG  | C1-C2-N2 | 2.26  | 113.99      | 110.43   |
| 3   | K     | 4   | MAN  | O5-C1-C2 | 2.22  | 116.09      | 110.79   |
| 3   | H     | 4   | MAN  | O5-C1-C2 | 2.21  | 116.06      | 110.79   |
| 3   | N     | 4   | MAN  | O5-C1-C2 | 2.21  | 116.06      | 110.79   |
| 3   | N     | 1   | NAG  | O6-C6-C5 | 2.21  | 118.85      | 111.33   |
| 3   | H     | 1   | NAG  | O6-C6-C5 | 2.20  | 118.83      | 111.33   |
| 3   | K     | 1   | NAG  | O6-C6-C5 | 2.20  | 118.83      | 111.33   |
| 3   | N     | 4   | MAN  | O4-C4-C3 | 2.18  | 115.52      | 110.38   |
| 3   | G     | 2   | NAG  | O4-C4-C5 | 2.17  | 114.68      | 109.32   |
| 3   | J     | 2   | NAG  | O4-C4-C5 | 2.17  | 114.68      | 109.32   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | H     | 4   | MAN  | O4-C4-C3 | 2.17  | 115.50      | 110.38   |
| 3   | K     | 4   | MAN  | O4-C4-C3 | 2.17  | 115.50      | 110.38   |
| 3   | M     | 2   | NAG  | O4-C4-C5 | 2.17  | 114.67      | 109.32   |
| 3   | K     | 3   | BMA  | C2-C3-C4 | 2.17  | 114.67      | 110.86   |
| 3   | H     | 3   | BMA  | C2-C3-C4 | 2.16  | 114.66      | 110.86   |
| 3   | M     | 3   | BMA  | O4-C4-C5 | 2.16  | 114.64      | 109.32   |
| 3   | G     | 2   | NAG  | C6-C5-C4 | -2.16 | 107.72      | 113.02   |
| 3   | G     | 4   | MAN  | O2-C2-C1 | 2.16  | 114.16      | 109.22   |
| 3   | J     | 2   | NAG  | C6-C5-C4 | -2.15 | 107.75      | 113.02   |
| 3   | M     | 2   | NAG  | C6-C5-C4 | -2.15 | 107.75      | 113.02   |
| 3   | G     | 3   | BMA  | O4-C4-C5 | 2.14  | 114.61      | 109.32   |
| 4   | I     | 2   | NAG  | O7-C7-C8 | -2.14 | 118.24      | 122.05   |
| 3   | J     | 4   | MAN  | O2-C2-C1 | 2.14  | 114.13      | 109.22   |
| 3   | N     | 4   | MAN  | O5-C5-C4 | 2.14  | 116.03      | 110.83   |
| 3   | M     | 4   | MAN  | O2-C2-C1 | 2.14  | 114.12      | 109.22   |
| 3   | N     | 3   | BMA  | C2-C3-C4 | 2.14  | 114.62      | 110.86   |
| 3   | K     | 4   | MAN  | O5-C5-C4 | 2.14  | 116.03      | 110.83   |
| 4   | L     | 2   | NAG  | O7-C7-C8 | -2.14 | 118.25      | 122.05   |
| 3   | J     | 3   | BMA  | O4-C4-C5 | 2.13  | 114.58      | 109.32   |
| 3   | H     | 4   | MAN  | O5-C5-C4 | 2.13  | 116.00      | 110.83   |
| 4   | O     | 2   | NAG  | O7-C7-C8 | -2.13 | 118.27      | 122.05   |
| 3   | N     | 4   | MAN  | O4-C4-C5 | 2.11  | 114.51      | 109.32   |
| 3   | M     | 4   | MAN  | O3-C3-C4 | 2.10  | 115.34      | 110.38   |
| 3   | H     | 4   | MAN  | O4-C4-C5 | 2.10  | 114.49      | 109.32   |
| 3   | K     | 4   | MAN  | O4-C4-C5 | 2.09  | 114.48      | 109.32   |
| 3   | G     | 4   | MAN  | O3-C3-C4 | 2.09  | 115.31      | 110.38   |
| 3   | J     | 4   | MAN  | O3-C3-C4 | 2.09  | 115.29      | 110.38   |
| 3   | K     | 5   | MAN  | O4-C4-C5 | 2.04  | 114.35      | 109.32   |
| 3   | H     | 5   | MAN  | O4-C4-C5 | 2.04  | 114.35      | 109.32   |
| 3   | N     | 5   | MAN  | O4-C4-C5 | 2.03  | 114.31      | 109.32   |

There are no chirality outliers.

All (63) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | G     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | G     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | G     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | H     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | H     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | H     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | J     | 2   | NAG  | C1-C2-N2-C7 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | J     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | J     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | K     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | K     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | K     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | M     | 2   | NAG  | C1-C2-N2-C7 |
| 3   | M     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | M     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | N     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | N     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | N     | 2   | NAG  | O7-C7-N2-C2 |
| 4   | I     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | I     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | L     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | L     | 1   | NAG  | O7-C7-N2-C2 |
| 4   | O     | 1   | NAG  | C8-C7-N2-C2 |
| 4   | O     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | G     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | J     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | M     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | G     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | G     | 5   | MAN  | O5-C5-C6-O6 |
| 3   | H     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | J     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | J     | 5   | MAN  | O5-C5-C6-O6 |
| 3   | K     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | M     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | M     | 5   | MAN  | O5-C5-C6-O6 |
| 3   | N     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | G     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | J     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | M     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | G     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | J     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | M     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | H     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | K     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | N     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | G     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | J     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | M     | 5   | MAN  | C4-C5-C6-O6 |
| 4   | L     | 2   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | O     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | G     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | J     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | M     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | L     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | O     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | K     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | H     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | N     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | H     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | N     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | K     | 5   | MAN  | C4-C5-C6-O6 |

There are no ring outliers.

24 monomers are involved in 31 short contacts:

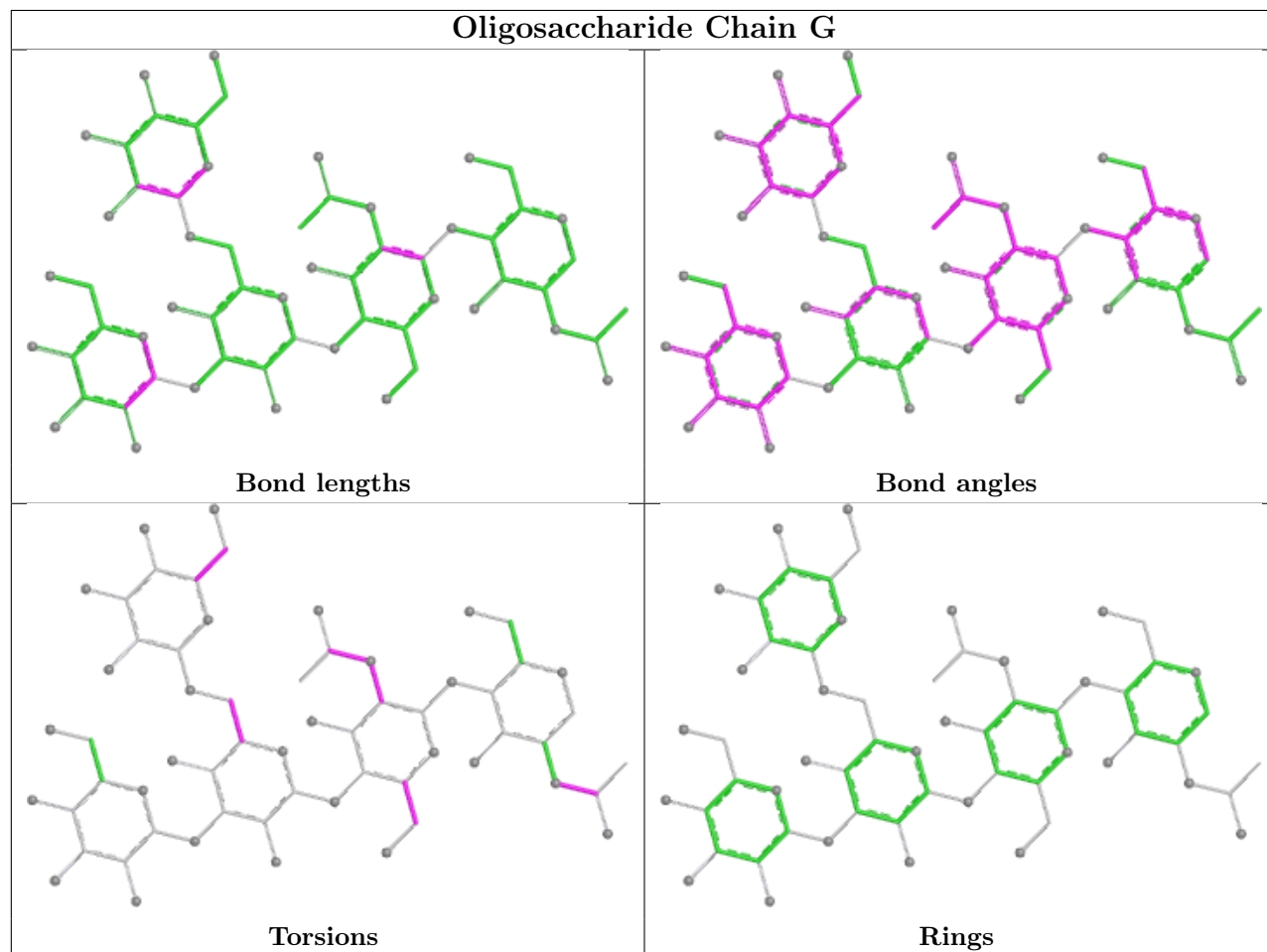
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | G     | 3   | BMA  | 3       | 0            |
| 3   | N     | 2   | NAG  | 1       | 0            |
| 3   | H     | 5   | MAN  | 3       | 0            |
| 3   | M     | 3   | BMA  | 4       | 0            |
| 3   | H     | 2   | NAG  | 1       | 0            |
| 3   | J     | 3   | BMA  | 3       | 0            |
| 3   | K     | 5   | MAN  | 3       | 0            |
| 4   | L     | 2   | NAG  | 1       | 0            |
| 4   | O     | 2   | NAG  | 1       | 0            |
| 3   | K     | 3   | BMA  | 2       | 0            |
| 3   | G     | 5   | MAN  | 3       | 0            |
| 3   | K     | 1   | NAG  | 2       | 0            |
| 3   | H     | 1   | NAG  | 2       | 0            |
| 3   | M     | 5   | MAN  | 4       | 0            |
| 3   | N     | 3   | BMA  | 2       | 0            |
| 3   | N     | 5   | MAN  | 3       | 0            |
| 3   | J     | 5   | MAN  | 3       | 0            |
| 3   | K     | 2   | NAG  | 1       | 0            |
| 4   | I     | 2   | NAG  | 1       | 0            |
| 4   | L     | 1   | NAG  | 2       | 0            |
| 3   | H     | 3   | BMA  | 2       | 0            |
| 3   | N     | 1   | NAG  | 2       | 0            |
| 4   | I     | 1   | NAG  | 2       | 0            |

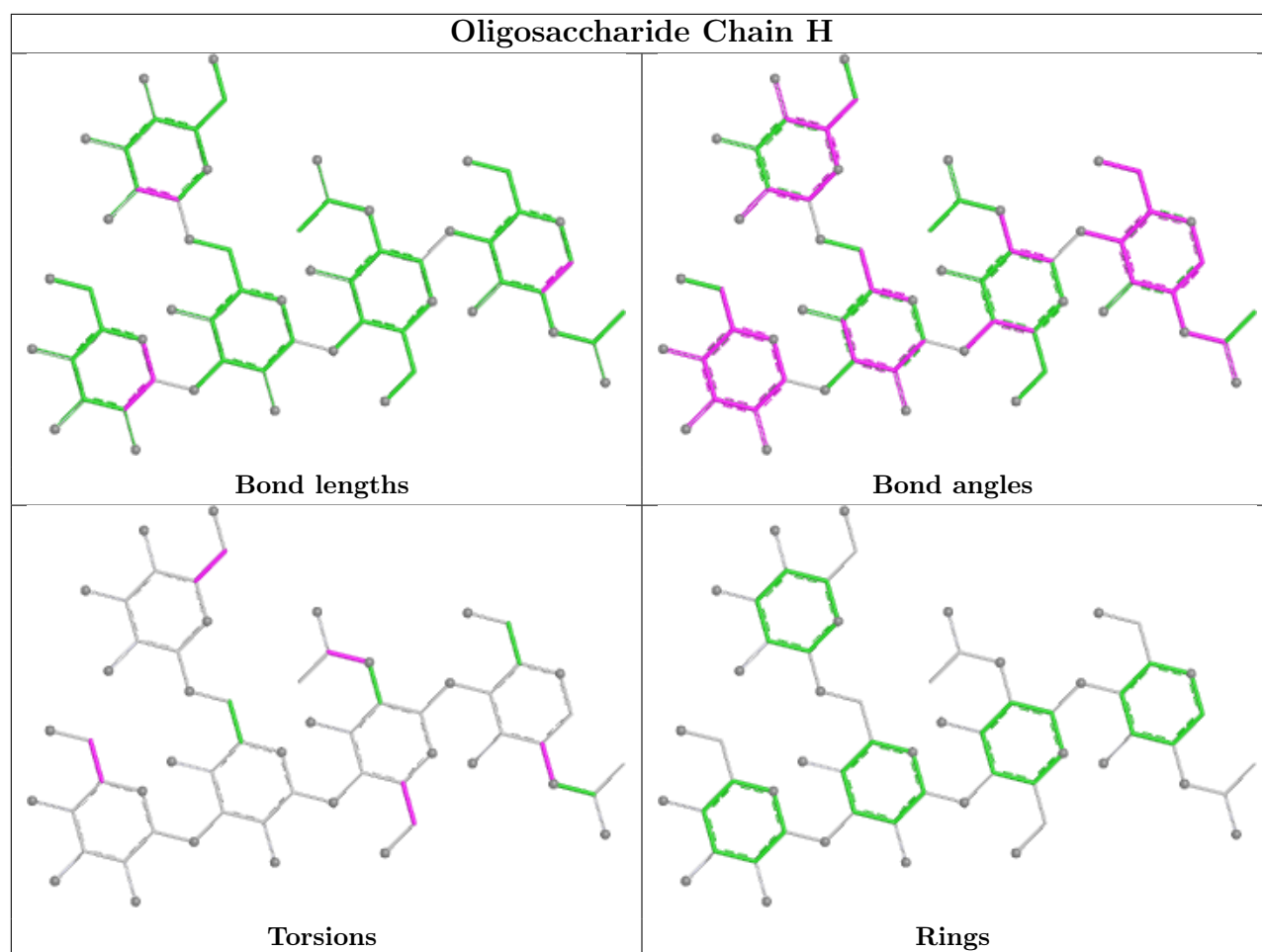
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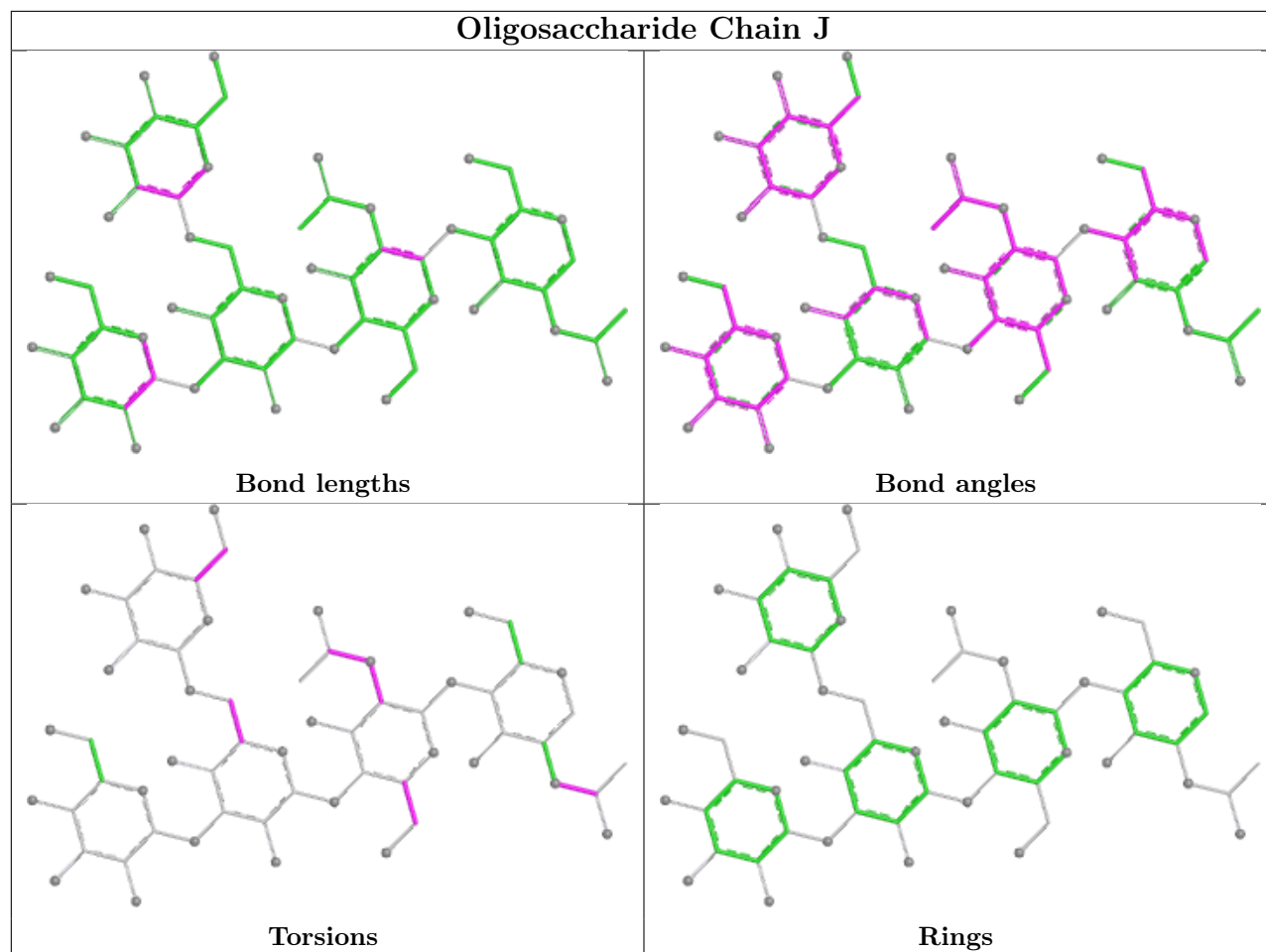
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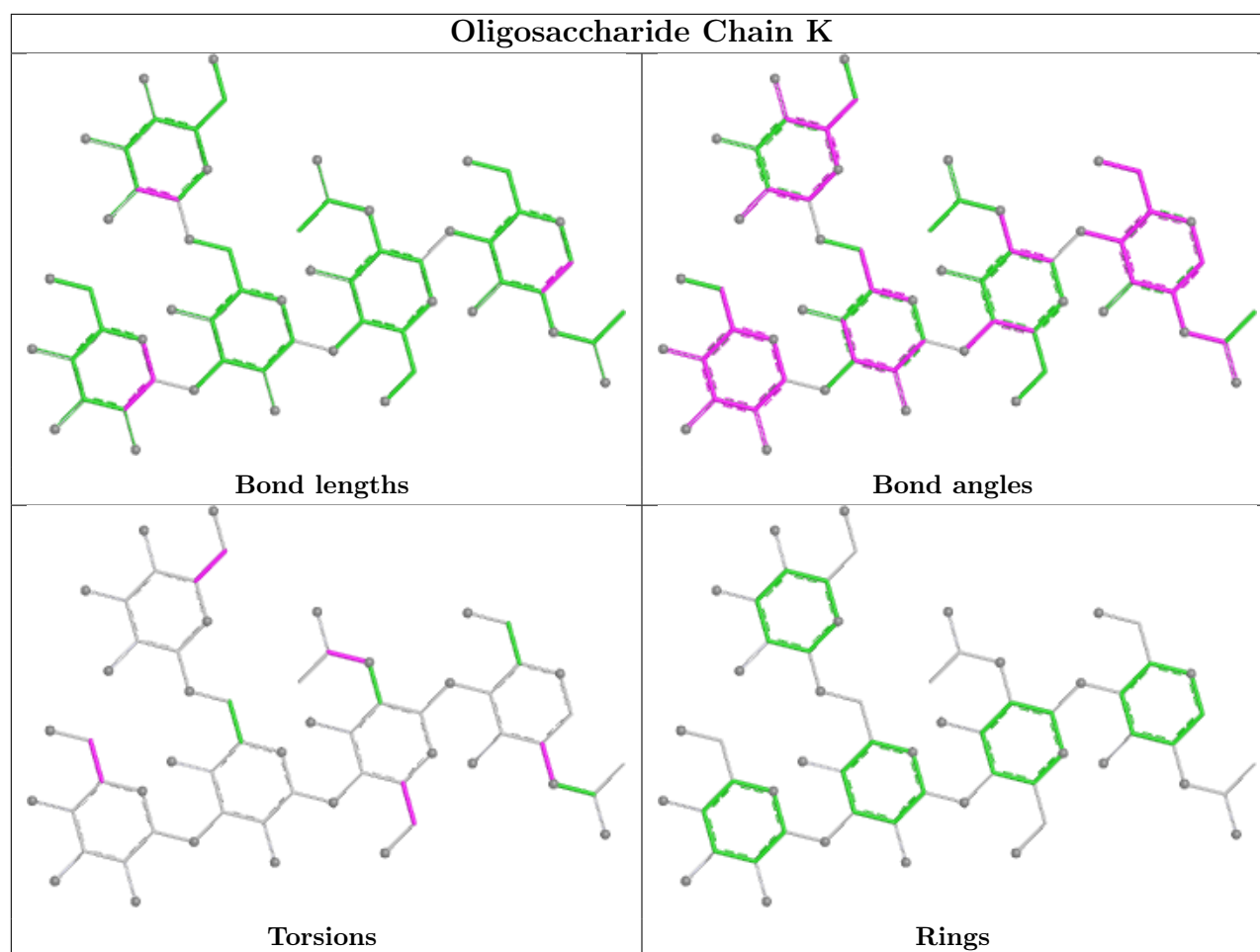
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | O     | 1   | NAG  | 2       | 0            |

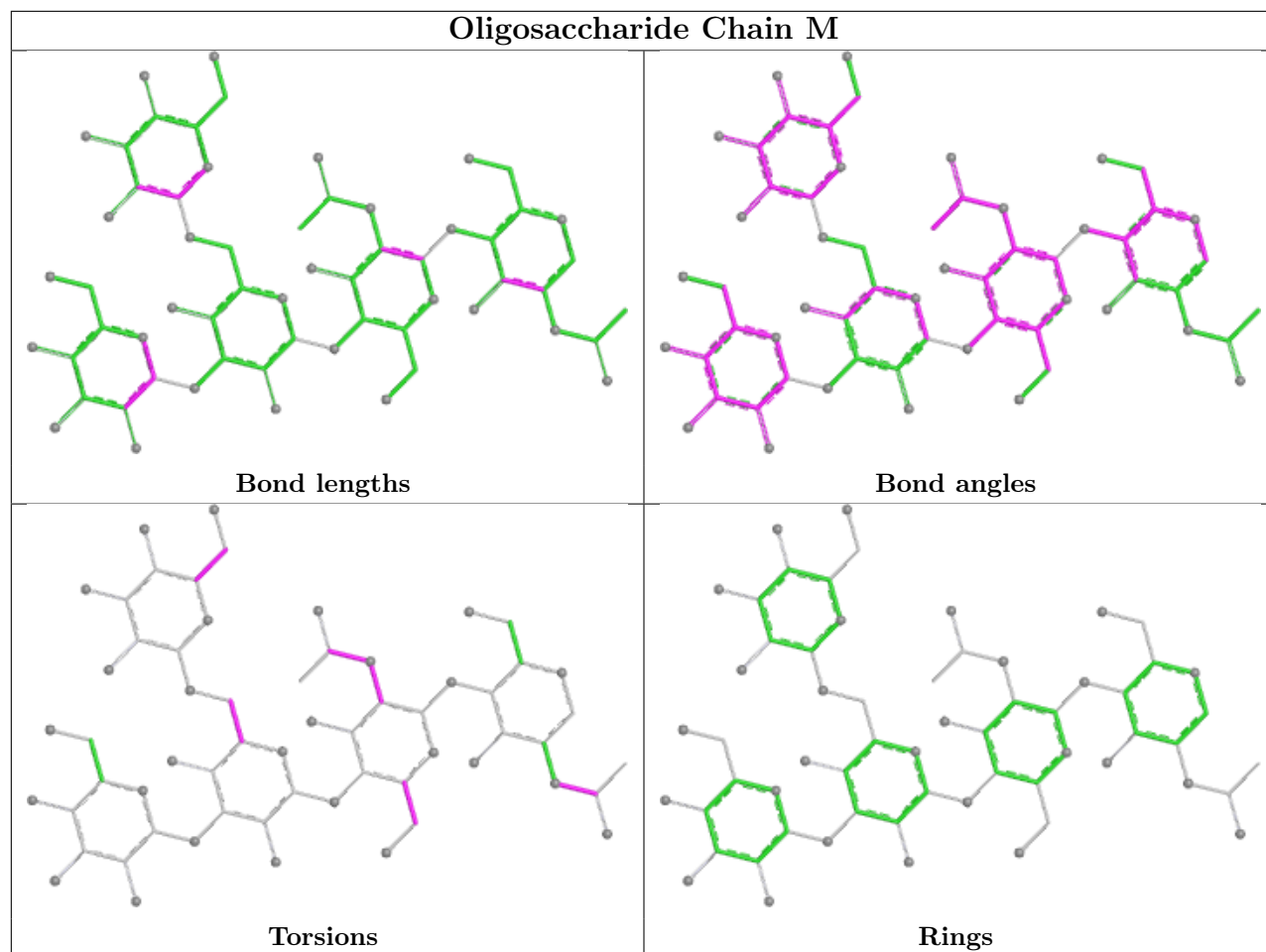
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



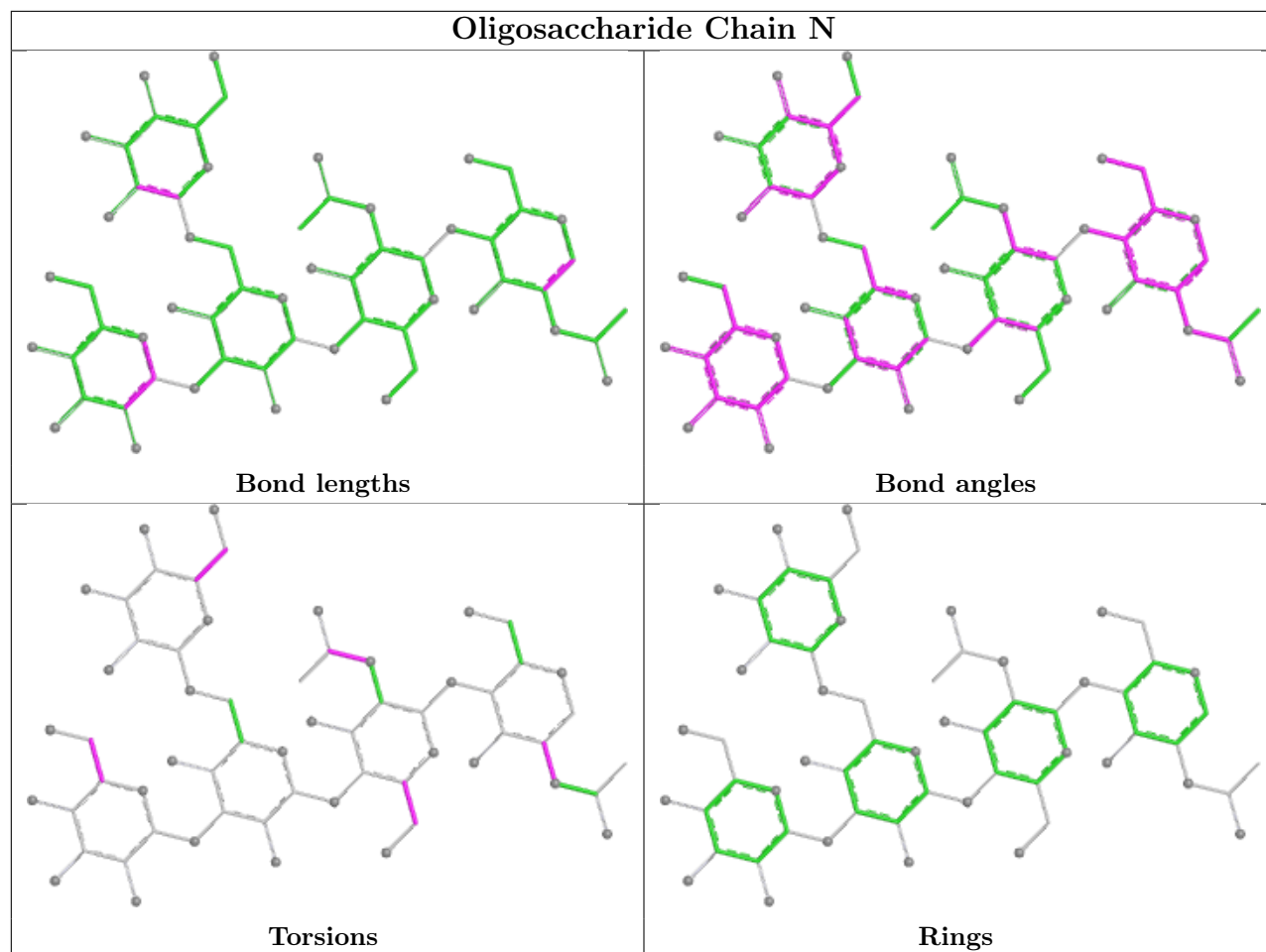


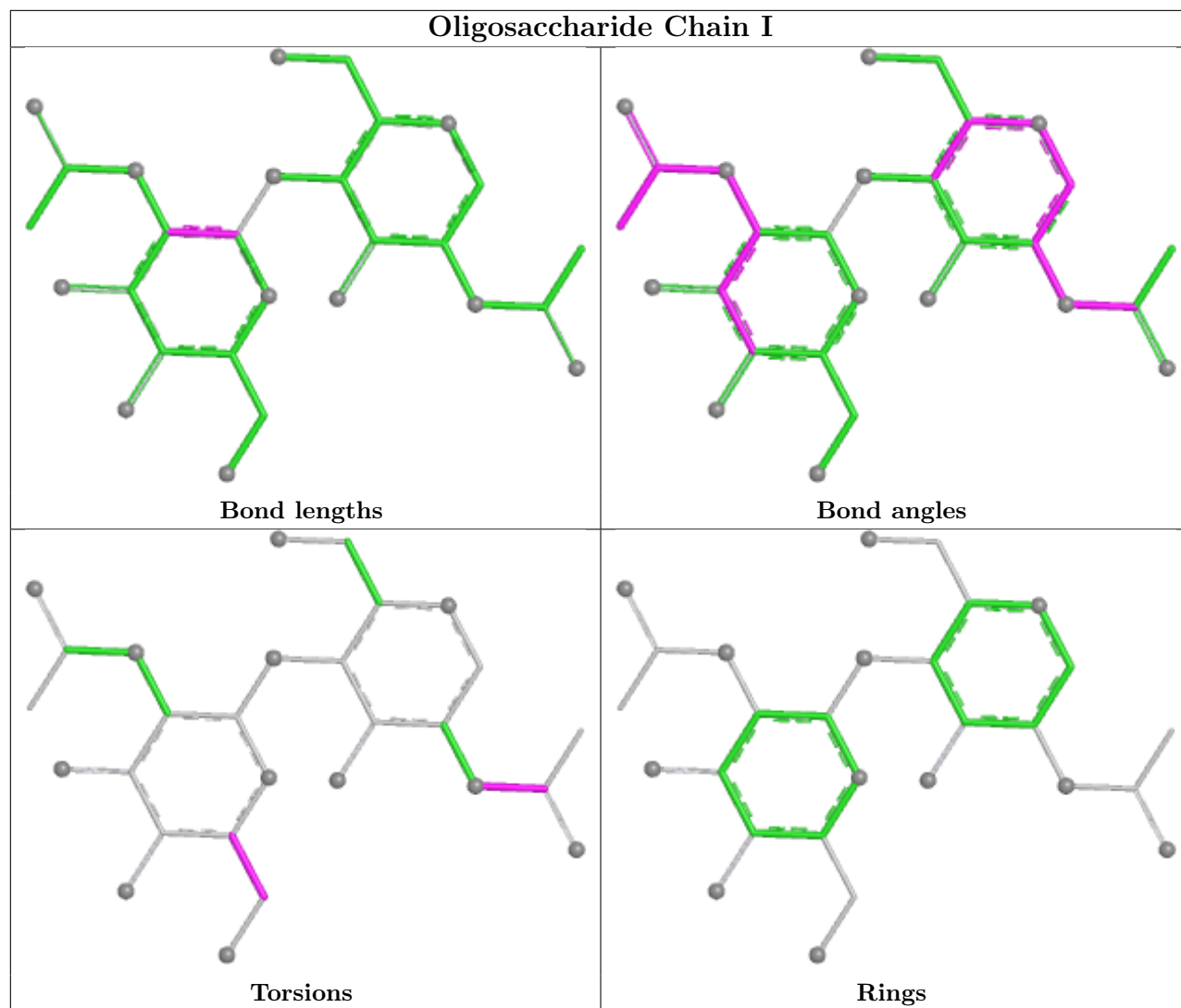


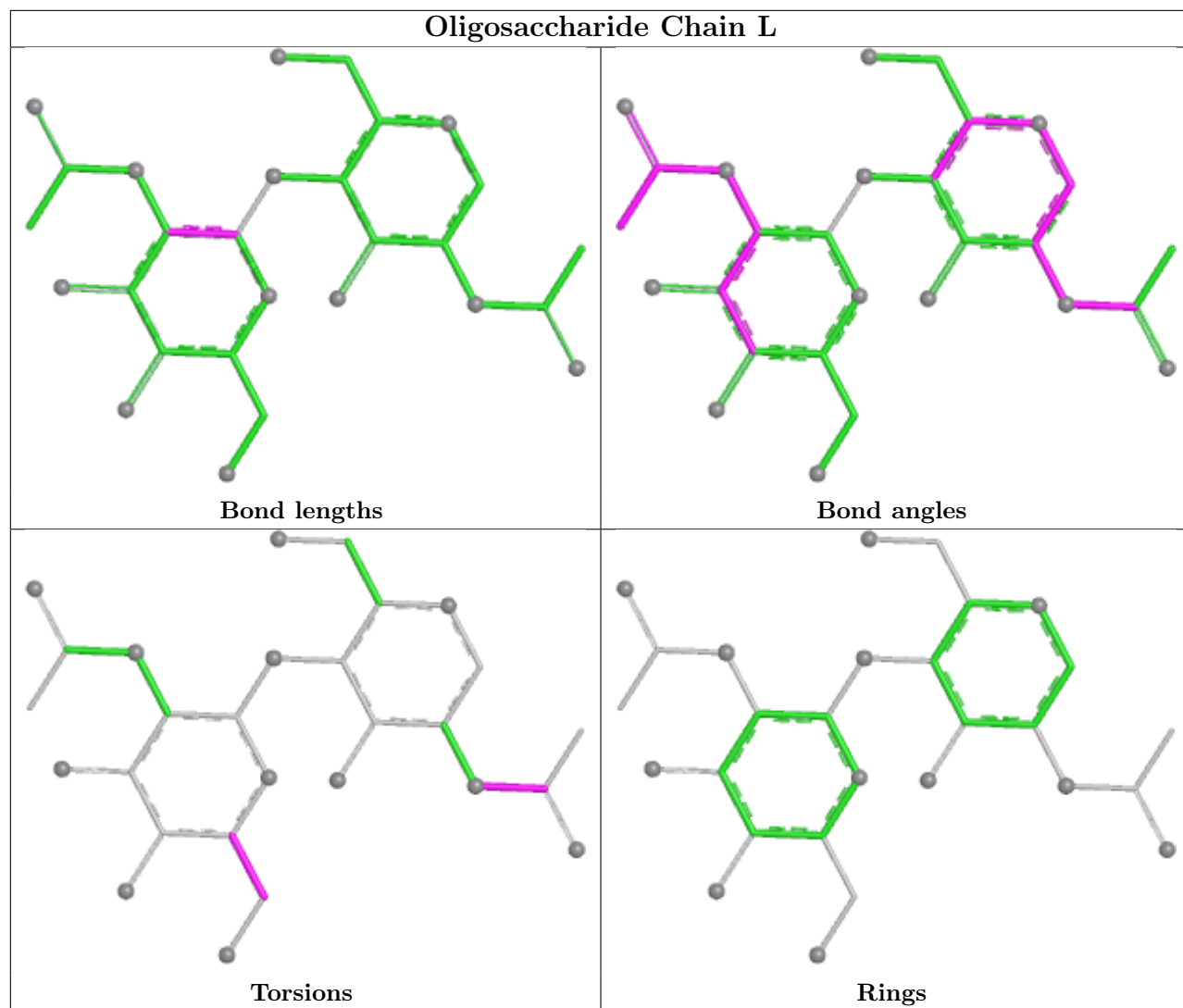


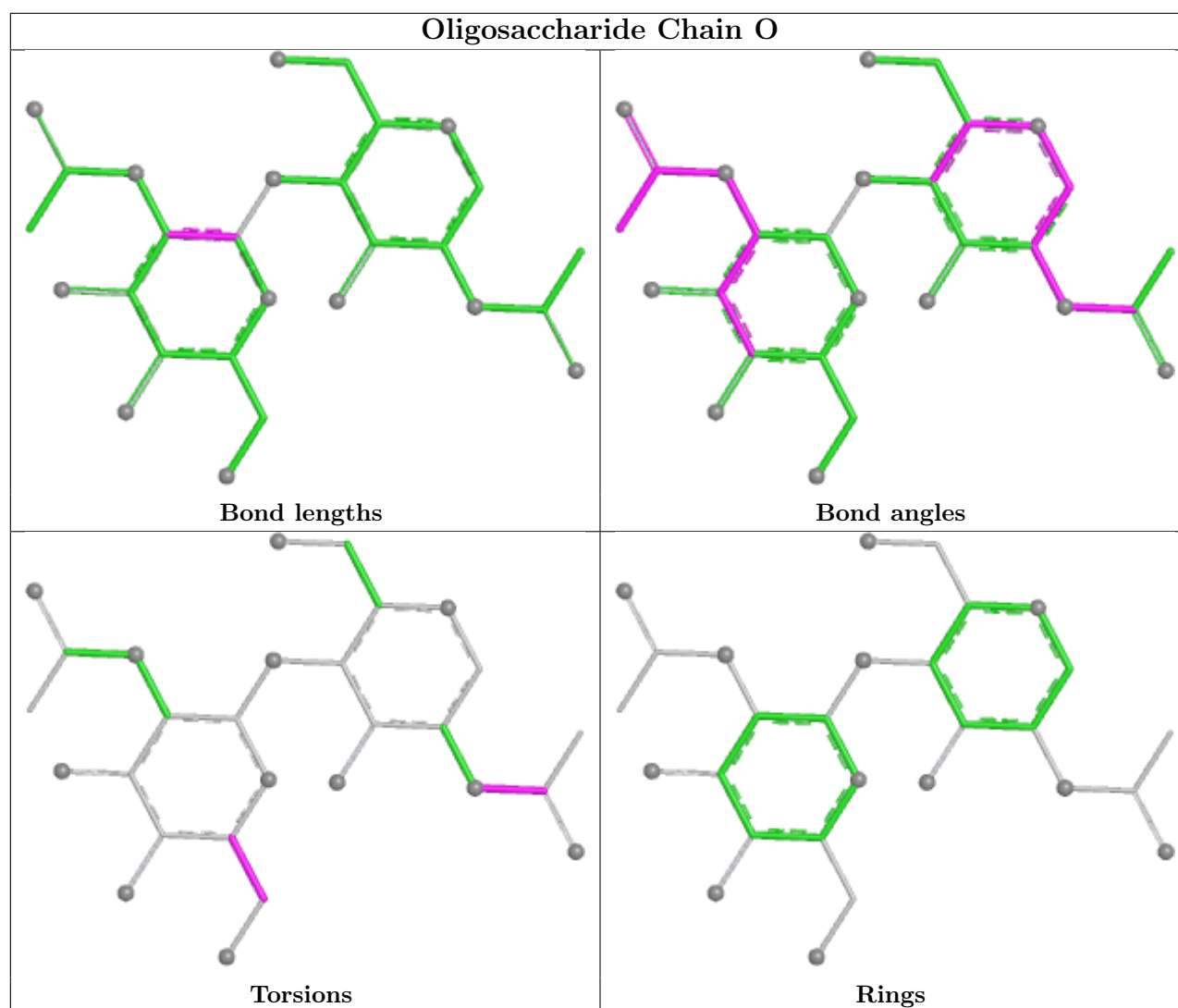












## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 6   | B12  | A     | 2007 | -    | 94,101,101   | 1.60 | 12 (12%)    | 149,166,166 | 2.53 | 42 (28%)    |
| 5   | NAG  | D     | 2013 | 2    | 14,14,15     | 0.63 | 0           | 17,19,21    | 1.99 | 5 (29%)     |
| 5   | NAG  | D     | 2007 | 2    | 14,14,15     | 0.54 | 0           | 17,19,21    | 1.09 | 2 (11%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | NAG  | B     | 2007 | 2    | 14,14,15     | 0.56 | 0        | 17,19,21    | 1.08 | 2 (11%)  |
| 5   | NAG  | B     | 2009 | 2    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.97 | 1 (5%)   |
| 5   | NAG  | A     | 2001 | 1    | 14,14,15     | 1.15 | 2 (14%)  | 17,19,21    | 2.44 | 7 (41%)  |
| 5   | NAG  | B     | 2008 | 2    | 14,14,15     | 0.60 | 0        | 17,19,21    | 1.13 | 2 (11%)  |
| 5   | NAG  | B     | 2012 | 2    | 14,14,15     | 0.66 | 0        | 17,19,21    | 2.19 | 3 (17%)  |
| 5   | NAG  | F     | 2008 | 2    | 14,14,15     | 0.59 | 0        | 17,19,21    | 1.13 | 2 (11%)  |
| 6   | B12  | C     | 2007 | -    | 94,101,101   | 1.60 | 13 (13%) | 149,166,166 | 2.54 | 41 (27%) |
| 6   | B12  | E     | 2007 | -    | 94,101,101   | 1.60 | 12 (12%) | 149,166,166 | 2.53 | 42 (28%) |
| 5   | NAG  | F     | 2007 | 2    | 14,14,15     | 0.56 | 0        | 17,19,21    | 1.09 | 2 (11%)  |
| 5   | NAG  | D     | 2001 | 2    | 14,14,15     | 0.97 | 1 (7%)   | 17,19,21    | 1.91 | 4 (23%)  |
| 5   | NAG  | B     | 2001 | 2    | 14,14,15     | 0.98 | 1 (7%)   | 17,19,21    | 1.90 | 4 (23%)  |
| 5   | NAG  | F     | 2001 | 2    | 14,14,15     | 0.99 | 1 (7%)   | 17,19,21    | 1.90 | 4 (23%)  |
| 5   | NAG  | F     | 2009 | 2    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.97 | 1 (5%)   |
| 5   | NAG  | D     | 2009 | 2    | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.97 | 1 (5%)   |
| 5   | NAG  | F     | 2013 | 2    | 14,14,15     | 0.67 | 1 (7%)   | 17,19,21    | 1.78 | 4 (23%)  |
| 5   | NAG  | B     | 2013 | 2    | 14,14,15     | 0.68 | 0        | 17,19,21    | 1.93 | 4 (23%)  |
| 5   | NAG  | F     | 2012 | 2    | 14,14,15     | 0.58 | 0        | 17,19,21    | 2.04 | 5 (29%)  |
| 5   | NAG  | D     | 2008 | 2    | 14,14,15     | 0.59 | 0        | 17,19,21    | 1.14 | 2 (11%)  |
| 5   | NAG  | C     | 2001 | 1    | 14,14,15     | 1.14 | 2 (14%)  | 17,19,21    | 2.45 | 7 (41%)  |
| 5   | NAG  | E     | 2001 | 1    | 14,14,15     | 1.16 | 2 (14%)  | 17,19,21    | 2.47 | 7 (41%)  |
| 5   | NAG  | D     | 2012 | 2    | 14,14,15     | 0.60 | 0        | 17,19,21    | 1.70 | 4 (23%)  |

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     |
|-----|------|-------|------|------|-----------|---------------|-----------|
| 6   | B12  | A     | 2007 | -    | 1/1/36/38 | 11/56/223/223 | 0/3/11/11 |
| 5   | NAG  | D     | 2013 | 2    | -         | 3/6/23/26     | 0/1/1/1   |
| 5   | NAG  | D     | 2007 | 2    | -         | 2/6/23/26     | 0/1/1/1   |
| 5   | NAG  | B     | 2007 | 2    | -         | 2/6/23/26     | 0/1/1/1   |
| 5   | NAG  | B     | 2009 | 2    | -         | 0/6/23/26     | 0/1/1/1   |
| 5   | NAG  | A     | 2001 | 1    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | B     | 2008 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | F     | 2008 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings     |
|-----|------|-------|------|------|-----------|---------------|-----------|
| 5   | NAG  | B     | 2012 | 2    | -         | 4/6/23/26     | 0/1/1/1   |
| 6   | B12  | C     | 2007 | -    | 1/1/36/38 | 11/56/223/223 | 0/3/11/11 |
| 6   | B12  | E     | 2007 | -    | 1/1/36/38 | 11/56/223/223 | 0/3/11/11 |
| 5   | NAG  | F     | 2007 | 2    | -         | 2/6/23/26     | 0/1/1/1   |
| 5   | NAG  | D     | 2001 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | B     | 2001 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | F     | 2001 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | F     | 2009 | 2    | -         | 0/6/23/26     | 0/1/1/1   |
| 5   | NAG  | D     | 2009 | 2    | -         | 0/6/23/26     | 0/1/1/1   |
| 5   | NAG  | F     | 2013 | 2    | -         | 3/6/23/26     | 0/1/1/1   |
| 5   | NAG  | B     | 2013 | 2    | -         | 3/6/23/26     | 0/1/1/1   |
| 5   | NAG  | F     | 2012 | 2    | -         | 4/6/23/26     | 0/1/1/1   |
| 5   | NAG  | D     | 2008 | 2    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | C     | 2001 | 1    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | E     | 2001 | 1    | 1/1/5/7   | 5/6/23/26     | 0/1/1/1   |
| 5   | NAG  | D     | 2012 | 2    | -         | 4/6/23/26     | 0/1/1/1   |

All (47) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | A     | 2007 | B12  | C19-N24 | -7.06 | 1.40        | 1.49     |
| 6   | C     | 2007 | B12  | C19-N24 | -7.04 | 1.40        | 1.49     |
| 6   | E     | 2007 | B12  | C19-N24 | -7.04 | 1.40        | 1.49     |
| 6   | A     | 2007 | B12  | C8B-C9B | 4.54  | 1.47        | 1.40     |
| 6   | E     | 2007 | B12  | C8B-C9B | 4.53  | 1.47        | 1.40     |
| 6   | E     | 2007 | B12  | C14-N23 | 4.52  | 1.41        | 1.35     |
| 6   | A     | 2007 | B12  | C14-N23 | 4.50  | 1.41        | 1.35     |
| 6   | C     | 2007 | B12  | C14-N23 | 4.50  | 1.41        | 1.35     |
| 6   | C     | 2007 | B12  | C8B-C9B | 4.49  | 1.47        | 1.40     |
| 6   | C     | 2007 | B12  | C8B-N1B | -4.38 | 1.30        | 1.39     |
| 6   | A     | 2007 | B12  | C8B-N1B | -4.36 | 1.30        | 1.39     |
| 6   | E     | 2007 | B12  | C8B-N1B | -4.35 | 1.30        | 1.39     |
| 6   | E     | 2007 | B12  | C9-N22  | 4.12  | 1.40        | 1.30     |
| 6   | A     | 2007 | B12  | C9-N22  | 4.10  | 1.40        | 1.30     |
| 6   | C     | 2007 | B12  | C9-N22  | 4.10  | 1.40        | 1.30     |
| 6   | C     | 2007 | B12  | C16-C15 | -3.88 | 1.33        | 1.44     |
| 6   | A     | 2007 | B12  | C16-C15 | -3.86 | 1.33        | 1.44     |
| 6   | E     | 2007 | B12  | C16-C15 | -3.86 | 1.33        | 1.44     |
| 6   | E     | 2007 | B12  | C11-N23 | 3.50  | 1.43        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | A     | 2007 | B12  | C11-N23 | 3.49  | 1.43        | 1.36     |
| 6   | C     | 2007 | B12  | C11-N23 | 3.48  | 1.43        | 1.36     |
| 6   | C     | 2007 | B12  | C6B-C5B | 3.05  | 1.48        | 1.40     |
| 6   | E     | 2007 | B12  | C6B-C5B | 3.05  | 1.48        | 1.40     |
| 6   | A     | 2007 | B12  | C6B-C5B | 3.04  | 1.48        | 1.40     |
| 5   | C     | 2001 | NAG  | C1-C2   | 3.01  | 1.56        | 1.52     |
| 5   | F     | 2001 | NAG  | C1-C2   | 2.93  | 1.56        | 1.52     |
| 5   | A     | 2001 | NAG  | C1-C2   | 2.89  | 1.56        | 1.52     |
| 5   | B     | 2001 | NAG  | C1-C2   | 2.87  | 1.56        | 1.52     |
| 5   | D     | 2001 | NAG  | C1-C2   | 2.81  | 1.56        | 1.52     |
| 5   | E     | 2001 | NAG  | C1-C2   | 2.64  | 1.55        | 1.52     |
| 6   | C     | 2007 | B12  | C2B-N3B | 2.39  | 1.36        | 1.31     |
| 6   | A     | 2007 | B12  | C2B-N3B | 2.37  | 1.36        | 1.31     |
| 6   | C     | 2007 | B12  | C1-C19  | -2.37 | 1.50        | 1.55     |
| 6   | E     | 2007 | B12  | C2B-N3B | 2.35  | 1.36        | 1.31     |
| 6   | A     | 2007 | B12  | C1-C19  | -2.34 | 1.50        | 1.55     |
| 6   | E     | 2007 | B12  | C1-C19  | -2.33 | 1.50        | 1.55     |
| 5   | A     | 2001 | NAG  | C2-N2   | 2.30  | 1.50        | 1.46     |
| 5   | E     | 2001 | NAG  | C2-N2   | 2.22  | 1.49        | 1.46     |
| 6   | E     | 2007 | B12  | C1-C2   | -2.17 | 1.53        | 1.58     |
| 6   | C     | 2007 | B12  | C1-C2   | -2.15 | 1.53        | 1.58     |
| 6   | A     | 2007 | B12  | C1-C2   | -2.15 | 1.53        | 1.58     |
| 6   | C     | 2007 | B12  | C10-C9  | 2.14  | 1.45        | 1.39     |
| 6   | A     | 2007 | B12  | C10-C9  | 2.12  | 1.45        | 1.39     |
| 6   | E     | 2007 | B12  | C10-C9  | 2.11  | 1.45        | 1.39     |
| 5   | C     | 2001 | NAG  | C2-N2   | 2.03  | 1.49        | 1.46     |
| 5   | F     | 2013 | NAG  | C1-C2   | 2.03  | 1.55        | 1.52     |
| 6   | C     | 2007 | B12  | C14-C15 | 2.00  | 1.47        | 1.38     |

All (198) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | E     | 2007 | B12  | C1-C19-N24  | 9.11  | 116.38      | 106.25   |
| 6   | A     | 2007 | B12  | C1-C19-N24  | 9.09  | 116.36      | 106.25   |
| 6   | C     | 2007 | B12  | C1-C19-N24  | 9.08  | 116.35      | 106.25   |
| 6   | C     | 2007 | B12  | C13-C12-C11 | -7.77 | 92.29       | 100.97   |
| 6   | C     | 2007 | B12  | C47-C12-C46 | 7.76  | 122.26      | 109.41   |
| 6   | C     | 2007 | B12  | C12-C11-C10 | -7.73 | 113.43      | 123.40   |
| 6   | A     | 2007 | B12  | C12-C11-C10 | -7.73 | 113.43      | 123.40   |
| 6   | A     | 2007 | B12  | C47-C12-C46 | 7.72  | 122.20      | 109.41   |
| 6   | A     | 2007 | B12  | C13-C12-C11 | -7.72 | 92.34       | 100.97   |
| 6   | E     | 2007 | B12  | C47-C12-C46 | 7.72  | 122.19      | 109.41   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | E     | 2007 | B12  | C12-C11-C10 | -7.70 | 113.48      | 123.40   |
| 6   | E     | 2007 | B12  | C13-C12-C11 | -7.69 | 92.37       | 100.97   |
| 6   | A     | 2007 | B12  | C46-C12-C13 | -7.50 | 82.36       | 112.74   |
| 6   | E     | 2007 | B12  | C46-C12-C13 | -7.49 | 82.36       | 112.74   |
| 6   | C     | 2007 | B12  | C46-C12-C13 | -7.49 | 82.37       | 112.74   |
| 6   | C     | 2007 | B12  | C12-C11-N23 | 6.96  | 121.41      | 111.83   |
| 6   | A     | 2007 | B12  | C12-C11-N23 | 6.94  | 121.38      | 111.83   |
| 6   | E     | 2007 | B12  | C12-C11-N23 | 6.91  | 121.35      | 111.83   |
| 6   | C     | 2007 | B12  | C20-C1-C19  | -6.61 | 102.98      | 109.35   |
| 6   | E     | 2007 | B12  | C20-C1-C19  | -6.57 | 103.03      | 109.35   |
| 6   | A     | 2007 | B12  | C20-C1-C19  | -6.56 | 103.03      | 109.35   |
| 6   | C     | 2007 | B12  | C1-C19-C18  | 6.15  | 131.87      | 121.90   |
| 6   | A     | 2007 | B12  | C1-C19-C18  | 6.13  | 131.84      | 121.90   |
| 6   | E     | 2007 | B12  | C1-C19-C18  | 6.13  | 131.84      | 121.90   |
| 5   | B     | 2012 | NAG  | C1-O5-C5    | 5.52  | 119.58      | 112.19   |
| 5   | B     | 2012 | NAG  | O5-C1-C2    | -5.45 | 102.85      | 111.29   |
| 6   | A     | 2007 | B12  | C18-C19-N24 | 5.21  | 110.16      | 102.33   |
| 6   | E     | 2007 | B12  | C18-C19-N24 | 5.20  | 110.14      | 102.33   |
| 6   | C     | 2007 | B12  | C18-C19-N24 | 5.20  | 110.14      | 102.33   |
| 6   | C     | 2007 | B12  | C12-C13-C14 | 5.18  | 110.77      | 102.26   |
| 6   | E     | 2007 | B12  | C12-C13-C14 | 5.15  | 110.72      | 102.26   |
| 6   | A     | 2007 | B12  | C12-C13-C14 | 5.14  | 110.72      | 102.26   |
| 5   | F     | 2012 | NAG  | O5-C1-C2    | -5.13 | 103.35      | 111.29   |
| 5   | F     | 2001 | NAG  | O5-C1-C2    | -5.11 | 103.39      | 111.29   |
| 5   | D     | 2001 | NAG  | O5-C1-C2    | -5.10 | 103.40      | 111.29   |
| 5   | A     | 2001 | NAG  | C1-C2-N2    | 5.07  | 118.43      | 110.43   |
| 5   | B     | 2001 | NAG  | O5-C1-C2    | -5.05 | 103.48      | 111.29   |
| 5   | E     | 2001 | NAG  | C1-C2-N2    | 5.03  | 118.35      | 110.43   |
| 6   | A     | 2007 | B12  | C55-C17-C16 | -4.99 | 106.83      | 116.59   |
| 6   | E     | 2007 | B12  | C55-C17-C16 | -4.99 | 106.84      | 116.59   |
| 6   | C     | 2007 | B12  | C55-C17-C16 | -4.99 | 106.85      | 116.59   |
| 6   | C     | 2007 | B12  | C30-C3-C2   | -4.93 | 108.12      | 119.00   |
| 5   | C     | 2001 | NAG  | C1-C2-N2    | 4.93  | 118.20      | 110.43   |
| 6   | A     | 2007 | B12  | C30-C3-C2   | -4.93 | 108.14      | 119.00   |
| 6   | E     | 2007 | B12  | C30-C3-C2   | -4.93 | 108.14      | 119.00   |
| 6   | C     | 2007 | B12  | C2-C1-C19   | 4.79  | 126.06      | 118.61   |
| 6   | E     | 2007 | B12  | C2-C1-C19   | 4.79  | 126.06      | 118.61   |
| 6   | A     | 2007 | B12  | C2-C1-C19   | 4.77  | 126.03      | 118.61   |
| 5   | D     | 2013 | NAG  | O5-C1-C2    | -4.74 | 103.95      | 111.29   |
| 6   | C     | 2007 | B12  | C2-C1-N21   | 4.64  | 108.23      | 101.78   |
| 6   | A     | 2007 | B12  | C2-C1-N21   | 4.63  | 108.21      | 101.78   |
| 6   | E     | 2007 | B12  | C2-C1-N21   | 4.63  | 108.21      | 101.78   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | C     | 2001 | NAG  | O5-C1-C2    | 4.55  | 118.34      | 111.29   |
| 5   | E     | 2001 | NAG  | O5-C1-C2    | 4.54  | 118.31      | 111.29   |
| 5   | B     | 2013 | NAG  | O5-C1-C2    | -4.50 | 104.32      | 111.29   |
| 6   | A     | 2007 | B12  | C47-C12-C13 | -4.42 | 94.82       | 112.74   |
| 6   | E     | 2007 | B12  | C47-C12-C13 | -4.41 | 94.84       | 112.74   |
| 6   | C     | 2007 | B12  | C47-C12-C13 | -4.41 | 94.85       | 112.74   |
| 6   | A     | 2007 | B12  | O3-C2P-C1P  | 4.41  | 115.68      | 106.94   |
| 6   | C     | 2007 | B12  | O3-C2P-C1P  | 4.40  | 115.66      | 106.94   |
| 6   | E     | 2007 | B12  | O3-C2P-C1P  | 4.40  | 115.65      | 106.94   |
| 5   | A     | 2001 | NAG  | O5-C1-C2    | 4.29  | 117.92      | 111.29   |
| 5   | A     | 2001 | NAG  | O7-C7-C8    | -4.13 | 114.71      | 122.05   |
| 5   | E     | 2001 | NAG  | O7-C7-C8    | -3.91 | 115.10      | 122.05   |
| 5   | F     | 2013 | NAG  | O5-C1-C2    | -3.90 | 105.25      | 111.29   |
| 6   | C     | 2007 | B12  | C2-C26-C27  | -3.85 | 104.48      | 115.19   |
| 6   | A     | 2007 | B12  | C2-C26-C27  | -3.85 | 104.49      | 115.19   |
| 6   | E     | 2007 | B12  | C2-C26-C27  | -3.85 | 104.50      | 115.19   |
| 6   | E     | 2007 | B12  | C20-C1-C2   | -3.81 | 106.99      | 113.28   |
| 6   | E     | 2007 | B12  | C54-C17-C18 | -3.81 | 107.52      | 112.99   |
| 6   | A     | 2007 | B12  | C20-C1-C2   | -3.81 | 107.00      | 113.28   |
| 6   | C     | 2007 | B12  | C54-C17-C18 | -3.80 | 107.53      | 112.99   |
| 6   | C     | 2007 | B12  | C20-C1-C2   | -3.80 | 107.01      | 113.28   |
| 6   | A     | 2007 | B12  | C54-C17-C18 | -3.80 | 107.54      | 112.99   |
| 5   | F     | 2012 | NAG  | C1-O5-C5    | 3.70  | 117.14      | 112.19   |
| 6   | C     | 2007 | B12  | C9-C10-C11  | -3.63 | 120.78      | 125.97   |
| 6   | E     | 2007 | B12  | C9-C10-C11  | -3.62 | 120.79      | 125.97   |
| 5   | D     | 2012 | NAG  | C1-O5-C5    | 3.62  | 117.04      | 112.19   |
| 6   | A     | 2007 | B12  | C9-C10-C11  | -3.62 | 120.79      | 125.97   |
| 5   | E     | 2001 | NAG  | O7-C7-N2    | 3.48  | 128.12      | 121.98   |
| 6   | C     | 2007 | B12  | C4B-C9B-C8B | -3.45 | 116.99      | 120.16   |
| 5   | D     | 2012 | NAG  | O5-C1-C2    | -3.45 | 105.95      | 111.29   |
| 6   | A     | 2007 | B12  | C4B-C9B-C8B | -3.44 | 117.00      | 120.16   |
| 6   | A     | 2007 | B12  | C4B-C9B-N3B | 3.42  | 136.27      | 130.51   |
| 6   | C     | 2007 | B12  | C4B-C9B-N3B | 3.41  | 136.25      | 130.51   |
| 6   | E     | 2007 | B12  | C4B-C9B-N3B | 3.40  | 136.24      | 130.51   |
| 6   | A     | 2007 | B12  | C8B-N1B-C2B | 3.40  | 109.34      | 106.26   |
| 6   | C     | 2007 | B12  | C8B-N1B-C2B | 3.39  | 109.34      | 106.26   |
| 6   | E     | 2007 | B12  | C4B-C9B-C8B | -3.39 | 117.05      | 120.16   |
| 6   | E     | 2007 | B12  | C8B-N1B-C2B | 3.38  | 109.33      | 106.26   |
| 5   | C     | 2001 | NAG  | O7-C7-N2    | 3.34  | 127.88      | 121.98   |
| 5   | C     | 2001 | NAG  | O6-C6-C5    | -3.27 | 100.19      | 111.33   |
| 5   | E     | 2001 | NAG  | O6-C6-C5    | -3.21 | 100.41      | 111.33   |
| 5   | A     | 2001 | NAG  | O7-C7-N2    | 3.21  | 127.65      | 121.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | D     | 2013 | NAG  | C1-O5-C5    | 3.20  | 116.47      | 112.19   |
| 5   | B     | 2013 | NAG  | O5-C5-C6    | 3.17  | 113.84      | 107.66   |
| 6   | E     | 2007 | B12  | C8B-N1B-C1R | -3.17 | 120.04      | 125.41   |
| 6   | E     | 2007 | B12  | O6R-C4R-C5R | -3.17 | 102.51      | 109.22   |
| 6   | A     | 2007 | B12  | C8B-N1B-C1R | -3.17 | 120.05      | 125.41   |
| 6   | A     | 2007 | B12  | O6R-C4R-C5R | -3.16 | 102.53      | 109.22   |
| 6   | C     | 2007 | B12  | O6R-C4R-C5R | -3.16 | 102.54      | 109.22   |
| 6   | C     | 2007 | B12  | C8B-N1B-C1R | -3.16 | 120.07      | 125.41   |
| 5   | C     | 2001 | NAG  | O3-C3-C4    | -3.14 | 102.97      | 110.38   |
| 5   | D     | 2013 | NAG  | O5-C5-C6    | 3.14  | 113.77      | 107.66   |
| 5   | B     | 2012 | NAG  | O3-C3-C2    | 3.12  | 115.87      | 109.40   |
| 5   | C     | 2001 | NAG  | O7-C7-C8    | -3.09 | 116.55      | 122.05   |
| 5   | F     | 2013 | NAG  | C1-O5-C5    | 3.07  | 116.29      | 112.19   |
| 6   | E     | 2007 | B12  | C8B-C9B-N3B | -3.04 | 106.71      | 110.00   |
| 6   | A     | 2007 | B12  | C8B-C9B-N3B | -3.03 | 106.73      | 110.00   |
| 6   | C     | 2007 | B12  | C8B-C9B-N3B | -3.00 | 106.75      | 110.00   |
| 5   | B     | 2013 | NAG  | C1-O5-C5    | 2.99  | 116.19      | 112.19   |
| 5   | F     | 2013 | NAG  | O5-C5-C6    | 2.99  | 113.48      | 107.66   |
| 6   | A     | 2007 | B12  | C26-C2-C1   | 2.97  | 114.59      | 110.00   |
| 5   | F     | 2001 | NAG  | C1-O5-C5    | 2.97  | 116.16      | 112.19   |
| 5   | D     | 2001 | NAG  | C1-O5-C5    | 2.96  | 116.16      | 112.19   |
| 6   | E     | 2007 | B12  | C26-C2-C1   | 2.96  | 114.58      | 110.00   |
| 6   | C     | 2007 | B12  | C26-C2-C1   | 2.95  | 114.56      | 110.00   |
| 5   | B     | 2001 | NAG  | C1-O5-C5    | 2.94  | 116.13      | 112.19   |
| 6   | A     | 2007 | B12  | O8R-C5R-C4R | -2.87 | 101.56      | 111.33   |
| 6   | C     | 2007 | B12  | O8R-C5R-C4R | -2.86 | 101.58      | 111.33   |
| 6   | E     | 2007 | B12  | O8R-C5R-C4R | -2.85 | 101.61      | 111.33   |
| 5   | A     | 2001 | NAG  | O6-C6-C5    | -2.82 | 101.74      | 111.33   |
| 6   | A     | 2007 | B12  | C46-C12-C11 | 2.77  | 119.98      | 110.08   |
| 6   | E     | 2007 | B12  | C46-C12-C11 | 2.77  | 119.97      | 110.08   |
| 6   | C     | 2007 | B12  | C46-C12-C11 | 2.76  | 119.94      | 110.08   |
| 5   | B     | 2013 | NAG  | C1-C2-N2    | 2.73  | 114.74      | 110.43   |
| 5   | E     | 2001 | NAG  | O3-C3-C4    | -2.70 | 104.01      | 110.38   |
| 6   | C     | 2007 | B12  | C9B-C8B-N1B | 2.64  | 106.47      | 105.30   |
| 6   | E     | 2007 | B12  | C9B-C8B-N1B | 2.62  | 106.47      | 105.30   |
| 5   | D     | 2007 | NAG  | C2-N2-C7    | -2.60 | 119.42      | 122.90   |
| 5   | A     | 2001 | NAG  | C4-C3-C2    | 2.59  | 114.82      | 111.02   |
| 6   | C     | 2007 | B12  | C18-C17-C16 | 2.59  | 103.81      | 100.69   |
| 5   | F     | 2007 | NAG  | C2-N2-C7    | -2.59 | 119.43      | 122.90   |
| 6   | A     | 2007 | B12  | C9B-C8B-N1B | 2.58  | 106.45      | 105.30   |
| 6   | A     | 2007 | B12  | C18-C17-C16 | 2.58  | 103.80      | 100.69   |
| 5   | B     | 2007 | NAG  | C2-N2-C7    | -2.58 | 119.45      | 122.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | E     | 2007 | B12  | C18-C17-C16 | 2.55  | 103.77      | 100.69   |
| 5   | D     | 2008 | NAG  | C1-C2-N2    | 2.52  | 114.40      | 110.43   |
| 5   | A     | 2001 | NAG  | O3-C3-C4    | -2.52 | 104.45      | 110.38   |
| 5   | F     | 2013 | NAG  | C1-C2-N2    | 2.49  | 114.36      | 110.43   |
| 5   | B     | 2008 | NAG  | C1-C2-N2    | 2.49  | 114.36      | 110.43   |
| 5   | F     | 2008 | NAG  | C1-C2-N2    | 2.47  | 114.33      | 110.43   |
| 5   | E     | 2001 | NAG  | C4-C3-C2    | 2.45  | 114.61      | 111.02   |
| 6   | C     | 2007 | B12  | C1-C2-C3    | 2.44  | 104.67      | 101.60   |
| 6   | A     | 2007 | B12  | C1-C2-C3    | 2.44  | 104.66      | 101.60   |
| 6   | C     | 2007 | B12  | C7-C6-N22   | 2.43  | 112.36      | 107.94   |
| 5   | B     | 2001 | NAG  | O7-C7-C8    | -2.42 | 117.74      | 122.05   |
| 6   | E     | 2007 | B12  | C1-C2-C3    | 2.42  | 104.65      | 101.60   |
| 5   | F     | 2001 | NAG  | O7-C7-C8    | -2.42 | 117.74      | 122.05   |
| 5   | D     | 2001 | NAG  | O7-C7-C8    | -2.40 | 117.77      | 122.05   |
| 6   | A     | 2007 | B12  | C7-C6-N22   | 2.40  | 112.31      | 107.94   |
| 6   | E     | 2007 | B12  | C7-C6-N22   | 2.40  | 112.30      | 107.94   |
| 6   | C     | 2007 | B12  | C7-C6-C5    | -2.39 | 124.34      | 128.07   |
| 5   | F     | 2012 | NAG  | C1-C2-N2    | -2.37 | 106.69      | 110.43   |
| 6   | A     | 2007 | B12  | C7-C6-C5    | -2.36 | 124.38      | 128.07   |
| 6   | E     | 2007 | B12  | C25-C2-C3   | -2.35 | 106.94      | 112.91   |
| 6   | A     | 2007 | B12  | C25-C2-C3   | -2.35 | 106.94      | 112.91   |
| 6   | C     | 2007 | B12  | C25-C2-C3   | -2.34 | 106.96      | 112.91   |
| 6   | E     | 2007 | B12  | C7-C6-C5    | -2.33 | 124.43      | 128.07   |
| 5   | F     | 2012 | NAG  | O3-C3-C2    | 2.32  | 114.22      | 109.40   |
| 5   | B     | 2001 | NAG  | C1-C2-N2    | 2.32  | 114.09      | 110.43   |
| 5   | D     | 2001 | NAG  | C1-C2-N2    | 2.30  | 114.06      | 110.43   |
| 5   | D     | 2013 | NAG  | C1-C2-N2    | 2.29  | 114.04      | 110.43   |
| 5   | F     | 2001 | NAG  | C1-C2-N2    | 2.27  | 114.02      | 110.43   |
| 5   | D     | 2013 | NAG  | C2-N2-C7    | -2.27 | 119.85      | 122.90   |
| 5   | F     | 2007 | NAG  | C1-O5-C5    | 2.24  | 115.19      | 112.19   |
| 5   | B     | 2007 | NAG  | C1-O5-C5    | 2.22  | 115.17      | 112.19   |
| 5   | D     | 2007 | NAG  | C1-O5-C5    | 2.22  | 115.16      | 112.19   |
| 5   | D     | 2012 | NAG  | O4-C4-C3    | -2.20 | 105.20      | 110.38   |
| 5   | D     | 2008 | NAG  | O5-C1-C2    | -2.18 | 107.91      | 111.29   |
| 5   | D     | 2012 | NAG  | O3-C3-C2    | 2.18  | 113.92      | 109.40   |
| 5   | B     | 2008 | NAG  | O5-C1-C2    | -2.17 | 107.93      | 111.29   |
| 6   | E     | 2007 | B12  | C47-C12-C11 | 2.17  | 117.84      | 110.08   |
| 5   | F     | 2008 | NAG  | O5-C1-C2    | -2.17 | 107.94      | 111.29   |
| 5   | B     | 2009 | NAG  | C4-C3-C2    | -2.17 | 107.84      | 111.02   |
| 6   | A     | 2007 | B12  | C47-C12-C11 | 2.17  | 117.82      | 110.08   |
| 6   | C     | 2007 | B12  | C47-C12-C11 | 2.16  | 117.79      | 110.08   |
| 5   | D     | 2009 | NAG  | C4-C3-C2    | -2.15 | 107.86      | 111.02   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | F     | 2009 | NAG  | C4-C3-C2    | -2.15 | 107.86      | 111.02   |
| 5   | F     | 2012 | NAG  | O3-C3-C4    | -2.15 | 105.30      | 110.38   |
| 5   | C     | 2001 | NAG  | C1-O5-C5    | 2.10  | 115.01      | 112.19   |
| 6   | E     | 2007 | B12  | C8-C7-C6    | 2.09  | 104.47      | 100.92   |
| 6   | A     | 2007 | B12  | C8-C7-C6    | 2.08  | 104.45      | 100.92   |
| 6   | E     | 2007 | B12  | C36-C7-C8   | -2.08 | 108.21      | 112.05   |
| 6   | C     | 2007 | B12  | C8-C7-C6    | 2.05  | 104.40      | 100.92   |
| 6   | A     | 2007 | B12  | C36-C7-C8   | -2.05 | 108.26      | 112.05   |
| 6   | C     | 2007 | B12  | C36-C7-C8   | -2.04 | 108.27      | 112.05   |
| 6   | E     | 2007 | B12  | O44-C43-N45 | -2.04 | 117.08      | 122.53   |
| 6   | E     | 2007 | B12  | C55-C17-C18 | 2.04  | 115.01      | 111.12   |
| 6   | A     | 2007 | B12  | O44-C43-N45 | -2.03 | 117.11      | 122.53   |
| 6   | C     | 2007 | B12  | C7-C37-C38  | -2.03 | 108.27      | 114.28   |
| 6   | A     | 2007 | B12  | C55-C17-C18 | 2.02  | 114.98      | 111.12   |
| 6   | A     | 2007 | B12  | C7-C37-C38  | -2.02 | 108.30      | 114.28   |
| 6   | E     | 2007 | B12  | C56-C55-C17 | -2.02 | 111.69      | 115.58   |
| 6   | E     | 2007 | B12  | C7-C37-C38  | -2.01 | 108.33      | 114.28   |
| 6   | C     | 2007 | B12  | C55-C17-C18 | 2.01  | 114.96      | 111.12   |
| 6   | C     | 2007 | B12  | O44-C43-N45 | -2.01 | 117.17      | 122.53   |
| 6   | A     | 2007 | B12  | C56-C55-C17 | -2.00 | 111.72      | 115.58   |

All (12) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 5   | A     | 2001 | NAG  | C1   |
| 5   | B     | 2001 | NAG  | C1   |
| 5   | B     | 2008 | NAG  | C1   |
| 5   | C     | 2001 | NAG  | C1   |
| 5   | D     | 2001 | NAG  | C1   |
| 5   | D     | 2008 | NAG  | C1   |
| 5   | E     | 2001 | NAG  | C1   |
| 5   | F     | 2001 | NAG  | C1   |
| 5   | F     | 2008 | NAG  | C1   |
| 6   | A     | 2007 | B12  | C19  |
| 6   | C     | 2007 | B12  | C19  |
| 6   | E     | 2007 | B12  | C19  |

All (105) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | A     | 2001 | NAG  | C8-C7-N2-C2 |
| 5   | A     | 2001 | NAG  | O7-C7-N2-C2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | B     | 2001 | NAG  | C3-C2-N2-C7     |
| 5   | B     | 2001 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2001 | NAG  | O7-C7-N2-C2     |
| 5   | B     | 2008 | NAG  | C1-C2-N2-C7     |
| 5   | B     | 2008 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2008 | NAG  | O7-C7-N2-C2     |
| 5   | B     | 2012 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2012 | NAG  | O7-C7-N2-C2     |
| 5   | B     | 2013 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2013 | NAG  | O7-C7-N2-C2     |
| 5   | C     | 2001 | NAG  | C8-C7-N2-C2     |
| 5   | C     | 2001 | NAG  | O7-C7-N2-C2     |
| 5   | D     | 2001 | NAG  | C3-C2-N2-C7     |
| 5   | D     | 2001 | NAG  | C8-C7-N2-C2     |
| 5   | D     | 2001 | NAG  | O7-C7-N2-C2     |
| 5   | D     | 2008 | NAG  | C1-C2-N2-C7     |
| 5   | D     | 2008 | NAG  | C8-C7-N2-C2     |
| 5   | D     | 2008 | NAG  | O7-C7-N2-C2     |
| 5   | D     | 2012 | NAG  | C8-C7-N2-C2     |
| 5   | D     | 2012 | NAG  | O7-C7-N2-C2     |
| 5   | D     | 2013 | NAG  | C8-C7-N2-C2     |
| 5   | D     | 2013 | NAG  | O7-C7-N2-C2     |
| 5   | E     | 2001 | NAG  | C8-C7-N2-C2     |
| 5   | E     | 2001 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2001 | NAG  | C3-C2-N2-C7     |
| 5   | F     | 2001 | NAG  | C8-C7-N2-C2     |
| 5   | F     | 2001 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2008 | NAG  | C1-C2-N2-C7     |
| 5   | F     | 2008 | NAG  | C8-C7-N2-C2     |
| 5   | F     | 2008 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2012 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2013 | NAG  | C8-C7-N2-C2     |
| 5   | F     | 2013 | NAG  | O7-C7-N2-C2     |
| 6   | A     | 2007 | B12  | C42-C41-C8-C9   |
| 6   | A     | 2007 | B12  | C16-C17-C55-C56 |
| 6   | A     | 2007 | B12  | C18-C17-C55-C56 |
| 6   | C     | 2007 | B12  | C42-C41-C8-C9   |
| 6   | C     | 2007 | B12  | C16-C17-C55-C56 |
| 6   | C     | 2007 | B12  | C18-C17-C55-C56 |
| 6   | E     | 2007 | B12  | C42-C41-C8-C9   |
| 6   | E     | 2007 | B12  | C16-C17-C55-C56 |
| 6   | E     | 2007 | B12  | C18-C17-C55-C56 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | B     | 2007 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2007 | NAG  | O7-C7-N2-C2     |
| 5   | D     | 2007 | NAG  | C8-C7-N2-C2     |
| 5   | D     | 2007 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2007 | NAG  | C8-C7-N2-C2     |
| 5   | F     | 2007 | NAG  | O7-C7-N2-C2     |
| 5   | F     | 2012 | NAG  | C8-C7-N2-C2     |
| 5   | B     | 2008 | NAG  | O5-C5-C6-O6     |
| 5   | D     | 2008 | NAG  | O5-C5-C6-O6     |
| 5   | F     | 2008 | NAG  | O5-C5-C6-O6     |
| 5   | B     | 2001 | NAG  | O5-C5-C6-O6     |
| 5   | D     | 2001 | NAG  | O5-C5-C6-O6     |
| 5   | F     | 2001 | NAG  | O5-C5-C6-O6     |
| 5   | D     | 2012 | NAG  | O5-C5-C6-O6     |
| 5   | B     | 2008 | NAG  | C4-C5-C6-O6     |
| 5   | D     | 2008 | NAG  | C4-C5-C6-O6     |
| 5   | F     | 2008 | NAG  | C4-C5-C6-O6     |
| 5   | B     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | D     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | F     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | F     | 2012 | NAG  | O5-C5-C6-O6     |
| 5   | B     | 2012 | NAG  | O5-C5-C6-O6     |
| 6   | A     | 2007 | B12  | C42-C41-C8-C7   |
| 6   | C     | 2007 | B12  | C42-C41-C8-C7   |
| 6   | E     | 2007 | B12  | C42-C41-C8-C7   |
| 5   | C     | 2001 | NAG  | O5-C5-C6-O6     |
| 5   | E     | 2001 | NAG  | O5-C5-C6-O6     |
| 5   | C     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | E     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | B     | 2013 | NAG  | O5-C5-C6-O6     |
| 5   | D     | 2013 | NAG  | O5-C5-C6-O6     |
| 5   | F     | 2013 | NAG  | O5-C5-C6-O6     |
| 6   | C     | 2007 | B12  | O58-C57-N59-C1P |
| 6   | A     | 2007 | B12  | O58-C57-N59-C1P |
| 6   | E     | 2007 | B12  | O58-C57-N59-C1P |
| 5   | A     | 2001 | NAG  | O5-C5-C6-O6     |
| 6   | A     | 2007 | B12  | C56-C57-N59-C1P |
| 6   | C     | 2007 | B12  | C56-C57-N59-C1P |
| 6   | E     | 2007 | B12  | C56-C57-N59-C1P |
| 6   | A     | 2007 | B12  | C14-C13-C48-C49 |
| 6   | C     | 2007 | B12  | C14-C13-C48-C49 |
| 6   | E     | 2007 | B12  | C14-C13-C48-C49 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | B     | 2012 | NAG  | C4-C5-C6-O6     |
| 5   | A     | 2001 | NAG  | C3-C2-N2-C7     |
| 5   | C     | 2001 | NAG  | C3-C2-N2-C7     |
| 5   | E     | 2001 | NAG  | C3-C2-N2-C7     |
| 6   | A     | 2007 | B12  | N59-C1P-C2P-C3P |
| 6   | C     | 2007 | B12  | N59-C1P-C2P-C3P |
| 6   | E     | 2007 | B12  | N59-C1P-C2P-C3P |
| 6   | A     | 2007 | B12  | N59-C1P-C2P-O3  |
| 6   | C     | 2007 | B12  | N59-C1P-C2P-O3  |
| 6   | E     | 2007 | B12  | N59-C1P-C2P-O3  |
| 5   | D     | 2012 | NAG  | C4-C5-C6-O6     |
| 5   | A     | 2001 | NAG  | C4-C5-C6-O6     |
| 5   | F     | 2012 | NAG  | C4-C5-C6-O6     |
| 6   | A     | 2007 | B12  | C18-C60-C61-O63 |
| 6   | C     | 2007 | B12  | C18-C60-C61-O63 |
| 6   | E     | 2007 | B12  | C18-C60-C61-O63 |
| 6   | A     | 2007 | B12  | C3R-O2-P-O4     |
| 6   | C     | 2007 | B12  | C3R-O2-P-O4     |
| 6   | E     | 2007 | B12  | C3R-O2-P-O4     |

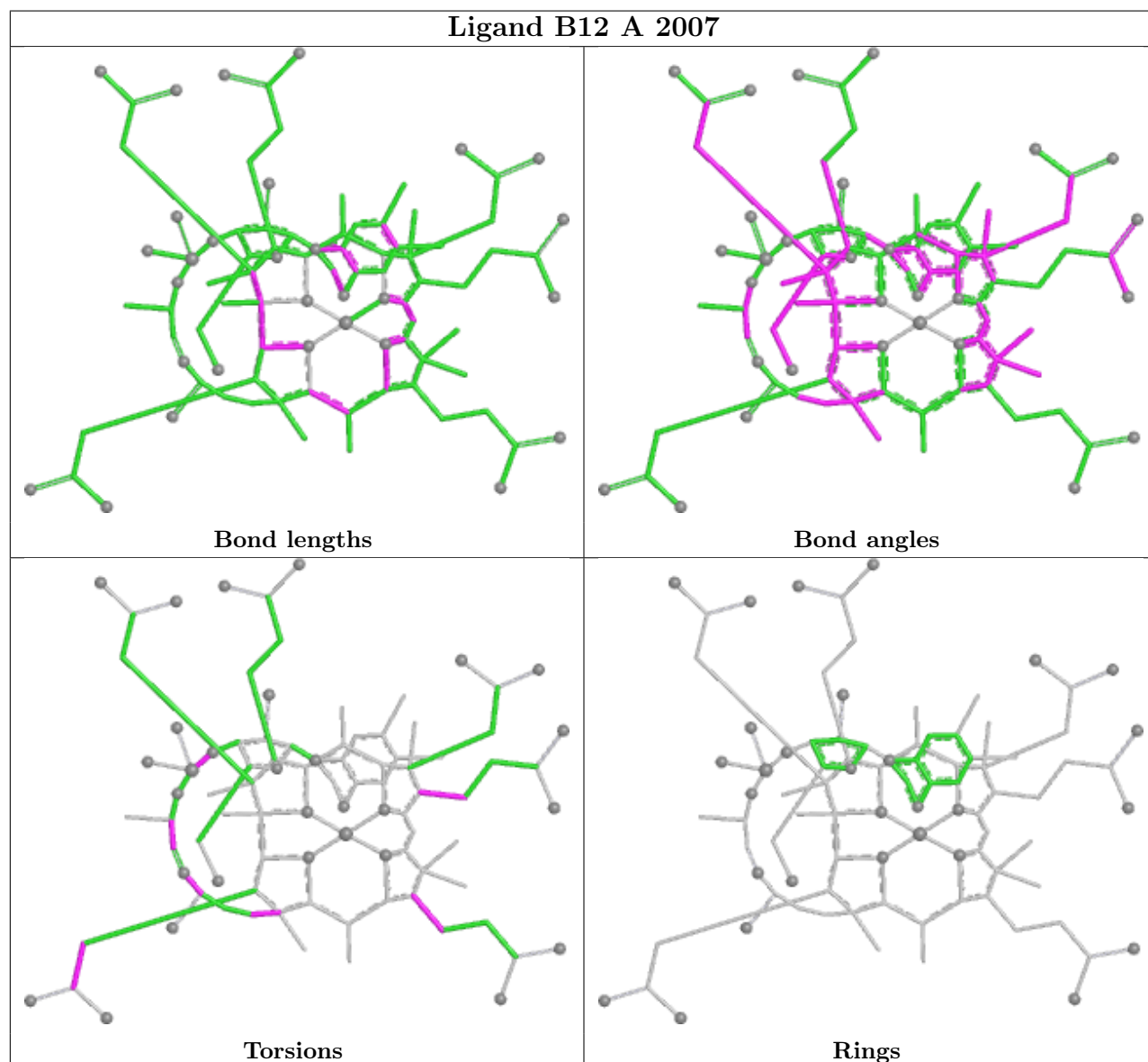
There are no ring outliers.

18 monomers are involved in 124 short contacts:

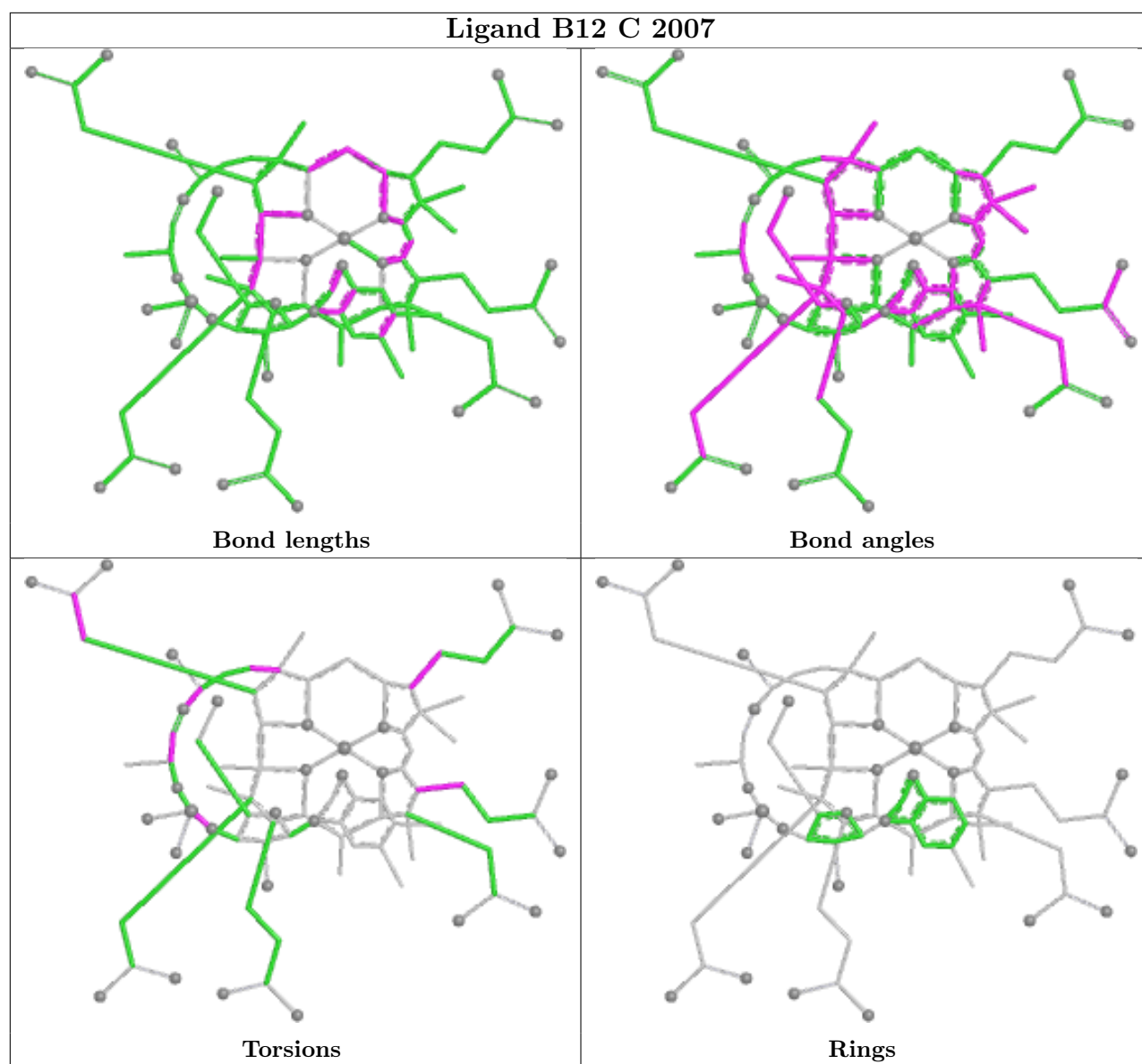
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | A     | 2007 | B12  | 29      | 0            |
| 5   | D     | 2013 | NAG  | 2       | 0            |
| 5   | B     | 2009 | NAG  | 2       | 0            |
| 5   | A     | 2001 | NAG  | 7       | 0            |
| 5   | B     | 2008 | NAG  | 2       | 0            |
| 5   | F     | 2008 | NAG  | 2       | 0            |
| 6   | C     | 2007 | B12  | 26      | 0            |
| 6   | E     | 2007 | B12  | 25      | 0            |
| 5   | D     | 2001 | NAG  | 1       | 0            |
| 5   | B     | 2001 | NAG  | 1       | 0            |
| 5   | F     | 2001 | NAG  | 1       | 0            |
| 5   | F     | 2009 | NAG  | 3       | 0            |
| 5   | D     | 2009 | NAG  | 2       | 0            |
| 5   | F     | 2013 | NAG  | 2       | 0            |
| 5   | B     | 2013 | NAG  | 2       | 0            |
| 5   | D     | 2008 | NAG  | 2       | 0            |
| 5   | C     | 2001 | NAG  | 8       | 0            |
| 5   | E     | 2001 | NAG  | 7       | 0            |

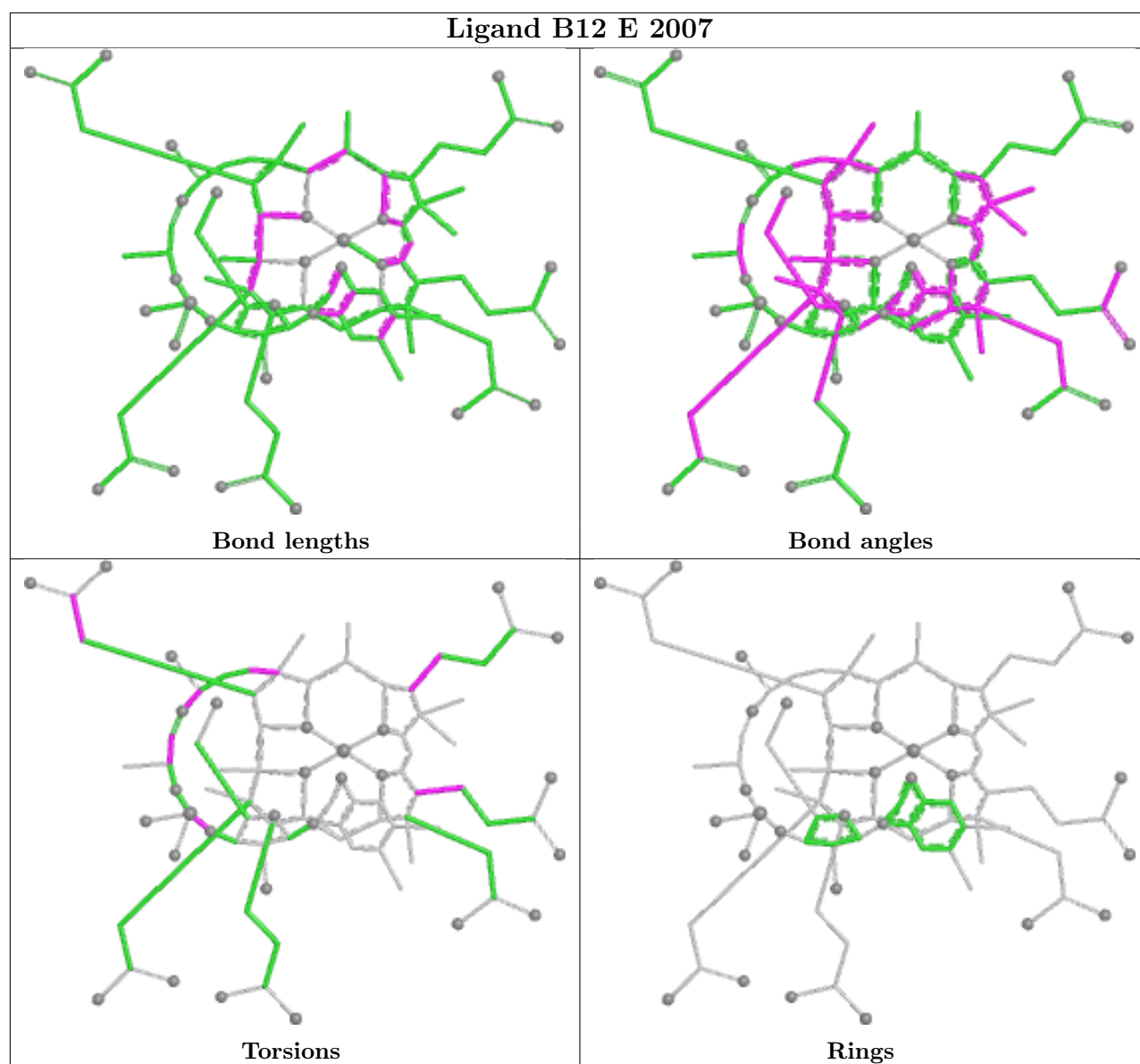


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|-----------|-----------------------|--------|
| 1   | A     | 385/393 (97%)   | -1.22  | 0 100 100 | 47, 77, 133, 281      | 1 (0%) |
| 1   | C     | 385/393 (97%)   | -1.23  | 0 100 100 | 47, 76, 139, 284      | 1 (0%) |
| 1   | E     | 385/393 (97%)   | -1.19  | 0 100 100 | 50, 77, 140, 256      | 1 (0%) |
| 2   | B     | 457/457 (100%)  | -1.02  | 0 100 100 | 59, 111, 172, 219     | 0      |
| 2   | D     | 457/457 (100%)  | -1.02  | 0 100 100 | 59, 110, 176, 228     | 0      |
| 2   | F     | 457/457 (100%)  | -1.07  | 0 100 100 | 61, 111, 178, 259     | 0      |
| All | All   | 2526/2550 (99%) | -1.12  | 0 100 100 | 47, 95, 170, 284      | 3 (0%) |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | NAG  | N     | 2   | 14/15 | 0.93 | 0.09 | 163,175,188,193            | 0     |
| 3   | MAN  | M     | 5   | 11/12 | 0.94 | 0.11 | 181,190,197,200            | 0     |
| 3   | MAN  | K     | 4   | 11/12 | 0.95 | 0.06 | 172,185,203,208            | 0     |
| 3   | MAN  | K     | 5   | 11/12 | 0.95 | 0.07 | 190,201,222,227            | 0     |
| 3   | MAN  | J     | 4   | 11/12 | 0.95 | 0.07 | 160,166,178,180            | 0     |
| 3   | MAN  | J     | 5   | 11/12 | 0.95 | 0.09 | 196,201,205,206            | 0     |

*Continued on next page...*

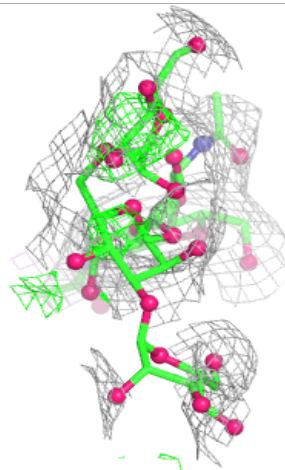
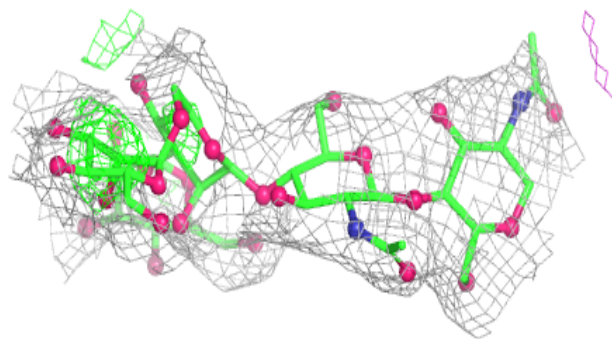
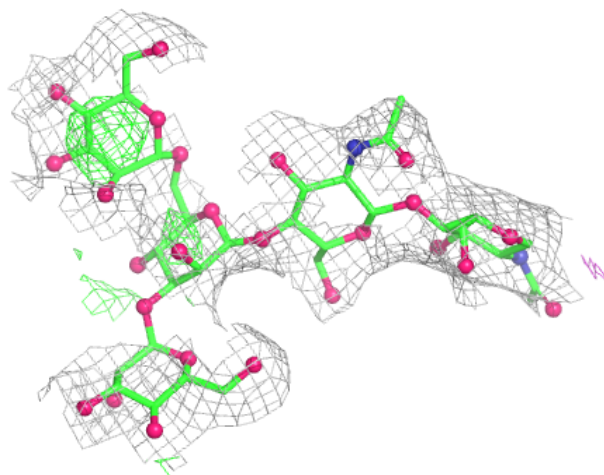
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | MAN  | G     | 4   | 11/12 | 0.96 | 0.06 | 162,165,175,180             | 0     |
| 3   | MAN  | G     | 5   | 11/12 | 0.96 | 0.07 | 190,195,201,202             | 0     |
| 3   | BMA  | K     | 3   | 11/12 | 0.96 | 0.05 | 167,179,190,190             | 0     |
| 3   | NAG  | H     | 2   | 14/15 | 0.96 | 0.07 | 159,171,180,183             | 0     |
| 3   | BMA  | H     | 3   | 11/12 | 0.96 | 0.05 | 167,178,184,188             | 0     |
| 3   | MAN  | H     | 4   | 11/12 | 0.96 | 0.06 | 181,194,208,211             | 0     |
| 3   | MAN  | H     | 5   | 11/12 | 0.96 | 0.08 | 184,197,219,223             | 0     |
| 3   | MAN  | N     | 4   | 11/12 | 0.96 | 0.05 | 188,194,206,206             | 0     |
| 3   | MAN  | N     | 5   | 11/12 | 0.96 | 0.06 | 192,201,209,213             | 0     |
| 4   | NAG  | I     | 2   | 14/15 | 0.96 | 0.05 | 150,155,171,178             | 0     |
| 3   | NAG  | M     | 2   | 14/15 | 0.97 | 0.14 | 89,97,107,109               | 0     |
| 3   | BMA  | N     | 3   | 11/12 | 0.97 | 0.06 | 173,182,191,193             | 0     |
| 3   | BMA  | M     | 3   | 11/12 | 0.97 | 0.05 | 129,131,147,153             | 0     |
| 3   | MAN  | M     | 4   | 11/12 | 0.97 | 0.06 | 169,175,195,202             | 0     |
| 3   | NAG  | K     | 2   | 14/15 | 0.97 | 0.09 | 151,172,184,186             | 0     |
| 4   | NAG  | L     | 2   | 14/15 | 0.97 | 0.06 | 163,170,176,178             | 0     |
| 3   | NAG  | G     | 2   | 14/15 | 0.98 | 0.10 | 90,95,103,104               | 0     |
| 3   | NAG  | M     | 1   | 14/15 | 0.98 | 0.18 | 53,78,96,106                | 0     |
| 3   | BMA  | G     | 3   | 11/12 | 0.98 | 0.05 | 128,134,138,144             | 0     |
| 3   | NAG  | J     | 1   | 14/15 | 0.98 | 0.15 | 59,75,86,91                 | 0     |
| 3   | NAG  | J     | 2   | 14/15 | 0.98 | 0.10 | 89,98,103,104               | 0     |
| 3   | BMA  | J     | 3   | 11/12 | 0.98 | 0.06 | 138,144,154,155             | 0     |
| 4   | NAG  | O     | 1   | 14/15 | 0.98 | 0.06 | 119,136,140,142             | 0     |
| 4   | NAG  | O     | 2   | 14/15 | 0.98 | 0.05 | 160,167,171,175             | 0     |
| 4   | NAG  | I     | 1   | 14/15 | 0.99 | 0.05 | 121,132,136,139             | 0     |
| 3   | NAG  | H     | 1   | 14/15 | 0.99 | 0.04 | 113,122,130,135             | 0     |
| 4   | NAG  | L     | 1   | 14/15 | 0.99 | 0.07 | 125,138,141,143             | 0     |
| 3   | NAG  | G     | 1   | 14/15 | 0.99 | 0.12 | 58,73,97,103                | 0     |
| 3   | NAG  | K     | 1   | 14/15 | 0.99 | 0.04 | 107,122,135,136             | 0     |
| 3   | NAG  | N     | 1   | 14/15 | 0.99 | 0.04 | 119,123,127,130             | 0     |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

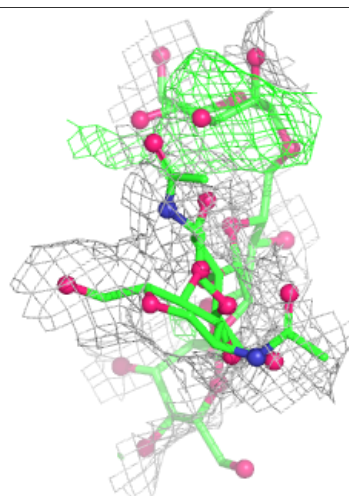
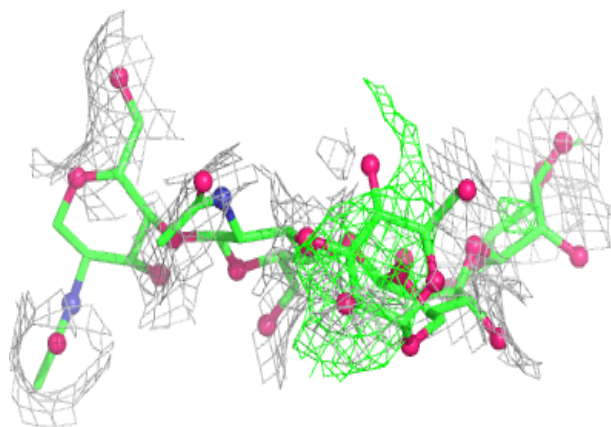
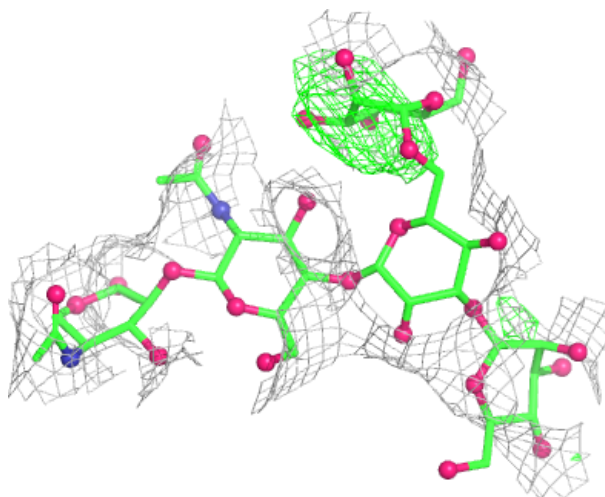
**Electron density around Chain G:**

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



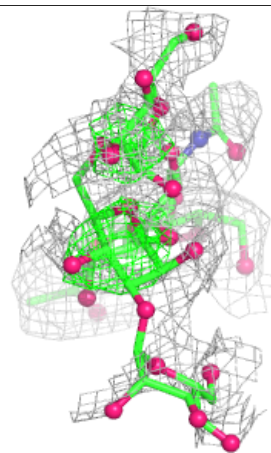
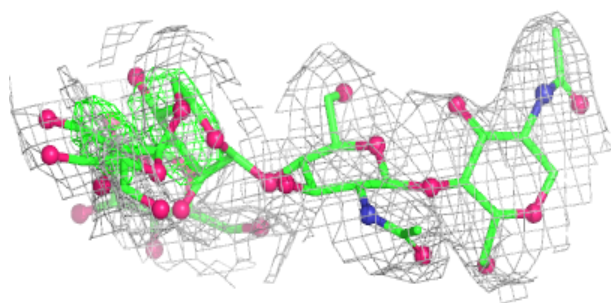
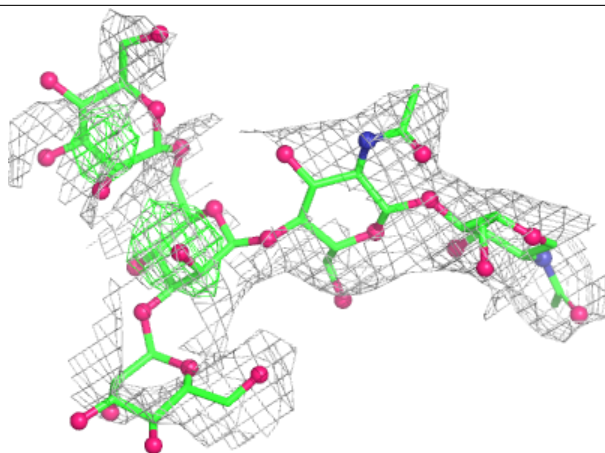
**Electron density around Chain H:**

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



**Electron density around Chain J:**

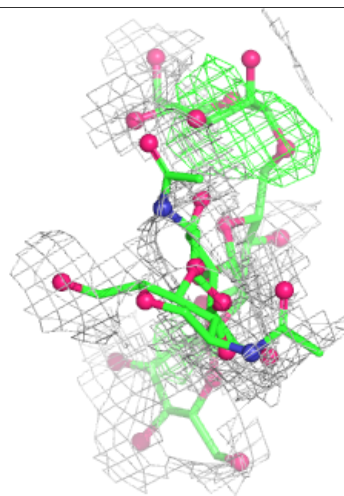
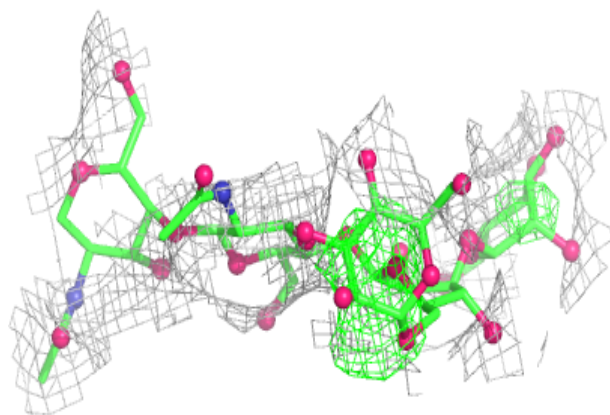
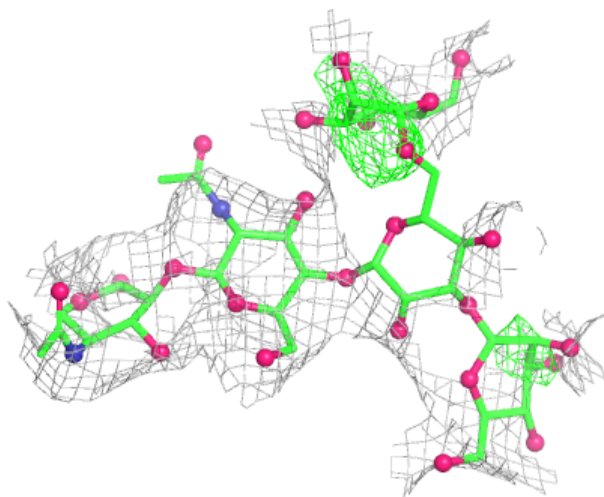
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain K:**

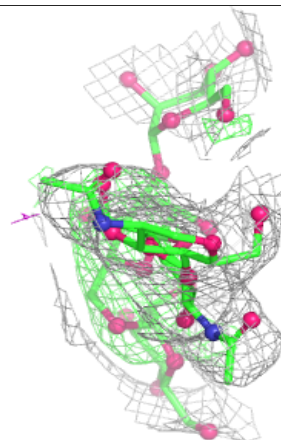
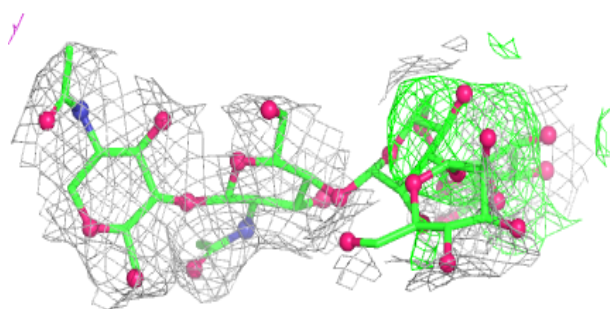
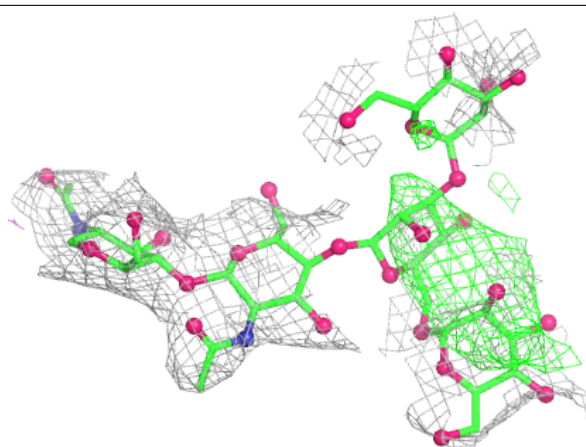
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





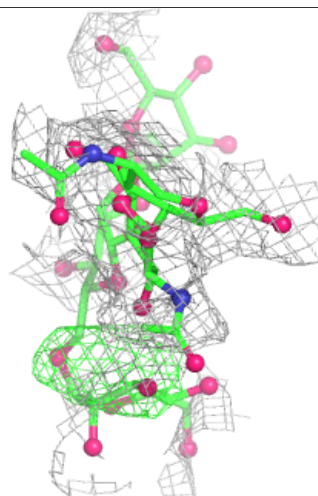
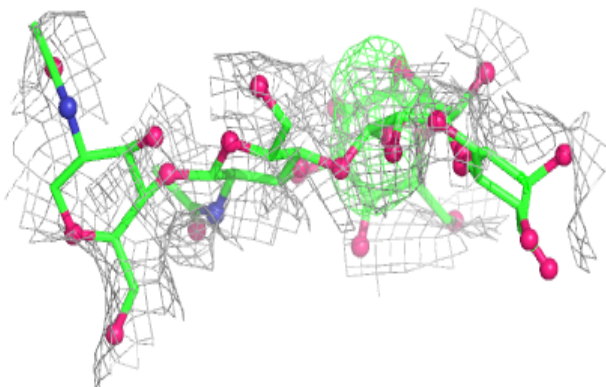
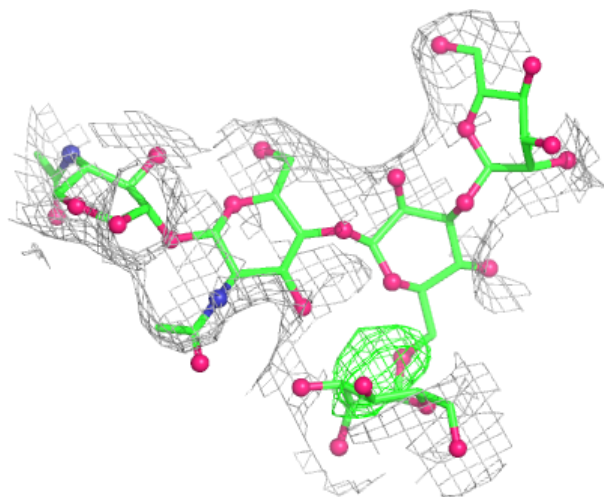
**Electron density around Chain M:**

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



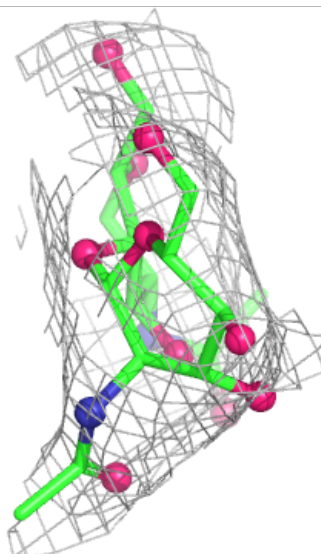
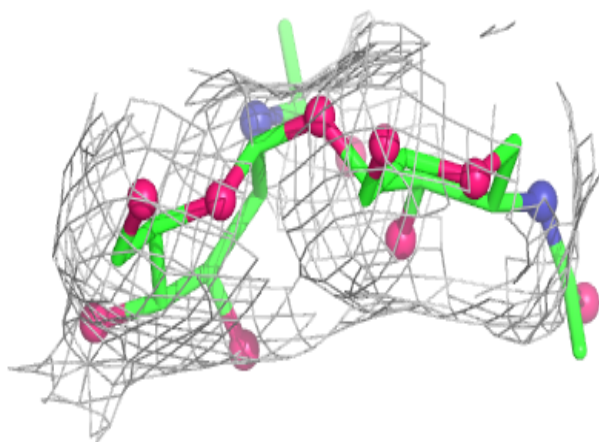
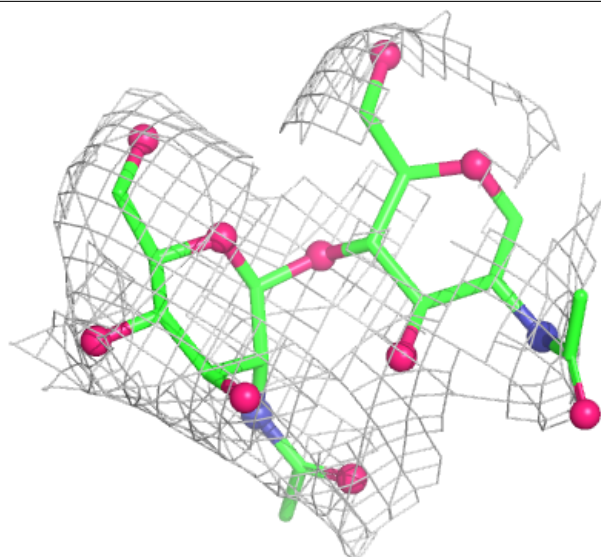
**Electron density around Chain N:**

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



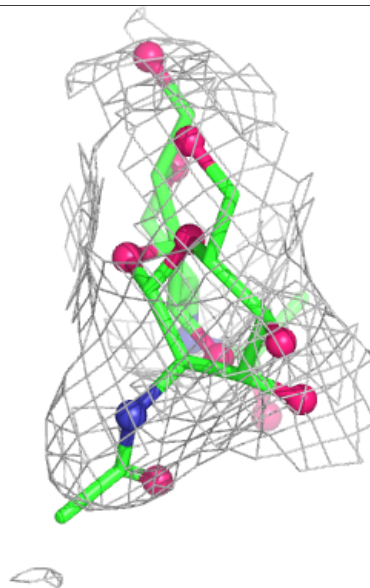
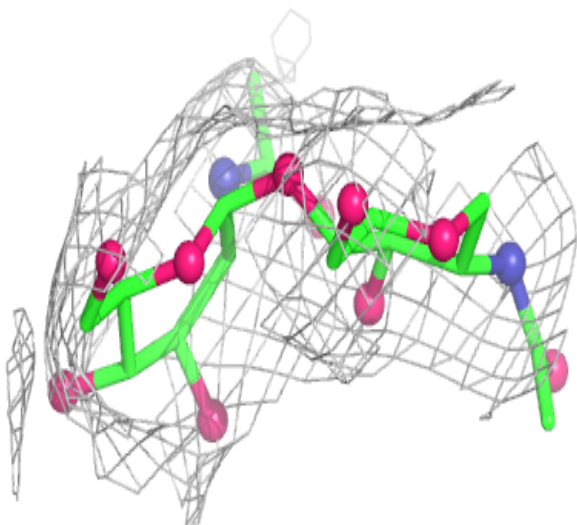
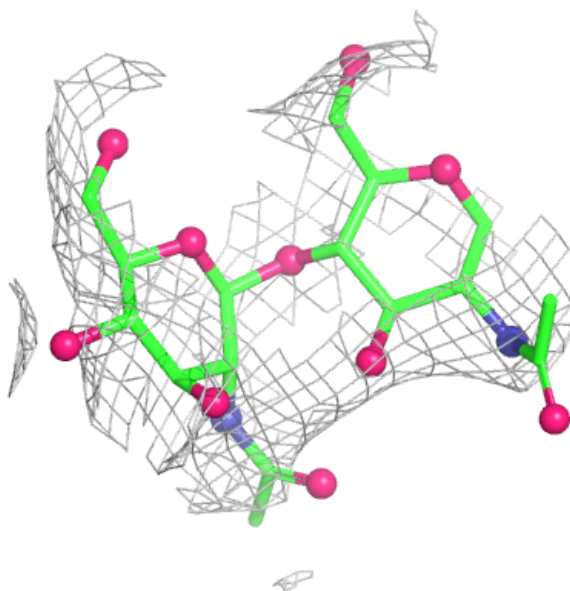
**Electron density around Chain I:**

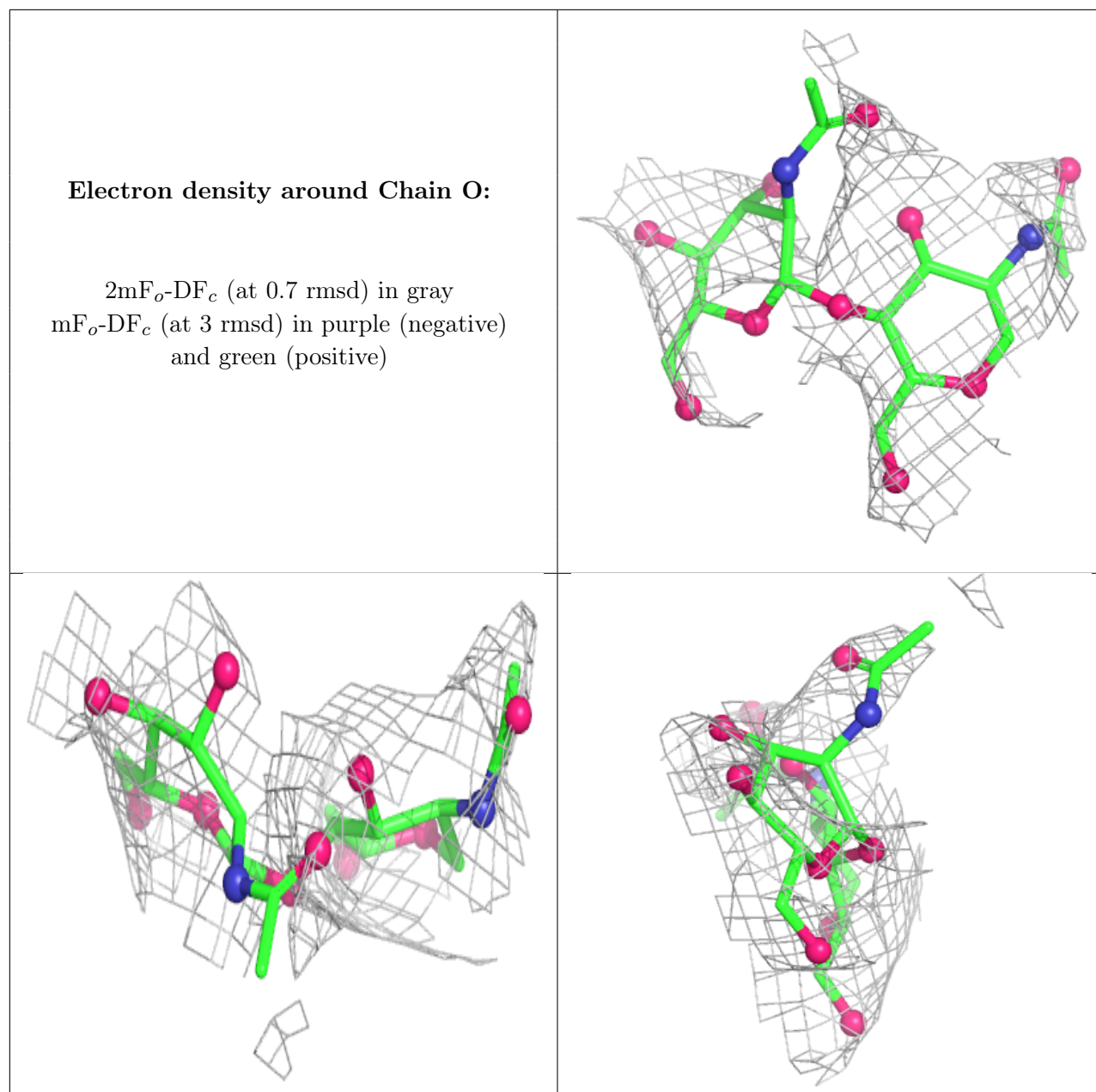
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain L:**

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





## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 5   | NAG  | B     | 2009 | 14/15 | 0.91 | 0.08 | 185,193,199,199            | 0     |
| 5   | NAG  | D     | 2001 | 14/15 | 0.92 | 0.07 | 187,191,196,197            | 0     |
| 5   | NAG  | D     | 2008 | 14/15 | 0.93 | 0.09 | 196,203,209,210            | 0     |

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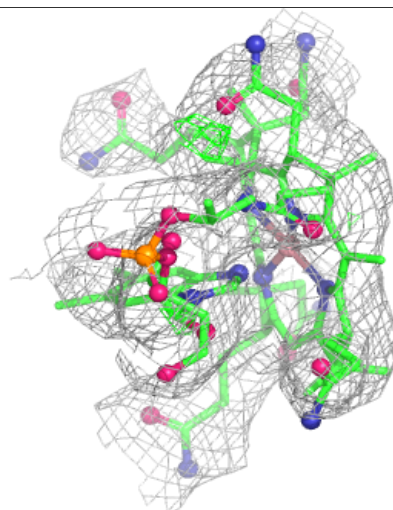
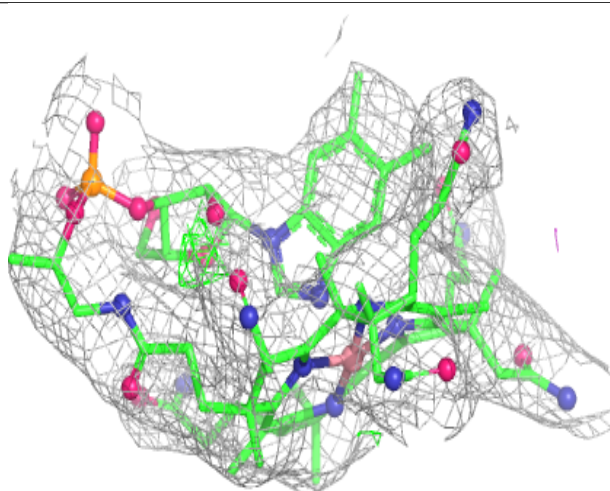
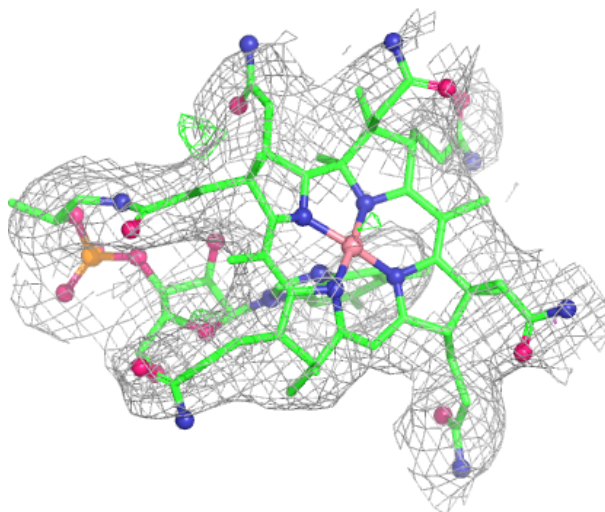
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | NAG  | F     | 2009 | 14/15 | 0.93 | 0.06 | 185,189,191,192             | 0     |
| 5   | NAG  | B     | 2001 | 14/15 | 0.94 | 0.09 | 195,202,205,206             | 0     |
| 5   | NAG  | F     | 2001 | 14/15 | 0.95 | 0.08 | 192,198,201,203             | 0     |
| 5   | NAG  | B     | 2008 | 14/15 | 0.95 | 0.08 | 196,198,198,199             | 0     |
| 5   | NAG  | F     | 2012 | 14/15 | 0.95 | 0.08 | 139,157,192,194             | 0     |
| 5   | NAG  | E     | 2001 | 14/15 | 0.96 | 0.16 | 50,55,60,61                 | 14    |
| 5   | NAG  | D     | 2007 | 14/15 | 0.96 | 0.08 | 166,193,216,223             | 0     |
| 5   | NAG  | F     | 2008 | 14/15 | 0.96 | 0.05 | 190,198,203,205             | 0     |
| 5   | NAG  | D     | 2009 | 14/15 | 0.96 | 0.06 | 188,192,195,195             | 0     |
| 5   | NAG  | D     | 2012 | 14/15 | 0.96 | 0.08 | 145,163,197,200             | 0     |
| 5   | NAG  | A     | 2001 | 14/15 | 0.97 | 0.15 | 50,54,57,60                 | 14    |
| 5   | NAG  | F     | 2007 | 14/15 | 0.97 | 0.09 | 151,172,188,195             | 0     |
| 5   | NAG  | B     | 2012 | 14/15 | 0.97 | 0.07 | 146,163,198,200             | 0     |
| 5   | NAG  | D     | 2013 | 14/15 | 0.97 | 0.05 | 168,182,187,189             | 0     |
| 5   | NAG  | C     | 2001 | 14/15 | 0.97 | 0.14 | 45,49,52,54                 | 14    |
| 5   | NAG  | F     | 2013 | 14/15 | 0.97 | 0.07 | 162,176,180,183             | 0     |
| 5   | NAG  | B     | 2007 | 14/15 | 0.98 | 0.08 | 149,179,202,211             | 0     |
| 5   | NAG  | B     | 2013 | 14/15 | 0.98 | 0.05 | 157,169,174,176             | 0     |
| 7   | CA   | B     | 2014 | 1/1   | 0.98 | 0.04 | 140,140,140,140             | 0     |
| 7   | CA   | D     | 2014 | 1/1   | 0.98 | 0.04 | 163,163,163,163             | 0     |
| 7   | CA   | B     | 2017 | 1/1   | 0.99 | 0.04 | 82,82,82,82                 | 0     |
| 7   | CA   | B     | 2016 | 1/1   | 0.99 | 0.03 | 147,147,147,147             | 0     |
| 7   | CA   | D     | 2016 | 1/1   | 0.99 | 0.04 | 139,139,139,139             | 0     |
| 7   | CA   | D     | 2017 | 1/1   | 0.99 | 0.02 | 79,79,79,79                 | 0     |
| 7   | CA   | F     | 2014 | 1/1   | 0.99 | 0.03 | 151,151,151,151             | 0     |
| 7   | CA   | F     | 2016 | 1/1   | 0.99 | 0.04 | 144,144,144,144             | 0     |
| 7   | CA   | F     | 2017 | 1/1   | 0.99 | 0.05 | 80,80,80,80                 | 0     |
| 7   | CA   | B     | 2015 | 1/1   | 1.00 | 0.02 | 54,54,54,54                 | 0     |
| 6   | B12  | C     | 2007 | 91/91 | 1.00 | 0.04 | 46,65,81,88                 | 0     |
| 6   | B12  | E     | 2007 | 91/91 | 1.00 | 0.04 | 40,66,91,95                 | 0     |
| 7   | CA   | F     | 2015 | 1/1   | 1.00 | 0.03 | 58,58,58,58                 | 0     |
| 6   | B12  | A     | 2007 | 91/91 | 1.00 | 0.04 | 45,64,92,100                | 0     |
| 7   | CA   | D     | 2015 | 1/1   | 1.00 | 0.02 | 60,60,60,60                 | 0     |

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



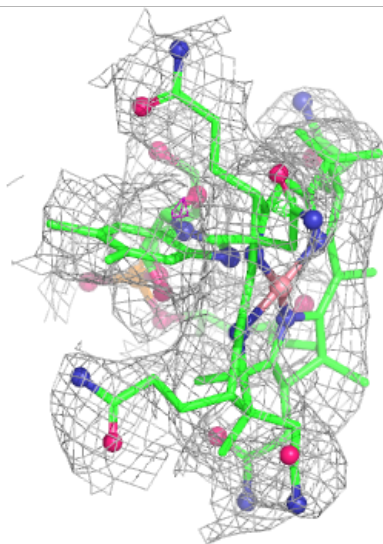
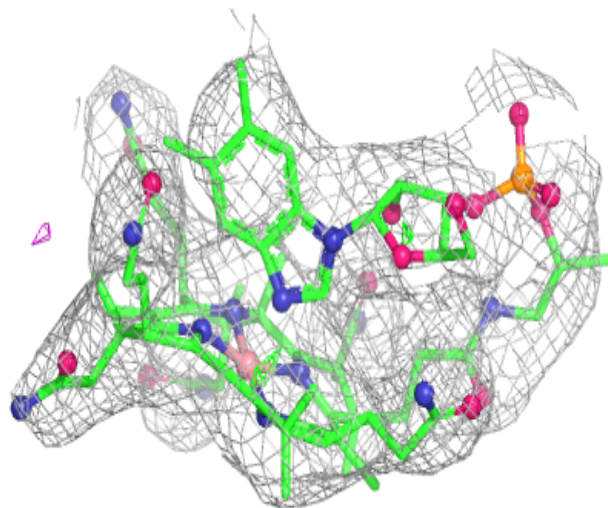
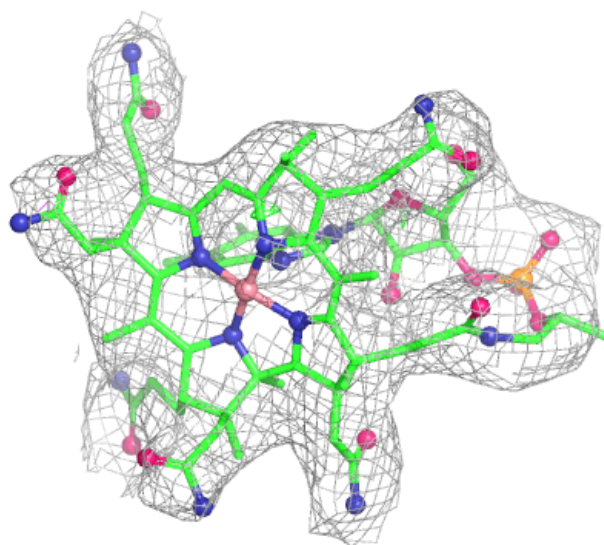
**Electron density around B12 C 2007:**

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



**Electron density around B12 E 2007:**

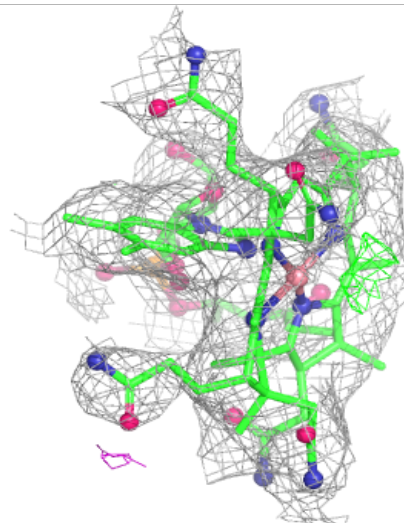
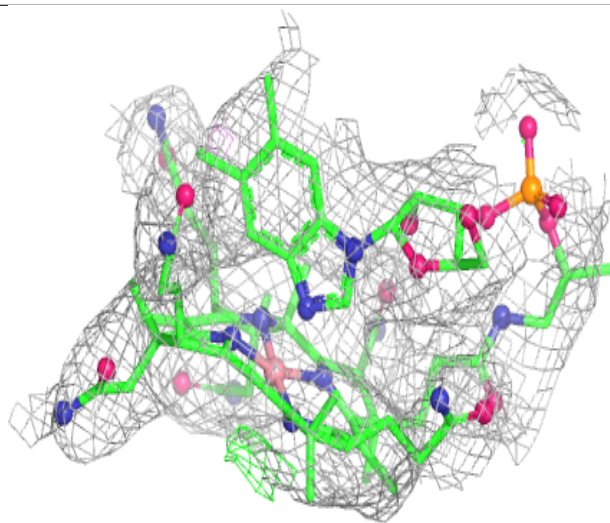
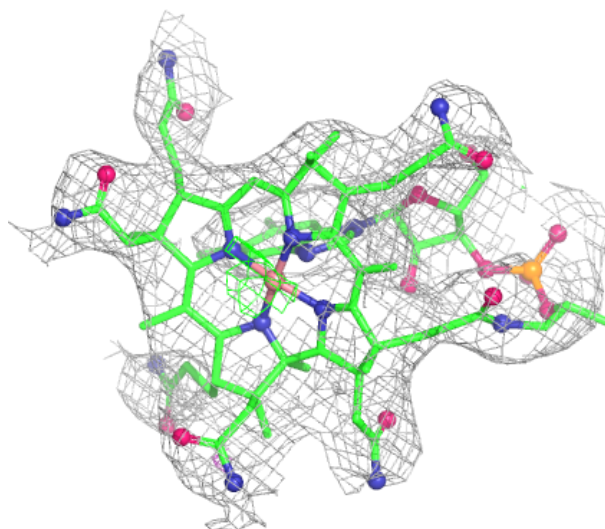
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around B12 A 2007:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.