



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:54 am BST

PDB ID : 3V4T  
Title : E. cloacae C115D MURA liganded with UNAG  
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.  
Deposited on : 2011-12-15  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

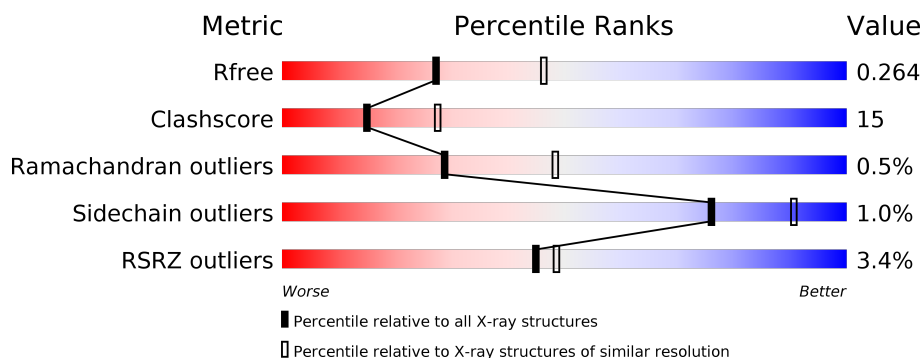
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 4661 (2.50-2.50)                                      |
| Clashscore            | 141614                      | 5346 (2.50-2.50)                                      |
| Ramachandran outliers | 138981                      | 5231 (2.50-2.50)                                      |
| Sidechain outliers    | 138945                      | 5233 (2.50-2.50)                                      |
| RSRZ outliers         | 127900                      | 4559 (2.50-2.50)                                      |

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 on 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     | 419    | <div> <div>10%</div> <div>74%</div> <div>26%</div> </div> |
| 1   | B     | 419    | <div> <div>10%</div> <div>61%</div> <div>38%</div> </div> |
| 1   | C     | 419    | <div> <div>2%</div> <div>69%</div> <div>30%</div> </div>  |
| 1   | D     | 419    | <div> <div>3%</div> <div>70%</div> <div>29%</div> </div>  |
| 1   | E     | 419    | <div> <div>4%</div> <div>68%</div> <div>31%</div> </div>  |
| 1   | F     | 419    | <div> <div>2%</div> <div>78%</div> <div>21%</div> </div>  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 419    |  |
| 1   | H     | 419    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | ACT  | C     | 502 | -         | -        | X       | -                |
| 3   | ACT  | C     | 503 | -         | -        | X       | -                |
| 3   | ACT  | E     | 502 | -         | -        | X       | -                |
| 3   | ACT  | E     | 504 | -         | -        | -       | X                |
| 3   | ACT  | F     | 502 | -         | -        | -       | X                |
| 3   | ACT  | F     | 503 | -         | -        | X       | -                |
| 4   | EDO  | E     | 510 | -         | -        | -       | X                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26190 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | B     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | C     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | D     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | E     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | F     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | G     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |
| 1   | H     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3144  | 1977 | 554 | 600 | 13 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

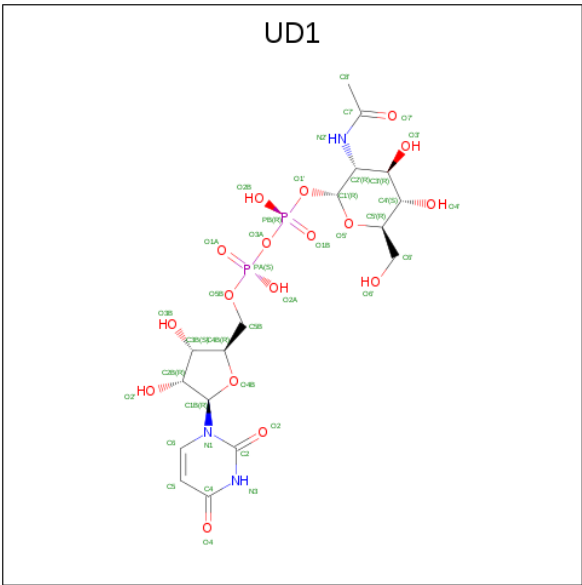
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| A     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| B     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| B     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| C     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| C     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| D     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| D     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| E     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| E     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| F     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| F     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| G     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| G     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |
| H     | 67      | IAS      | ASN    | SEE REMARK 999      | UNP P33038 |
| H     | 115     | ASP      | CYS    | ENGINEERED MUTATION | UNP P33038 |

- Molecule 2 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>3</sub>O<sub>17</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 39    | 17 | 3 | 17 | 2 |         |         |

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



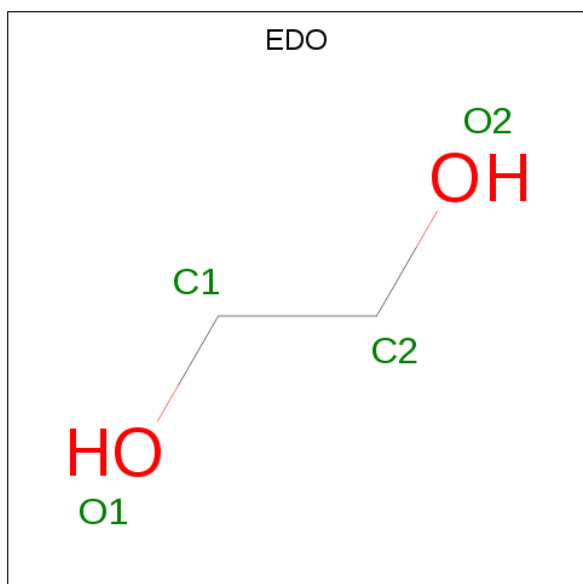
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>4 2 2 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 67       | Total O<br>67 67 | 0       | 0       |

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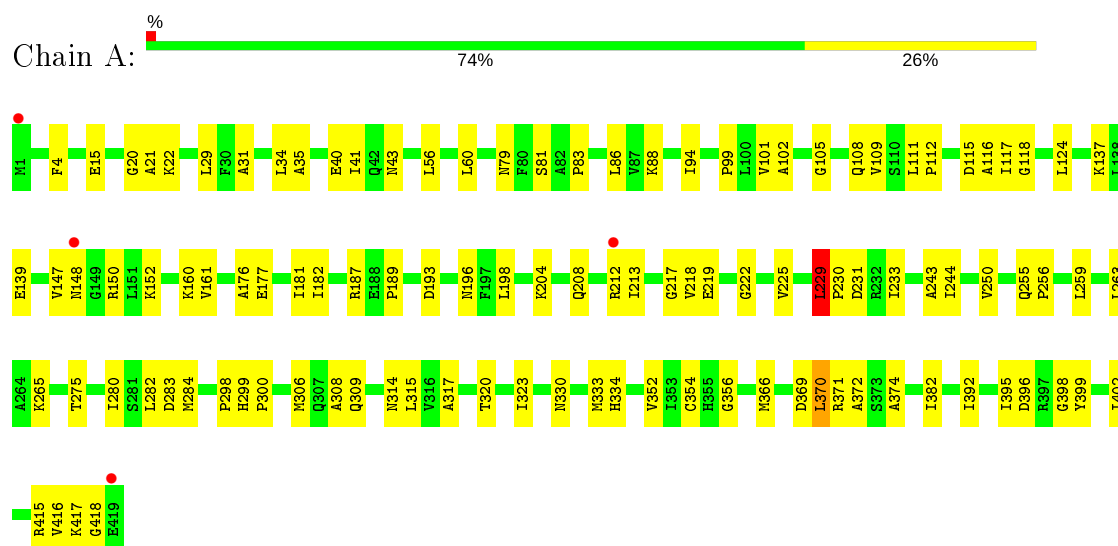
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5   | B     | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 5   | C     | 53       | Total<br>53 | O<br>53 | 0       | 0       |
| 5   | D     | 61       | Total<br>61 | O<br>61 | 0       | 0       |
| 5   | E     | 66       | Total<br>66 | O<br>66 | 0       | 0       |
| 5   | F     | 60       | Total<br>60 | O<br>60 | 0       | 0       |
| 5   | G     | 67       | Total<br>67 | O<br>67 | 0       | 0       |
| 5   | H     | 63       | Total<br>63 | O<br>63 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

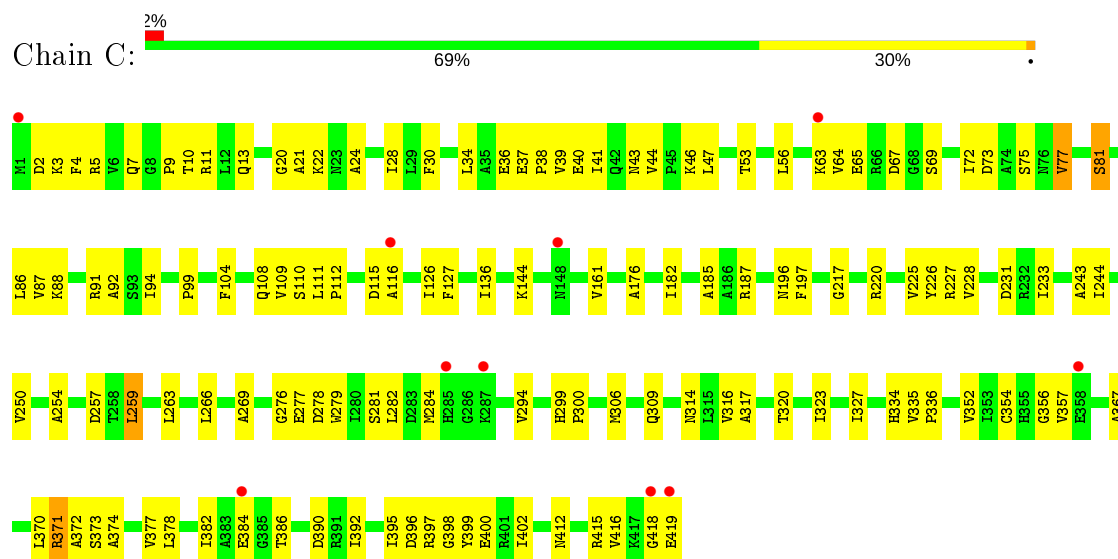
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



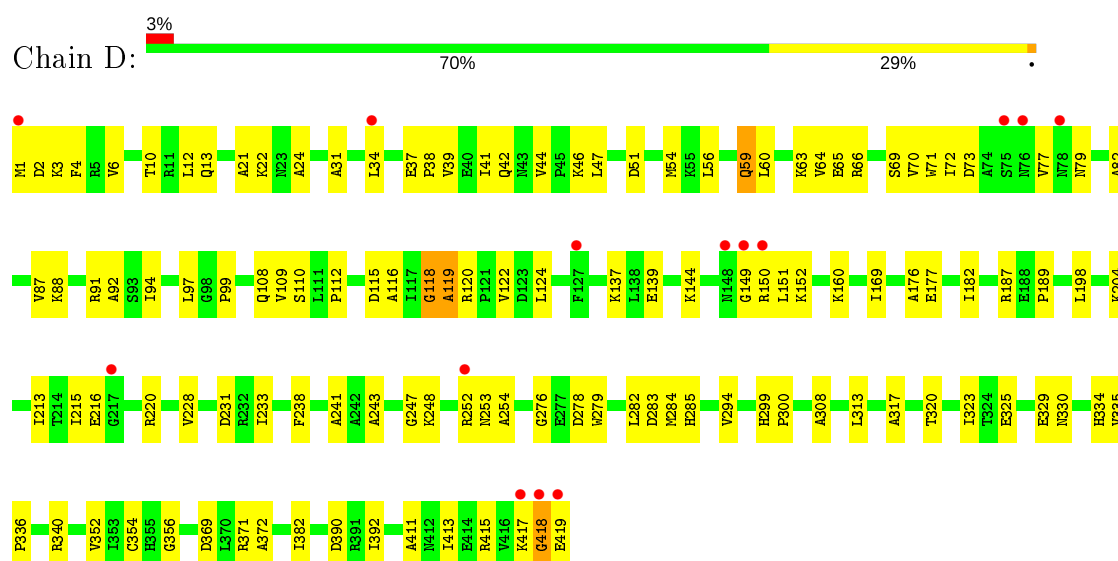
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



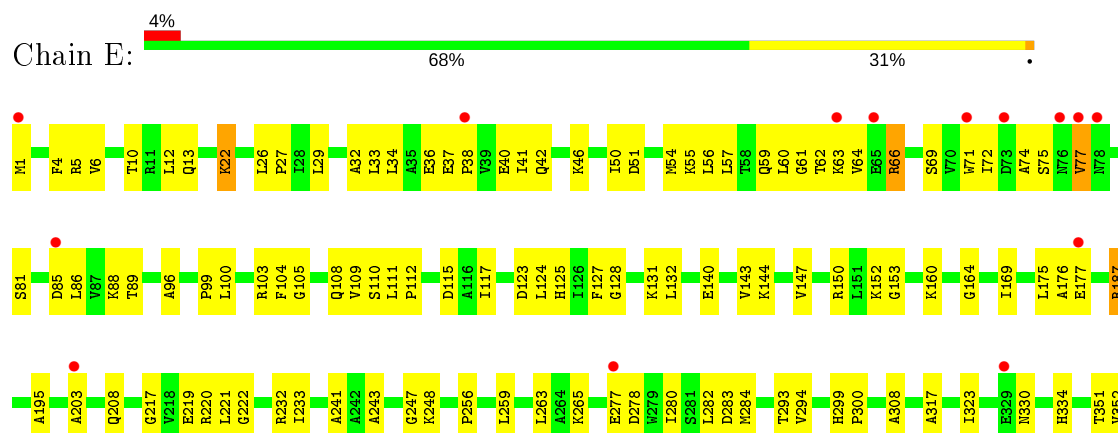
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

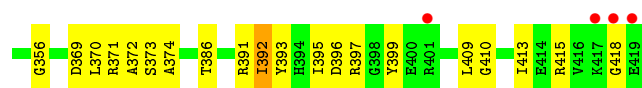


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

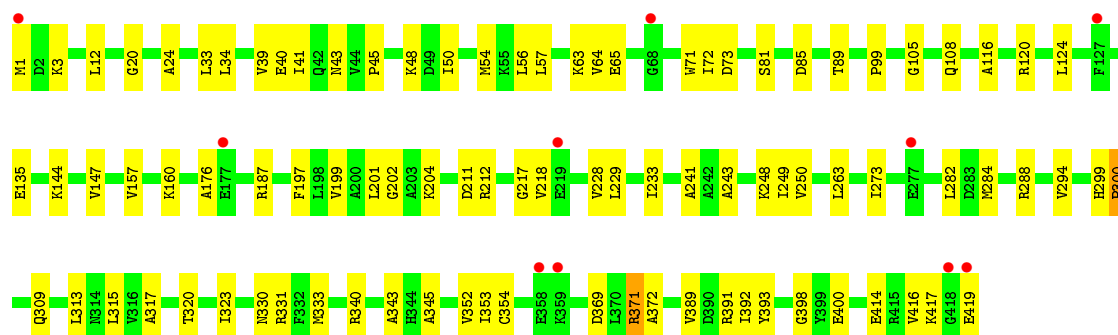
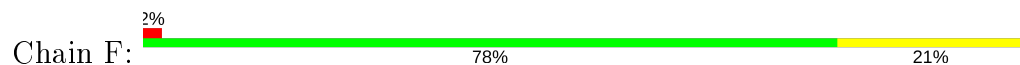


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

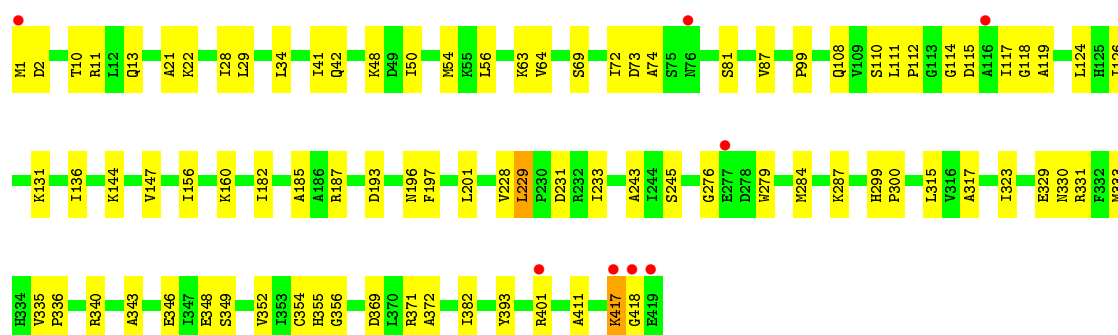
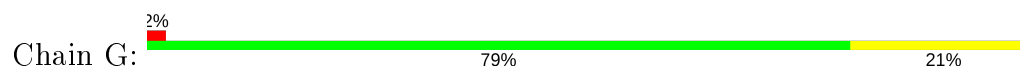




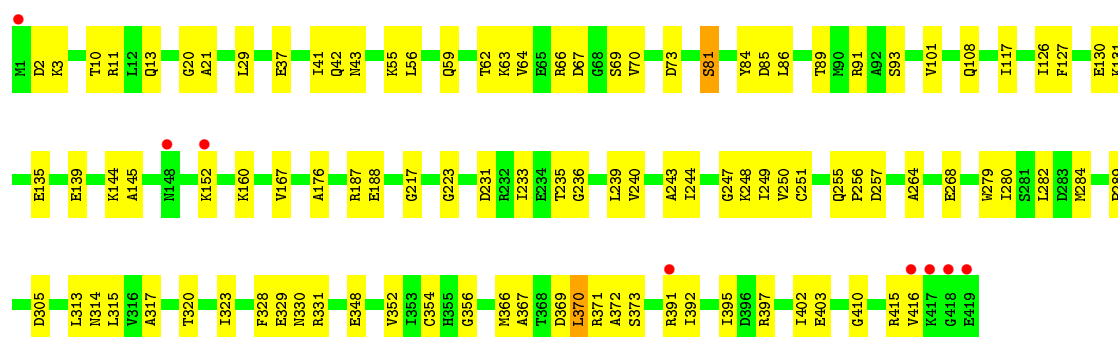
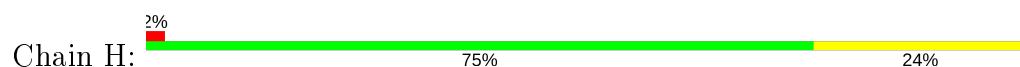
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 83.05Å 153.14Å 131.68Å<br>90.00° 102.36° 90.00°             | Depositor        |
| Resolution (Å)  | 19.77 – 2.50<br>19.77 – 2.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (19.77-2.50)<br>99.7 (19.77-2.50)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | 0.05  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.46 (at 2.50Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.208 , 0.271<br>0.198 , 0.264                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1216 reflections (1.10%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 39.3  | Xtriage          |
| Anisotropy  | 0.279   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.39 , 52.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 26190   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.63% 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: UD1, EDO, IAS, ACT

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.56         | 1/3180 (0.0%)  | 0.91        | 1/4308 (0.0%)  |
| 1   | B     | 0.53         | 3/3180 (0.1%)  | 0.89        | 2/4308 (0.0%)  |
| 1   | C     | 0.49         | 0/3180         | 0.88        | 1/4308 (0.0%)  |
| 1   | D     | 0.49         | 0/3180         | 0.90        | 0/4308         |
| 1   | E     | 0.50         | 1/3180 (0.0%)  | 0.89        | 1/4308 (0.0%)  |
| 1   | F     | 0.51         | 1/3180 (0.0%)  | 0.89        | 0/4308         |
| 1   | G     | 0.52         | 0/3180         | 0.89        | 2/4308 (0.0%)  |
| 1   | H     | 0.49         | 0/3180         | 0.89        | 2/4308 (0.0%)  |
| All | All   | 0.51         | 6/25440 (0.0%) | 0.89        | 9/34464 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | A     | 300 | PRO  | N-CD    | -12.67 | 1.30        | 1.47     |
| 1   | B     | 300 | PRO  | N-CD    | -12.44 | 1.30        | 1.47     |
| 1   | F     | 300 | PRO  | N-CD    | -11.88 | 1.31        | 1.47     |
| 1   | B     | 38  | PRO  | N-CD    | -10.56 | 1.33        | 1.47     |
| 1   | E     | 277 | GLU  | CG-CD   | 5.46   | 1.60        | 1.51     |
| 1   | B     | 279 | TRP  | NE1-CE2 | -5.03  | 1.31        | 1.37     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 370 | LEU  | CA-CB-CG | 8.73  | 135.39      | 115.30   |
| 1   | A     | 229 | LEU  | CA-CB-CG | 6.67  | 130.64      | 115.30   |
| 1   | B     | 81  | SER  | N-CA-C   | 5.83  | 126.74      | 111.00   |
| 1   | G     | 287 | LYS  | N-CA-C   | 5.79  | 126.63      | 111.00   |
| 1   | B     | 276 | GLY  | N-CA-C   | -5.43 | 99.53       | 113.10   |
| 1   | C     | 81  | SER  | N-CA-C   | 5.19  | 125.02      | 111.00   |
| 1   | G     | 417 | LYS  | N-CA-C   | 5.19  | 125.02      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | E     | 247 | GLY  | N-CA-C | 5.18 | 126.05      | 113.10   |
| 1   | H     | 81  | SER  | N-CA-C | 5.10 | 124.77      | 111.00   |

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     | 3144  | 0        | 3215     | 92      | 0            |
| 1   | B     | 3144  | 0        | 3215     | 136     | 1            |
| 1   | C     | 3144  | 0        | 3215     | 108     | 0            |
| 1   | D     | 3144  | 0        | 3215     | 95      | 0            |
| 1   | E     | 3144  | 0        | 3215     | 112     | 0            |
| 1   | F     | 3144  | 0        | 3215     | 74      | 0            |
| 1   | G     | 3144  | 0        | 3215     | 76      | 0            |
| 1   | H     | 3144  | 0        | 3215     | 99      | 1            |
| 2   | A     | 39    | 0        | 25       | 1       | 0            |
| 2   | B     | 39    | 0        | 25       | 0       | 0            |
| 2   | C     | 39    | 0        | 25       | 0       | 0            |
| 2   | D     | 39    | 0        | 25       | 0       | 0            |
| 2   | E     | 39    | 0        | 25       | 0       | 0            |
| 2   | F     | 39    | 0        | 25       | 0       | 0            |
| 2   | G     | 39    | 0        | 25       | 0       | 0            |
| 2   | H     | 39    | 0        | 25       | 0       | 0            |
| 3   | A     | 16    | 0        | 12       | 0       | 0            |
| 3   | B     | 4     | 0        | 3        | 0       | 0            |
| 3   | C     | 8     | 0        | 6        | 4       | 0            |
| 3   | D     | 8     | 0        | 6        | 0       | 0            |
| 3   | E     | 12    | 0        | 9        | 2       | 0            |
| 3   | F     | 12    | 0        | 9        | 3       | 0            |
| 3   | H     | 20    | 0        | 15       | 2       | 0            |
| 4   | A     | 16    | 0        | 24       | 2       | 0            |
| 4   | B     | 12    | 0        | 18       | 0       | 0            |
| 4   | C     | 16    | 0        | 24       | 0       | 0            |
| 4   | D     | 28    | 0        | 42       | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | E     | 28    | 0        | 42       | 1       | 0            |
| 4   | F     | 20    | 0        | 30       | 1       | 0            |
| 4   | G     | 28    | 0        | 42       | 1       | 0            |
| 4   | H     | 28    | 0        | 42       | 3       | 0            |
| 5   | A     | 67    | 0        | 0        | 0       | 0            |
| 5   | B     | 33    | 0        | 0        | 1       | 0            |
| 5   | C     | 53    | 0        | 0        | 4       | 0            |
| 5   | D     | 61    | 0        | 0        | 1       | 0            |
| 5   | E     | 66    | 0        | 0        | 3       | 0            |
| 5   | F     | 60    | 0        | 0        | 2       | 0            |
| 5   | G     | 67    | 0        | 0        | 5       | 0            |
| 5   | H     | 63    | 0        | 0        | 4       | 0            |
| All | All   | 26190 | 0        | 26244    | 784     | 1            |

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 15.

All (784) 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:G:1:MET:O      | 1:G:418:GLY:HA2  | 1.20                     | 1.28              |
| 1:B:418:GLY:O    | 1:B:419:GLU:HG3  | 1.11                     | 1.24              |
| 1:A:395:ILE:CD1  | 1:A:402:ILE:HG21 | 1.66                     | 1.24              |
| 1:C:418:GLY:CA   | 1:C:419:GLU:O    | 1.83                     | 1.24              |
| 1:A:395:ILE:HD11 | 1:A:402:ILE:CG2  | 1.69                     | 1.23              |
| 1:C:392:ILE:O    | 1:C:395:ILE:HG22 | 1.11                     | 1.22              |
| 1:C:418:GLY:HA3  | 1:C:419:GLU:O    | 1.40                     | 1.21              |
| 1:G:1:MET:O      | 1:G:418:GLY:CA   | 1.90                     | 1.20              |
| 1:B:418:GLY:O    | 1:B:419:GLU:CG   | 1.93                     | 1.16              |
| 1:C:392:ILE:O    | 1:C:395:ILE:CG2  | 2.03                     | 1.05              |
| 1:A:392:ILE:O    | 1:A:395:ILE:HG22 | 1.56                     | 1.05              |
| 1:C:395:ILE:HD11 | 1:C:402:ILE:HG21 | 1.04                     | 1.03              |
| 1:B:81:SER:HB3   | 1:B:108:GLN:HG3  | 1.42                     | 1.02              |
| 1:C:418:GLY:HA2  | 1:C:419:GLU:O    | 1.58                     | 1.01              |
| 1:D:120:ARG:HH22 | 4:D:510:EDO:H12  | 1.26                     | 1.01              |
| 1:C:395:ILE:CD1  | 1:C:402:ILE:HG21 | 1.92                     | 0.98              |
| 1:B:15:GLU:HG2   | 1:B:250:VAL:HB   | 1.40                     | 0.98              |
| 1:F:108:GLN:HG2  | 1:F:144:LYS:HG2  | 1.47                     | 0.97              |
| 1:G:118:GLY:HA3  | 1:G:329:GLU:OE1  | 1.63                     | 0.97              |
| 1:E:34:LEU:HD21  | 1:E:99:PRO:HA    | 1.46                     | 0.96              |
| 1:C:56:LEU:HB2   | 1:C:86:LEU:HD13  | 1.48                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:233:ILE:HG21 | 1:D:371:ARG:HD2  | 1.48                     | 0.94              |
| 1:C:395:ILE:HD11 | 1:C:402:ILE:CG2  | 1.97                     | 0.93              |
| 1:G:108:GLN:HG2  | 1:G:144:LYS:HG2  | 1.51                     | 0.93              |
| 1:H:108:GLN:HG2  | 1:H:144:LYS:HG2  | 1.51                     | 0.93              |
| 1:C:4:PHE:HE2    | 1:C:395:ILE:HD13 | 1.34                     | 0.92              |
| 1:H:370:LEU:HD12 | 1:H:397:ARG:HD3  | 1.51                     | 0.91              |
| 1:H:2:ASP:HB3    | 1:H:392:ILE:HD11 | 1.53                     | 0.90              |
| 1:H:370:LEU:CD1  | 1:H:397:ARG:HD3  | 2.03                     | 0.89              |
| 1:C:63:LYS:HB3   | 1:C:73:ASP:HB3   | 1.55                     | 0.88              |
| 1:G:323:ILE:HB   | 1:G:352:VAL:HG12 | 1.54                     | 0.87              |
| 1:D:369:ASP:HB3  | 1:D:372:ALA:HB3  | 1.55                     | 0.87              |
| 1:D:94:ILE:HA    | 1:D:109:VAL:HG11 | 1.58                     | 0.85              |
| 1:D:177:GLU:HG2  | 4:D:508:EDO:H21  | 1.58                     | 0.84              |
| 1:G:2:ASP:OD1    | 1:G:417:LYS:HG2  | 1.78                     | 0.83              |
| 1:F:331:ARG:H    | 3:F:503:ACT:H2   | 1.43                     | 0.83              |
| 1:A:259:LEU:HD12 | 1:A:263:LEU:HG   | 1.61                     | 0.82              |
| 1:D:41:ILE:O     | 1:D:69:SER:HB2   | 1.79                     | 0.82              |
| 1:F:369:ASP:HB3  | 1:F:372:ALA:HB3  | 1.62                     | 0.82              |
| 1:G:1:MET:O      | 1:G:418:GLY:N    | 2.12                     | 0.81              |
| 1:A:306:MET:HE1  | 1:A:309:GLN:NE2  | 1.96                     | 0.81              |
| 1:H:42:GLN:HA    | 1:H:69:SER:HB3   | 1.62                     | 0.80              |
| 1:G:118:GLY:CA   | 1:G:329:GLU:OE1  | 2.28                     | 0.80              |
| 1:C:367:ALA:HB1  | 1:C:373:SER:HB3  | 1.62                     | 0.80              |
| 1:B:64:VAL:O     | 1:B:65:GLU:HG3   | 1.84                     | 0.77              |
| 1:G:243:ALA:HA   | 1:G:284:MET:HG3  | 1.67                     | 0.77              |
| 1:G:81:SER:HB3   | 1:G:108:GLN:HB2  | 1.66                     | 0.77              |
| 1:B:47:LEU:HB2   | 1:B:50:ILE:HG12  | 1.65                     | 0.77              |
| 1:E:243:ALA:HA   | 1:E:284:MET:CG   | 2.14                     | 0.77              |
| 1:F:212:ARG:HD2  | 5:F:660:HOH:O    | 1.83                     | 0.77              |
| 1:H:243:ALA:HA   | 1:H:284:MET:CG   | 2.15                     | 0.76              |
| 1:B:4:PHE:CD1    | 1:B:392:ILE:HD13 | 2.20                     | 0.76              |
| 1:C:4:PHE:CE2    | 1:C:395:ILE:HD13 | 2.20                     | 0.76              |
| 1:D:108:GLN:HG2  | 1:D:144:LYS:HG2  | 1.69                     | 0.75              |
| 1:E:34:LEU:HD21  | 1:E:99:PRO:CA    | 2.17                     | 0.75              |
| 1:H:108:GLN:CG   | 1:H:144:LYS:HG2  | 2.17                     | 0.75              |
| 1:B:244:ILE:HD12 | 1:B:382:ILE:HD13 | 1.68                     | 0.74              |
| 1:C:418:GLY:CA   | 1:C:419:GLU:C    | 2.52                     | 0.74              |
| 1:E:55:LYS:HE3   | 1:E:86:LEU:HD21  | 1.69                     | 0.74              |
| 1:C:370:LEU:HG   | 1:C:371:ARG:HG2  | 1.70                     | 0.74              |
| 1:E:36:GLU:HG2   | 1:E:103:ARG:HH21 | 1.53                     | 0.73              |
| 1:E:36:GLU:O     | 1:E:75:SER:HB3   | 1.89                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:41:ILE:HG22  | 1:C:44:VAL:CG2   | 2.19                     | 0.72              |
| 1:E:1:MET:N      | 1:E:418:GLY:HA2  | 2.04                     | 0.72              |
| 1:G:233:ILE:HG21 | 1:G:371:ARG:HD2  | 1.71                     | 0.72              |
| 1:F:48:LYS:NZ    | 1:F:393:TYR:HB2  | 2.03                     | 0.72              |
| 1:C:257:ASP:HB3  | 3:C:502:ACT:H1   | 1.72                     | 0.72              |
| 1:D:323:ILE:HB   | 1:D:352:VAL:CG1  | 2.20                     | 0.72              |
| 1:D:91:ARG:NH2   | 1:D:120:ARG:O    | 2.22                     | 0.72              |
| 1:B:37:GLU:HB2   | 1:B:223:GLY:H    | 1.55                     | 0.71              |
| 1:G:323:ILE:HB   | 1:G:352:VAL:CG1  | 2.18                     | 0.71              |
| 1:A:259:LEU:CD1  | 1:A:263:LEU:HG   | 2.20                     | 0.71              |
| 1:C:3:LYS:HD3    | 1:C:390:ASP:OD1  | 1.89                     | 0.71              |
| 1:G:48:LYS:NZ    | 1:G:393:TYR:HB2  | 2.06                     | 0.71              |
| 1:B:259:LEU:HD12 | 1:B:263:LEU:HG   | 1.70                     | 0.71              |
| 1:E:127:PHE:CZ   | 1:E:131:LYS:HE2  | 2.24                     | 0.71              |
| 1:A:181:ILE:HG21 | 1:A:212:ARG:HD2  | 1.72                     | 0.71              |
| 1:F:331:ARG:N    | 3:F:503:ACT:H2   | 2.05                     | 0.71              |
| 1:B:63:LYS:HB3   | 1:B:73:ASP:HB3   | 1.72                     | 0.71              |
| 1:F:33:LEU:HD21  | 1:F:57:LEU:HD22  | 1.73                     | 0.71              |
| 1:H:243:ALA:HA   | 1:H:284:MET:HG2  | 1.73                     | 0.70              |
| 1:A:29:LEU:HD23  | 1:A:41:ILE:CD1   | 2.21                     | 0.70              |
| 1:C:9:PRO:HD3    | 1:C:384:GLU:HG3  | 1.73                     | 0.70              |
| 1:H:315:LEU:HD23 | 1:H:354:CYS:HB3  | 1.72                     | 0.70              |
| 1:A:334:HIS:HB3  | 1:A:372:ALA:HB1  | 1.73                     | 0.70              |
| 1:C:108:GLN:HG2  | 1:C:144:LYS:HG2  | 1.74                     | 0.70              |
| 1:C:327:ILE:HD12 | 3:C:503:ACT:H1   | 1.73                     | 0.70              |
| 1:G:10:THR:HG21  | 1:G:411:ALA:HA   | 1.71                     | 0.70              |
| 1:C:7:GLN:HB2    | 1:C:412:ASN:ND2  | 2.06                     | 0.70              |
| 1:B:4:PHE:CE1    | 1:B:392:ILE:HD12 | 2.27                     | 0.70              |
| 1:G:346:GLU:OE2  | 1:G:355:HIS:NE2  | 2.21                     | 0.70              |
| 1:A:395:ILE:CD1  | 1:A:402:ILE:CG2  | 2.49                     | 0.69              |
| 1:B:21:ALA:HA    | 1:B:231:ASP:HB2  | 1.72                     | 0.69              |
| 1:D:323:ILE:HB   | 1:D:352:VAL:HG13 | 1.73                     | 0.69              |
| 1:E:370:LEU:H    | 1:E:370:LEU:HD23 | 1.58                     | 0.69              |
| 1:A:176:ALA:O    | 1:A:217:GLY:HA3  | 1.91                     | 0.69              |
| 1:G:315:LEU:HD13 | 1:G:343:ALA:HB1  | 1.75                     | 0.68              |
| 1:G:333:MET:HG3  | 5:G:663:HOH:O    | 1.92                     | 0.68              |
| 1:C:176:ALA:O    | 1:C:217:GLY:HA3  | 1.92                     | 0.68              |
| 1:C:396:ASP:CG   | 1:C:415:ARG:HH22 | 1.95                     | 0.68              |
| 1:B:418:GLY:O    | 1:B:419:GLU:CB   | 2.41                     | 0.68              |
| 1:A:229:LEU:HB2  | 1:A:230:PRO:HD2  | 1.75                     | 0.68              |
| 1:E:22:LYS:HZ1   | 3:E:502:ACT:H2   | 1.58                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:417:LYS:HG2  | 1:B:418:GLY:N    | 2.09                     | 0.68              |
| 1:C:81:SER:HB3   | 1:C:108:GLN:HB2  | 1.75                     | 0.68              |
| 1:A:29:LEU:HD23  | 1:A:41:ILE:HD12  | 1.74                     | 0.68              |
| 1:B:417:LYS:HG2  | 1:B:418:GLY:H    | 1.57                     | 0.68              |
| 1:E:103:ARG:NH1  | 1:E:104:PHE:HZ   | 1.91                     | 0.67              |
| 1:E:369:ASP:HB3  | 1:E:372:ALA:HB3  | 1.76                     | 0.67              |
| 1:E:108:GLN:HG2  | 1:E:144:LYS:HG2  | 1.75                     | 0.67              |
| 1:F:176:ALA:O    | 1:F:217:GLY:HA3  | 1.95                     | 0.67              |
| 1:B:4:PHE:CD1    | 1:B:392:ILE:CD1  | 2.78                     | 0.67              |
| 1:G:243:ALA:HA   | 1:G:284:MET:CG   | 2.25                     | 0.66              |
| 1:C:416:VAL:HG12 | 1:C:418:GLY:H    | 1.60                     | 0.66              |
| 1:F:369:ASP:CB   | 1:F:372:ALA:HB3  | 2.25                     | 0.66              |
| 1:D:149:GLY:O    | 1:D:150:ARG:HD3  | 1.96                     | 0.66              |
| 1:D:42:GLN:HA    | 1:D:69:SER:HB3   | 1.78                     | 0.66              |
| 1:E:36:GLU:HG2   | 1:E:103:ARG:NH2  | 2.11                     | 0.66              |
| 1:A:323:ILE:HB   | 1:A:352:VAL:CG1  | 2.26                     | 0.66              |
| 1:E:105:GLY:HA2  | 1:E:147:VAL:HG12 | 1.78                     | 0.66              |
| 1:H:370:LEU:CD1  | 1:H:397:ARG:CD   | 2.74                     | 0.66              |
| 1:A:229:LEU:HB2  | 1:A:230:PRO:CD   | 2.27                     | 0.66              |
| 1:H:369:ASP:HB3  | 1:H:372:ALA:HB3  | 1.78                     | 0.66              |
| 1:A:181:ILE:CG2  | 1:A:212:ARG:HD2  | 2.25                     | 0.65              |
| 1:F:243:ALA:HA   | 1:F:284:MET:CG   | 2.26                     | 0.65              |
| 1:A:317:ALA:O    | 1:A:356:GLY:HA3  | 1.96                     | 0.65              |
| 1:B:176:ALA:O    | 1:B:217:GLY:HA3  | 1.95                     | 0.65              |
| 1:A:370:LEU:O    | 1:A:371:ARG:HD2  | 1.96                     | 0.65              |
| 1:B:401:ARG:HG2  | 5:B:616:HOH:O    | 1.96                     | 0.65              |
| 1:D:137:LYS:HE3  | 1:D:139:GLU:OE1  | 1.97                     | 0.65              |
| 1:G:126:ILE:HG23 | 1:G:136:ILE:HD13 | 1.77                     | 0.65              |
| 1:E:243:ALA:HA   | 1:E:284:MET:HG2  | 1.78                     | 0.65              |
| 1:F:81:SER:HB3   | 1:F:108:GLN:HB2  | 1.79                     | 0.65              |
| 1:H:395:ILE:HG21 | 1:H:402:ILE:HG21 | 1.79                     | 0.64              |
| 1:C:227:ARG:HD2  | 5:C:637:HOH:O    | 1.97                     | 0.64              |
| 1:C:396:ASP:OD2  | 1:C:415:ARG:NH2  | 2.21                     | 0.64              |
| 1:E:393:TYR:O    | 1:E:397:ARG:HG3  | 1.97                     | 0.64              |
| 1:H:63:LYS:HB3   | 1:H:73:ASP:HB3   | 1.80                     | 0.64              |
| 1:A:243:ALA:HA   | 1:A:284:MET:CG   | 2.26                     | 0.64              |
| 1:B:118:GLY:CA   | 1:B:329:GLU:OE2  | 2.46                     | 0.64              |
| 1:E:128:GLY:HA3  | 1:E:169:ILE:HD11 | 1.79                     | 0.64              |
| 1:E:243:ALA:HA   | 1:E:284:MET:HG3  | 1.78                     | 0.64              |
| 1:F:243:ALA:HA   | 1:F:284:MET:HG3  | 1.77                     | 0.64              |
| 1:A:111:LEU:HD12 | 1:A:112:PRO:HD2  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:3:LYS:HA     | 1:F:392:ILE:HG23 | 1.80                     | 0.64              |
| 1:D:112:PRO:HA   | 4:D:509:EDO:H22  | 1.80                     | 0.64              |
| 1:B:29:LEU:HD23  | 1:B:41:ILE:HD12  | 1.79                     | 0.63              |
| 1:D:82:ALA:HB3   | 1:D:109:VAL:HG13 | 1.80                     | 0.63              |
| 1:D:243:ALA:HA   | 1:D:284:MET:CG   | 2.27                     | 0.63              |
| 1:B:74:ALA:O     | 1:B:77:VAL:HG23  | 1.97                     | 0.63              |
| 1:H:108:GLN:NE2  | 1:H:144:LYS:HE2  | 2.13                     | 0.63              |
| 1:H:41:ILE:O     | 1:H:69:SER:HB2   | 1.98                     | 0.63              |
| 1:D:38:PRO:HG3   | 1:D:73:ASP:OD2   | 1.97                     | 0.63              |
| 1:A:243:ALA:HA   | 1:A:284:MET:HG3  | 1.80                     | 0.63              |
| 1:C:34:LEU:HD21  | 1:C:99:PRO:HA    | 1.81                     | 0.63              |
| 1:G:41:ILE:O     | 1:G:69:SER:HB2   | 1.99                     | 0.63              |
| 1:G:196:ASN:HB3  | 4:G:505:EDO:H12  | 1.80                     | 0.63              |
| 1:G:29:LEU:HD23  | 1:G:41:ILE:HD12  | 1.81                     | 0.63              |
| 1:C:24:ALA:HB3   | 1:C:228:VAL:HG13 | 1.81                     | 0.62              |
| 1:H:10:THR:HG21  | 1:H:410:GLY:O    | 1.99                     | 0.62              |
| 1:B:418:GLY:C    | 1:B:419:GLU:HG3  | 2.11                     | 0.62              |
| 1:B:34:LEU:HD22  | 1:B:175:LEU:HD11 | 1.82                     | 0.62              |
| 1:E:282:LEU:C    | 1:E:282:LEU:HD23 | 2.20                     | 0.62              |
| 1:A:306:MET:CE   | 1:A:309:GLN:NE2  | 2.61                     | 0.62              |
| 1:B:152:LYS:HD2  | 1:B:177:GLU:O    | 1.99                     | 0.62              |
| 1:G:369:ASP:HB3  | 1:G:372:ALA:HB3  | 1.82                     | 0.62              |
| 1:F:204:LYS:HE3  | 1:F:218:VAL:HG12 | 1.82                     | 0.62              |
| 1:A:320:THR:HG21 | 1:C:320:THR:HG21 | 1.81                     | 0.61              |
| 1:D:108:GLN:HG3  | 5:D:646:HOH:O    | 1.98                     | 0.61              |
| 1:E:46:LYS:HG2   | 1:E:66:ARG:NH1   | 2.15                     | 0.61              |
| 1:E:22:LYS:NZ    | 3:E:502:ACT:H2   | 2.16                     | 0.61              |
| 1:G:48:LYS:HZ3   | 1:G:393:TYR:HB2  | 1.65                     | 0.61              |
| 1:B:2:ASP:OD2    | 1:B:415:ARG:HD3  | 2.01                     | 0.61              |
| 1:F:63:LYS:HB3   | 1:F:73:ASP:HB3   | 1.81                     | 0.61              |
| 1:G:335:VAL:HB   | 1:G:336:PRO:HD3  | 1.83                     | 0.61              |
| 1:D:120:ARG:HH22 | 4:D:510:EDO:C1   | 2.07                     | 0.61              |
| 1:D:92:ALA:HA    | 4:D:504:EDO:H12  | 1.82                     | 0.61              |
| 1:F:323:ILE:HB   | 1:F:352:VAL:HG13 | 1.83                     | 0.61              |
| 1:B:39:VAL:HG22  | 1:B:223:GLY:HA2  | 1.81                     | 0.60              |
| 1:H:370:LEU:HD11 | 1:H:397:ARG:NE   | 2.16                     | 0.60              |
| 1:H:313:LEU:C    | 1:H:313:LEU:HD23 | 2.22                     | 0.60              |
| 1:B:334:HIS:HB3  | 1:B:372:ALA:HB1  | 1.83                     | 0.60              |
| 1:B:3:LYS:HG3    | 1:B:3:LYS:O      | 2.02                     | 0.60              |
| 1:B:367:ALA:HB1  | 1:B:373:SER:OG   | 2.01                     | 0.60              |
| 1:D:124:LEU:HD11 | 1:D:160:LYS:HG2  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:373:SER:HB3  | 1:B:395:ILE:HG12 | 1.83                     | 0.60              |
| 1:B:4:PHE:CD2    | 1:B:413:ILE:HD11 | 2.36                     | 0.60              |
| 1:F:3:LYS:HB2    | 1:F:389:VAL:O    | 2.00                     | 0.60              |
| 1:H:81:SER:HB3   | 1:H:108:GLN:HB2  | 1.83                     | 0.60              |
| 1:A:369:ASP:C    | 1:A:371:ARG:H    | 2.05                     | 0.59              |
| 1:H:176:ALA:O    | 1:H:217:GLY:HA3  | 2.02                     | 0.59              |
| 1:E:41:ILE:O     | 1:E:69:SER:HB2   | 2.03                     | 0.59              |
| 1:E:5:ARG:NH1    | 1:E:386:THR:HG21 | 2.17                     | 0.59              |
| 1:A:150:ARG:HH12 | 1:A:219:GLU:HA   | 1.67                     | 0.59              |
| 1:G:340:ARG:HG2  | 1:G:340:ARG:HH11 | 1.66                     | 0.59              |
| 1:G:348:GLU:O    | 1:G:349:SER:HB3  | 2.03                     | 0.59              |
| 1:E:150:ARG:HB2  | 1:E:177:GLU:CG   | 2.30                     | 0.59              |
| 1:H:366:MET:CE   | 1:H:391:ARG:HD2  | 2.32                     | 0.59              |
| 1:A:204:LYS:HE2  | 1:A:218:VAL:HG12 | 1.84                     | 0.59              |
| 1:A:306:MET:HE1  | 1:A:309:GLN:HE21 | 1.65                     | 0.59              |
| 1:D:63:LYS:HB3   | 1:D:73:ASP:HB3   | 1.84                     | 0.59              |
| 1:A:40:GLU:HB3   | 1:A:225:VAL:HG22 | 1.84                     | 0.59              |
| 1:A:116:ALA:O    | 1:A:330:ASN:ND2  | 2.35                     | 0.59              |
| 1:B:48:LYS:HE3   | 1:B:397:ARG:HG2  | 1.85                     | 0.59              |
| 1:E:323:ILE:HB   | 1:E:352:VAL:HG13 | 1.85                     | 0.59              |
| 1:E:152:LYS:HD2  | 1:E:153:GLY:N    | 2.18                     | 0.59              |
| 1:G:317:ALA:O    | 1:G:356:GLY:HA3  | 2.03                     | 0.59              |
| 1:B:4:PHE:CE1    | 1:B:392:ILE:CD1  | 2.85                     | 0.58              |
| 1:C:4:PHE:HE2    | 1:C:395:ILE:CD1  | 2.12                     | 0.58              |
| 1:A:259:LEU:HD12 | 1:A:263:LEU:CG   | 2.31                     | 0.58              |
| 1:C:233:ILE:HG23 | 1:C:306:MET:HE3  | 1.84                     | 0.58              |
| 1:B:34:LEU:HD22  | 1:B:175:LEU:CD1  | 2.33                     | 0.58              |
| 1:D:64:VAL:HG22  | 1:D:72:ILE:HD13  | 1.85                     | 0.58              |
| 1:H:243:ALA:HA   | 1:H:284:MET:HG3  | 1.84                     | 0.58              |
| 1:C:36:GLU:OE1   | 1:C:220:ARG:NE   | 2.35                     | 0.58              |
| 1:F:48:LYS:HZ1   | 1:F:393:TYR:HB2  | 1.68                     | 0.58              |
| 1:H:85:ASP:O     | 1:H:89:THR:HG23  | 2.03                     | 0.58              |
| 1:A:370:LEU:HD12 | 1:A:370:LEU:O    | 2.03                     | 0.58              |
| 1:H:152:LYS:HE3  | 5:H:627:HOH:O    | 2.03                     | 0.58              |
| 1:B:4:PHE:H      | 1:B:392:ILE:HG21 | 1.68                     | 0.57              |
| 1:C:334:HIS:HB3  | 1:C:372:ALA:HB1  | 1.85                     | 0.57              |
| 1:G:1:MET:C      | 1:G:418:GLY:HA2  | 2.14                     | 0.57              |
| 1:F:197:PHE:CZ   | 1:F:201:LEU:HD11 | 2.40                     | 0.57              |
| 1:G:124:LEU:HD11 | 1:G:160:LYS:HG2  | 1.85                     | 0.57              |
| 1:B:118:GLY:HA3  | 1:B:329:GLU:OE2  | 2.03                     | 0.57              |
| 1:B:56:LEU:HB2   | 1:B:86:LEU:HD13  | 1.84                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:LEU:HD12 | 1:C:263:LEU:HG   | 1.86                     | 0.57              |
| 1:D:41:ILE:HG22  | 1:D:44:VAL:CG2   | 2.35                     | 0.57              |
| 1:D:66:ARG:HB3   | 1:D:70:VAL:HG22  | 1.86                     | 0.57              |
| 1:F:391:ARG:HB3  | 1:F:393:TYR:CE2  | 2.40                     | 0.57              |
| 1:A:333:MET:CE   | 1:A:333:MET:HA   | 2.35                     | 0.57              |
| 1:E:152:LYS:HD2  | 1:E:153:GLY:H    | 1.70                     | 0.57              |
| 1:E:373:SER:HB2  | 1:E:395:ILE:CD1  | 2.35                     | 0.57              |
| 1:E:40:GLU:OE2   | 1:E:71:TRP:NE1   | 2.38                     | 0.57              |
| 1:F:315:LEU:HD21 | 1:F:345:ALA:HB2  | 1.85                     | 0.57              |
| 1:A:15:GLU:HG2   | 1:A:250:VAL:HB   | 1.86                     | 0.56              |
| 1:E:103:ARG:NH1  | 1:E:104:PHE:CZ   | 2.72                     | 0.56              |
| 1:F:48:LYS:HZ3   | 1:F:393:TYR:HB2  | 1.70                     | 0.56              |
| 1:E:105:GLY:HA2  | 1:E:147:VAL:CG1  | 2.33                     | 0.56              |
| 1:F:3:LYS:NZ     | 1:F:419:GLU:C    | 2.58                     | 0.56              |
| 1:C:306:MET:HE2  | 1:C:306:MET:HA   | 1.88                     | 0.56              |
| 1:E:127:PHE:CE2  | 1:E:131:LYS:HE2  | 2.41                     | 0.56              |
| 1:A:395:ILE:HD11 | 1:A:402:ILE:HG21 | 0.75                     | 0.56              |
| 1:D:243:ALA:HA   | 1:D:284:MET:HG3  | 1.88                     | 0.56              |
| 1:A:395:ILE:HG23 | 1:A:396:ASP:N    | 2.21                     | 0.56              |
| 1:E:248:LYS:HD2  | 1:E:283:ASP:OD2  | 2.05                     | 0.56              |
| 1:B:314:ASN:HB3  | 1:B:354:CYS:HB2  | 1.87                     | 0.56              |
| 1:D:64:VAL:HG22  | 1:D:72:ILE:CD1   | 2.36                     | 0.55              |
| 1:B:17:THR:HA    | 1:B:252:ARG:HB2  | 1.87                     | 0.55              |
| 1:A:94:ILE:HA    | 1:A:109:VAL:HG11 | 1.88                     | 0.55              |
| 1:B:417:LYS:CG   | 1:B:418:GLY:H    | 2.19                     | 0.55              |
| 1:B:29:LEU:HD23  | 1:B:41:ILE:CD1   | 2.37                     | 0.55              |
| 1:G:81:SER:HB3   | 1:G:108:GLN:CB   | 2.36                     | 0.55              |
| 1:H:127:PHE:CE2  | 1:H:131:LYS:HD2  | 2.41                     | 0.55              |
| 1:E:330:ASN:OD1  | 1:H:330:ASN:HB2  | 2.06                     | 0.55              |
| 1:A:81:SER:HB3   | 1:A:108:GLN:HB2  | 1.89                     | 0.55              |
| 1:B:372:ALA:O    | 1:B:375:SER:N    | 2.39                     | 0.55              |
| 1:C:182:ILE:HG22 | 1:C:185:ALA:HB2  | 1.89                     | 0.55              |
| 1:C:250:VAL:HG22 | 1:C:281:SER:HB2  | 1.88                     | 0.55              |
| 1:D:56:LEU:HD23  | 1:D:56:LEU:C     | 2.26                     | 0.55              |
| 1:E:36:GLU:OE1   | 1:E:220:ARG:HB2  | 2.07                     | 0.55              |
| 1:H:323:ILE:HB   | 1:H:352:VAL:CG1  | 2.37                     | 0.55              |
| 1:B:40:GLU:HG3   | 1:B:71:TRP:NE1   | 2.22                     | 0.55              |
| 1:C:370:LEU:HD11 | 1:C:399:TYR:CD1  | 2.42                     | 0.54              |
| 1:D:94:ILE:HD12  | 1:D:122:VAL:HG11 | 1.89                     | 0.54              |
| 1:H:117:ILE:CG2  | 1:H:331:ARG:HG3  | 2.36                     | 0.54              |
| 3:H:503:ACT:H2   | 5:H:606:HOH:O    | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:LEU:C     | 1:A:56:LEU:HD23  | 2.27                     | 0.54              |
| 1:B:21:ALA:HB2   | 1:B:231:ASP:HA   | 1.90                     | 0.54              |
| 1:D:152:LYS:HD2  | 1:D:177:GLU:O    | 2.07                     | 0.54              |
| 1:D:313:LEU:C    | 1:D:313:LEU:HD23 | 2.27                     | 0.54              |
| 1:G:64:VAL:HG22  | 1:G:72:ILE:HD13  | 1.89                     | 0.54              |
| 1:B:48:LYS:NZ    | 1:B:393:TYR:HB2  | 2.22                     | 0.54              |
| 1:E:103:ARG:HH11 | 1:E:104:PHE:HZ   | 1.55                     | 0.54              |
| 1:E:373:SER:HB2  | 1:E:395:ILE:HD11 | 1.89                     | 0.54              |
| 1:H:248:LYS:NZ   | 1:H:248:LYS:HB3  | 2.23                     | 0.54              |
| 1:H:56:LEU:HD23  | 1:H:56:LEU:C     | 2.28                     | 0.54              |
| 1:C:77:VAL:HB    | 1:C:104:PHE:CZ   | 2.43                     | 0.54              |
| 1:F:56:LEU:HD23  | 1:F:56:LEU:C     | 2.27                     | 0.54              |
| 1:E:56:LEU:HD23  | 1:E:56:LEU:O     | 2.07                     | 0.54              |
| 1:F:323:ILE:HB   | 1:F:352:VAL:CG1  | 2.38                     | 0.54              |
| 1:B:126:ILE:O    | 1:B:130:GLU:HG3  | 2.07                     | 0.54              |
| 1:B:9:PRO:HD3    | 1:B:384:GLU:HA   | 1.89                     | 0.54              |
| 1:E:323:ILE:HB   | 1:E:352:VAL:CG1  | 2.37                     | 0.54              |
| 1:F:120:ARG:HB3  | 5:F:622:HOH:O    | 2.07                     | 0.54              |
| 1:B:97:LEU:O     | 1:B:97:LEU:HD12  | 2.08                     | 0.53              |
| 1:H:188:GLU:N    | 1:H:188:GLU:OE1  | 2.41                     | 0.53              |
| 1:B:244:ILE:HA   | 1:B:289:PRO:HG2  | 1.89                     | 0.53              |
| 1:C:127:PHE:HB2  | 5:C:641:HOH:O    | 2.07                     | 0.53              |
| 1:D:299:HIS:ND1  | 1:D:300:PRO:HA   | 2.24                     | 0.53              |
| 1:E:124:LEU:HD11 | 1:E:160:LYS:HG3  | 1.90                     | 0.53              |
| 1:G:56:LEU:HD23  | 1:G:56:LEU:O     | 2.08                     | 0.53              |
| 1:A:115:ASP:HB3  | 1:A:118:GLY:O    | 2.08                     | 0.53              |
| 1:A:31:ALA:HB1   | 1:A:198:LEU:HD21 | 1.90                     | 0.53              |
| 1:C:317:ALA:O    | 1:C:356:GLY:HA3  | 2.08                     | 0.53              |
| 1:E:150:ARG:HH12 | 1:E:219:GLU:HA   | 1.73                     | 0.53              |
| 1:G:111:LEU:HD12 | 1:G:112:PRO:HD2  | 1.91                     | 0.53              |
| 1:B:395:ILE:HG21 | 1:B:402:ILE:HG21 | 1.91                     | 0.53              |
| 1:C:299:HIS:CG   | 1:C:300:PRO:HA   | 2.43                     | 0.53              |
| 1:H:3:LYS:HB2    | 1:H:416:VAL:HB   | 1.91                     | 0.53              |
| 1:H:62:THR:HG22  | 1:H:64:VAL:HG22  | 1.90                     | 0.53              |
| 1:F:416:VAL:HG12 | 1:F:417:LYS:N    | 2.23                     | 0.53              |
| 1:H:317:ALA:O    | 1:H:356:GLY:HA3  | 2.09                     | 0.53              |
| 1:B:317:ALA:O    | 1:B:356:GLY:HA3  | 2.09                     | 0.53              |
| 1:B:45:PRO:O     | 1:B:50:ILE:HG13  | 2.09                     | 0.53              |
| 1:E:74:ALA:O     | 1:E:77:VAL:HG23  | 2.09                     | 0.53              |
| 1:B:46:LYS:N     | 1:B:400:GLU:OE1  | 2.35                     | 0.53              |
| 1:D:46:LYS:HG2   | 1:D:66:ARG:CZ    | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:243:ALA:HA   | 1:B:284:MET:HG3  | 1.91                     | 0.52              |
| 1:C:233:ILE:HG23 | 1:C:306:MET:CE   | 2.39                     | 0.52              |
| 1:E:5:ARG:HH12   | 1:E:386:THR:HG21 | 1.73                     | 0.52              |
| 1:A:181:ILE:HG23 | 1:A:212:ARG:CG   | 2.40                     | 0.52              |
| 1:C:111:LEU:HD12 | 1:C:112:PRO:HD2  | 1.90                     | 0.52              |
| 1:A:306:MET:HA   | 1:A:306:MET:HE2  | 1.91                     | 0.52              |
| 1:E:64:VAL:HG13  | 1:E:72:ILE:HD11  | 1.91                     | 0.52              |
| 1:H:21:ALA:HA    | 1:H:231:ASP:HB2  | 1.91                     | 0.52              |
| 1:D:118:GLY:O    | 1:D:119:ALA:HB3  | 2.09                     | 0.52              |
| 1:A:152:LYS:HD2  | 1:A:177:GLU:O    | 2.09                     | 0.52              |
| 1:C:316:VAL:HG23 | 1:C:316:VAL:O    | 2.08                     | 0.52              |
| 1:A:416:VAL:HG12 | 1:A:418:GLY:H    | 1.74                     | 0.52              |
| 1:B:97:LEU:HD11  | 1:B:145:ALA:HB3  | 1.92                     | 0.52              |
| 1:E:150:ARG:HB2  | 1:E:177:GLU:HG3  | 1.91                     | 0.52              |
| 1:B:213:ILE:HG22 | 1:B:215:ILE:HD11 | 1.91                     | 0.52              |
| 1:C:243:ALA:HA   | 1:C:284:MET:HG3  | 1.92                     | 0.52              |
| 1:C:40:GLU:HB3   | 1:C:225:VAL:HG22 | 1.92                     | 0.52              |
| 1:B:108:GLN:NE2  | 1:B:144:LYS:HE2  | 2.24                     | 0.52              |
| 1:B:249:ILE:HG12 | 1:B:250:VAL:N    | 2.24                     | 0.52              |
| 1:E:299:HIS:CG   | 1:E:300:PRO:HA   | 2.45                     | 0.52              |
| 1:C:41:ILE:HD11  | 1:C:197:PHE:CE1  | 2.45                     | 0.52              |
| 1:E:330:ASN:CG   | 1:H:330:ASN:HB2  | 2.29                     | 0.52              |
| 1:F:33:LEU:HD21  | 1:F:57:LEU:CD2   | 2.38                     | 0.52              |
| 1:B:87:VAL:HG21  | 1:B:110:SER:HB3  | 1.91                     | 0.52              |
| 1:D:1:MET:N      | 1:D:418:GLY:O    | 2.43                     | 0.52              |
| 1:H:37:GLU:HB2   | 1:H:223:GLY:N    | 2.25                     | 0.52              |
| 1:H:370:LEU:HD11 | 1:H:397:ARG:CZ   | 2.40                     | 0.52              |
| 1:A:137:LYS:NZ   | 1:A:139:GLU:OE2  | 2.42                     | 0.51              |
| 1:A:34:LEU:HD21  | 1:A:99:PRO:HA    | 1.91                     | 0.51              |
| 1:C:126:ILE:HG23 | 1:C:136:ILE:HG21 | 1.92                     | 0.51              |
| 1:B:119:ALA:N    | 1:B:329:GLU:OE2  | 2.44                     | 0.51              |
| 1:A:101:VAL:HG13 | 1:A:102:ALA:N    | 2.25                     | 0.51              |
| 1:C:233:ILE:CG2  | 1:C:306:MET:HE3  | 2.41                     | 0.51              |
| 1:E:111:LEU:HD13 | 1:E:143:VAL:CG2  | 2.40                     | 0.51              |
| 1:E:330:ASN:HB2  | 1:H:330:ASN:OD1  | 2.10                     | 0.51              |
| 1:F:105:GLY:HA2  | 1:F:147:VAL:HG12 | 1.92                     | 0.51              |
| 1:A:275:THR:HG22 | 1:A:280:ILE:HG12 | 1.92                     | 0.51              |
| 1:E:278:ASP:OD1  | 1:E:278:ASP:N    | 2.42                     | 0.51              |
| 1:A:124:LEU:HD11 | 1:A:160:LYS:HG2  | 1.93                     | 0.51              |
| 1:B:220:ARG:O    | 1:B:221:LEU:HD23 | 2.11                     | 0.51              |
| 1:D:4:PHE:HE1    | 1:D:415:ARG:HB2  | 1.75                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:123:ASP:HA   | 4:E:508:EDO:H21  | 1.93                     | 0.51              |
| 1:D:204:LYS:HB2  | 1:D:216:GLU:HB3  | 1.92                     | 0.51              |
| 1:E:57:LEU:O     | 1:E:62:THR:HB    | 2.11                     | 0.51              |
| 1:D:12:LEU:HD12  | 1:D:241:ALA:HB1  | 1.92                     | 0.51              |
| 1:E:369:ASP:CB   | 1:E:372:ALA:HB3  | 2.40                     | 0.51              |
| 1:D:369:ASP:CB   | 1:D:372:ALA:HB3  | 2.35                     | 0.51              |
| 1:D:254:ALA:O    | 1:D:278:ASP:HA   | 2.11                     | 0.51              |
| 1:G:299:HIS:ND1  | 1:G:300:PRO:HA   | 2.26                     | 0.51              |
| 1:C:276:GLY:HA3  | 1:C:279:TRP:NE1  | 2.26                     | 0.50              |
| 1:A:259:LEU:CD1  | 1:A:263:LEU:CG   | 2.88                     | 0.50              |
| 1:D:299:HIS:CG   | 1:D:300:PRO:HA   | 2.46                     | 0.50              |
| 1:E:115:ASP:OD2  | 1:E:117:ILE:HG12 | 2.12                     | 0.50              |
| 1:G:21:ALA:HA    | 1:G:231:ASP:HB2  | 1.92                     | 0.50              |
| 1:G:42:GLN:HA    | 1:G:69:SER:HB3   | 1.92                     | 0.50              |
| 1:H:240:VAL:O    | 1:H:244:ILE:HG12 | 2.12                     | 0.50              |
| 1:H:282:LEU:C    | 1:H:282:LEU:HD23 | 2.32                     | 0.50              |
| 1:A:115:ASP:OD2  | 1:A:116:ALA:N    | 2.45                     | 0.50              |
| 1:D:13:GLN:HA    | 1:D:248:LYS:O    | 2.10                     | 0.50              |
| 1:F:340:ARG:HG2  | 1:F:340:ARG:HH11 | 1.74                     | 0.50              |
| 1:G:131:LYS:HD3  | 1:G:156:ILE:HG23 | 1.94                     | 0.50              |
| 1:B:5:ARG:NE     | 1:B:416:VAL:HG21 | 2.26                     | 0.50              |
| 1:D:10:THR:HG21  | 1:D:411:ALA:HA   | 1.92                     | 0.50              |
| 1:E:124:LEU:HD11 | 1:E:160:LYS:CG   | 2.42                     | 0.50              |
| 1:E:176:ALA:O    | 1:E:217:GLY:HA3  | 2.12                     | 0.50              |
| 1:C:36:GLU:O     | 1:C:75:SER:HB3   | 2.12                     | 0.50              |
| 1:H:62:THR:HG22  | 1:H:64:VAL:CG2   | 2.42                     | 0.50              |
| 1:B:21:ALA:HA    | 1:B:231:ASP:CB   | 2.42                     | 0.49              |
| 1:A:81:SER:CB    | 1:A:108:GLN:HB2  | 2.42                     | 0.49              |
| 1:C:294:VAL:HB   | 1:C:323:ILE:HD13 | 1.93                     | 0.49              |
| 1:A:21:ALA:HA    | 1:A:231:ASP:HB2  | 1.94                     | 0.49              |
| 1:B:180:THR:HB   | 1:B:215:ILE:HB   | 1.94                     | 0.49              |
| 1:B:296:THR:HA   | 1:B:302:PHE:O    | 2.12                     | 0.49              |
| 1:B:37:GLU:HB2   | 1:B:223:GLY:N    | 2.23                     | 0.49              |
| 1:F:50:ILE:O     | 1:F:54:MET:HG3   | 2.11                     | 0.49              |
| 1:B:48:LYS:HZ2   | 1:B:393:TYR:HB2  | 1.76                     | 0.49              |
| 1:E:152:LYS:CE   | 5:E:632:HOH:O    | 2.60                     | 0.49              |
| 1:E:152:LYS:HE3  | 5:E:632:HOH:O    | 2.11                     | 0.49              |
| 1:F:294:VAL:HB   | 1:F:323:ILE:HD13 | 1.94                     | 0.49              |
| 1:H:329:GLU:HG2  | 1:H:330:ASN:H    | 1.76                     | 0.49              |
| 1:B:35:ALA:O     | 1:B:74:ALA:HB3   | 2.13                     | 0.49              |
| 1:C:94:ILE:HA    | 1:C:109:VAL:HG11 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:271:ALA:HB2  | 1:B:284:MET:SD   | 2.52                     | 0.49              |
| 1:C:399:TYR:CD2  | 1:C:402:ILE:HD12 | 2.47                     | 0.49              |
| 1:E:4:PHE:CD2    | 1:E:392:ILE:HG21 | 2.48                     | 0.49              |
| 1:G:87:VAL:HG21  | 1:G:110:SER:HB3  | 1.95                     | 0.49              |
| 1:C:357:VAL:HG13 | 5:C:606:HOH:O    | 2.11                     | 0.49              |
| 1:F:24:ALA:HB3   | 1:F:228:VAL:HG13 | 1.93                     | 0.49              |
| 1:H:366:MET:HE3  | 1:H:391:ARG:HD2  | 1.94                     | 0.49              |
| 1:C:243:ALA:HA   | 1:C:284:MET:CG   | 2.43                     | 0.49              |
| 1:E:46:LYS:HG2   | 1:E:66:ARG:CZ    | 2.43                     | 0.49              |
| 1:H:367:ALA:HB1  | 1:H:373:SER:CB   | 2.43                     | 0.49              |
| 1:C:87:VAL:HG21  | 1:C:110:SER:HB3  | 1.94                     | 0.48              |
| 1:F:330:ASN:HB2  | 1:G:330:ASN:HB2  | 1.95                     | 0.48              |
| 1:B:35:ALA:HB2   | 1:B:201:LEU:HD13 | 1.95                     | 0.48              |
| 1:E:1:MET:H2     | 1:E:418:GLY:HA2  | 1.78                     | 0.48              |
| 1:A:282:LEU:HD23 | 1:A:282:LEU:C    | 2.34                     | 0.48              |
| 1:B:299:HIS:CG   | 1:B:300:PRO:HA   | 2.48                     | 0.48              |
| 1:B:360:LEU:O    | 1:B:384:GLU:N    | 2.44                     | 0.48              |
| 1:D:276:GLY:HA3  | 1:D:279:TRP:NE1  | 2.28                     | 0.48              |
| 1:G:340:ARG:CG   | 1:G:340:ARG:HH11 | 2.26                     | 0.48              |
| 1:C:220:ARG:HH11 | 1:C:220:ARG:HG3  | 1.78                     | 0.48              |
| 1:E:294:VAL:HB   | 1:E:323:ILE:HD13 | 1.96                     | 0.48              |
| 1:E:373:SER:CB   | 1:E:395:ILE:HD11 | 2.43                     | 0.48              |
| 1:D:150:ARG:HG3  | 4:D:508:EDO:O1   | 2.14                     | 0.48              |
| 1:H:21:ALA:HA    | 1:H:231:ASP:CB   | 2.44                     | 0.48              |
| 1:B:234:GLU:HG3  | 1:B:238:PHE:CE2  | 2.49                     | 0.48              |
| 1:D:22:LYS:HD3   | 1:D:371:ARG:NH1  | 2.28                     | 0.48              |
| 1:F:45:PRO:HA    | 1:F:400:GLU:OE1  | 2.14                     | 0.48              |
| 1:G:114:GLY:HA2  | 1:G:119:ALA:O    | 2.13                     | 0.48              |
| 1:H:348:GLU:HA   | 1:H:348:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:83:PRO:HD2   | 1:A:86:LEU:HD12  | 1.96                     | 0.48              |
| 1:B:117:ILE:HD11 | 1:B:120:ARG:NH1  | 2.28                     | 0.48              |
| 1:F:331:ARG:H    | 3:F:503:ACT:CH3  | 2.22                     | 0.48              |
| 1:G:160:LYS:HE3  | 5:G:655:HOH:O    | 2.13                     | 0.48              |
| 1:C:91:ARG:HG3   | 5:C:646:HOH:O    | 2.13                     | 0.48              |
| 1:F:330:ASN:CB   | 1:G:330:ASN:HB2  | 2.44                     | 0.48              |
| 1:A:233:ILE:HG23 | 1:A:306:MET:CE   | 2.44                     | 0.48              |
| 1:C:46:LYS:N     | 1:C:400:GLU:OE1  | 2.30                     | 0.48              |
| 1:D:417:LYS:O    | 1:D:419:GLU:N    | 2.41                     | 0.48              |
| 1:B:220:ARG:HG3  | 1:B:220:ARG:HH11 | 1.79                     | 0.47              |
| 1:B:234:GLU:OE2  | 1:B:238:PHE:HE2  | 1.97                     | 0.47              |
| 1:B:407:ARG:HG3  | 1:B:411:ALA:O    | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:309:GLN:N    | 1:C:309:GLN:OE1  | 2.44                     | 0.47              |
| 1:C:373:SER:O    | 1:C:377:VAL:HG23 | 2.13                     | 0.47              |
| 1:E:308:ALA:HA   | 1:E:334:HIS:NE2  | 2.29                     | 0.47              |
| 1:B:60:LEU:HD22  | 1:B:79:ASN:O     | 2.15                     | 0.47              |
| 1:C:108:GLN:CG   | 1:C:144:LYS:HG2  | 2.43                     | 0.47              |
| 1:C:88:LYS:HE3   | 1:C:88:LYS:HB3   | 1.40                     | 0.47              |
| 1:D:115:ASP:OD2  | 1:D:116:ALA:N    | 2.48                     | 0.47              |
| 1:F:320:THR:HG21 | 1:H:320:THR:HG21 | 1.96                     | 0.47              |
| 1:F:3:LYS:HZ1    | 1:F:419:GLU:C    | 2.17                     | 0.47              |
| 1:B:276:GLY:HA3  | 1:B:279:TRP:NE1  | 2.29                     | 0.47              |
| 1:B:30:PHE:CE1   | 1:B:96:ALA:HB2   | 2.49                     | 0.47              |
| 1:C:37:GLU:HB3   | 1:C:38:PRO:CD    | 2.44                     | 0.47              |
| 1:D:37:GLU:OE2   | 1:D:220:ARG:NH2  | 2.47                     | 0.47              |
| 1:B:273:ILE:O    | 1:B:274:GLU:HG2  | 2.15                     | 0.47              |
| 1:E:56:LEU:C     | 1:E:56:LEU:HD23  | 2.34                     | 0.47              |
| 1:E:64:VAL:HG13  | 1:E:72:ILE:CD1   | 2.45                     | 0.47              |
| 1:D:37:GLU:O     | 1:D:39:VAL:HG23  | 2.14                     | 0.47              |
| 1:E:125:HIS:CE1  | 1:E:164:GLY:C    | 2.88                     | 0.47              |
| 1:H:369:ASP:CB   | 1:H:372:ALA:HB3  | 2.43                     | 0.47              |
| 1:C:276:GLY:HA3  | 1:C:279:TRP:CE2  | 2.48                     | 0.47              |
| 1:E:6:VAL:HG22   | 1:E:413:ILE:HG13 | 1.96                     | 0.47              |
| 1:B:13:GLN:HA    | 1:B:248:LYS:O    | 2.15                     | 0.47              |
| 1:E:128:GLY:HA3  | 1:E:169:ILE:CD1  | 2.45                     | 0.47              |
| 1:E:42:GLN:HA    | 1:E:69:SER:CB    | 2.45                     | 0.47              |
| 1:E:96:ALA:O     | 1:E:99:PRO:HD2   | 2.14                     | 0.47              |
| 1:G:333:MET:O    | 1:G:336:PRO:HD2  | 2.15                     | 0.47              |
| 1:A:282:LEU:HD23 | 1:A:283:ASP:N    | 2.30                     | 0.47              |
| 1:B:282:LEU:HD21 | 1:B:284:MET:HG2  | 1.95                     | 0.47              |
| 1:B:299:HIS:ND1  | 1:B:300:PRO:HA   | 2.30                     | 0.47              |
| 1:D:97:LEU:HB2   | 1:D:109:VAL:HG21 | 1.97                     | 0.47              |
| 1:D:91:ARG:NH2   | 1:D:120:ARG:HB3  | 2.30                     | 0.47              |
| 1:D:6:VAL:HG22   | 1:D:413:ILE:HG13 | 1.96                     | 0.47              |
| 1:E:111:LEU:HD13 | 1:E:143:VAL:HG21 | 1.97                     | 0.47              |
| 1:E:10:THR:HG21  | 1:E:410:GLY:O    | 2.15                     | 0.47              |
| 1:G:108:GLN:HG3  | 5:G:635:HOH:O    | 2.15                     | 0.47              |
| 1:H:248:LYS:CB   | 1:H:248:LYS:NZ   | 2.78                     | 0.47              |
| 1:H:255:GLN:HG2  | 1:H:257:ASP:OD1  | 2.14                     | 0.47              |
| 1:A:20:GLY:HA3   | 1:A:43:ASN:O     | 2.15                     | 0.47              |
| 1:H:81:SER:CB    | 1:H:108:GLN:HB2  | 2.44                     | 0.47              |
| 1:A:323:ILE:HB   | 1:A:352:VAL:HG13 | 1.97                     | 0.47              |
| 1:C:115:ASP:CG   | 1:C:116:ALA:H    | 2.17                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:299:HIS:ND1  | 1:C:300:PRO:HA   | 2.30                     | 0.47              |
| 1:D:22:LYS:HB2   | 1:D:47:LEU:CD1   | 2.44                     | 0.47              |
| 1:H:29:LEU:HD23  | 1:H:41:ILE:CD1   | 2.45                     | 0.47              |
| 1:B:124:LEU:HD11 | 1:B:160:LYS:HG2  | 1.95                     | 0.47              |
| 1:D:169:ILE:HG22 | 1:D:182:ILE:HD11 | 1.97                     | 0.47              |
| 1:E:103:ARG:HB2  | 1:E:175:LEU:CD1  | 2.44                     | 0.47              |
| 1:F:248:LYS:HA   | 1:F:282:LEU:O    | 2.15                     | 0.47              |
| 1:F:85:ASP:O     | 1:F:89:THR:HG23  | 2.15                     | 0.47              |
| 1:B:236:GLY:O    | 1:B:240:VAL:HG23 | 2.15                     | 0.46              |
| 1:D:325:GLU:CG   | 1:D:329:GLU:H    | 2.28                     | 0.46              |
| 1:G:74:ALA:HB3   | 5:G:637:HOH:O    | 2.15                     | 0.46              |
| 1:H:251:CYS:O    | 1:H:279:TRP:HA   | 2.15                     | 0.46              |
| 1:H:233:ILE:HD12 | 1:H:305:ASP:HB2  | 1.95                     | 0.46              |
| 1:H:370:LEU:HD11 | 1:H:397:ARG:CD   | 2.43                     | 0.46              |
| 1:B:273:ILE:HG22 | 1:B:274:GLU:N    | 2.30                     | 0.46              |
| 1:C:277:GLU:HG3  | 3:C:502:ACT:O    | 2.15                     | 0.46              |
| 1:C:3:LYS:CD     | 1:C:390:ASP:OD1  | 2.62                     | 0.46              |
| 1:D:325:GLU:HG3  | 1:D:329:GLU:H    | 1.80                     | 0.46              |
| 1:F:233:ILE:HG21 | 1:F:371:ARG:CD   | 2.46                     | 0.46              |
| 1:G:369:ASP:CB   | 1:G:372:ALA:HB3  | 2.45                     | 0.46              |
| 1:A:315:LEU:HD23 | 1:A:354:CYS:HB3  | 1.96                     | 0.46              |
| 1:C:323:ILE:HB   | 1:C:352:VAL:HG12 | 1.97                     | 0.46              |
| 1:F:249:ILE:HG12 | 1:F:250:VAL:N    | 2.30                     | 0.46              |
| 1:D:243:ALA:HA   | 1:D:284:MET:HG2  | 1.96                     | 0.46              |
| 1:E:59:GLN:C     | 1:E:61:GLY:H     | 2.18                     | 0.46              |
| 1:F:157:VAL:O    | 4:F:509:EDO:H22  | 2.15                     | 0.46              |
| 1:G:63:LYS:HB3   | 1:G:73:ASP:HB3   | 1.97                     | 0.46              |
| 1:B:41:ILE:O     | 1:B:69:SER:HB2   | 2.16                     | 0.46              |
| 1:C:266:LEU:O    | 1:C:269:ALA:HB3  | 2.16                     | 0.46              |
| 1:D:116:ALA:O    | 1:D:330:ASN:ND2  | 2.38                     | 0.46              |
| 1:D:60:LEU:O     | 1:D:77:VAL:HG13  | 2.16                     | 0.46              |
| 1:F:41:ILE:HG23  | 1:F:228:VAL:HG23 | 1.97                     | 0.46              |
| 1:B:282:LEU:HD23 | 1:B:282:LEU:C    | 2.35                     | 0.46              |
| 1:F:288:ARG:NH2  | 1:F:317:ALA:O    | 2.48                     | 0.46              |
| 1:H:160:LYS:HA   | 5:H:653:HOH:O    | 2.16                     | 0.46              |
| 1:H:84:TYR:CE1   | 4:H:507:EDO:H12  | 2.50                     | 0.46              |
| 1:D:21:ALA:HA    | 1:D:231:ASP:HB2  | 1.98                     | 0.46              |
| 1:D:417:LYS:C    | 1:D:419:GLU:H    | 2.18                     | 0.46              |
| 1:E:1:MET:H3     | 1:E:418:GLY:HA2  | 1.76                     | 0.46              |
| 1:E:88:LYS:HG2   | 1:E:88:LYS:O     | 2.15                     | 0.46              |
| 1:F:353:ILE:HD12 | 1:F:353:ILE:N    | 2.31                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:193:ASP:CG   | 1:G:229:LEU:HD22 | 2.36                     | 0.46              |
| 1:H:108:GLN:CD   | 1:H:144:LYS:HE2  | 2.36                     | 0.46              |
| 1:B:37:GLU:O     | 1:B:38:PRO:C     | 2.53                     | 0.46              |
| 1:H:264:ALA:O    | 1:H:268:GLU:HG3  | 2.16                     | 0.46              |
| 1:H:66:ARG:HB3   | 1:H:70:VAL:HG22  | 1.97                     | 0.46              |
| 1:C:367:ALA:CB   | 1:C:373:SER:HB3  | 2.40                     | 0.46              |
| 1:E:36:GLU:OE1   | 1:E:220:ARG:NE   | 2.49                     | 0.46              |
| 1:G:331:ARG:NH2  | 1:G:371:ARG:HB2  | 2.30                     | 0.46              |
| 1:A:147:VAL:HG13 | 1:A:147:VAL:O    | 2.16                     | 0.46              |
| 1:B:213:ILE:HG22 | 1:B:215:ILE:CD1  | 2.45                     | 0.46              |
| 1:G:315:LEU:HD23 | 1:G:354:CYS:HB3  | 1.98                     | 0.46              |
| 1:H:249:ILE:HG12 | 1:H:250:VAL:N    | 2.31                     | 0.46              |
| 1:H:320:THR:HA   | 1:H:354:CYS:O    | 2.16                     | 0.46              |
| 1:B:14:GLY:O     | 1:B:249:ILE:HA   | 2.16                     | 0.45              |
| 1:C:20:GLY:HA3   | 1:C:43:ASN:O     | 2.16                     | 0.45              |
| 1:C:47:LEU:HB3   | 1:C:397:ARG:O    | 2.16                     | 0.45              |
| 1:D:213:ILE:HG22 | 1:D:215:ILE:HD11 | 1.97                     | 0.45              |
| 1:D:39:VAL:HG12  | 1:D:41:ILE:HD12  | 1.98                     | 0.45              |
| 1:F:299:HIS:CG   | 1:F:300:PRO:HA   | 2.51                     | 0.45              |
| 1:H:248:LYS:HZ3  | 1:H:248:LYS:HB3  | 1.80                     | 0.45              |
| 1:D:51:ASP:HA    | 1:D:54:MET:CE    | 2.46                     | 0.45              |
| 1:B:20:GLY:HA3   | 1:B:43:ASN:O     | 2.16                     | 0.45              |
| 1:D:12:LEU:O     | 1:D:247:GLY:HA3  | 2.16                     | 0.45              |
| 1:D:42:GLN:HA    | 1:D:69:SER:CB    | 2.46                     | 0.45              |
| 1:F:416:VAL:CG1  | 1:F:417:LYS:N    | 2.79                     | 0.45              |
| 1:G:48:LYS:HZ1   | 1:G:393:TYR:HB2  | 1.81                     | 0.45              |
| 1:H:126:ILE:O    | 1:H:130:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:4:PHE:HE2    | 1:A:395:ILE:HD13 | 1.80                     | 0.45              |
| 1:B:85:ASP:HA    | 1:B:88:LYS:HE2   | 1.97                     | 0.45              |
| 1:E:26:LEU:N     | 1:E:27:PRO:HD2   | 2.32                     | 0.45              |
| 1:F:124:LEU:HD11 | 1:F:160:LYS:HG2  | 1.97                     | 0.45              |
| 1:F:34:LEU:HD21  | 1:F:99:PRO:HA    | 1.97                     | 0.45              |
| 1:G:28:ILE:HD12  | 1:G:228:VAL:HG22 | 1.99                     | 0.45              |
| 1:B:335:VAL:HB   | 1:B:336:PRO:CD   | 2.47                     | 0.45              |
| 1:F:313:LEU:HD23 | 1:F:313:LEU:C    | 2.37                     | 0.45              |
| 1:F:116:ALA:HB1  | 1:F:333:MET:HE1  | 1.98                     | 0.45              |
| 1:H:367:ALA:HB1  | 1:H:373:SER:HB2  | 1.97                     | 0.45              |
| 1:H:20:GLY:HA3   | 1:H:43:ASN:O     | 2.16                     | 0.45              |
| 1:B:376:LEU:O    | 1:B:379:ALA:HB3  | 2.17                     | 0.45              |
| 1:D:59:GLN:OE1   | 1:D:79:ASN:ND2   | 2.49                     | 0.45              |
| 1:F:108:GLN:HG2  | 1:F:144:LYS:CG   | 2.34                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:115:ASP:OD2  | 1:G:117:ILE:HG12 | 2.17                     | 0.45              |
| 1:G:299:HIS:CG   | 1:G:300:PRO:HA   | 2.51                     | 0.45              |
| 1:A:105:GLY:HA2  | 1:A:147:VAL:CG1  | 2.47                     | 0.45              |
| 1:B:111:LEU:HD12 | 1:B:112:PRO:HD2  | 1.98                     | 0.45              |
| 1:B:316:VAL:HG23 | 1:B:316:VAL:O    | 2.17                     | 0.45              |
| 1:C:22:LYS:HD2   | 1:C:398:GLY:HA2  | 1.97                     | 0.45              |
| 1:F:309:GLN:OE1  | 1:F:309:GLN:N    | 2.39                     | 0.45              |
| 1:E:5:ARG:NH1    | 5:E:641:HOH:O    | 2.40                     | 0.45              |
| 1:G:108:GLN:CD   | 1:G:144:LYS:HE2  | 2.37                     | 0.45              |
| 1:G:11:ARG:HD3   | 1:G:13:GLN:OE1   | 2.17                     | 0.45              |
| 1:G:197:PHE:CZ   | 1:G:201:LEU:HD11 | 2.52                     | 0.45              |
| 1:G:401:ARG:HA   | 5:G:642:HOH:O    | 2.17                     | 0.45              |
| 1:C:21:ALA:HA    | 1:C:231:ASP:HB2  | 1.98                     | 0.44              |
| 1:D:31:ALA:HB1   | 1:D:198:LEU:HD21 | 1.98                     | 0.44              |
| 1:F:299:HIS:ND1  | 1:F:300:PRO:HA   | 2.32                     | 0.44              |
| 1:H:59:GLN:NE2   | 1:H:86:LEU:HD11  | 2.32                     | 0.44              |
| 1:C:220:ARG:HG3  | 1:C:220:ARG:NH1  | 2.33                     | 0.44              |
| 1:C:395:ILE:HG23 | 1:C:396:ASP:N    | 2.32                     | 0.44              |
| 1:E:265:LYS:HE3  | 1:E:293:THR:O    | 2.17                     | 0.44              |
| 1:E:374:ALA:HB2  | 1:E:399:TYR:CE1  | 2.52                     | 0.44              |
| 1:E:187:ARG:HD2  | 1:F:211:ASP:OD2  | 2.17                     | 0.44              |
| 1:F:12:LEU:CD1   | 1:F:241:ALA:HB1  | 2.46                     | 0.44              |
| 1:G:276:GLY:HA3  | 1:G:279:TRP:CE2  | 2.53                     | 0.44              |
| 1:B:115:ASP:HB3  | 1:B:120:ARG:HD3  | 2.00                     | 0.44              |
| 1:F:64:VAL:HG13  | 1:F:72:ILE:HD13  | 2.00                     | 0.44              |
| 1:G:34:LEU:HD21  | 1:G:99:PRO:HA    | 2.00                     | 0.44              |
| 1:H:314:ASN:HD22 | 1:H:323:ILE:HD11 | 1.82                     | 0.44              |
| 1:A:181:ILE:HG23 | 1:A:212:ARG:HG3  | 1.99                     | 0.44              |
| 1:G:131:LYS:HE3  | 1:G:156:ILE:HG12 | 2.00                     | 0.44              |
| 1:G:331:ARG:HG2  | 1:G:331:ARG:O    | 2.18                     | 0.44              |
| 1:B:127:PHE:CZ   | 1:B:131:LYS:HE3  | 2.53                     | 0.44              |
| 1:B:218:VAL:HG21 | 1:B:221:LEU:HD21 | 2.00                     | 0.44              |
| 1:B:5:ARG:HE     | 1:B:416:VAL:HG21 | 1.81                     | 0.44              |
| 1:B:87:VAL:HG11  | 1:B:110:SER:O    | 2.17                     | 0.44              |
| 1:D:320:THR:HA   | 1:D:354:CYS:O    | 2.16                     | 0.44              |
| 1:E:37:GLU:HB3   | 1:E:38:PRO:CD    | 2.48                     | 0.44              |
| 1:E:50:ILE:O     | 1:E:54:MET:HG3   | 2.17                     | 0.44              |
| 1:H:167:VAL:HG12 | 4:H:508:EDO:H22  | 1.98                     | 0.44              |
| 1:A:366:MET:CE   | 1:D:88:LYS:HD2   | 2.48                     | 0.44              |
| 1:B:81:SER:CB    | 1:B:108:GLN:HG3  | 2.30                     | 0.44              |
| 1:B:372:ALA:O    | 1:B:373:SER:C    | 2.56                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:124:LEU:HD11 | 1:D:160:LYS:CG   | 2.48                     | 0.44              |
| 1:H:367:ALA:CB   | 1:H:373:SER:HB2  | 2.48                     | 0.44              |
| 1:H:392:ILE:HD12 | 1:H:415:ARG:NH1  | 2.33                     | 0.44              |
| 1:H:13:GLN:HA    | 1:H:248:LYS:O    | 2.18                     | 0.44              |
| 1:E:109:VAL:HG12 | 1:E:110:SER:O    | 2.17                     | 0.44              |
| 1:H:11:ARG:HD3   | 1:H:247:GLY:HA2  | 2.00                     | 0.44              |
| 1:C:374:ALA:O    | 1:C:378:LEU:HG   | 2.18                     | 0.44              |
| 1:E:233:ILE:HG21 | 1:E:371:ARG:HD3  | 2.00                     | 0.44              |
| 1:E:12:LEU:HD12  | 1:E:241:ALA:HB1  | 2.00                     | 0.43              |
| 1:G:193:ASP:CB   | 1:G:229:LEU:HD22 | 2.48                     | 0.43              |
| 1:H:101:VAL:HG11 | 1:H:145:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:374:ALA:HB2  | 1:A:399:TYR:CE1  | 2.53                     | 0.43              |
| 1:B:193:ASP:CG   | 1:B:229:LEU:HD22 | 2.38                     | 0.43              |
| 1:B:308:ALA:HA   | 1:B:334:HIS:NE2  | 2.32                     | 0.43              |
| 1:F:369:ASP:CG   | 1:F:372:ALA:HB3  | 2.38                     | 0.43              |
| 1:F:39:VAL:HG12  | 1:F:40:GLU:N     | 2.32                     | 0.43              |
| 1:G:64:VAL:HG22  | 1:G:72:ILE:CD1   | 2.49                     | 0.43              |
| 1:H:67:IAS:CG    | 1:H:69:SER:N     | 2.81                     | 0.43              |
| 1:B:24:ALA:HB3   | 1:B:228:VAL:HG13 | 1.99                     | 0.43              |
| 1:D:3:LYS:HE2    | 1:D:390:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:323:ILE:HB   | 1:A:352:VAL:HG12 | 1.98                     | 0.43              |
| 1:A:395:ILE:CG2  | 1:A:396:ASP:N    | 2.81                     | 0.43              |
| 1:B:108:GLN:HB3  | 1:B:144:LYS:HG2  | 1.99                     | 0.43              |
| 1:D:340:ARG:HG2  | 1:D:340:ARG:HH11 | 1.83                     | 0.43              |
| 1:D:41:ILE:HG22  | 1:D:44:VAL:HG23  | 1.99                     | 0.43              |
| 1:F:320:THR:HA   | 1:F:354:CYS:O    | 2.19                     | 0.43              |
| 1:A:244:ILE:HD12 | 1:A:382:ILE:HD13 | 2.01                     | 0.43              |
| 1:B:16:VAL:CG1   | 1:B:249:ILE:HD11 | 2.48                     | 0.43              |
| 1:B:220:ARG:HG3  | 1:B:220:ARG:NH1  | 2.33                     | 0.43              |
| 1:D:87:VAL:HG11  | 1:D:110:SER:O    | 2.18                     | 0.43              |
| 1:E:396:ASP:CG   | 1:E:415:ARG:HH22 | 2.22                     | 0.43              |
| 1:G:56:LEU:HD23  | 1:G:56:LEU:C     | 2.39                     | 0.43              |
| 1:D:335:VAL:HB   | 1:D:336:PRO:CD   | 2.48                     | 0.43              |
| 1:E:1:MET:C      | 1:E:418:GLY:HA2  | 2.39                     | 0.43              |
| 1:H:289:PRO:HD3  | 5:H:601:HOH:O    | 2.18                     | 0.43              |
| 1:A:35:ALA:HB1   | 1:A:222:GLY:O    | 2.19                     | 0.43              |
| 1:A:22:LYS:HD3   | 1:A:398:GLY:HA2  | 2.01                     | 0.43              |
| 1:B:416:VAL:HG12 | 1:B:417:LYS:N    | 2.33                     | 0.43              |
| 1:E:256:PRO:HG3  | 1:E:280:ILE:HG13 | 2.00                     | 0.43              |
| 1:A:265:LYS:HA   | 1:A:265:LYS:HD3  | 1.78                     | 0.43              |
| 1:D:151:LEU:O    | 1:D:176:ALA:HB1  | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:189:PRO:HD3  | 1:D:299:HIS:CD2  | 2.54                     | 0.43              |
| 1:D:317:ALA:O    | 1:D:356:GLY:HA3  | 2.18                     | 0.43              |
| 1:G:371:ARG:HD3  | 1:G:371:ARG:HA   | 1.75                     | 0.43              |
| 1:A:161:VAL:HG11 | 1:A:298:PRO:HB3  | 2.00                     | 0.42              |
| 1:A:308:ALA:HA   | 1:A:334:HIS:NE2  | 2.34                     | 0.42              |
| 1:B:32:ALA:O     | 1:B:34:LEU:N     | 2.52                     | 0.42              |
| 1:C:335:VAL:HB   | 1:C:336:PRO:CD   | 2.49                     | 0.42              |
| 1:C:64:VAL:HG13  | 1:C:72:ILE:CD1   | 2.49                     | 0.42              |
| 1:D:238:PHE:O    | 1:D:241:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:182:ILE:O    | 1:A:212:ARG:HA   | 2.19                     | 0.42              |
| 1:A:4:PHE:HE1    | 1:A:415:ARG:HB2  | 1.83                     | 0.42              |
| 1:B:315:LEU:O    | 1:B:357:VAL:HG22 | 2.18                     | 0.42              |
| 1:D:2:ASP:HB3    | 1:D:392:ILE:HD11 | 2.01                     | 0.42              |
| 1:E:51:ASP:HA    | 1:E:54:MET:HE2   | 2.01                     | 0.42              |
| 1:E:63:LYS:O     | 1:E:72:ILE:HA    | 2.19                     | 0.42              |
| 1:G:118:GLY:HA2  | 1:G:329:GLU:OE1  | 2.14                     | 0.42              |
| 1:B:323:ILE:HB   | 1:B:352:VAL:HG13 | 2.01                     | 0.42              |
| 1:C:254:ALA:O    | 1:C:278:ASP:HA   | 2.20                     | 0.42              |
| 1:C:282:LEU:HD23 | 1:C:282:LEU:C    | 2.40                     | 0.42              |
| 1:D:94:ILE:CD1   | 1:D:122:VAL:HG11 | 2.49                     | 0.42              |
| 1:E:259:LEU:HD12 | 1:E:263:LEU:HG   | 2.01                     | 0.42              |
| 1:E:29:LEU:O     | 1:E:32:ALA:HB3   | 2.20                     | 0.42              |
| 1:E:85:ASP:O     | 1:E:89:THR:HG23  | 2.19                     | 0.42              |
| 1:F:33:LEU:CD2   | 1:F:57:LEU:HD22  | 2.46                     | 0.42              |
| 1:A:230:PRO:HG2  | 1:A:255:GLN:HB2  | 2.01                     | 0.42              |
| 1:A:117:ILE:HG21 | 1:A:369:ASP:OD2  | 2.19                     | 0.42              |
| 1:C:30:PHE:CZ    | 1:C:53:THR:HG23  | 2.54                     | 0.42              |
| 1:D:308:ALA:HA   | 1:D:334:HIS:NE2  | 2.34                     | 0.42              |
| 1:E:265:LYS:HA   | 1:E:265:LYS:HD3  | 1.84                     | 0.42              |
| 1:E:323:ILE:O    | 1:E:351:THR:HA   | 2.20                     | 0.42              |
| 1:H:235:THR:O    | 1:H:239:LEU:HG   | 2.19                     | 0.42              |
| 1:B:313:LEU:C    | 1:B:313:LEU:HD23 | 2.40                     | 0.42              |
| 1:B:315:LEU:HD21 | 1:B:345:ALA:HB2  | 2.01                     | 0.42              |
| 1:E:232:ARG:HB2  | 1:E:259:LEU:HD23 | 2.01                     | 0.42              |
| 1:H:402:ILE:HG23 | 1:H:403:GLU:N    | 2.35                     | 0.42              |
| 1:C:11:ARG:HD3   | 1:C:13:GLN:OE1   | 2.20                     | 0.42              |
| 1:C:370:LEU:HD11 | 1:C:399:TYR:CE1  | 2.54                     | 0.42              |
| 1:F:414:GLU:HG2  | 1:F:416:VAL:HG23 | 2.02                     | 0.42              |
| 1:F:20:GLY:HA3   | 1:F:43:ASN:O     | 2.19                     | 0.42              |
| 1:F:64:VAL:C     | 1:F:65:GLU:HG3   | 2.40                     | 0.42              |
| 1:H:42:GLN:HA    | 1:H:69:SER:CB    | 2.41                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:21:ALA:HA    | 1:A:231:ASP:CB   | 2.49                     | 0.42              |
| 1:C:136:ILE:HA   | 1:C:144:LYS:O    | 2.20                     | 0.42              |
| 1:D:34:LEU:HD21  | 1:D:99:PRO:HA    | 2.00                     | 0.42              |
| 1:A:333:MET:HE3  | 1:A:333:MET:HA   | 2.00                     | 0.42              |
| 1:B:77:VAL:HB    | 1:B:104:PHE:CZ   | 2.55                     | 0.42              |
| 1:B:264:ALA:O    | 1:B:268:GLU:HG3  | 2.19                     | 0.42              |
| 1:C:5:ARG:NH1    | 1:C:386:THR:HG21 | 2.35                     | 0.42              |
| 1:C:28:ILE:HG23  | 1:C:197:PHE:CD2  | 2.54                     | 0.42              |
| 1:C:24:ALA:CB    | 1:C:228:VAL:HG13 | 2.48                     | 0.42              |
| 1:C:244:ILE:HD12 | 1:C:382:ILE:HD13 | 2.01                     | 0.42              |
| 1:D:213:ILE:HG22 | 1:D:215:ILE:CD1  | 2.50                     | 0.42              |
| 1:E:111:LEU:HA   | 1:E:112:PRO:HD3  | 1.90                     | 0.42              |
| 1:E:132:LEU:HA   | 1:E:132:LEU:HD23 | 1.87                     | 0.42              |
| 1:E:317:ALA:O    | 1:E:356:GLY:HA3  | 2.20                     | 0.42              |
| 1:G:182:ILE:HG22 | 1:G:185:ALA:HB2  | 2.00                     | 0.42              |
| 1:H:2:ASP:HB3    | 1:H:392:ILE:CD1  | 2.38                     | 0.42              |
| 1:H:370:LEU:HD12 | 1:H:397:ARG:CD   | 2.35                     | 0.42              |
| 1:H:91:ARG:C     | 1:H:93:SER:H     | 2.23                     | 0.42              |
| 1:A:189:PRO:HD3  | 1:A:299:HIS:CD2  | 2.55                     | 0.42              |
| 1:B:4:PHE:CE2    | 1:B:413:ILE:HD11 | 2.55                     | 0.42              |
| 1:B:83:PRO:CG    | 1:B:86:LEU:HD12  | 2.50                     | 0.42              |
| 1:D:294:VAL:HB   | 1:D:323:ILE:HD13 | 2.00                     | 0.42              |
| 1:D:382:ILE:HD12 | 4:D:507:EDO:H22  | 2.01                     | 0.42              |
| 1:H:55:LYS:HA    | 4:H:510:EDO:H22  | 2.02                     | 0.42              |
| 1:B:197:PHE:O    | 1:B:201:LEU:HG   | 2.20                     | 0.41              |
| 1:C:392:ILE:HB   | 1:C:395:ILE:HG21 | 2.01                     | 0.41              |
| 1:C:64:VAL:O     | 1:C:65:GLU:HG3   | 2.20                     | 0.41              |
| 2:A:501:UD1:H5'2 | 4:A:507:EDO:O2   | 2.20                     | 0.41              |
| 1:B:369:ASP:C    | 1:B:371:ARG:H    | 2.23                     | 0.41              |
| 1:E:103:ARG:HG2  | 1:E:104:PHE:CE1  | 2.54                     | 0.41              |
| 1:E:81:SER:HB3   | 1:E:108:GLN:HB2  | 2.02                     | 0.41              |
| 1:F:282:LEU:C    | 1:F:282:LEU:HD23 | 2.40                     | 0.41              |
| 1:H:256:PRO:HG3  | 1:H:280:ILE:CG1  | 2.50                     | 0.41              |
| 1:H:66:ARG:CB    | 1:H:70:VAL:HG22  | 2.50                     | 0.41              |
| 1:B:189:PRO:HD3  | 1:B:299:HIS:CD2  | 2.55                     | 0.41              |
| 1:B:273:ILE:CG2  | 1:B:274:GLU:N    | 2.84                     | 0.41              |
| 1:B:30:PHE:HE1   | 1:B:96:ALA:HB2   | 1.85                     | 0.41              |
| 1:G:245:SER:HB3  | 1:G:382:ILE:HG22 | 2.01                     | 0.41              |
| 1:H:117:ILE:HG22 | 1:H:331:ARG:HG3  | 2.01                     | 0.41              |
| 1:H:56:LEU:HB2   | 1:H:86:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:298:PRO:HA   | 4:A:507:EDO:H11  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:SER:HA    | 1:A:108:GLN:O    | 2.20                     | 0.41              |
| 1:E:203:ALA:HB2  | 1:E:221:LEU:HD21 | 2.03                     | 0.41              |
| 1:H:366:MET:HE2  | 1:H:391:ARG:HD2  | 2.01                     | 0.41              |
| 1:H:2:ASP:C      | 1:H:392:ILE:HG12 | 2.41                     | 0.41              |
| 1:C:37:GLU:HB3   | 1:C:38:PRO:HD2   | 2.02                     | 0.41              |
| 1:E:195:ALA:HB3  | 1:E:208:GLN:HG3  | 2.02                     | 0.41              |
| 1:G:22:LYS:HD3   | 1:G:371:ARG:NH2  | 2.35                     | 0.41              |
| 1:G:50:ILE:O     | 1:G:54:MET:HG3   | 2.20                     | 0.41              |
| 1:H:236:GLY:O    | 1:H:240:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:88:LYS:HG2   | 1:A:88:LYS:O     | 2.21                     | 0.41              |
| 1:B:415:ARG:HG2  | 1:B:415:ARG:O    | 2.19                     | 0.41              |
| 1:D:282:LEU:HD23 | 1:D:282:LEU:C    | 2.40                     | 0.41              |
| 1:F:199:VAL:O    | 1:F:202:GLY:N    | 2.49                     | 0.41              |
| 1:H:29:LEU:HD23  | 1:H:41:ILE:HD13  | 2.03                     | 0.41              |
| 1:A:208:GLN:HA   | 1:A:213:ILE:HG12 | 2.03                     | 0.41              |
| 1:B:54:MET:HG2   | 1:B:64:VAL:HG11  | 2.02                     | 0.41              |
| 1:C:161:VAL:O    | 3:C:503:ACT:H2   | 2.21                     | 0.41              |
| 1:D:252:ARG:O    | 1:D:253:ASN:HB2  | 2.21                     | 0.41              |
| 1:F:204:LYS:HG3  | 1:F:218:VAL:HG11 | 2.02                     | 0.41              |
| 1:A:60:LEU:HA    | 1:A:79:ASN:HB3   | 2.03                     | 0.41              |
| 1:B:66:ARG:HD2   | 1:B:70:VAL:HG22  | 2.03                     | 0.41              |
| 1:C:196:ASN:HB2  | 1:C:226:TYR:OH   | 2.20                     | 0.41              |
| 1:D:12:LEU:CD1   | 1:D:241:ALA:HB1  | 2.51                     | 0.41              |
| 1:D:65:GLU:HG3   | 1:D:71:TRP:HB2   | 2.02                     | 0.41              |
| 1:H:370:LEU:HD12 | 1:H:397:ARG:HB2  | 2.03                     | 0.41              |
| 1:A:256:PRO:HG3  | 1:A:280:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:373:SER:HB3  | 1:B:395:ILE:CG1  | 2.51                     | 0.41              |
| 1:E:42:GLN:HA    | 1:E:69:SER:HB2   | 2.02                     | 0.41              |
| 1:C:314:ASN:HB3  | 1:C:354:CYS:HB2  | 2.03                     | 0.41              |
| 1:C:392:ILE:C    | 1:C:395:ILE:HG22 | 2.15                     | 0.41              |
| 1:C:39:VAL:HG12  | 1:C:41:ILE:CD1   | 2.50                     | 0.41              |
| 1:E:13:GLN:O     | 1:E:409:LEU:HA   | 2.21                     | 0.41              |
| 1:F:371:ARG:NH2  | 1:F:398:GLY:O    | 2.54                     | 0.41              |
| 1:G:131:LYS:HB3  | 1:G:131:LYS:HE3  | 1.94                     | 0.41              |
| 1:B:16:VAL:HG11  | 1:B:249:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:67:IAS:CG    | 1:C:69:SER:N     | 2.84                     | 0.41              |
| 1:D:283:ASP:OD2  | 1:D:285:HIS:CE1  | 2.74                     | 0.41              |
| 1:F:263:LEU:HD22 | 1:F:273:ILE:HD13 | 2.02                     | 0.41              |
| 1:G:340:ARG:NH1  | 1:G:340:ARG:CG   | 2.83                     | 0.41              |
| 1:H:370:LEU:CD1  | 1:H:397:ARG:CZ   | 2.99                     | 0.41              |
| 1:H:91:ARG:C     | 1:H:93:SER:N     | 2.73                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:ASP:C    | 1:A:371:ARG:N    | 2.74                     | 0.40              |
| 1:B:57:LEU:HD23  | 1:B:57:LEU:HA    | 1.92                     | 0.40              |
| 1:C:2:ASP:HB3    | 1:C:392:ILE:HD11 | 2.03                     | 0.40              |
| 1:C:4:PHE:CD1    | 1:C:392:ILE:HD13 | 2.56                     | 0.40              |
| 1:D:91:ARG:NH2   | 1:D:120:ARG:CB   | 2.84                     | 0.40              |
| 1:E:330:ASN:HB2  | 1:H:330:ASN:CG   | 2.42                     | 0.40              |
| 1:E:57:LEU:O     | 1:E:62:THR:CB    | 2.69                     | 0.40              |
| 1:H:117:ILE:HD12 | 1:H:328:PHE:CD2  | 2.56                     | 0.40              |
| 1:H:56:LEU:HD23  | 1:H:56:LEU:O     | 2.20                     | 0.40              |
| 1:A:196:ASN:OD1  | 1:A:208:GLN:NE2  | 2.55                     | 0.40              |
| 1:E:33:LEU:HD13  | 1:E:100:LEU:HD21 | 2.03                     | 0.40              |
| 1:F:315:LEU:HD22 | 1:F:343:ALA:HB1  | 2.01                     | 0.40              |
| 1:G:147:VAL:HG13 | 1:G:147:VAL:O    | 2.20                     | 0.40              |
| 1:H:63:LYS:HG2   | 3:H:504:ACT:H3   | 2.03                     | 0.40              |
| 1:A:314:ASN:ND2  | 1:A:323:ILE:HD11 | 2.36                     | 0.40              |
| 1:B:190:GLU:N    | 1:B:190:GLU:OE1  | 2.50                     | 0.40              |
| 1:C:367:ALA:HB1  | 1:C:373:SER:CB   | 2.44                     | 0.40              |
| 1:A:233:ILE:HG23 | 1:A:306:MET:HE3  | 2.03                     | 0.40              |
| 1:A:4:PHE:HA     | 1:A:4:PHE:HD1    | 1.79                     | 0.40              |
| 1:B:395:ILE:HG21 | 1:B:402:ILE:CG2  | 2.52                     | 0.40              |
| 1:B:401:ARG:HB3  | 1:B:404:ASP:OD2  | 2.21                     | 0.40              |
| 1:D:24:ALA:HB3   | 1:D:228:VAL:HG13 | 2.03                     | 0.40              |
| 1:F:1:MET:CE     | 1:F:391:ARG:HG2  | 2.50                     | 0.40              |
| 1:C:4:PHE:CG     | 1:C:392:ILE:HG21 | 2.56                     | 0.40              |
| 1:F:40:GLU:CD    | 1:F:71:TRP:HE1   | 2.25                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:B:419:GLU:O | 1:H:139:GLU:OE2[2_456] | 1.89                     | 0.31              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 415/419 (99%)   | 398 (96%)  | 14 (3%)  | 3 (1%)   | 22          | 39  |
| 1   | B     | 415/419 (99%)   | 386 (93%)  | 26 (6%)  | 3 (1%)   | 22          | 39  |
| 1   | C     | 415/419 (99%)   | 404 (97%)  | 9 (2%)   | 2 (0%)   | 29          | 48  |
| 1   | D     | 415/419 (99%)   | 398 (96%)  | 14 (3%)  | 3 (1%)   | 22          | 39  |
| 1   | E     | 415/419 (99%)   | 389 (94%)  | 21 (5%)  | 5 (1%)   | 13          | 24  |
| 1   | F     | 415/419 (99%)   | 399 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| 1   | G     | 415/419 (99%)   | 400 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | H     | 415/419 (99%)   | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| All | All   | 3320/3352 (99%) | 3171 (96%) | 133 (4%) | 16 (0%)  | 29          | 48  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 119 | ALA  |
| 1   | E     | 60  | LEU  |
| 1   | E     | 77  | VAL  |
| 1   | B     | 33  | LEU  |
| 1   | A     | 417 | LYS  |
| 1   | B     | 92  | ALA  |
| 1   | B     | 370 | LEU  |
| 1   | C     | 92  | ALA  |
| 1   | D     | 118 | GLY  |
| 1   | E     | 140 | GLU  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 370 | LEU  |
| 1   | D     | 418 | GLY  |
| 1   | E     | 222 | GLY  |
| 1   | C     | 77  | VAL  |
| 1   | E     | 392 | ILE  |

### 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     | 329/329 (100%)   | 326 (99%)  | 3 (1%)   | 78          | 92 |
| 1   | B     | 329/329 (100%)   | 324 (98%)  | 5 (2%)   | 65          | 85 |
| 1   | C     | 329/329 (100%)   | 325 (99%)  | 4 (1%)   | 71          | 88 |
| 1   | D     | 329/329 (100%)   | 327 (99%)  | 2 (1%)   | 86          | 95 |
| 1   | E     | 329/329 (100%)   | 325 (99%)  | 4 (1%)   | 71          | 88 |
| 1   | F     | 329/329 (100%)   | 325 (99%)  | 4 (1%)   | 71          | 88 |
| 1   | G     | 329/329 (100%)   | 327 (99%)  | 2 (1%)   | 86          | 95 |
| 1   | H     | 329/329 (100%)   | 326 (99%)  | 3 (1%)   | 78          | 92 |
| All | All   | 2632/2632 (100%) | 2605 (99%) | 27 (1%)  | 76          | 90 |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 187 | ARG  |
| 1   | A     | 193 | ASP  |
| 1   | A     | 229 | LEU  |
| 1   | B     | 187 | ARG  |
| 1   | B     | 193 | ASP  |
| 1   | B     | 278 | ASP  |
| 1   | B     | 307 | GLN  |
| 1   | B     | 371 | ARG  |
| 1   | C     | 10  | THR  |
| 1   | C     | 187 | ARG  |
| 1   | C     | 259 | LEU  |
| 1   | C     | 371 | ARG  |
| 1   | D     | 59  | GLN  |
| 1   | D     | 187 | ARG  |
| 1   | E     | 22  | LYS  |
| 1   | E     | 66  | ARG  |
| 1   | E     | 187 | ARG  |
| 1   | E     | 391 | ARG  |
| 1   | F     | 135 | GLU  |
| 1   | F     | 187 | ARG  |
| 1   | F     | 229 | LEU  |
| 1   | F     | 371 | ARG  |
| 1   | G     | 187 | ARG  |
| 1   | G     | 229 | LEU  |
| 1   | H     | 135 | GLU  |
| 1   | H     | 187 | ARG  |
| 1   | H     | 371 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 79  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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 | $\# Z  > 2$ |
| 1   | IAS  | G     | 67  | 1    | 4,7,8        | 0.84 | 0           | 2,8,10      | 1.22 | 0           |
| 1   | IAS  | H     | 67  | 1    | 4,7,8        | 0.69 | 0           | 2,8,10      | 1.15 | 0           |
| 1   | IAS  | E     | 67  | 1    | 4,7,8        | 0.67 | 0           | 2,8,10      | 1.22 | 0           |
| 1   | IAS  | C     | 67  | 1    | 4,7,8        | 0.63 | 0           | 2,8,10      | 1.26 | 0           |
| 1   | IAS  | A     | 67  | 1    | 4,7,8        | 0.62 | 0           | 2,8,10      | 1.16 | 0           |
| 1   | IAS  | F     | 67  | 1    | 4,7,8        | 0.71 | 0           | 2,8,10      | 1.38 | 0           |
| 1   | IAS  | D     | 67  | 1    | 4,7,8        | 0.78 | 0           | 2,8,10      | 1.06 | 0           |
| 1   | IAS  | B     | 67  | 1    | 4,7,8        | 0.58 | 0           | 2,8,10      | 1.23 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | IAS  | G     | 67  | 1    | -       | 0/3/7/8  | -     |
| 1   | IAS  | H     | 67  | 1    | -       | 0/3/7/8  | -     |
| 1   | IAS  | E     | 67  | 1    | -       | 0/3/7/8  | -     |
| 1   | IAS  | C     | 67  | 1    | -       | 0/3/7/8  | -     |
| 1   | IAS  | A     | 67  | 1    | -       | 0/3/7/8  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1   | IAS  | F     | 67  | 1    | -       | 0/3/7/8  | -     |
| 1   | IAS  | D     | 67  | 1    | -       | 1/3/7/8  | -     |
| 1   | IAS  | B     | 67  | 1    | -       | 0/3/7/8  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 1   | D     | 67  | IAS  | C-CA-CB-CG |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | H     | 67  | IAS  | 1       | 0            |
| 1   | C     | 67  | IAS  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

72 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ACT  | F     | 503 | -    | 1,3,3        | 1.74 | 0        | 0,3,3       | 0.00 | -        |
| 3   | ACT  | A     | 503 | -    | 1,3,3        | 2.11 | 1 (100%) | 0,3,3       | 0.00 | -        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | UD1  | E     | 501 | -    | 34,41,41     | 1.96 | 11 (32%) | 45,62,62    | 1.39 | 5 (11%)  |
| 4   | EDO  | E     | 508 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.24 | 0        |
| 2   | UD1  | H     | 501 | -    | 34,41,41     | 2.08 | 12 (35%) | 45,62,62    | 1.39 | 6 (13%)  |
| 4   | EDO  | A     | 509 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | D     | 507 | -    | 3,3,3        | 0.44 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | E     | 505 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.31 | 0        |
| 4   | EDO  | G     | 502 | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.31 | 0        |
| 4   | EDO  | D     | 506 | -    | 3,3,3        | 0.65 | 0        | 2,2,2       | 0.20 | 0        |
| 4   | EDO  | A     | 506 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.34 | 0        |
| 3   | ACT  | H     | 502 | -    | 1,3,3        | 2.19 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | D     | 508 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.23 | 0        |
| 3   | ACT  | D     | 502 | -    | 1,3,3        | 2.61 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | H     | 513 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.29 | 0        |
| 4   | EDO  | B     | 505 | -    | 3,3,3        | 0.42 | 0        | 2,2,2       | 0.36 | 0        |
| 4   | EDO  | C     | 507 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.31 | 0        |
| 3   | ACT  | A     | 502 | -    | 1,3,3        | 3.37 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | H     | 506 | -    | 1,3,3        | 2.85 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | D     | 503 | -    | 1,3,3        | 2.17 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | H     | 504 | -    | 1,3,3        | 1.39 | 0        | 0,3,3       | 0.00 | -        |
| 4   | EDO  | C     | 505 | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.24 | 0        |
| 2   | UD1  | C     | 501 | -    | 34,41,41     | 2.01 | 10 (29%) | 45,62,62    | 1.34 | 5 (11%)  |
| 3   | ACT  | A     | 504 | -    | 1,3,3        | 2.57 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | H     | 503 | -    | 1,3,3        | 0.66 | 0        | 0,3,3       | 0.00 | -        |
| 4   | EDO  | C     | 506 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.28 | 0        |
| 4   | EDO  | G     | 508 | -    | 3,3,3        | 0.89 | 0        | 2,2,2       | 0.30 | 0        |
| 4   | EDO  | G     | 506 | -    | 3,3,3        | 0.55 | 0        | 2,2,2       | 0.28 | 0        |
| 4   | EDO  | F     | 508 | -    | 3,3,3        | 0.49 | 0        | 2,2,2       | 0.31 | 0        |
| 4   | EDO  | E     | 511 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.28 | 0        |
| 3   | ACT  | E     | 502 | -    | 1,3,3        | 1.76 | 0        | 0,3,3       | 0.00 | -        |
| 4   | EDO  | E     | 507 | -    | 3,3,3        | 0.63 | 0        | 2,2,2       | 0.25 | 0        |
| 4   | EDO  | F     | 505 | -    | 3,3,3        | 0.45 | 0        | 2,2,2       | 0.34 | 0        |
| 4   | EDO  | C     | 504 | -    | 3,3,3        | 0.44 | 0        | 2,2,2       | 0.30 | 0        |
| 2   | UD1  | F     | 501 | -    | 34,41,41     | 1.87 | 10 (29%) | 45,62,62    | 1.38 | 5 (11%)  |
| 4   | EDO  | H     | 512 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.33 | 0        |
| 2   | UD1  | D     | 501 | -    | 34,41,41     | 1.94 | 10 (29%) | 45,62,62    | 1.41 | 5 (11%)  |
| 4   | EDO  | H     | 508 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.26 | 0        |
| 2   | UD1  | G     | 501 | -    | 34,41,41     | 1.84 | 9 (26%)  | 45,62,62    | 1.38 | 5 (11%)  |
| 4   | EDO  | B     | 503 | -    | 3,3,3        | 0.35 | 0        | 2,2,2       | 0.45 | 0        |
| 4   | EDO  | D     | 510 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.35 | 0        |
| 4   | EDO  | H     | 510 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.30 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ACT  | A     | 505 | -    | 1,3,3        | 2.58 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | F     | 509 | -    | 3,3,3        | 0.56 | 0        | 2,2,2       | 0.33 | 0        |
| 4   | EDO  | H     | 511 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.33 | 0        |
| 4   | EDO  | D     | 509 | -    | 3,3,3        | 0.45 | 0        | 2,2,2       | 0.32 | 0        |
| 3   | ACT  | F     | 504 | -    | 1,3,3        | 2.67 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | H     | 507 | -    | 3,3,3        | 0.47 | 0        | 2,2,2       | 0.28 | 0        |
| 4   | EDO  | B     | 504 | -    | 3,3,3        | 0.44 | 0        | 2,2,2       | 0.35 | 0        |
| 2   | UD1  | A     | 501 | -    | 34,41,41     | 1.92 | 10 (29%) | 45,62,62    | 1.36 | 5 (11%)  |
| 4   | EDO  | E     | 509 | -    | 3,3,3        | 0.35 | 0        | 2,2,2       | 0.35 | 0        |
| 3   | ACT  | C     | 503 | -    | 1,3,3        | 2.90 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | G     | 504 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.24 | 0        |
| 4   | EDO  | D     | 504 | -    | 3,3,3        | 0.40 | 0        | 2,2,2       | 0.41 | 0        |
| 4   | EDO  | G     | 505 | -    | 3,3,3        | 0.48 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | A     | 508 | -    | 3,3,3        | 0.50 | 0        | 2,2,2       | 0.30 | 0        |
| 3   | ACT  | F     | 502 | -    | 1,3,3        | 2.52 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | E     | 503 | -    | 1,3,3        | 2.18 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | G     | 507 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.23 | 0        |
| 3   | ACT  | E     | 504 | -    | 1,3,3        | 2.21 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | H     | 509 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.29 | 0        |
| 4   | EDO  | A     | 507 | -    | 3,3,3        | 0.46 | 0        | 2,2,2       | 0.37 | 0        |
| 4   | EDO  | E     | 506 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.26 | 0        |
| 4   | EDO  | E     | 510 | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.20 | 0        |
| 3   | ACT  | H     | 505 | -    | 1,3,3        | 2.53 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | G     | 503 | -    | 3,3,3        | 0.48 | 0        | 2,2,2       | 0.34 | 0        |
| 4   | EDO  | D     | 505 | -    | 3,3,3        | 0.35 | 0        | 2,2,2       | 0.39 | 0        |
| 3   | ACT  | B     | 502 | -    | 1,3,3        | 2.46 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 3   | ACT  | C     | 502 | -    | 1,3,3        | 2.23 | 1 (100%) | 0,3,3       | 0.00 | -        |
| 4   | EDO  | F     | 507 | -    | 3,3,3        | 0.49 | 0        | 2,2,2       | 0.28 | 0        |
| 2   | UD1  | B     | 501 | -    | 34,41,41     | 2.00 | 13 (38%) | 45,62,62    | 1.38 | 6 (13%)  |
| 4   | EDO  | F     | 506 | -    | 3,3,3        | 0.48 | 0        | 2,2,2       | 0.34 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | EDO  | H     | 507 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | C     | 504 | -    | -       | 0/1/1/1    | -       |
| 2   | UD1  | E     | 501 | -    | -       | 6/24/63/63 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | EDO  | E     | 508 | -    | -       | 1/1/1/1    | -       |
| 2   | UD1  | H     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | A     | 509 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | D     | 507 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | E     | 505 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | G     | 502 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | D     | 506 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | A     | 506 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | E     | 509 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | H     | 512 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | H     | 513 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | B     | 505 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | C     | 507 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | C     | 505 | -    | -       | 1/1/1/1    | -       |
| 2   | UD1  | C     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | F     | 507 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | C     | 506 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | G     | 508 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | G     | 506 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | F     | 508 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | E     | 511 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | E     | 507 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | F     | 505 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | H     | 510 | -    | -       | 1/1/1/1    | -       |
| 2   | UD1  | F     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 2   | UD1  | D     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | H     | 508 | -    | -       | 0/1/1/1    | -       |
| 2   | UD1  | G     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | B     | 503 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | D     | 510 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | F     | 509 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | H     | 511 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | D     | 509 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | D     | 508 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | H     | 509 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | B     | 504 | -    | -       | 0/1/1/1    | -       |
| 2   | UD1  | A     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | G     | 504 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | D     | 504 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | G     | 505 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | A     | 508 | -    | -       | 1/1/1/1    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | EDO  | A     | 507 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | E     | 506 | -    | -       | 1/1/1/1    | -       |
| 4   | EDO  | E     | 510 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | G     | 503 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | D     | 505 | -    | -       | 0/1/1/1    | -       |
| 4   | EDO  | G     | 507 | -    | -       | 0/1/1/1    | -       |
| 2   | UD1  | B     | 501 | -    | -       | 5/24/63/63 | 0/3/3/3 |
| 4   | EDO  | F     | 506 | -    | -       | 1/1/1/1    | -       |

All (101) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 501 | UD1  | C6-N1   | 6.09  | 1.43        | 1.35     |
| 2   | C     | 501 | UD1  | C6-N1   | 6.00  | 1.43        | 1.35     |
| 2   | E     | 501 | UD1  | C6-N1   | 5.46  | 1.42        | 1.35     |
| 2   | D     | 501 | UD1  | C6-N1   | 5.31  | 1.42        | 1.35     |
| 2   | B     | 501 | UD1  | C6-N1   | 5.27  | 1.42        | 1.35     |
| 2   | G     | 501 | UD1  | C6-N1   | 5.20  | 1.42        | 1.35     |
| 2   | F     | 501 | UD1  | C6-N1   | 5.11  | 1.42        | 1.35     |
| 2   | A     | 501 | UD1  | C6-N1   | 4.68  | 1.41        | 1.35     |
| 2   | C     | 501 | UD1  | C4-N3   | 4.53  | 1.40        | 1.33     |
| 2   | D     | 501 | UD1  | C4-N3   | 4.49  | 1.40        | 1.33     |
| 2   | A     | 501 | UD1  | C4-N3   | 4.05  | 1.40        | 1.33     |
| 2   | H     | 501 | UD1  | C4-N3   | 3.91  | 1.39        | 1.33     |
| 2   | G     | 501 | UD1  | C4-N3   | 3.77  | 1.39        | 1.33     |
| 2   | B     | 501 | UD1  | C2B-C1B | -3.70 | 1.48        | 1.53     |
| 2   | E     | 501 | UD1  | C4-N3   | 3.65  | 1.39        | 1.33     |
| 2   | H     | 501 | UD1  | C2B-C1B | -3.60 | 1.48        | 1.53     |
| 2   | F     | 501 | UD1  | C4-N3   | 3.53  | 1.39        | 1.33     |
| 2   | A     | 501 | UD1  | O5'-C5' | 3.40  | 1.52        | 1.44     |
| 2   | D     | 501 | UD1  | O5'-C5' | 3.39  | 1.52        | 1.44     |
| 3   | A     | 502 | ACT  | CH3-C   | 3.37  | 1.53        | 1.48     |
| 2   | B     | 501 | UD1  | C4-N3   | 3.36  | 1.38        | 1.33     |
| 2   | E     | 501 | UD1  | O3B-C3B | 3.03  | 1.50        | 1.43     |
| 2   | E     | 501 | UD1  | C2B-C1B | -2.91 | 1.49        | 1.53     |
| 3   | C     | 503 | ACT  | CH3-C   | 2.90  | 1.52        | 1.48     |
| 3   | H     | 506 | ACT  | CH3-C   | 2.85  | 1.52        | 1.48     |
| 2   | G     | 501 | UD1  | O5'-C5' | 2.84  | 1.51        | 1.44     |
| 2   | A     | 501 | UD1  | O2'-C2B | 2.81  | 1.49        | 1.43     |
| 2   | H     | 501 | UD1  | O3'-C3' | 2.80  | 1.49        | 1.43     |
| 2   | F     | 501 | UD1  | O2'-C2B | 2.80  | 1.49        | 1.43     |
| 2   | E     | 501 | UD1  | O5'-C5' | 2.78  | 1.51        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 501 | UD1  | C2B-C1B | -2.77 | 1.49        | 1.53     |
| 2   | H     | 501 | UD1  | PB-O1B  | -2.76 | 1.41        | 1.50     |
| 2   | C     | 501 | UD1  | PB-O2B  | -2.70 | 1.42        | 1.55     |
| 2   | B     | 501 | UD1  | O3B-C3B | 2.70  | 1.49        | 1.43     |
| 2   | B     | 501 | UD1  | O5'-C5' | 2.68  | 1.50        | 1.44     |
| 3   | F     | 504 | ACT  | CH3-C   | 2.67  | 1.52        | 1.48     |
| 2   | C     | 501 | UD1  | O3B-C3B | 2.63  | 1.49        | 1.43     |
| 2   | A     | 501 | UD1  | O4'-C4' | 2.63  | 1.49        | 1.43     |
| 2   | A     | 501 | UD1  | C2B-C1B | -2.62 | 1.49        | 1.53     |
| 3   | D     | 502 | ACT  | CH3-C   | 2.61  | 1.52        | 1.48     |
| 3   | A     | 505 | ACT  | CH3-C   | 2.58  | 1.52        | 1.48     |
| 2   | H     | 501 | UD1  | O5'-C5' | 2.58  | 1.50        | 1.44     |
| 2   | G     | 501 | UD1  | O2'-C2B | 2.58  | 1.49        | 1.43     |
| 2   | C     | 501 | UD1  | O2'-C2B | 2.57  | 1.49        | 1.43     |
| 3   | A     | 504 | ACT  | CH3-C   | 2.57  | 1.52        | 1.48     |
| 2   | G     | 501 | UD1  | PB-O2B  | -2.56 | 1.43        | 1.55     |
| 2   | H     | 501 | UD1  | C1'-C2' | 2.53  | 1.57        | 1.53     |
| 3   | H     | 505 | ACT  | CH3-C   | 2.53  | 1.52        | 1.48     |
| 3   | F     | 502 | ACT  | CH3-C   | 2.52  | 1.52        | 1.48     |
| 2   | A     | 501 | UD1  | O3B-C3B | 2.50  | 1.48        | 1.43     |
| 2   | E     | 501 | UD1  | O2'-C2B | 2.49  | 1.48        | 1.43     |
| 2   | D     | 501 | UD1  | C8'-C7' | 2.48  | 1.55        | 1.50     |
| 2   | D     | 501 | UD1  | O2'-C2B | 2.47  | 1.48        | 1.43     |
| 2   | H     | 501 | UD1  | O2'-C2B | 2.46  | 1.48        | 1.43     |
| 2   | G     | 501 | UD1  | C8'-C7' | 2.46  | 1.55        | 1.50     |
| 3   | B     | 502 | ACT  | CH3-C   | 2.46  | 1.51        | 1.48     |
| 2   | D     | 501 | UD1  | O3'-C3' | 2.46  | 1.48        | 1.43     |
| 2   | C     | 501 | UD1  | O5'-C5' | 2.45  | 1.50        | 1.44     |
| 2   | C     | 501 | UD1  | C8'-C7' | 2.43  | 1.55        | 1.50     |
| 2   | A     | 501 | UD1  | C8'-C7' | 2.41  | 1.55        | 1.50     |
| 2   | B     | 501 | UD1  | C4'-C5' | 2.40  | 1.58        | 1.53     |
| 2   | A     | 501 | UD1  | PB-O2B  | -2.40 | 1.44        | 1.55     |
| 2   | H     | 501 | UD1  | O3B-C3B | 2.40  | 1.48        | 1.43     |
| 2   | F     | 501 | UD1  | O3B-C3B | 2.39  | 1.48        | 1.43     |
| 2   | F     | 501 | UD1  | O5'-C5' | 2.39  | 1.50        | 1.44     |
| 2   | F     | 501 | UD1  | PB-O1B  | -2.37 | 1.42        | 1.50     |
| 2   | E     | 501 | UD1  | PB-O2B  | -2.37 | 1.44        | 1.55     |
| 2   | F     | 501 | UD1  | PB-O2B  | -2.37 | 1.44        | 1.55     |
| 2   | G     | 501 | UD1  | PB-O1B  | -2.36 | 1.42        | 1.50     |
| 2   | E     | 501 | UD1  | C8'-C7' | 2.33  | 1.55        | 1.50     |
| 2   | C     | 501 | UD1  | PB-O1B  | -2.29 | 1.42        | 1.50     |
| 2   | A     | 501 | UD1  | C2'-N2' | 2.28  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 501 | UD1  | O3'-C3' | 2.26  | 1.48        | 1.43     |
| 2   | D     | 501 | UD1  | PB-O2B  | -2.25 | 1.44        | 1.55     |
| 2   | B     | 501 | UD1  | O2'-C2B | 2.23  | 1.48        | 1.43     |
| 2   | D     | 501 | UD1  | C3B-C4B | 2.23  | 1.58        | 1.53     |
| 3   | C     | 502 | ACT  | CH3-C   | 2.23  | 1.51        | 1.48     |
| 2   | B     | 501 | UD1  | O4'-C4' | 2.22  | 1.48        | 1.43     |
| 3   | E     | 504 | ACT  | CH3-C   | 2.21  | 1.51        | 1.48     |
| 2   | B     | 501 | UD1  | O3'-C3' | 2.21  | 1.48        | 1.43     |
| 2   | B     | 501 | UD1  | C3B-C4B | 2.19  | 1.58        | 1.53     |
| 2   | B     | 501 | UD1  | C8'-C7' | 2.19  | 1.55        | 1.50     |
| 2   | B     | 501 | UD1  | PB-O2B  | -2.19 | 1.45        | 1.55     |
| 3   | H     | 502 | ACT  | CH3-C   | 2.19  | 1.51        | 1.48     |
| 2   | H     | 501 | UD1  | PB-O2B  | -2.19 | 1.45        | 1.55     |
| 2   | F     | 501 | UD1  | PA-O2A  | -2.18 | 1.45        | 1.55     |
| 2   | B     | 501 | UD1  | C1'-C2' | 2.18  | 1.56        | 1.53     |
| 3   | E     | 503 | ACT  | CH3-C   | 2.18  | 1.51        | 1.48     |
| 2   | G     | 501 | UD1  | O3'-C3' | 2.17  | 1.48        | 1.43     |
| 2   | H     | 501 | UD1  | C8'-C7' | 2.17  | 1.55        | 1.50     |
| 3   | D     | 503 | ACT  | CH3-C   | 2.17  | 1.51        | 1.48     |
| 2   | D     | 501 | UD1  | O5'-C1' | 2.15  | 1.47        | 1.41     |
| 2   | D     | 501 | UD1  | PB-O1B  | -2.13 | 1.43        | 1.50     |
| 2   | E     | 501 | UD1  | PB-O1B  | -2.12 | 1.43        | 1.50     |
| 2   | E     | 501 | UD1  | O5'-C1' | 2.12  | 1.47        | 1.41     |
| 2   | H     | 501 | UD1  | C3B-C4B | 2.11  | 1.58        | 1.53     |
| 3   | A     | 503 | ACT  | CH3-C   | 2.11  | 1.51        | 1.48     |
| 2   | F     | 501 | UD1  | O3'-C3' | 2.09  | 1.47        | 1.43     |
| 2   | C     | 501 | UD1  | O3'-C3' | 2.06  | 1.47        | 1.43     |
| 2   | F     | 501 | UD1  | C8'-C7' | 2.03  | 1.54        | 1.50     |
| 2   | G     | 501 | UD1  | O4'-C4' | 2.00  | 1.47        | 1.43     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 501 | UD1  | C5-C4-N3    | -3.70 | 115.17      | 123.31   |
| 2   | B     | 501 | UD1  | C5-C4-N3    | -3.65 | 115.29      | 123.31   |
| 2   | A     | 501 | UD1  | C5-C4-N3    | -3.63 | 115.33      | 123.31   |
| 2   | G     | 501 | UD1  | C5-C4-N3    | -3.59 | 115.41      | 123.31   |
| 2   | D     | 501 | UD1  | C5-C4-N3    | -3.56 | 115.47      | 123.31   |
| 2   | H     | 501 | UD1  | C5-C4-N3    | -3.54 | 115.52      | 123.31   |
| 2   | E     | 501 | UD1  | C5-C4-N3    | -3.51 | 115.58      | 123.31   |
| 2   | H     | 501 | UD1  | O3B-C3B-C4B | 3.46  | 121.06      | 111.05   |
| 2   | B     | 501 | UD1  | O3B-C3B-C4B | 3.44  | 121.00      | 111.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 501 | UD1  | C5-C4-N3    | -3.43 | 115.77      | 123.31   |
| 2   | G     | 501 | UD1  | O3B-C3B-C4B | 3.15  | 120.17      | 111.05   |
| 2   | D     | 501 | UD1  | O3B-C3B-C4B | 3.11  | 120.05      | 111.05   |
| 2   | E     | 501 | UD1  | O3B-C3B-C4B | 3.05  | 119.87      | 111.05   |
| 2   | G     | 501 | UD1  | O2'-C2B-C1B | 3.05  | 122.11      | 110.85   |
| 2   | C     | 501 | UD1  | O3B-C3B-C4B | 3.05  | 119.86      | 111.05   |
| 2   | E     | 501 | UD1  | O3A-PB-O1'  | 3.04  | 108.61      | 102.48   |
| 2   | A     | 501 | UD1  | O3B-C3B-C4B | 3.02  | 119.77      | 111.05   |
| 2   | A     | 501 | UD1  | O2'-C2B-C3B | 2.97  | 121.42      | 111.82   |
| 2   | D     | 501 | UD1  | O2'-C2B-C1B | 2.97  | 121.82      | 110.85   |
| 2   | F     | 501 | UD1  | O2'-C2B-C3B | 2.93  | 121.30      | 111.82   |
| 2   | B     | 501 | UD1  | O2'-C2B-C3B | 2.93  | 121.29      | 111.82   |
| 2   | G     | 501 | UD1  | O3A-PB-O1'  | 2.90  | 108.34      | 102.48   |
| 2   | F     | 501 | UD1  | O3A-PB-O1'  | 2.89  | 108.32      | 102.48   |
| 2   | B     | 501 | UD1  | O3A-PB-O1'  | 2.89  | 108.32      | 102.48   |
| 2   | E     | 501 | UD1  | O2'-C2B-C3B | 2.86  | 121.08      | 111.82   |
| 2   | E     | 501 | UD1  | O2'-C2B-C1B | 2.85  | 121.36      | 110.85   |
| 2   | F     | 501 | UD1  | O3B-C3B-C4B | 2.84  | 119.25      | 111.05   |
| 2   | H     | 501 | UD1  | O3A-PB-O1'  | 2.82  | 108.18      | 102.48   |
| 2   | H     | 501 | UD1  | O2'-C2B-C3B | 2.81  | 120.93      | 111.82   |
| 2   | C     | 501 | UD1  | O2'-C2B-C3B | 2.81  | 120.92      | 111.82   |
| 2   | A     | 501 | UD1  | O3A-PB-O1'  | 2.81  | 108.15      | 102.48   |
| 2   | D     | 501 | UD1  | O3A-PB-O1'  | 2.80  | 108.12      | 102.48   |
| 2   | D     | 501 | UD1  | O2'-C2B-C3B | 2.76  | 120.74      | 111.82   |
| 2   | G     | 501 | UD1  | O2'-C2B-C3B | 2.64  | 120.37      | 111.82   |
| 2   | H     | 501 | UD1  | O2'-C2B-C1B | 2.64  | 120.60      | 110.85   |
| 2   | C     | 501 | UD1  | O2'-C2B-C1B | 2.61  | 120.48      | 110.85   |
| 2   | F     | 501 | UD1  | O2'-C2B-C1B | 2.59  | 120.43      | 110.85   |
| 2   | A     | 501 | UD1  | O2'-C2B-C1B | 2.55  | 120.28      | 110.85   |
| 2   | B     | 501 | UD1  | O2'-C2B-C1B | 2.26  | 119.20      | 110.85   |
| 2   | B     | 501 | UD1  | C2B-C3B-C4B | -2.18 | 98.41       | 102.64   |
| 2   | H     | 501 | UD1  | C4'-C3'-C2' | -2.14 | 107.20      | 110.34   |
| 2   | C     | 501 | UD1  | O3A-PB-O1'  | 2.03  | 106.58      | 102.48   |

There are no chirality outliers.

All (63) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 2   | E     | 501 | UD1  | C5B-O5B-PA-O1A |
| 2   | E     | 501 | UD1  | C5B-O5B-PA-O2A |
| 2   | H     | 501 | UD1  | C5B-O5B-PA-O1A |
| 2   | H     | 501 | UD1  | C5B-O5B-PA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | C     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 2   | F     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | F     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 2   | D     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | D     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 2   | G     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | G     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 2   | A     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | A     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 2   | B     | 501 | UD1  | C5B-O5B-PA-O1A  |
| 2   | B     | 501 | UD1  | C5B-O5B-PA-O2A  |
| 4   | G     | 508 | EDO  | O1-C1-C2-O2     |
| 4   | E     | 508 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 507 | EDO  | O1-C1-C2-O2     |
| 4   | G     | 506 | EDO  | O1-C1-C2-O2     |
| 4   | E     | 507 | EDO  | O1-C1-C2-O2     |
| 4   | H     | 510 | EDO  | O1-C1-C2-O2     |
| 4   | G     | 505 | EDO  | O1-C1-C2-O2     |
| 4   | F     | 506 | EDO  | O1-C1-C2-O2     |
| 4   | C     | 505 | EDO  | O1-C1-C2-O2     |
| 4   | E     | 506 | EDO  | O1-C1-C2-O2     |
| 2   | C     | 501 | UD1  | PB-O3A-PA-O1A   |
| 4   | E     | 511 | EDO  | O1-C1-C2-O2     |
| 4   | H     | 511 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 508 | EDO  | O1-C1-C2-O2     |
| 2   | E     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | C     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | F     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | D     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | G     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | A     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | B     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 4   | A     | 508 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 510 | EDO  | O1-C1-C2-O2     |
| 2   | D     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | A     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | B     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | B     | 501 | UD1  | C3'-C2'-N2'-C7' |
| 2   | E     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | F     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | G     | 501 | UD1  | PB-O3A-PA-O1A   |

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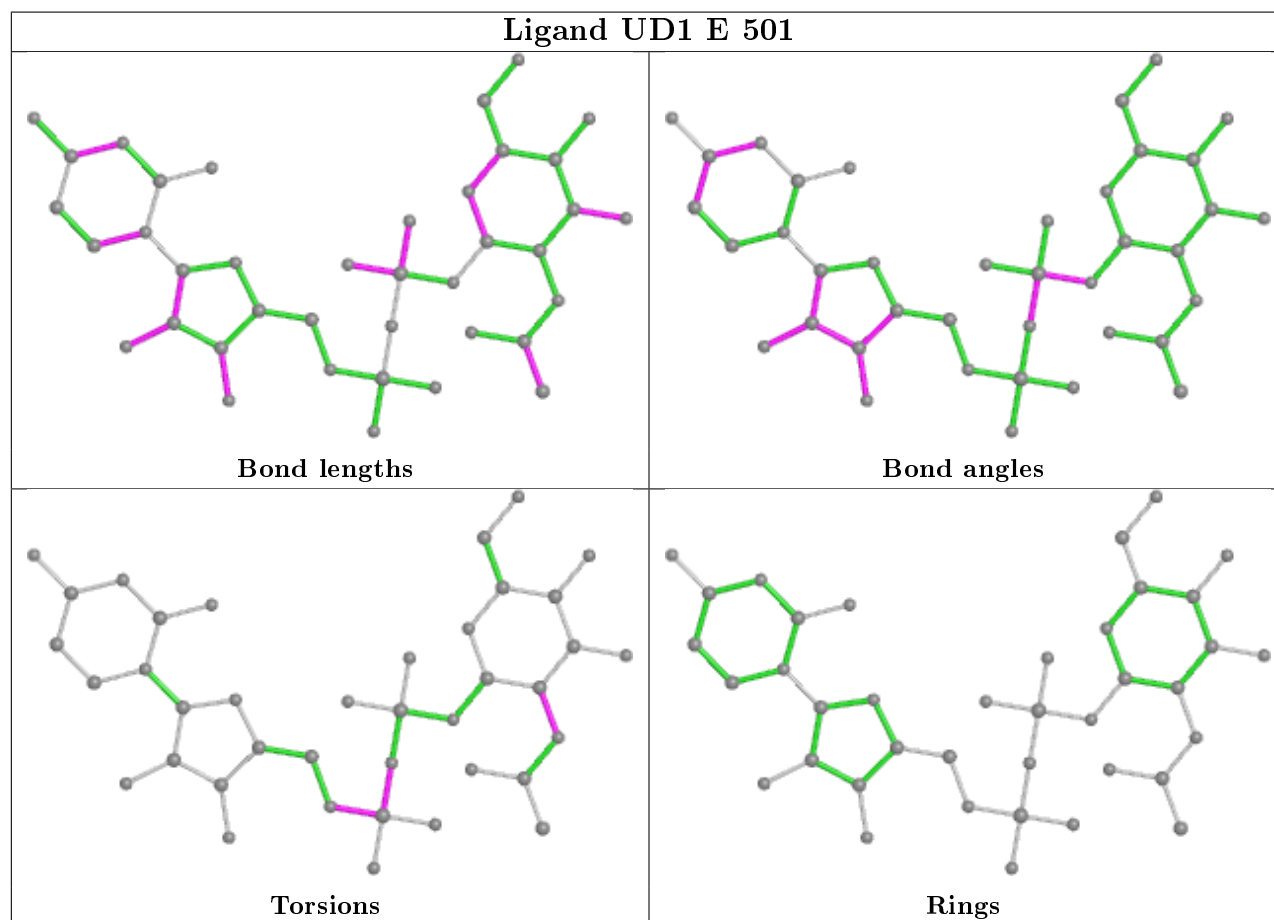
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | E     | 501 | UD1  | C3'-C2'-N2'-C7' |
| 4   | E     | 505 | EDO  | O1-C1-C2-O2     |
| 4   | B     | 505 | EDO  | O1-C1-C2-O2     |
| 4   | F     | 508 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 504 | EDO  | O1-C1-C2-O2     |
| 4   | A     | 507 | EDO  | O1-C1-C2-O2     |
| 2   | H     | 501 | UD1  | C5B-O5B-PA-O3A  |
| 2   | E     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | H     | 501 | UD1  | PB-O3A-PA-O1A   |
| 2   | H     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | F     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | D     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | G     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | A     | 501 | UD1  | PB-O3A-PA-O2A   |
| 2   | C     | 501 | UD1  | C3'-C2'-N2'-C7' |
| 4   | G     | 502 | EDO  | O1-C1-C2-O2     |
| 4   | D     | 506 | EDO  | O1-C1-C2-O2     |

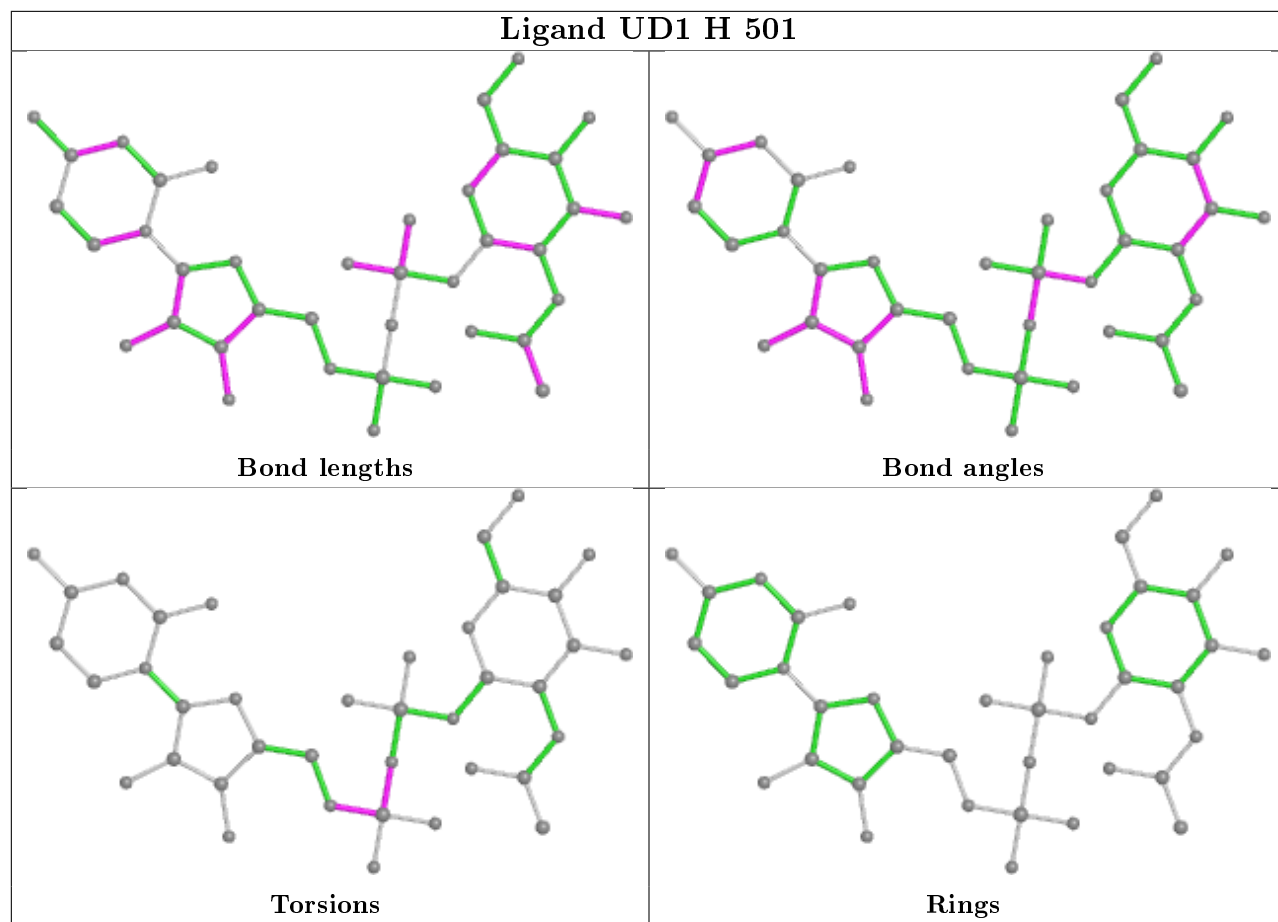
There are no ring outliers.

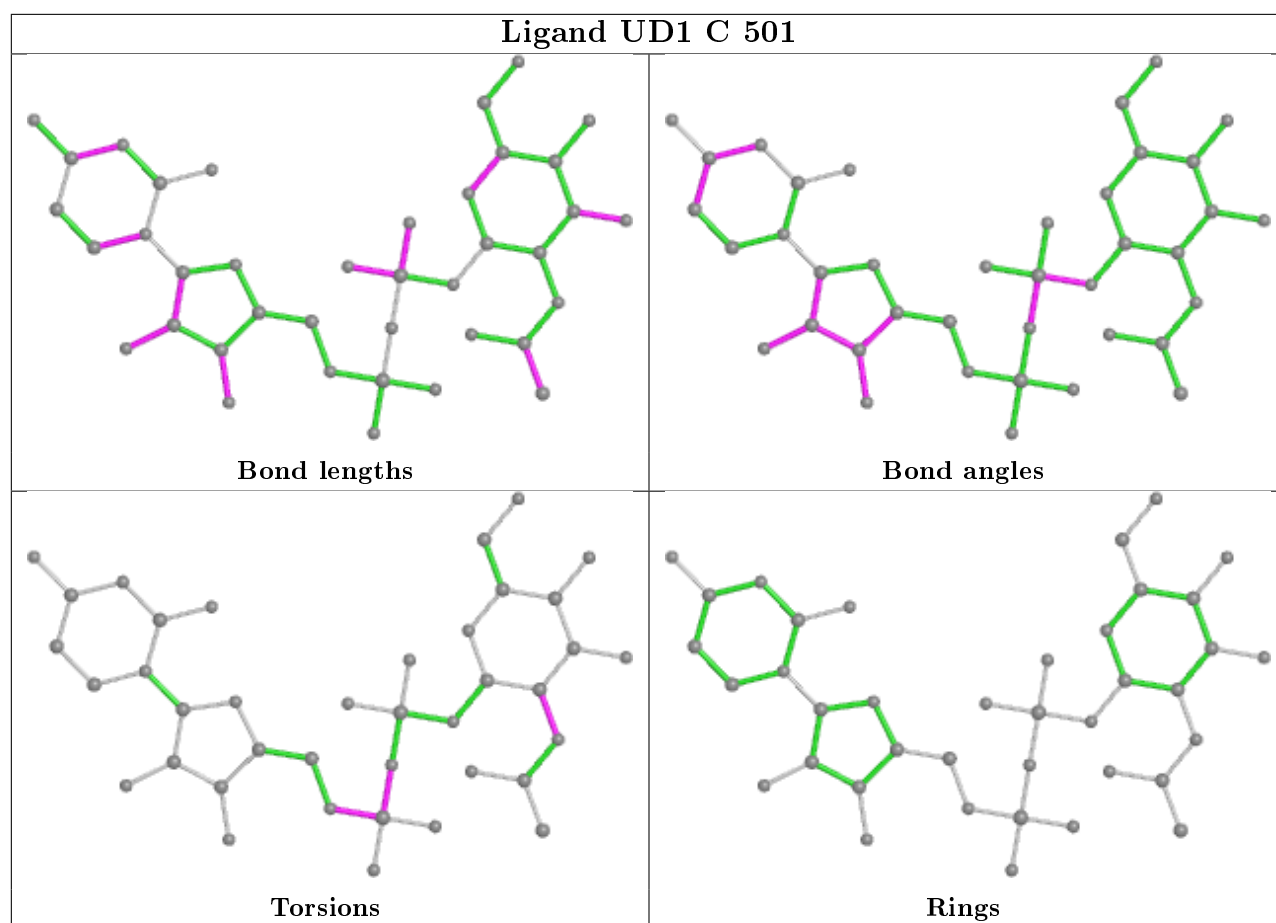
19 monomers are involved in 26 short contacts:

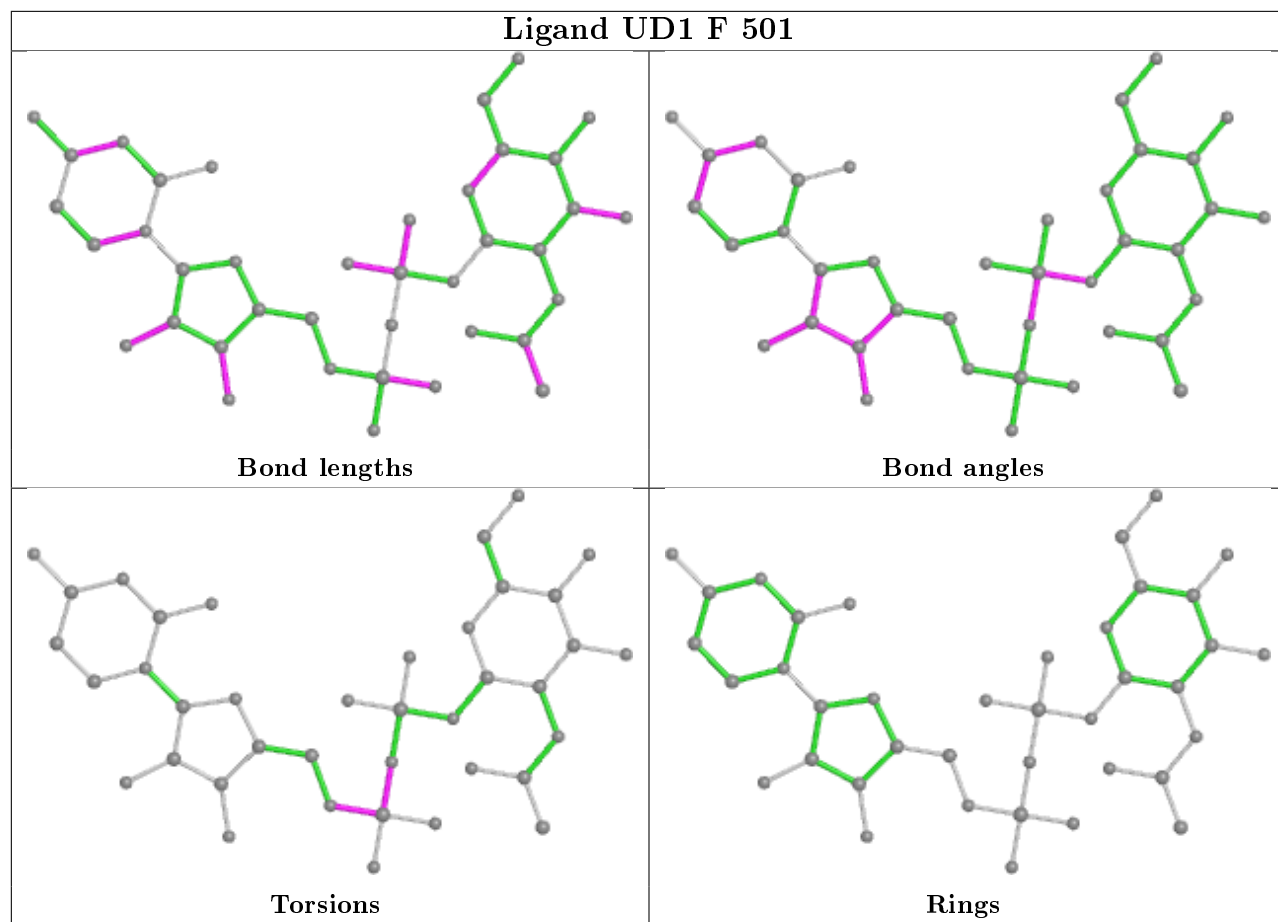
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | F     | 503 | ACT  | 3       | 0            |
| 4   | E     | 508 | EDO  | 1       | 0            |
| 4   | D     | 507 | EDO  | 1       | 0            |
| 4   | D     | 508 | EDO  | 2       | 0            |
| 3   | H     | 504 | ACT  | 1       | 0            |
| 3   | H     | 503 | ACT  | 1       | 0            |
| 3   | E     | 502 | ACT  | 2       | 0            |
| 4   | H     | 508 | EDO  | 1       | 0            |
| 4   | D     | 510 | EDO  | 2       | 0            |
| 4   | H     | 510 | EDO  | 1       | 0            |
| 4   | F     | 509 | EDO  | 1       | 0            |
| 4   | D     | 509 | EDO  | 1       | 0            |
| 4   | H     | 507 | EDO  | 1       | 0            |
| 2   | A     | 501 | UD1  | 1       | 0            |
| 3   | C     | 503 | ACT  | 2       | 0            |
| 4   | D     | 504 | EDO  | 1       | 0            |
| 4   | G     | 505 | EDO  | 1       | 0            |
| 4   | A     | 507 | EDO  | 2       | 0            |
| 3   | C     | 502 | ACT  | 2       | 0            |

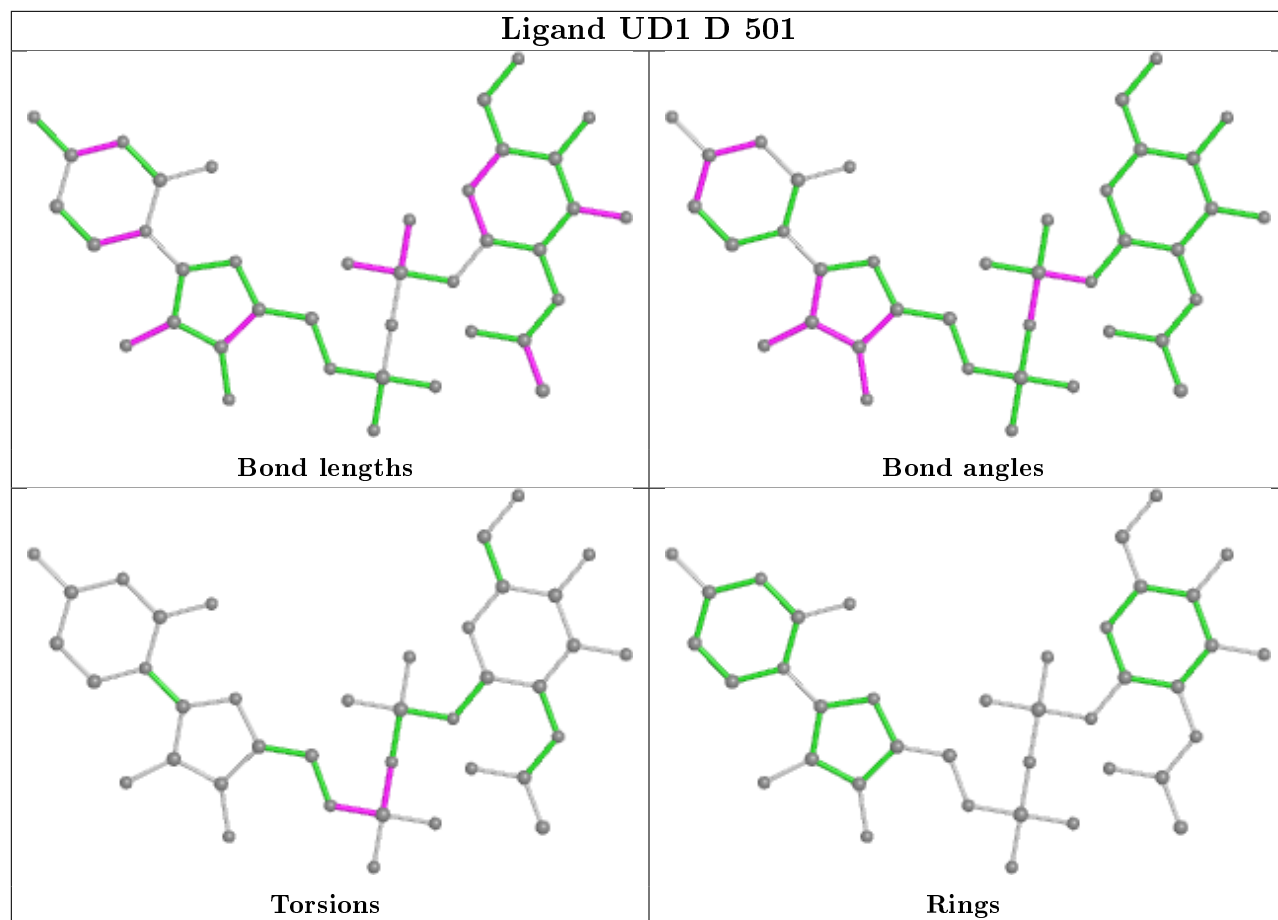
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

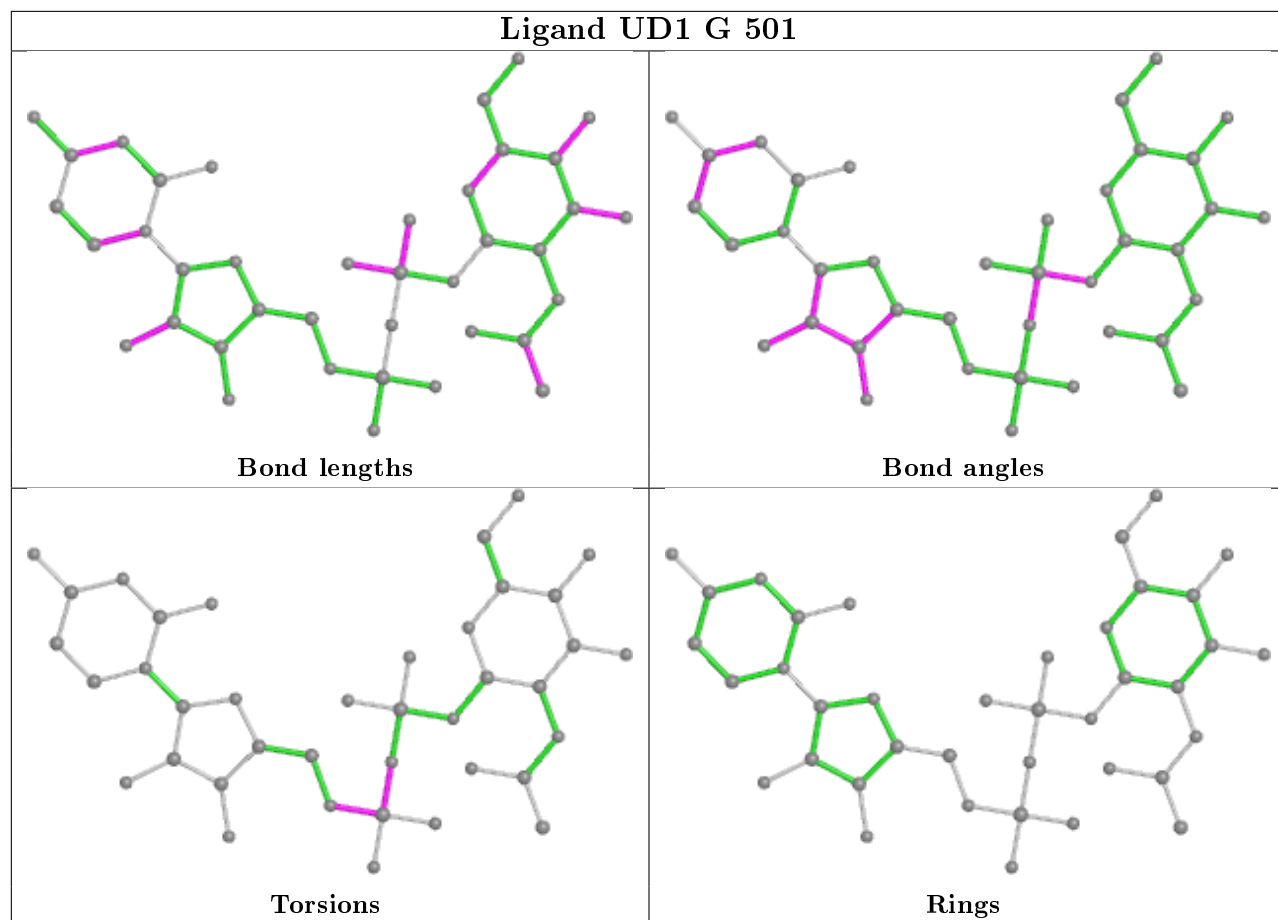


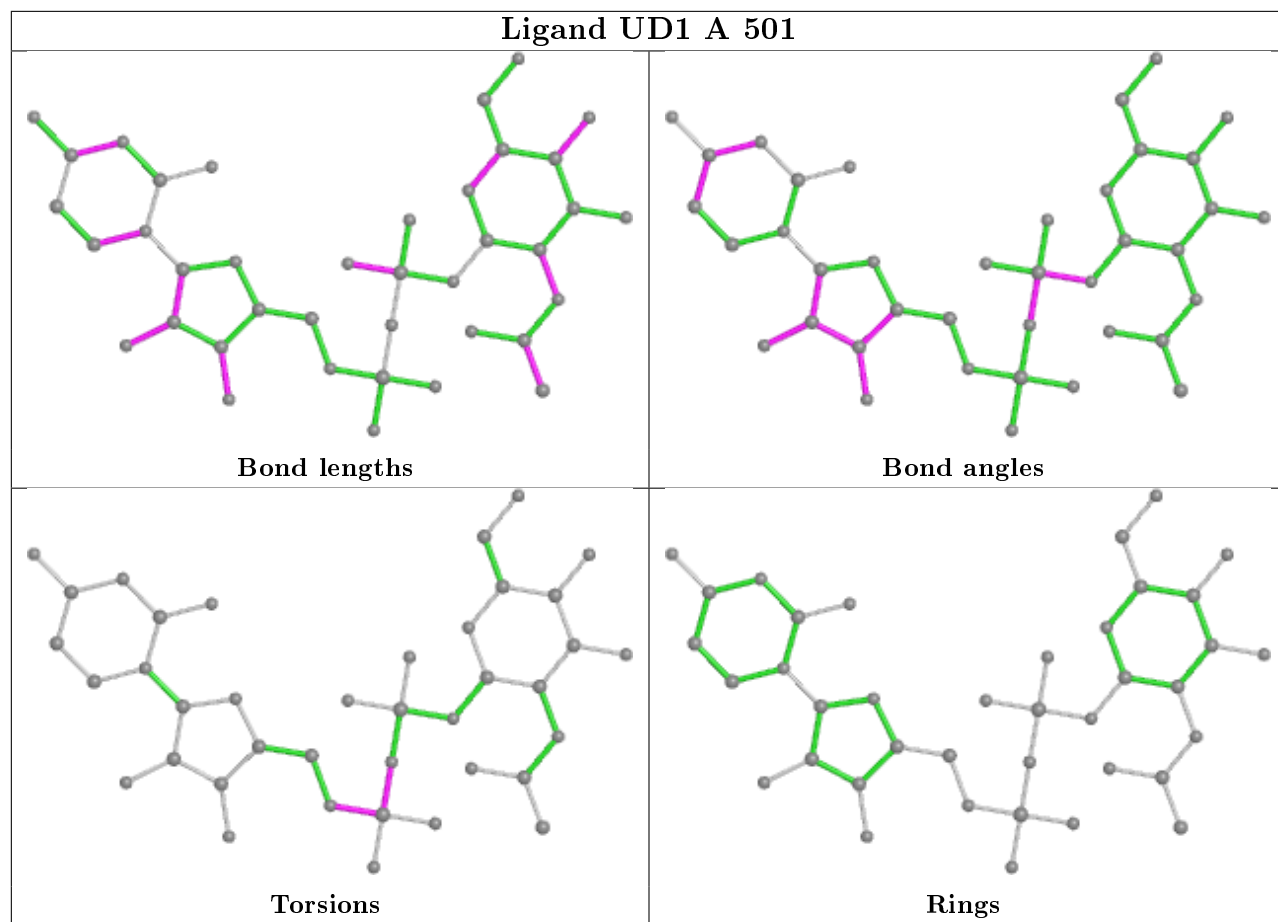




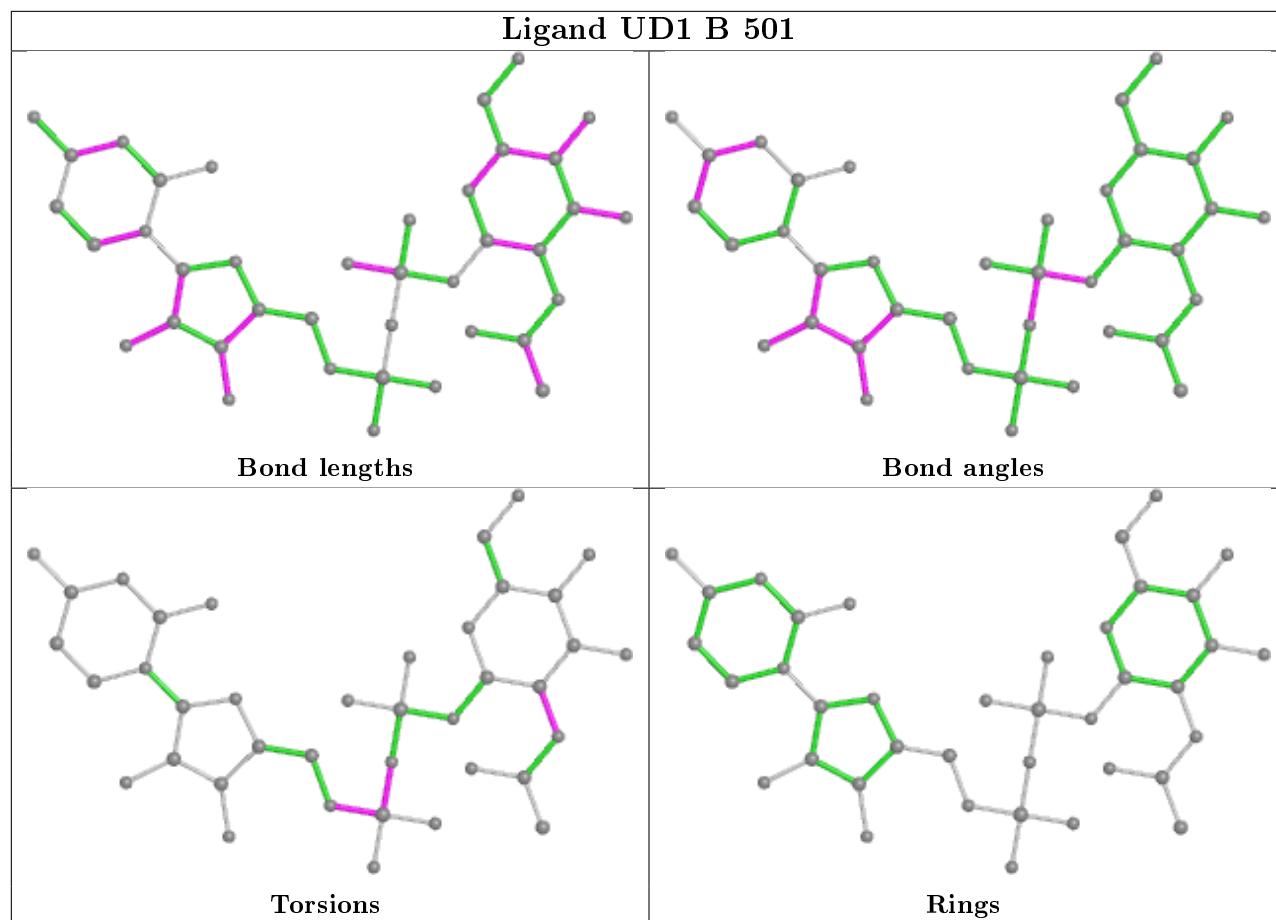












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | G     | 1                |
| 1   | D     | 1                |
| 1   | E     | 1                |
| 1   | H     | 1                |
| 1   | B     | 1                |
| 1   | C     | 1                |
| 1   | A     | 1                |
| 1   | F     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | D     | 67:IAS    | C      | 68:GLY    | N      | 4.54         |
| 1     | A     | 67:IAS    | C      | 68:GLY    | N      | 4.43         |
| 1     | C     | 67:IAS    | C      | 68:GLY    | N      | 4.41         |
| 1     | H     | 67:IAS    | C      | 68:GLY    | N      | 4.41         |
| 1     | B     | 67:IAS    | C      | 68:GLY    | N      | 4.39         |
| 1     | F     | 67:IAS    | C      | 68:GLY    | N      | 4.38         |
| 1     | E     | 67:IAS    | C      | 68:GLY    | N      | 4.33         |
| 1     | G     | 67:IAS    | C      | 68:GLY    | N      | 4.30         |

## 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     | 418/419 (99%)   | -0.14  | 4 (0%) 82 84   | 22, 36, 52, 87        | 0     |
| 1   | B     | 418/419 (99%)   | 0.52   | 43 (10%) 6 6   | 30, 53, 75, 94        | 0     |
| 1   | C     | 418/419 (99%)   | -0.02  | 10 (2%) 59 62  | 24, 42, 58, 81        | 0     |
| 1   | D     | 418/419 (99%)   | -0.02  | 14 (3%) 46 50  | 22, 39, 58, 83        | 0     |
| 1   | E     | 418/419 (99%)   | 0.10   | 18 (4%) 35 38  | 19, 42, 71, 92        | 0     |
| 1   | F     | 418/419 (99%)   | -0.05  | 10 (2%) 59 62  | 24, 40, 58, 84        | 0     |
| 1   | G     | 418/419 (99%)   | -0.02  | 8 (1%) 66 69   | 22, 39, 56, 93        | 0     |
| 1   | H     | 418/419 (99%)   | -0.08  | 8 (1%) 66 69   | 19, 36, 52, 89        | 0     |
| All | All   | 3344/3352 (99%) | 0.04   | 115 (3%) 45 48 | 19, 40, 64, 94        | 0     |

All (115) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 419 | GLU  | 10.4 |
| 1   | B     | 418 | GLY  | 10.3 |
| 1   | H     | 419 | GLU  | 7.3  |
| 1   | B     | 419 | GLU  | 7.2  |
| 1   | G     | 419 | GLU  | 6.4  |
| 1   | B     | 417 | LYS  | 6.4  |
| 1   | H     | 418 | GLY  | 6.3  |
| 1   | H     | 417 | LYS  | 5.7  |
| 1   | F     | 419 | GLU  | 5.5  |
| 1   | E     | 418 | GLY  | 5.2  |
| 1   | G     | 418 | GLY  | 4.9  |
| 1   | A     | 419 | GLU  | 4.8  |
| 1   | E     | 419 | GLU  | 4.6  |
| 1   | A     | 1   | MET  | 4.3  |
| 1   | B     | 287 | LYS  | 4.1  |
| 1   | B     | 277 | GLU  | 4.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | E            | 277        | GLU         | 4.0         |
| 1          | D            | 419        | GLU         | 4.0         |
| 1          | F            | 418        | GLY         | 4.0         |
| 1          | E            | 417        | LYS         | 3.9         |
| 1          | E            | 63         | LYS         | 3.8         |
| 1          | D            | 418        | GLY         | 3.7         |
| 1          | C            | 287        | LYS         | 3.6         |
| 1          | D            | 1          | MET         | 3.6         |
| 1          | C            | 1          | MET         | 3.5         |
| 1          | B            | 359        | LYS         | 3.5         |
| 1          | D            | 148        | ASN         | 3.5         |
| 1          | B            | 401        | ARG         | 3.5         |
| 1          | E            | 65         | GLU         | 3.5         |
| 1          | D            | 76         | ASN         | 3.5         |
| 1          | D            | 149        | GLY         | 3.4         |
| 1          | H            | 1          | MET         | 3.4         |
| 1          | E            | 329        | GLU         | 3.3         |
| 1          | B            | 38         | PRO         | 3.3         |
| 1          | B            | 71         | TRP         | 3.2         |
| 1          | F            | 277        | GLU         | 3.2         |
| 1          | E            | 71         | TRP         | 3.2         |
| 1          | F            | 1          | MET         | 3.1         |
| 1          | B            | 63         | LYS         | 3.1         |
| 1          | B            | 358        | GLU         | 3.0         |
| 1          | G            | 417        | LYS         | 3.0         |
| 1          | F            | 127        | PHE         | 3.0         |
| 1          | B            | 2          | ASP         | 3.0         |
| 1          | B            | 61         | GLY         | 3.0         |
| 1          | B            | 285        | HIS         | 3.0         |
| 1          | F            | 177        | GLU         | 2.9         |
| 1          | B            | 83         | PRO         | 2.9         |
| 1          | B            | 248        | LYS         | 2.9         |
| 1          | E            | 1          | MET         | 2.9         |
| 1          | E            | 38         | PRO         | 2.9         |
| 1          | B            | 127        | PHE         | 2.9         |
| 1          | C            | 418        | GLY         | 2.9         |
| 1          | E            | 401        | ARG         | 2.9         |
| 1          | B            | 416        | VAL         | 2.8         |
| 1          | B            | 80         | PHE         | 2.8         |
| 1          | E            | 85         | ASP         | 2.8         |
| 1          | G            | 1          | MET         | 2.8         |
| 1          | F            | 219        | GLU         | 2.7         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 76  | ASN  | 2.7  |
| 1   | E     | 76  | ASN  | 2.7  |
| 1   | C     | 63  | LYS  | 2.7  |
| 1   | B     | 79  | ASN  | 2.6  |
| 1   | H     | 391 | ARG  | 2.6  |
| 1   | B     | 78  | ASN  | 2.6  |
| 1   | F     | 358 | GLU  | 2.6  |
| 1   | B     | 384 | GLU  | 2.5  |
| 1   | A     | 212 | ARG  | 2.5  |
| 1   | B     | 15  | GLU  | 2.5  |
| 1   | B     | 202 | GLY  | 2.5  |
| 1   | F     | 68  | GLY  | 2.5  |
| 1   | B     | 219 | GLU  | 2.5  |
| 1   | B     | 86  | LEU  | 2.4  |
| 1   | G     | 76  | ASN  | 2.4  |
| 1   | D     | 75  | SER  | 2.4  |
| 1   | D     | 252 | ARG  | 2.4  |
| 1   | B     | 42  | GLN  | 2.3  |
| 1   | D     | 417 | LYS  | 2.3  |
| 1   | E     | 78  | ASN  | 2.3  |
| 1   | C     | 384 | GLU  | 2.3  |
| 1   | B     | 252 | ARG  | 2.3  |
| 1   | B     | 46  | LYS  | 2.3  |
| 1   | B     | 7   | GLN  | 2.3  |
| 1   | D     | 34  | LEU  | 2.3  |
| 1   | B     | 243 | ALA  | 2.2  |
| 1   | C     | 285 | HIS  | 2.2  |
| 1   | F     | 359 | LYS  | 2.2  |
| 1   | G     | 116 | ALA  | 2.2  |
| 1   | C     | 358 | GLU  | 2.2  |
| 1   | E     | 203 | ALA  | 2.2  |
| 1   | A     | 148 | ASN  | 2.2  |
| 1   | B     | 318 | GLU  | 2.2  |
| 1   | B     | 217 | GLY  | 2.2  |
| 1   | G     | 277 | GLU  | 2.2  |
| 1   | H     | 148 | ASN  | 2.2  |
| 1   | B     | 9   | PRO  | 2.2  |
| 1   | E     | 77  | VAL  | 2.2  |
| 1   | D     | 217 | GLY  | 2.2  |
| 1   | D     | 78  | ASN  | 2.1  |
| 1   | D     | 150 | ARG  | 2.1  |
| 1   | G     | 401 | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 370 | LEU  | 2.1  |
| 1   | C     | 116 | ALA  | 2.1  |
| 1   | H     | 416 | VAL  | 2.1  |
| 1   | E     | 177 | GLU  | 2.1  |
| 1   | B     | 59  | GLN  | 2.1  |
| 1   | B     | 3   | LYS  | 2.1  |
| 1   | B     | 152 | LYS  | 2.1  |
| 1   | B     | 272 | ASP  | 2.1  |
| 1   | E     | 73  | ASP  | 2.1  |
| 1   | H     | 152 | LYS  | 2.1  |
| 1   | D     | 127 | PHE  | 2.1  |
| 1   | B     | 216 | GLU  | 2.1  |
| 1   | B     | 220 | ARG  | 2.0  |
| 1   | B     | 1   | MET  | 2.0  |
| 1   | C     | 148 | ASN  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | IAS  | E     | 67  | 8/9   | 0.86 | 0.30 | 68,70,71,72                | 0     |
| 1   | IAS  | D     | 67  | 8/9   | 0.87 | 0.27 | 56,57,61,62                | 0     |
| 1   | IAS  | F     | 67  | 8/9   | 0.92 | 0.24 | 59,60,62,64                | 0     |
| 1   | IAS  | B     | 67  | 8/9   | 0.92 | 0.36 | 73,74,76,76                | 0     |
| 1   | IAS  | G     | 67  | 8/9   | 0.93 | 0.20 | 36,38,41,42                | 0     |
| 1   | IAS  | C     | 67  | 8/9   | 0.93 | 0.20 | 49,52,52,53                | 0     |
| 1   | IAS  | A     | 67  | 8/9   | 0.93 | 0.11 | 34,36,37,37                | 0     |
| 1   | IAS  | H     | 67  | 8/9   | 0.97 | 0.12 | 34,35,37,38                | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | ACT  | A     | 505 | 4/4   | 0.67 | 0.38 | 72,72,73,73                | 0     |
| 3   | ACT  | E     | 504 | 4/4   | 0.72 | 0.41 | 81,81,82,82                | 0     |
| 3   | ACT  | A     | 502 | 4/4   | 0.72 | 0.25 | 47,51,51,51                | 0     |
| 4   | EDO  | D     | 508 | 4/4   | 0.72 | 0.19 | 58,59,60,60                | 0     |
| 4   | EDO  | G     | 506 | 4/4   | 0.74 | 0.28 | 57,58,58,58                | 0     |
| 4   | EDO  | E     | 508 | 4/4   | 0.77 | 0.22 | 54,54,55,55                | 0     |
| 3   | ACT  | F     | 502 | 4/4   | 0.77 | 0.47 | 69,69,70,70                | 0     |
| 4   | EDO  | E     | 510 | 4/4   | 0.78 | 0.45 | 59,62,63,63                | 0     |
| 3   | ACT  | C     | 502 | 4/4   | 0.79 | 0.35 | 74,75,75,76                | 0     |
| 4   | EDO  | G     | 505 | 4/4   | 0.80 | 0.29 | 62,63,64,64                | 0     |
| 3   | ACT  | A     | 503 | 4/4   | 0.81 | 0.35 | 67,68,68,69                | 0     |
| 3   | ACT  | H     | 505 | 4/4   | 0.81 | 0.32 | 57,58,59,60                | 0     |
| 4   | EDO  | C     | 505 | 4/4   | 0.83 | 0.19 | 51,54,55,56                | 0     |
| 3   | ACT  | D     | 502 | 4/4   | 0.84 | 0.22 | 52,54,55,56                | 0     |
| 4   | EDO  | H     | 510 | 4/4   | 0.84 | 0.28 | 56,58,59,60                | 0     |
| 4   | EDO  | D     | 507 | 4/4   | 0.84 | 0.28 | 58,59,59,61                | 0     |
| 4   | EDO  | F     | 506 | 4/4   | 0.84 | 0.17 | 59,59,61,61                | 0     |
| 4   | EDO  | E     | 511 | 4/4   | 0.85 | 0.15 | 62,64,65,65                | 0     |
| 4   | EDO  | F     | 509 | 4/4   | 0.85 | 0.25 | 44,45,47,49                | 0     |
| 3   | ACT  | F     | 503 | 4/4   | 0.85 | 0.36 | 49,52,52,52                | 0     |
| 4   | EDO  | F     | 508 | 4/4   | 0.85 | 0.24 | 59,62,62,63                | 0     |
| 4   | EDO  | F     | 507 | 4/4   | 0.85 | 0.17 | 60,63,63,64                | 0     |
| 4   | EDO  | G     | 507 | 4/4   | 0.85 | 0.21 | 48,49,50,51                | 0     |
| 3   | ACT  | H     | 506 | 4/4   | 0.86 | 0.21 | 57,57,58,58                | 0     |
| 4   | EDO  | D     | 510 | 4/4   | 0.87 | 0.20 | 44,47,48,51                | 0     |
| 3   | ACT  | F     | 504 | 4/4   | 0.87 | 0.29 | 68,70,70,70                | 0     |
| 3   | ACT  | B     | 502 | 4/4   | 0.87 | 0.23 | 69,71,71,71                | 0     |
| 4   | EDO  | G     | 508 | 4/4   | 0.88 | 0.25 | 46,47,48,49                | 0     |
| 4   | EDO  | G     | 504 | 4/4   | 0.88 | 0.18 | 45,45,46,47                | 0     |
| 4   | EDO  | E     | 506 | 4/4   | 0.88 | 0.21 | 48,48,50,52                | 0     |
| 3   | ACT  | C     | 503 | 4/4   | 0.88 | 0.36 | 52,53,55,56                | 0     |
| 4   | EDO  | D     | 506 | 4/4   | 0.88 | 0.27 | 48,50,52,53                | 0     |
| 3   | ACT  | H     | 504 | 4/4   | 0.89 | 0.24 | 58,58,58,59                | 0     |
| 4   | EDO  | H     | 511 | 4/4   | 0.89 | 0.17 | 54,56,57,58                | 0     |
| 4   | EDO  | A     | 509 | 4/4   | 0.89 | 0.26 | 55,56,56,56                | 0     |
| 3   | ACT  | E     | 503 | 4/4   | 0.89 | 0.32 | 74,75,75,75                | 0     |
| 4   | EDO  | B     | 505 | 4/4   | 0.89 | 0.30 | 59,59,59,60                | 0     |
| 4   | EDO  | H     | 509 | 4/4   | 0.89 | 0.19 | 58,58,59,61                | 0     |
| 3   | ACT  | H     | 502 | 4/4   | 0.89 | 0.32 | 55,57,58,58                | 0     |
| 3   | ACT  | D     | 503 | 4/4   | 0.90 | 0.23 | 68,68,69,69                | 0     |
| 4   | EDO  | E     | 507 | 4/4   | 0.90 | 0.23 | 45,46,47,47                | 0     |

*Continued on next page...*

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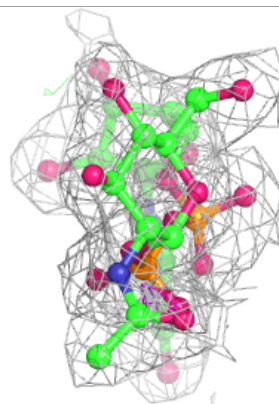
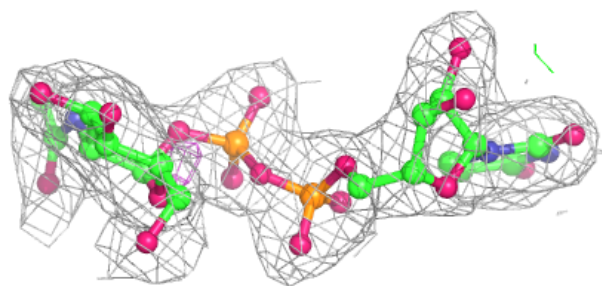
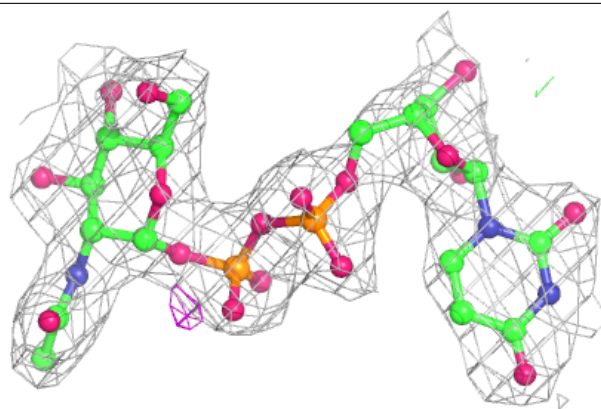
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | ACT  | E     | 502 | 4/4   | 0.91 | 0.17 | 63,64,64,65                 | 0     |
| 4   | EDO  | H     | 513 | 4/4   | 0.91 | 0.32 | 56,56,56,57                 | 0     |
| 4   | EDO  | G     | 503 | 4/4   | 0.91 | 0.15 | 51,51,51,53                 | 0     |
| 4   | EDO  | E     | 505 | 4/4   | 0.91 | 0.12 | 51,55,55,57                 | 0     |
| 4   | EDO  | C     | 506 | 4/4   | 0.92 | 0.22 | 55,57,57,58                 | 0     |
| 4   | EDO  | B     | 503 | 4/4   | 0.92 | 0.18 | 44,44,44,48                 | 0     |
| 3   | ACT  | A     | 504 | 4/4   | 0.92 | 0.20 | 52,54,54,56                 | 0     |
| 4   | EDO  | D     | 505 | 4/4   | 0.92 | 0.15 | 48,49,49,51                 | 0     |
| 4   | EDO  | C     | 507 | 4/4   | 0.93 | 0.32 | 54,54,54,54                 | 0     |
| 3   | ACT  | H     | 503 | 4/4   | 0.94 | 0.19 | 42,45,46,47                 | 0     |
| 4   | EDO  | D     | 504 | 4/4   | 0.94 | 0.17 | 39,40,41,43                 | 0     |
| 4   | EDO  | B     | 504 | 4/4   | 0.94 | 0.15 | 59,60,61,61                 | 0     |
| 4   | EDO  | A     | 506 | 4/4   | 0.94 | 0.17 | 32,34,35,39                 | 0     |
| 4   | EDO  | H     | 508 | 4/4   | 0.95 | 0.15 | 50,52,52,52                 | 0     |
| 4   | EDO  | H     | 512 | 4/4   | 0.95 | 0.15 | 34,36,36,39                 | 0     |
| 4   | EDO  | H     | 507 | 4/4   | 0.95 | 0.12 | 42,42,43,44                 | 0     |
| 4   | EDO  | A     | 508 | 4/4   | 0.96 | 0.11 | 53,53,54,54                 | 0     |
| 4   | EDO  | D     | 509 | 4/4   | 0.96 | 0.16 | 61,62,62,62                 | 0     |
| 4   | EDO  | A     | 507 | 4/4   | 0.96 | 0.42 | 35,35,37,40                 | 0     |
| 4   | EDO  | E     | 509 | 4/4   | 0.96 | 0.14 | 45,46,47,49                 | 0     |
| 2   | UD1  | A     | 501 | 39/39 | 0.97 | 0.11 | 18,29,37,41                 | 0     |
| 2   | UD1  | G     | 501 | 39/39 | 0.97 | 0.11 | 25,30,42,44                 | 0     |
| 2   | UD1  | E     | 501 | 39/39 | 0.97 | 0.11 | 23,30,35,35                 | 0     |
| 4   | EDO  | F     | 505 | 4/4   | 0.97 | 0.15 | 43,44,44,45                 | 0     |
| 4   | EDO  | G     | 502 | 4/4   | 0.97 | 0.13 | 35,36,37,39                 | 0     |
| 2   | UD1  | D     | 501 | 39/39 | 0.97 | 0.11 | 18,28,37,37                 | 0     |
| 2   | UD1  | B     | 501 | 39/39 | 0.97 | 0.12 | 31,38,42,44                 | 0     |
| 2   | UD1  | H     | 501 | 39/39 | 0.97 | 0.11 | 27,32,39,40                 | 0     |
| 4   | EDO  | C     | 504 | 4/4   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 2   | UD1  | F     | 501 | 39/39 | 0.98 | 0.11 | 24,32,37,40                 | 0     |
| 2   | UD1  | C     | 501 | 39/39 | 0.98 | 0.11 | 24,29,37,40                 | 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.

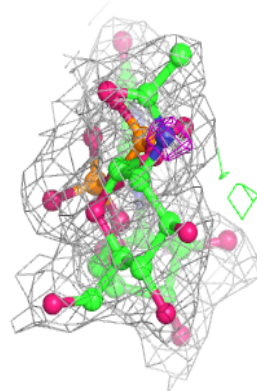
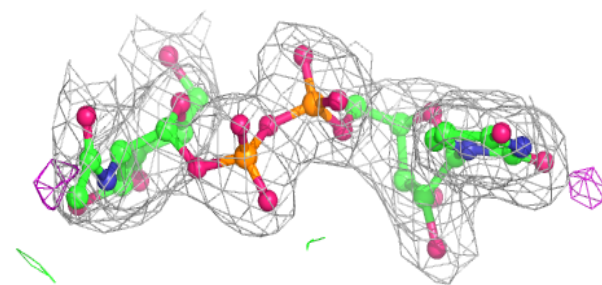
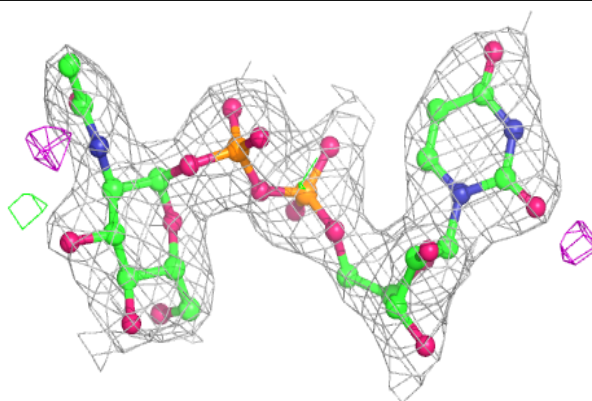


**Electron density around UD1 A 501:**

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

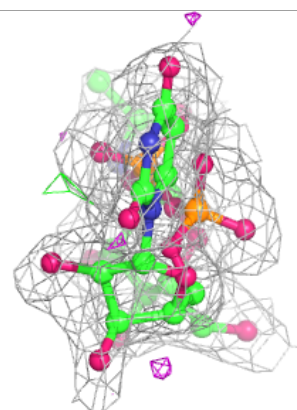
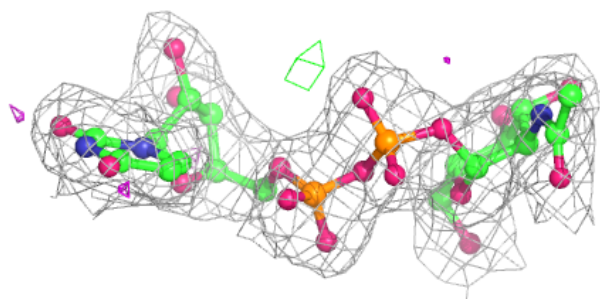
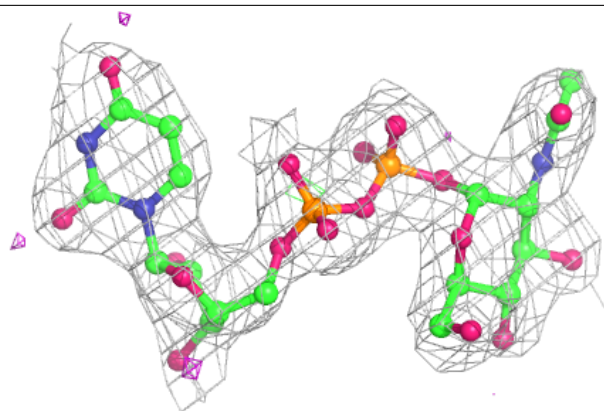
**Electron density around UD1 G 501:**

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

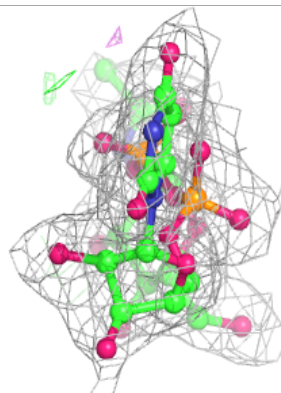
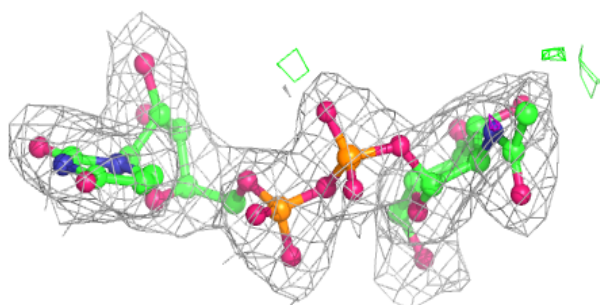
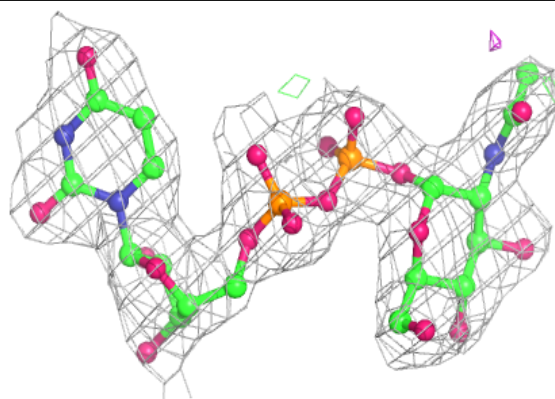


**Electron density around UD1 E 501:**

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

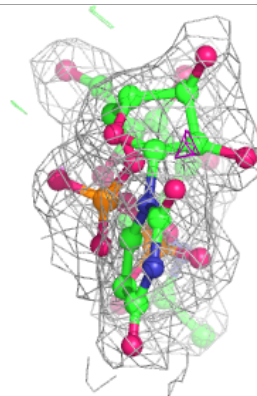
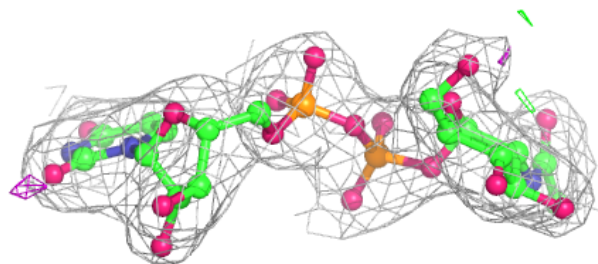
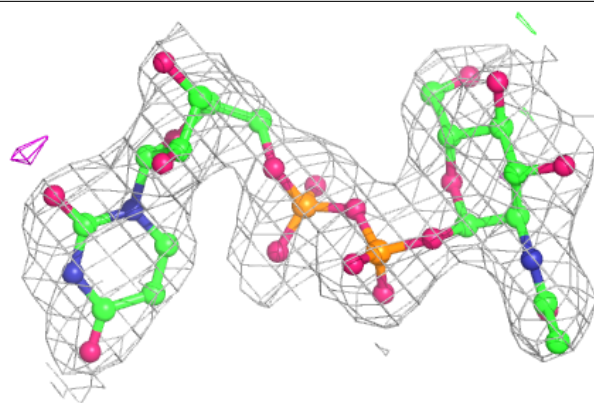
**Electron density around UD1 D 501:**

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

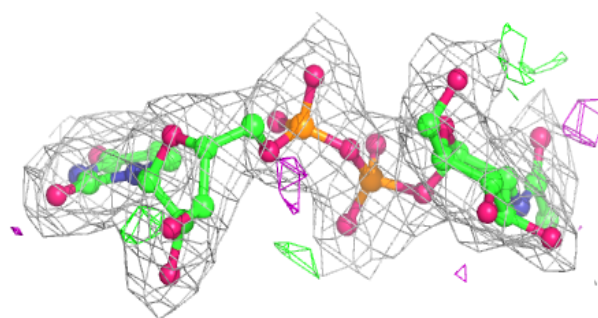
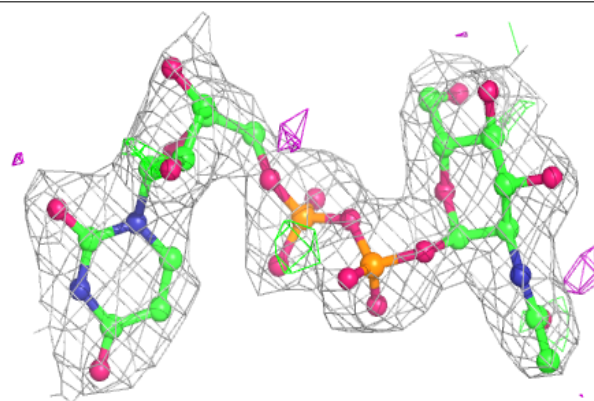


**Electron density around UD1 B 501:**

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

**Electron density around UD1 H 501:**

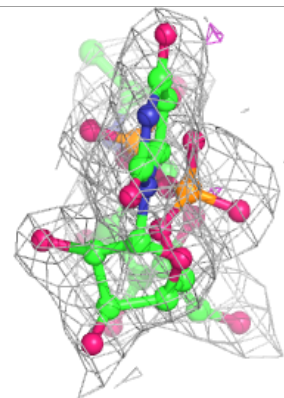
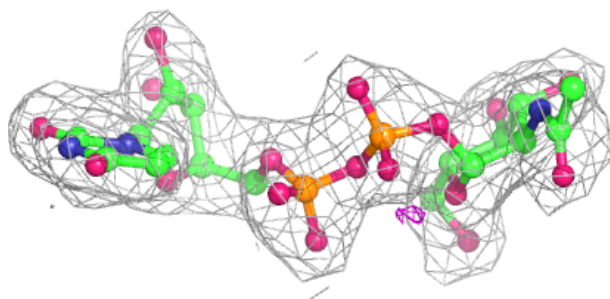
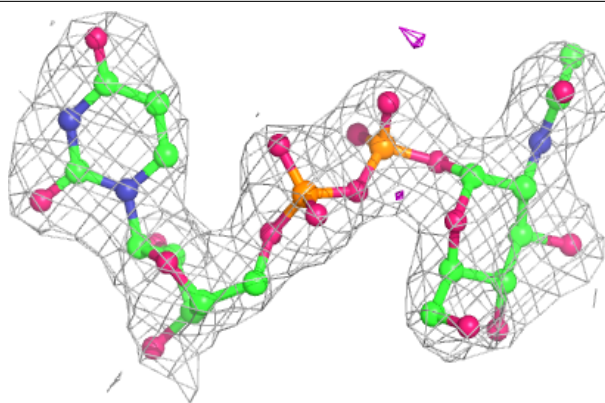
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



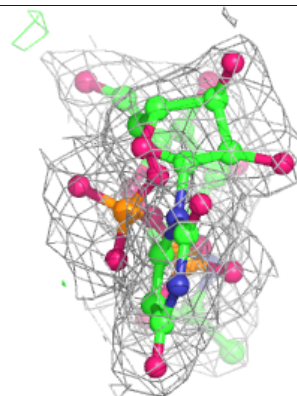
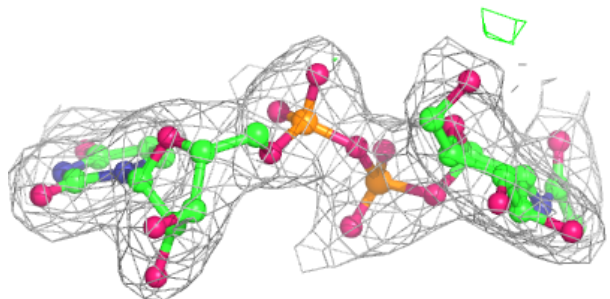
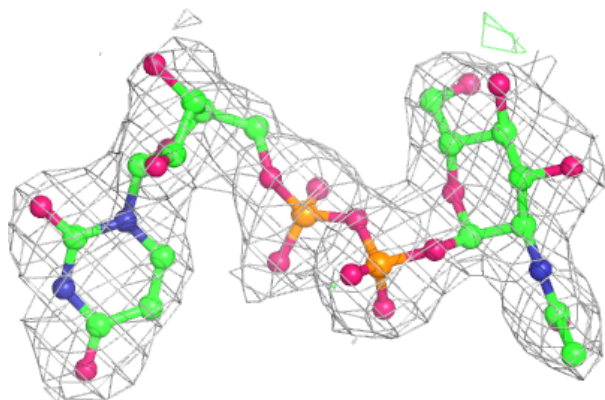


**Electron density around UD1 F 501:**

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

**Electron density around UD1 C 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.