



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:26 PM UTC

PDB ID : 7QUP / pdb\_00007qup  
EMDB ID : EMD-14150  
Title : D. melanogaster 13-protofilament microtubule  
Authors : Wagstaff, J.; Planelles-Herrero, V.J.; Derivery, E.; Lowe, J.  
Deposited on : 2022-01-18  
Resolution : 3.80 Å(reported)  
Based on initial model : 3J1T

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

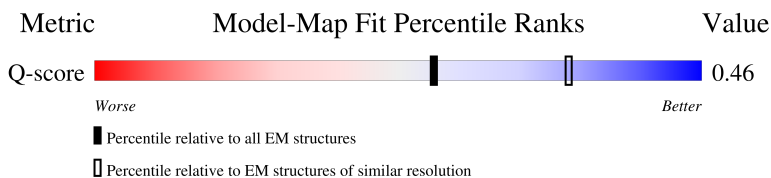
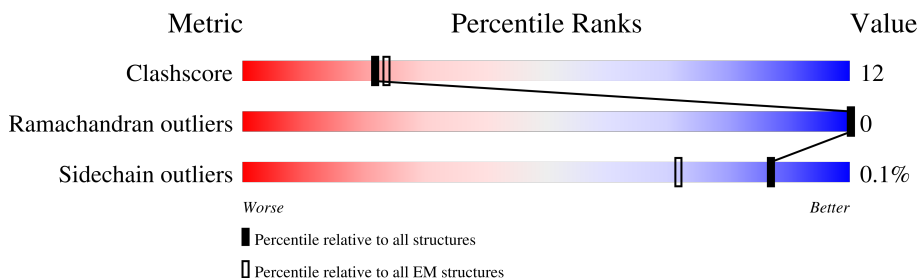
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | 10A   | 475    | <div> <div>5%</div> <div>66%</div> <div>24%</div> <div>10%</div> </div> |
| 1   | 10C   | 475    | <div> <div>67%</div> <div>23%</div> <div>10%</div> </div>               |
| 1   | 10E   | 475    | <div> <div>7%</div> <div>64%</div> <div>26%</div> <div>10%</div> </div> |
| 1   | 11A   | 475    | <div> <div>7%</div> <div>68%</div> <div>21%</div> <div>10%</div> </div> |

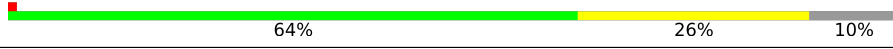
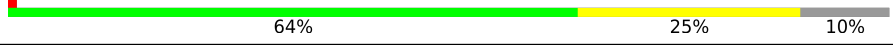
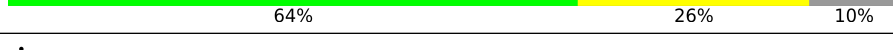
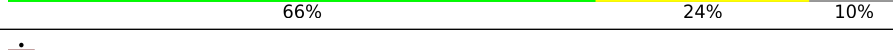
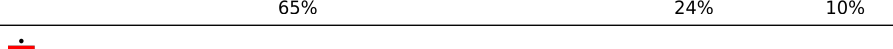
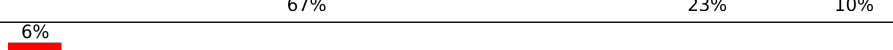
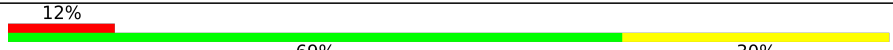
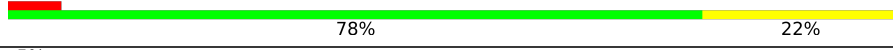
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 11C   | 475    |                  |
| 1   | 11E   | 475    |                  |
| 1   | 12A   | 475    |                  |
| 1   | 12C   | 475    |                  |
| 1   | 12E   | 475    |                  |
| 1   | 13A   | 475    |                  |
| 1   | 13C   | 475    |                  |
| 1   | 13E   | 475    |                  |
| 1   | 1A    | 475    |                  |
| 1   | 1C    | 475    |                  |
| 1   | 1E    | 475    |                  |
| 1   | 2A    | 475    |                  |
| 1   | 2C    | 475    |                  |
| 1   | 2E    | 475    |                  |
| 1   | 3A    | 475    |                  |
| 1   | 3C    | 475    |                  |
| 1   | 3E    | 475    |                  |
| 1   | 4A    | 475    |                  |
| 1   | 4C    | 475    |                  |
| 1   | 4E    | 475    |                  |
| 1   | 5A    | 475    |                  |
| 1   | 5C    | 475    |                  |
| 1   | 5E    | 475    |                  |
| 1   | 6A    | 475    |                  |
| 1   | 6C    | 475    |                  |

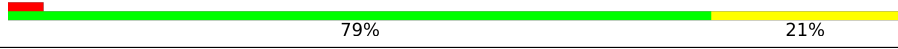
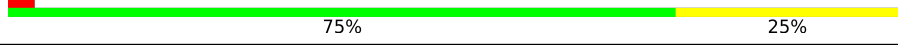
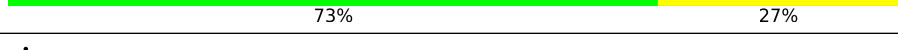
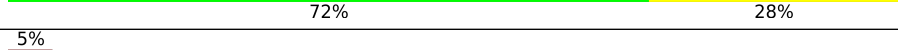
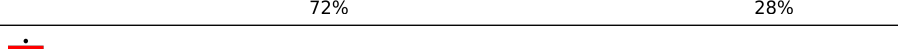
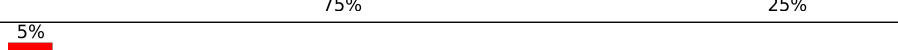
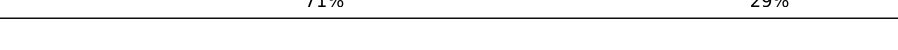
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 6E    | 475    |    |
| 1   | 7A    | 475    |    |
| 1   | 7C    | 475    |    |
| 1   | 7E    | 475    |    |
| 1   | 8A    | 475    |    |
| 1   | 8C    | 475    |    |
| 1   | 8E    | 475    |    |
| 1   | 9A    | 475    |    |
| 1   | 9C    | 475    |    |
| 1   | 9E    | 475    |    |
| 2   | 10B   | 425    |    |
| 2   | 10D   | 425    |  |
| 2   | 11B   | 425    |  |
| 2   | 11D   | 425    |  |
| 2   | 12B   | 425    |  |
| 2   | 12D   | 425    |  |
| 2   | 13B   | 425    |  |
| 2   | 13D   | 425    |  |
| 2   | 1B    | 425    |  |
| 2   | 1D    | 425    |  |
| 2   | 2B    | 425    |  |
| 2   | 2D    | 425    |  |
| 2   | 3B    | 425    |  |
| 2   | 3D    | 425    |  |
| 2   | 4B    | 425    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |  |
|-----|-------|--------|------------------------------------------------------------------------------------|--|
| 2   | 4D    | 425    |  |  |
| 2   | 5B    | 425    |  |  |
| 2   | 5D    | 425    |  |  |
| 2   | 6B    | 425    |  |  |
| 2   | 6D    | 425    |  |  |
| 2   | 7B    | 425    |  |  |
| 2   | 7D    | 425    |  |  |
| 2   | 8B    | 425    |  |  |
| 2   | 8D    | 425    |  |  |
| 2   | 9B    | 425    |  |  |
| 2   | 9D    | 425    |  |  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 219271 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tubulin alpha-1 chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 10A   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 10C   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 10E   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 11A   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 11C   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 11E   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 12A   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 12C   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 12E   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 13A   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 13C   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 13E   | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 1A    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 1C    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 1E    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 2A    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |
| 1   | 2C    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1   | 2E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 3A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 3C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 3E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 4A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 4C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 4E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 5A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 5C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 5E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 6A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 6C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 6E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 7A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 7C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 7E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 8A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 8C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 8E    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 9A    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |
| 1   | 9C    | 426      | Total<br>3342 | C<br>2121 | N<br>569 | O<br>631 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 9E    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3342  | 2121 | 569 | 631 | 21 |         |       |

There are 1521 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 10A   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 10A   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 10A   | -17     | GLU      | -      | expression tag        | UNP P06603 |
| 10A   | -16     | ASP      | -      | expression tag        | UNP P06603 |
| 10A   | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 10A   | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 10A   | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 10A   | -12     | PRO      | -      | expression tag        | UNP P06603 |
| 10A   | -11     | ARG      | -      | expression tag        | UNP P06603 |
| 10A   | -10     | LEU      | -      | expression tag        | UNP P06603 |
| 10A   | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 10A   | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 10A   | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 10A   | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 10A   | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 10A   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 10A   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 10A   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 10A   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 10A   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 10A   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 10A   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 10A   | 447     | ALA      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 10A   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 10A   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 10A   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 10C   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 10C   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 10C   | -17     | GLU      | -      | expression tag        | UNP P06603 |
| 10C   | -16     | ASP      | -      | expression tag        | UNP P06603 |
| 10C   | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 10C   | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 10C   | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 10C   | -12     | PRO      | -      | expression tag        | UNP P06603 |
| 10C   | -11     | ARG      | -      | expression tag        | UNP P06603 |
| 10C   | -10     | LEU      | -      | expression tag        | UNP P06603 |
| 10C   | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 10C   | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 10C   | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 10C   | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 10C   | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 10C   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 10C   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 10C   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 10C   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 10C   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 10C   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 10C   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 10C   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 10C   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 10C   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 10C   | 450     | TYR      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 10E   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 10E   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 10E   | -17     | GLU      | -      | expression tag        | UNP P06603 |
| 10E   | -16     | ASP      | -      | expression tag        | UNP P06603 |
| 10E   | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 10E   | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 10E   | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 10E   | -12     | PRO      | -      | expression tag        | UNP P06603 |
| 10E   | -11     | ARG      | -      | expression tag        | UNP P06603 |
| 10E   | -10     | LEU      | -      | expression tag        | UNP P06603 |
| 10E   | -9      | ILE      | -      | expression tag        | UNP P06603 |
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| 10E   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 10E   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 10E   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 10E   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 10E   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 10E   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 10E   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 10E   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 10E   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 10E   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 10E   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 10E   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 10E   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 10E   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 11A   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 11A   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 11A   | -22     | HIS      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 11A   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 11A   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 11A   | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 11A   | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 11A   | -17     | GLU      | -      | expression tag        | UNP P06603 |
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| 11A   | -15     | GLN      | -      | expression tag        | UNP P06603 |
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| 11A   | 444     | GLY      | -      | expression tag        | UNP P06603 |
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| 11A   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 11A   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 11A   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 11A   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 11A   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 11C   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 11C   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 11C   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 11C   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 11C   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 11C   | -19     | HIS      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 11C   | 444     | GLY      | -      | expression tag        | UNP P06603 |
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| 11C   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 11C   | 448     | GLU      | -      | expression tag        | UNP P06603 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 11E   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 11E   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 12A   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 12A   | -23     | HIS      | -      | expression tag        | UNP P06603 |
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| 12A   | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 12A   | -13     | ASP      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
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| 12A   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 12A   | 447     | ALA      | -      | expression tag        | UNP P06603 |
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| 12A   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 12C   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 12C   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 12C   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 12C   | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 12C   | -1      | ARG      | -      | expression tag        | UNP P06603 |
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| 12C   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 12C   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 12C   | 439     | SER      | -      | expression tag        | UNP P06603 |
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| 12C   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 12C   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 12C   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 12C   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 12C   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 12E   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 12E   | -23     | HIS      | -      | expression tag        | UNP P06603 |
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| 12E   | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 12E   | -7      | GLY      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 12E   | -6      | LYS      | -      | expression tag        | UNP P06603 |
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| 12E   | -2      | GLY      | -      | expression tag        | UNP P06603 |
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| 12E   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 12E   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 12E   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 12E   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 12E   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 13A   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 13A   | -23     | HIS      | -      | expression tag        | UNP P06603 |
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| 13A   | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 13A   | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 13A   | -17     | GLU      | -      | expression tag        | UNP P06603 |
| 13A   | -16     | ASP      | -      | expression tag        | UNP P06603 |
| 13A   | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 13A   | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 13A   | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 13A   | -12     | PRO      | -      | expression tag        | UNP P06603 |
| 13A   | -11     | ARG      | -      | expression tag        | UNP P06603 |
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| 13A   | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 13A   | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 13A   | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 13A   | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | -4      | GLY      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 13A   | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 13A   | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 13A   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 13A   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 13A   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 13A   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 13A   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 13A   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 13A   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 13A   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 13A   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 13A   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 13A   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 13C   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 13C   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 13C   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 13C   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 13C   | -20     | HIS      | -      | expression tag        | UNP P06603 |
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| 13C   | -9      | ILE      | -      | expression tag        | UNP P06603 |
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| 13C   | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 13C   | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | -1      | ARG      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 13C   | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 13C   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 13C   | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 13C   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 13C   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 13C   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 13C   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 13C   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 13C   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 13C   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 13C   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 13C   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 13E   | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 13E   | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 13E   | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 13E   | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 13E   | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 13E   | -19     | HIS      | -      | expression tag        | UNP P06603 |
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| 13E   | -17     | GLU      | -      | expression tag        | UNP P06603 |
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| 13E   | -9      | ILE      | -      | expression tag        | UNP P06603 |
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| 13E   | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 13E   | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 13E   | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 13E   | 437     | MET      | -      | expression tag        | UNP P06603 |
| 13E   | 438     | ASP      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 13E   | 439     | SER      | -      | expression tag        | UNP P06603 |
| 13E   | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 13E   | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 13E   | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 13E   | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 13E   | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 13E   | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 13E   | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 13E   | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 1A    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 1A    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 1A    | -22     | HIS      | -      | expression tag        | UNP P06603 |
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| 1A    | -10     | LEU      | -      | expression tag        | UNP P06603 |
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| 1A    | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 1A    | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 1A    | -5      | GLY      | -      | expression tag        | UNP P06603 |
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| 1A    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 1A    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 1A    | 437     | MET      | -      | expression tag        | UNP P06603 |
| 1A    | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 1A    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 1A    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | 441     | ASP      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 1A    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 1A    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 1A    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 1A    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 1A    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 1A    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 1A    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 1C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 1C    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 1C    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 1C    | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| 1C    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 1C    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 1C    | 437     | MET      | -      | expression tag        | UNP P06603 |
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| 1C    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 1C    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 1C    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 1C    | 444     | GLY      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 1C    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 1C    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 1C    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 1C    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 1C    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 1C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 1E    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 1E    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 1E    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 1E    | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| 1E    | -17     | GLU      | -      | expression tag        | UNP P06603 |
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| 1E    | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 1E    | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 1E    | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 1E    | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 1E    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 1E    | 437     | MET      | -      | expression tag        | UNP P06603 |
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| 1E    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 1E    | 440     | GLY      | -      | expression tag        | UNP P06603 |
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| 1E    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 1E    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 1E    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 1E    | 447     | ALA      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 1E    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 1E    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 1E    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 2A    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 2A    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 2A    | -22     | HIS      | -      | expression tag        | UNP P06603 |
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| 2A    | -17     | GLU      | -      | expression tag        | UNP P06603 |
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| 2A    | -15     | GLN      | -      | expression tag        | UNP P06603 |
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| 2A    | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 2A    | -5      | GLY      | -      | expression tag        | UNP P06603 |
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| 2A    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | -1      | ARG      | -      | expression tag        | UNP P06603 |
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| 2A    | 437     | MET      | -      | expression tag        | UNP P06603 |
| 2A    | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 2A    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 2A    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 2A    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 2A    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 2A    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 2A    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 2A    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 2A    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 2A    | 450     | TYR      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 2C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 2C    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -21     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -20     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 2C    | -17     | GLU      | -      | expression tag        | UNP P06603 |
| 2C    | -16     | ASP      | -      | expression tag        | UNP P06603 |
| 2C    | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 2C    | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 2C    | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 2C    | -12     | PRO      | -      | expression tag        | UNP P06603 |
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| 2C    | 437     | MET      | -      | expression tag        | UNP P06603 |
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| 2C    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 2C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 2E    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 2E    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 2E    | -22     | HIS      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 2E    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 2E    | 450     | TYR      | -      | expression tag        | UNP P06603 |
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| 3A    | -19     | HIS      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 3C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 4A    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 4C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 4C    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 4C    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 4C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 4E    | -24     | MET      | -      | initiating methionine | UNP P06603 |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 4E    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 4E    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 4E    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 4E    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 4E    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 4E    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 4E    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 4E    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 4E    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 4E    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 4E    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 4E    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 5A    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 5A    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 5A    | -22     | HIS      | -      | expression tag        | UNP P06603 |
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| 5A    | -15     | GLN      | -      | expression tag        | UNP P06603 |
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| 5A    | -11     | ARG      | -      | expression tag        | UNP P06603 |
| 5A    | -10     | LEU      | -      | expression tag        | UNP P06603 |
| 5A    | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 5A    | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 5A    | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 5A    | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | -1      | ARG      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 5A    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 5A    | 437     | MET      | -      | expression tag        | UNP P06603 |
| 5A    | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 5A    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 5A    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 5A    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 5A    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 5A    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 5A    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 5A    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 5A    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 5A    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 5C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 5C    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 5C    | -22     | HIS      | -      | expression tag        | UNP P06603 |
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| 5C    | -12     | PRO      | -      | expression tag        | UNP P06603 |
| 5C    | -11     | ARG      | -      | expression tag        | UNP P06603 |
| 5C    | -10     | LEU      | -      | expression tag        | UNP P06603 |
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| 5C    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 5C    | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 5C    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 5C    | 437     | MET      | -      | expression tag        | UNP P06603 |
| 5C    | 438     | ASP      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 5C    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 5C    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 5C    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 5C    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 5C    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 5C    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 5C    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 5C    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 5C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 5E    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 5E    | -23     | HIS      | -      | expression tag        | UNP P06603 |
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| 5E    | -2      | GLY      | -      | expression tag        | UNP P06603 |
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| 5E    | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 5E    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 5E    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 5E    | 441     | ASP      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 5E    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 5E    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 5E    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 5E    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 5E    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 5E    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 5E    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 5E    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 5E    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 6A    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 6A    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 6A    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 6A    | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| 6A    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 6A    | -5      | GLY      | -      | expression tag        | UNP P06603 |
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| 6A    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 6A    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 6A    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 6A    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 6A    | 437     | MET      | -      | expression tag        | UNP P06603 |
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| 6A    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 6A    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 6A    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 6A    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 6A    | 444     | GLY      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 6A    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 6A    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 6A    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 6A    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 6A    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 6A    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 6C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 6C    | -23     | HIS      | -      | expression tag        | UNP P06603 |
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| 6C    | -6      | LYS      | -      | expression tag        | UNP P06603 |
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| 6C    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 6C    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 6C    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 6C    | 0       | PRO      | -      | expression tag        | UNP P06603 |
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| 6C    | 440     | GLY      | -      | expression tag        | UNP P06603 |
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| 6C    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 6C    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 6C    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 6C    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 6C    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 6C    | 447     | ALA      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 6C    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 6C    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 6C    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 6E    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 6E    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 6E    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 6E    | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| 6E    | -16     | ASP      | -      | expression tag        | UNP P06603 |
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| 6E    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 6E    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 6E    | 0       | PRO      | -      | expression tag        | UNP P06603 |
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| 6E    | 439     | SER      | -      | expression tag        | UNP P06603 |
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| 6E    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 6E    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 6E    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 6E    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 6E    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 6E    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 6E    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 6E    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 6E    | 450     | TYR      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| 7A    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 7A    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 7A    | -22     | HIS      | -      | expression tag        | UNP P06603 |
| 7A    | -21     | HIS      | -      | expression tag        | UNP P06603 |
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| 7A    | -19     | HIS      | -      | expression tag        | UNP P06603 |
| 7A    | -18     | HIS      | -      | expression tag        | UNP P06603 |
| 7A    | -17     | GLU      | -      | expression tag        | UNP P06603 |
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| 7A    | -15     | GLN      | -      | expression tag        | UNP P06603 |
| 7A    | -14     | VAL      | -      | expression tag        | UNP P06603 |
| 7A    | -13     | ASP      | -      | expression tag        | UNP P06603 |
| 7A    | -12     | PRO      | -      | expression tag        | UNP P06603 |
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| 7A    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 7A    | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | -1      | ARG      | -      | expression tag        | UNP P06603 |
| 7A    | 0       | PRO      | -      | expression tag        | UNP P06603 |
| 7A    | 437     | MET      | -      | expression tag        | UNP P06603 |
| 7A    | 438     | ASP      | -      | expression tag        | UNP P06603 |
| 7A    | 439     | SER      | -      | expression tag        | UNP P06603 |
| 7A    | 440     | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | 441     | ASP      | -      | expression tag        | UNP P06603 |
| 7A    | 442     | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | 443     | GLU      | -      | expression tag        | UNP P06603 |
| 7A    | 444     | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | 445     | GLU      | -      | expression tag        | UNP P06603 |
| 7A    | 446     | GLY      | -      | expression tag        | UNP P06603 |
| 7A    | 447     | ALA      | -      | expression tag        | UNP P06603 |
| 7A    | 448     | GLU      | -      | expression tag        | UNP P06603 |
| 7A    | 449     | GLU      | -      | expression tag        | UNP P06603 |
| 7A    | 450     | TYR      | -      | expression tag        | UNP P06603 |
| 7C    | -24     | MET      | -      | initiating methionine | UNP P06603 |
| 7C    | -23     | HIS      | -      | expression tag        | UNP P06603 |
| 7C    | -22     | HIS      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
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| 9E    | -10     | LEU      | -      | expression tag        | UNP P06603 |
| 9E    | -9      | ILE      | -      | expression tag        | UNP P06603 |
| 9E    | -8      | ASP      | -      | expression tag        | UNP P06603 |
| 9E    | -7      | GLY      | -      | expression tag        | UNP P06603 |
| 9E    | -6      | LYS      | -      | expression tag        | UNP P06603 |
| 9E    | -5      | GLY      | -      | expression tag        | UNP P06603 |
| 9E    | -4      | GLY      | -      | expression tag        | UNP P06603 |
| 9E    | -3      | GLY      | -      | expression tag        | UNP P06603 |
| 9E    | -2      | GLY      | -      | expression tag        | UNP P06603 |
| 9E    | -1      | ARG      | -      | expression tag        | UNP P06603 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 9E    | 0       | PRO      | -      | expression tag | UNP P06603 |
| 9E    | 437     | MET      | -      | expression tag | UNP P06603 |
| 9E    | 438     | ASP      | -      | expression tag | UNP P06603 |
| 9E    | 439     | SER      | -      | expression tag | UNP P06603 |
| 9E    | 440     | GLY      | -      | expression tag | UNP P06603 |
| 9E    | 441     | ASP      | -      | expression tag | UNP P06603 |
| 9E    | 442     | GLY      | -      | expression tag | UNP P06603 |
| 9E    | 443     | GLU      | -      | expression tag | UNP P06603 |
| 9E    | 444     | GLY      | -      | expression tag | UNP P06603 |
| 9E    | 445     | GLU      | -      | expression tag | UNP P06603 |
| 9E    | 446     | GLY      | -      | expression tag | UNP P06603 |
| 9E    | 447     | ALA      | -      | expression tag | UNP P06603 |
| 9E    | 448     | GLU      | -      | expression tag | UNP P06603 |
| 9E    | 449     | GLU      | -      | expression tag | UNP P06603 |
| 9E    | 450     | TYR      | -      | expression tag | UNP P06603 |

- Molecule 2 is a protein called Tubulin beta-1 chain.

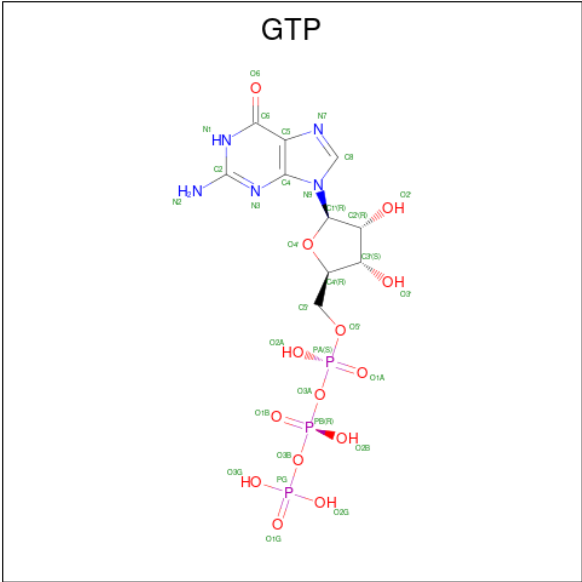
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 10B   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 10D   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 11B   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 11D   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 12B   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 12D   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 13B   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 13D   | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 1B    | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 1D    | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 2B    | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |
| 2   | 2D    | 425      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3343  | 2102 | 573 | 643 | 25 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | 3B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 3D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 4B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 4D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 5B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 5D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 6B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 6D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 7B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 7D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 8B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 8D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 9B    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |
| 2   | 9D    | 425      | Total<br>3343 | C<br>2102 | N<br>573 | O<br>643 | S<br>25 | 0       | 0     |

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | 10A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 10C   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 10E   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 11A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 11C   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 11E   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 12A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 12C   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 12E   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 13A   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 13C   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 13E   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1A    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1C    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 3   | 1E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 2A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 2C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 2E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 5A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 5C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 5E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 6A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 6C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 6E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 7A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 7C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 7E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 8A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 8C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | 8E    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 9A    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 9C    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 9E    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | 10A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 10C   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 10E   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 11A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 11C   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 11E   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 12A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 12C   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 12E   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 13A   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 13C   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 13E   | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1C    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1E    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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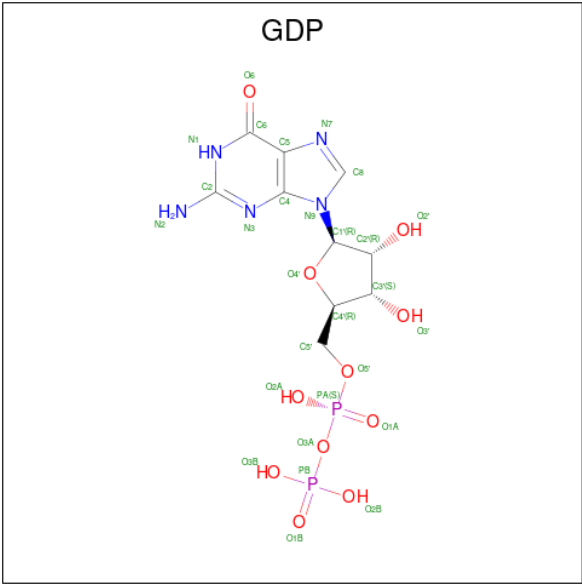
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | 2A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 5A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 5C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 5E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 6A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 6C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 6E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 7A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 7C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 7E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 8A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 8C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 8E    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | 9A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 9C    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 9E    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | 10B   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 10D   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 11B   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 11D   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 12B   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 12D   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 13B   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 13D   | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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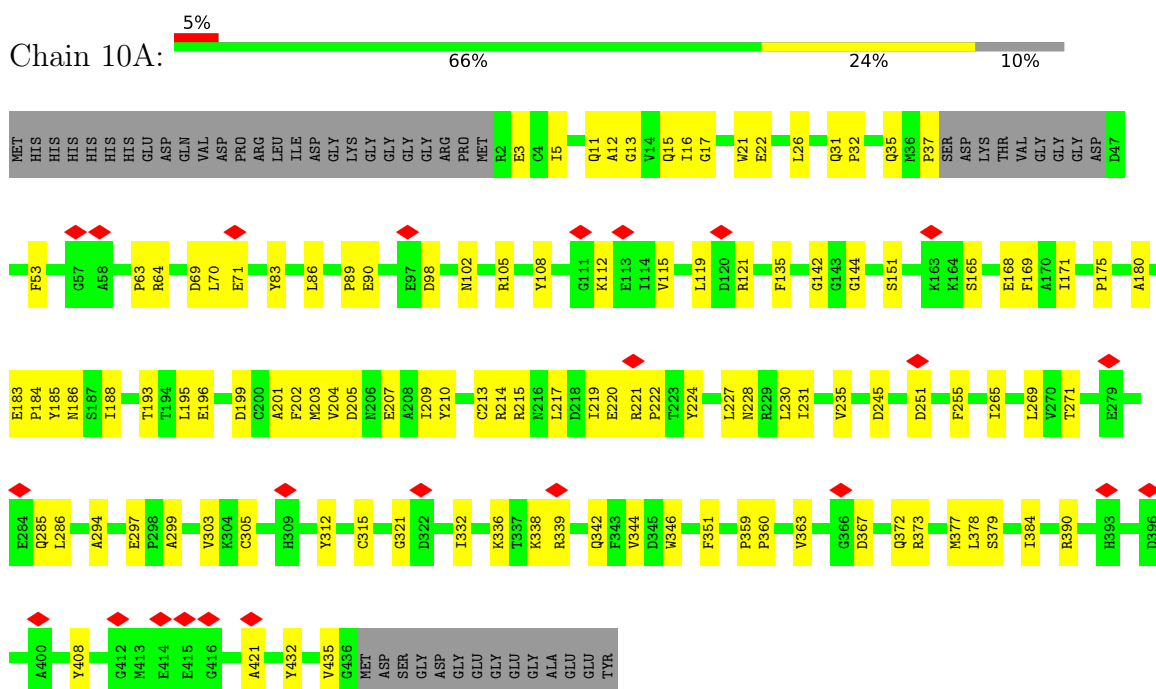
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | 1B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 1D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 5B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 5D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 6B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 6D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 7B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 7D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 8B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 8D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 9B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 9D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

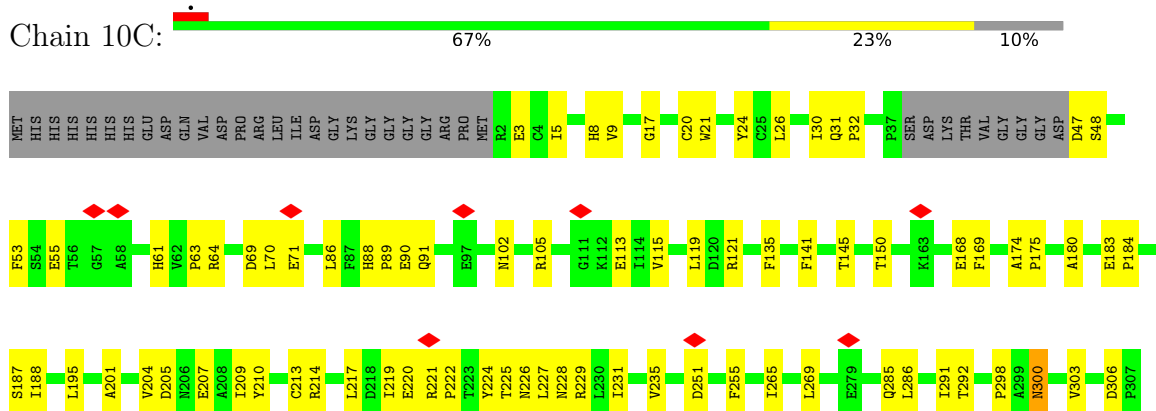
### 3 Residue-property plots [i](#)

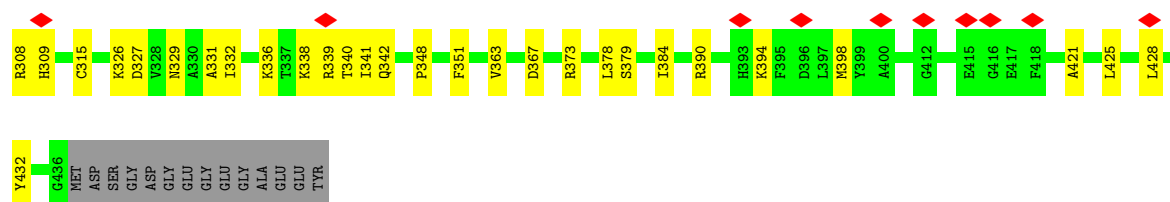
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Tubulin alpha-1 chain

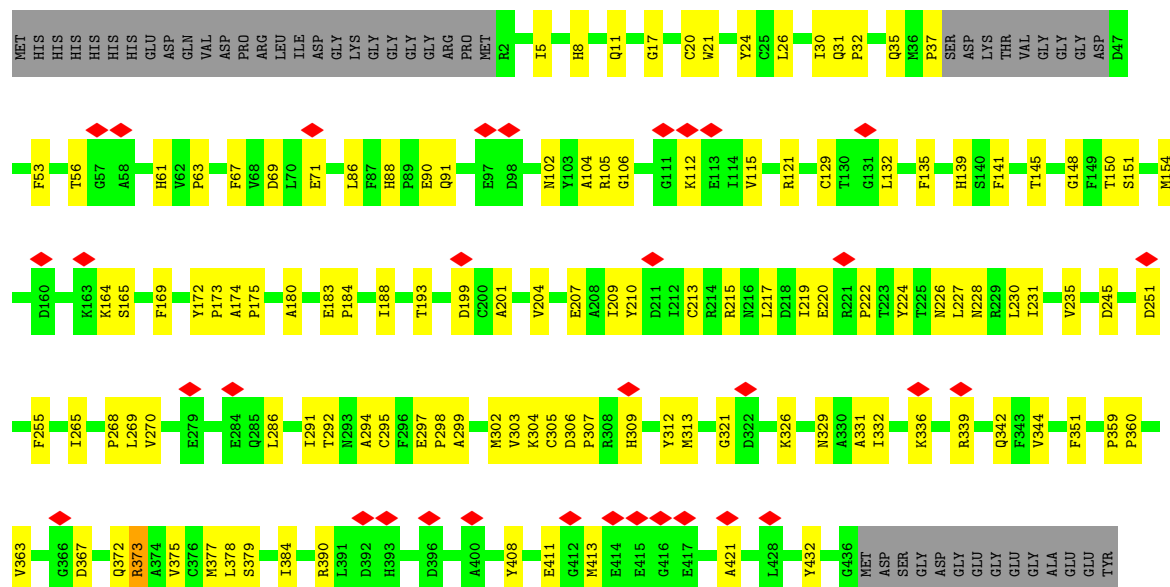


#### • Molecule 1: Tubulin alpha-1 chain

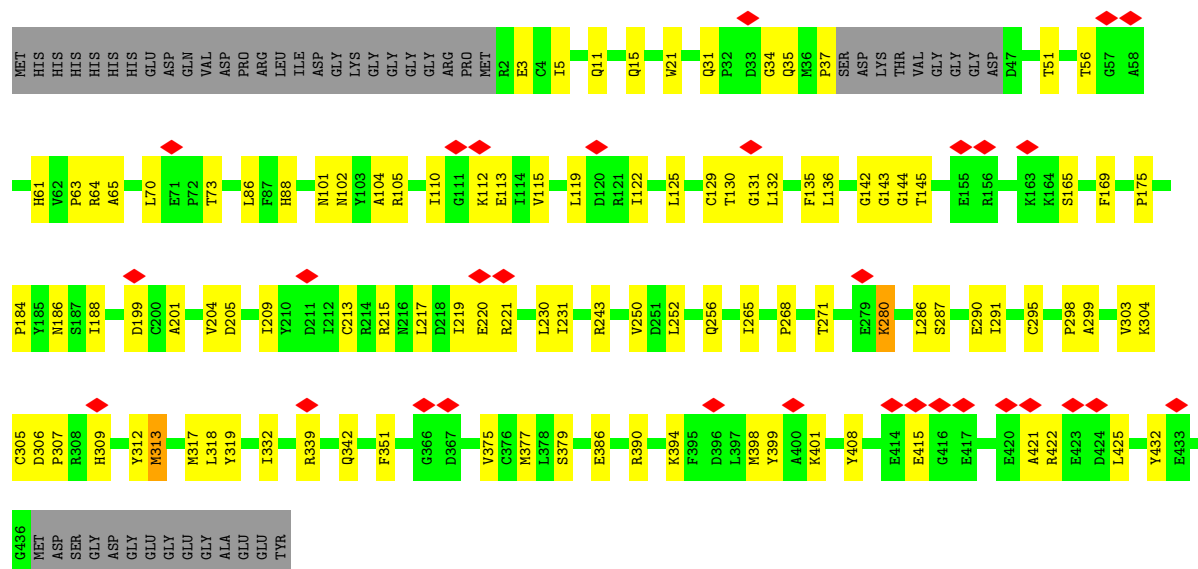




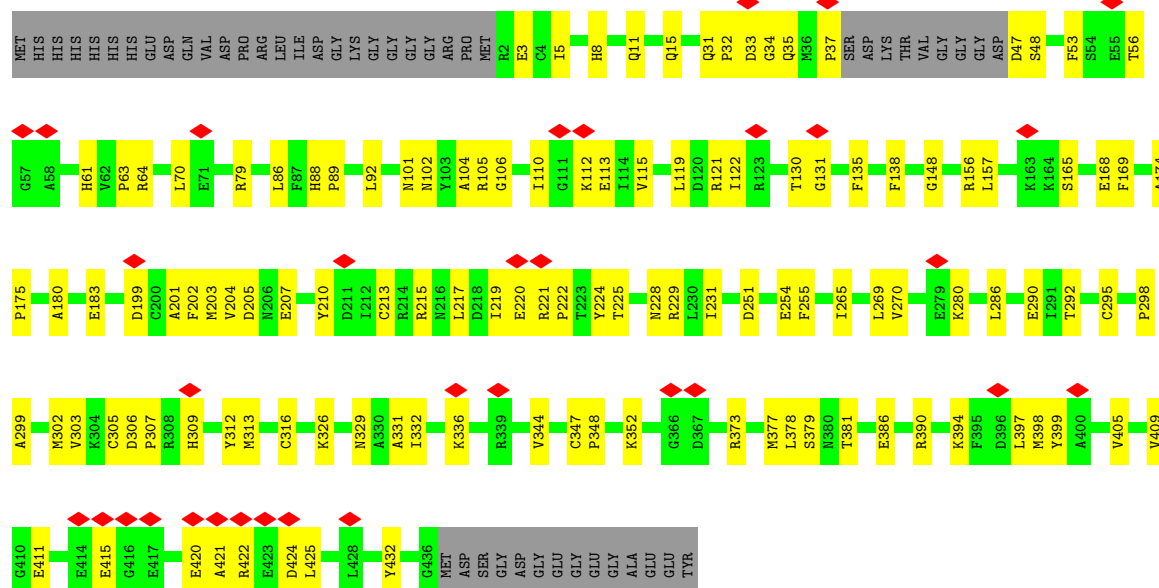
- Molecule 1: Tubulin alpha-1 chain



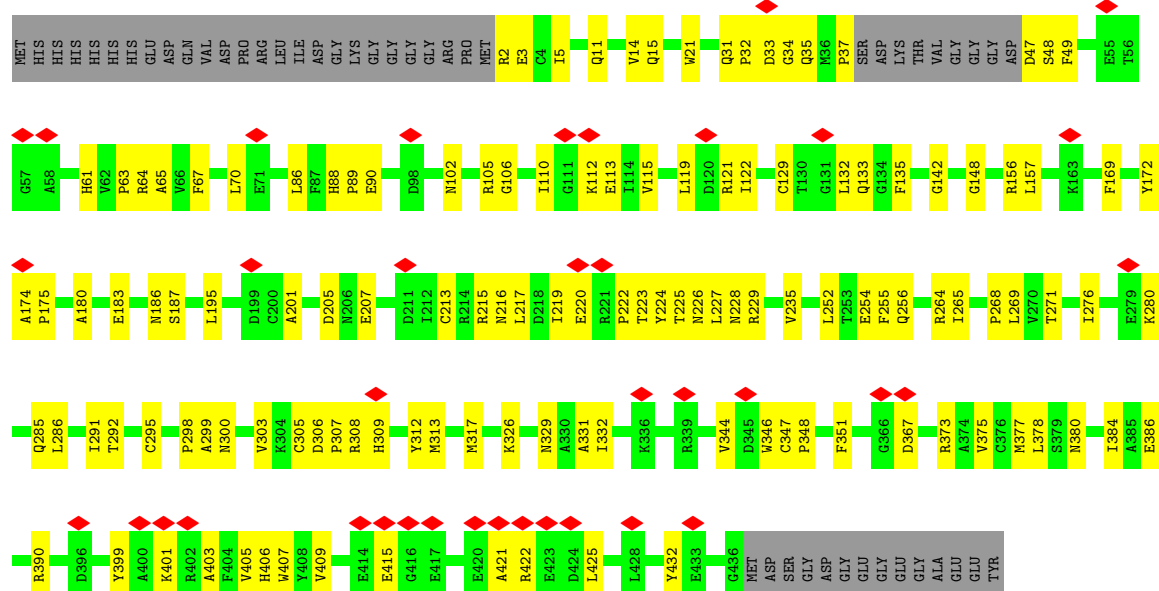
- Molecule 1: Tubulin alpha-1 chain



- Molecule 1: Tubulin alpha-1 chain

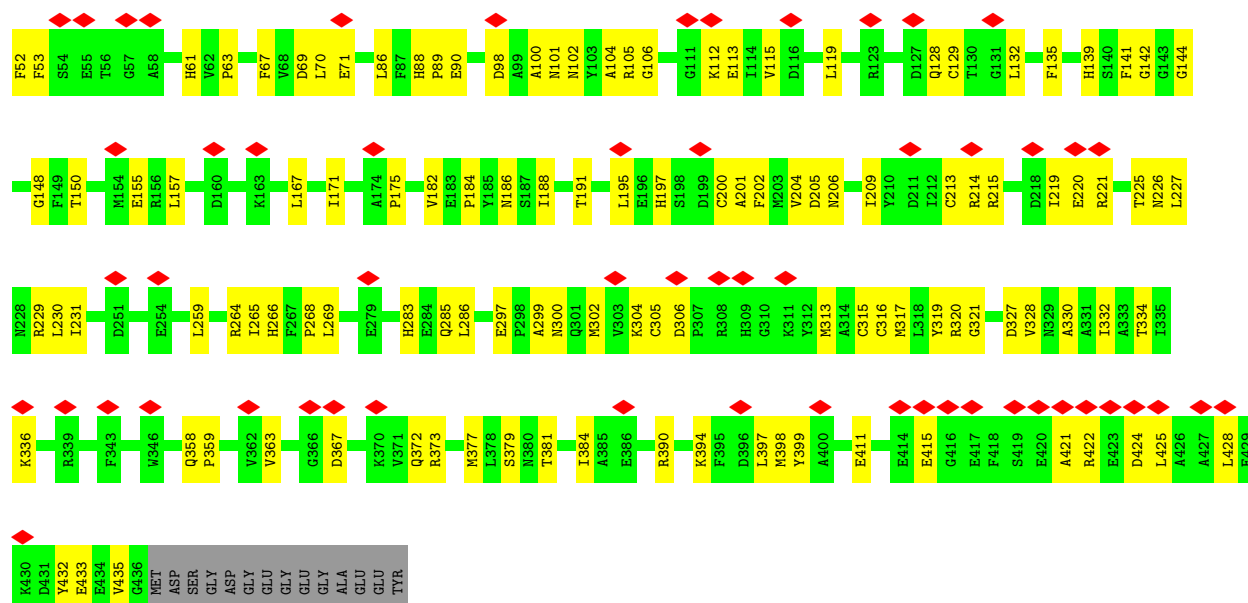


• Molecule 1: Tubulin alpha-1 chain

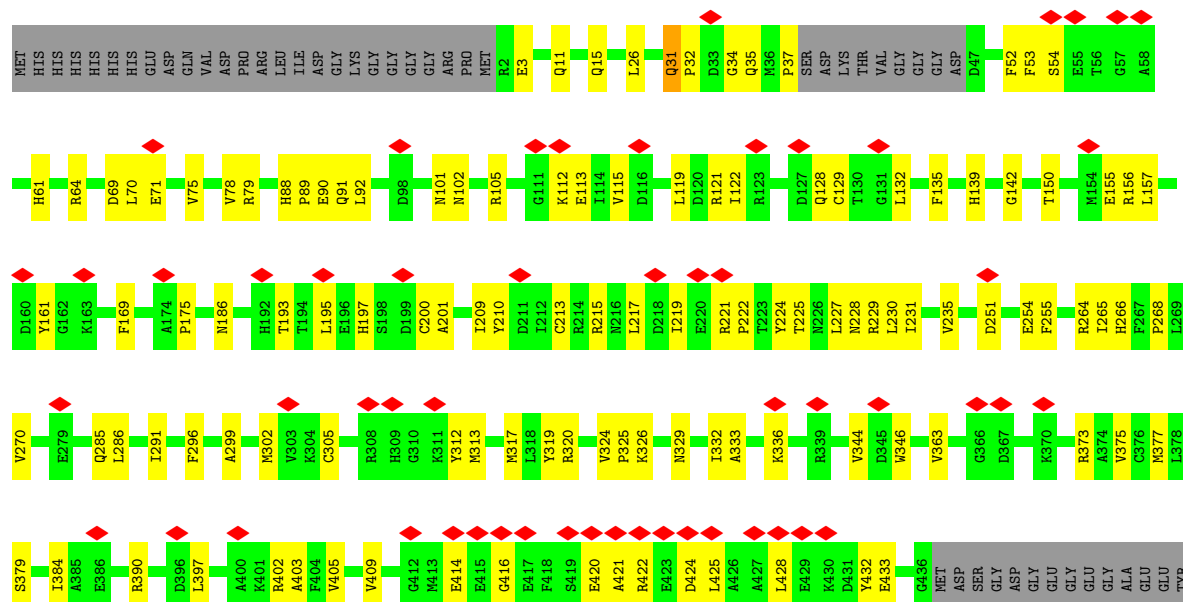


• Molecule 1: Tubulin alpha-1 chain

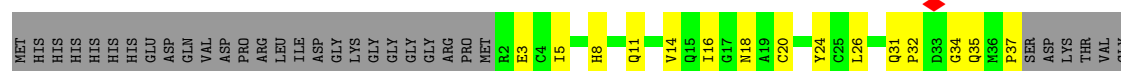


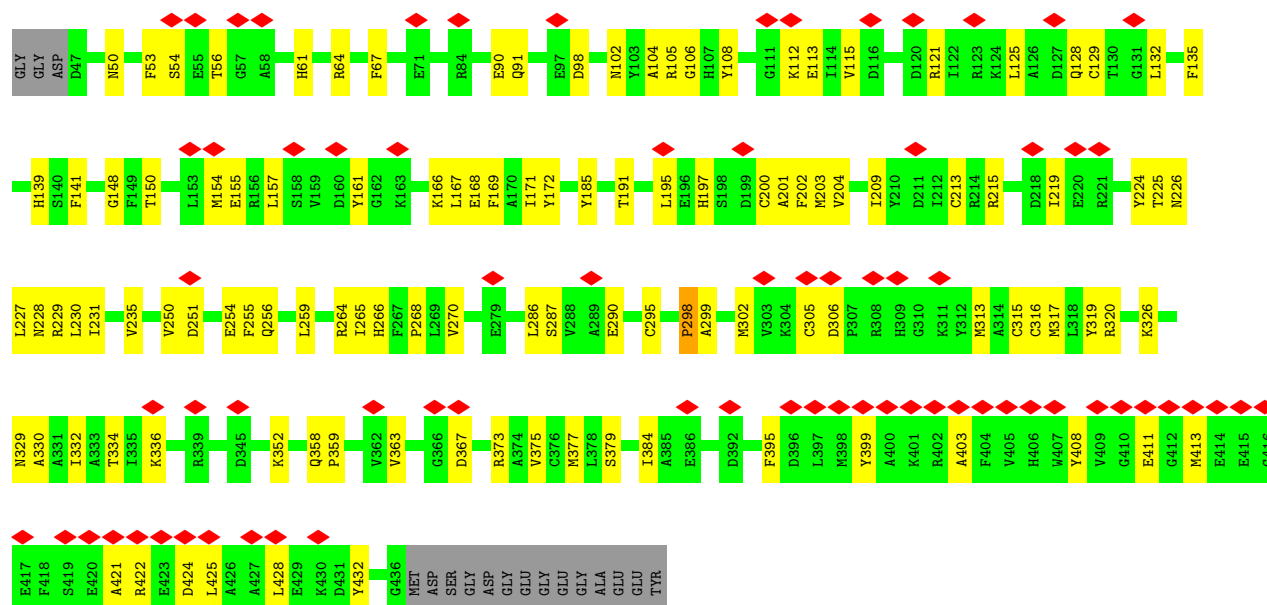


- Molecule 1: Tubulin alpha-1 chain

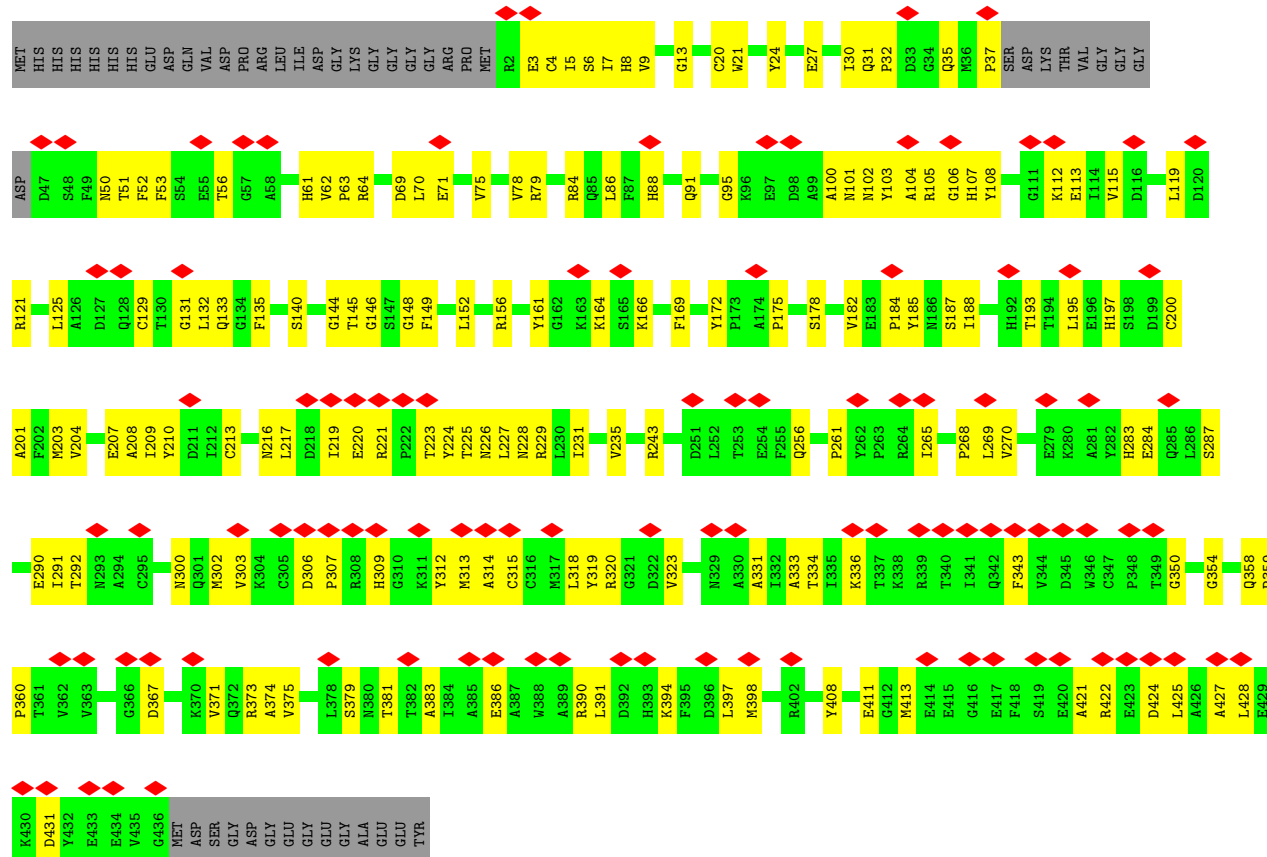


- Molecule 1: Tubulin alpha-1 chain

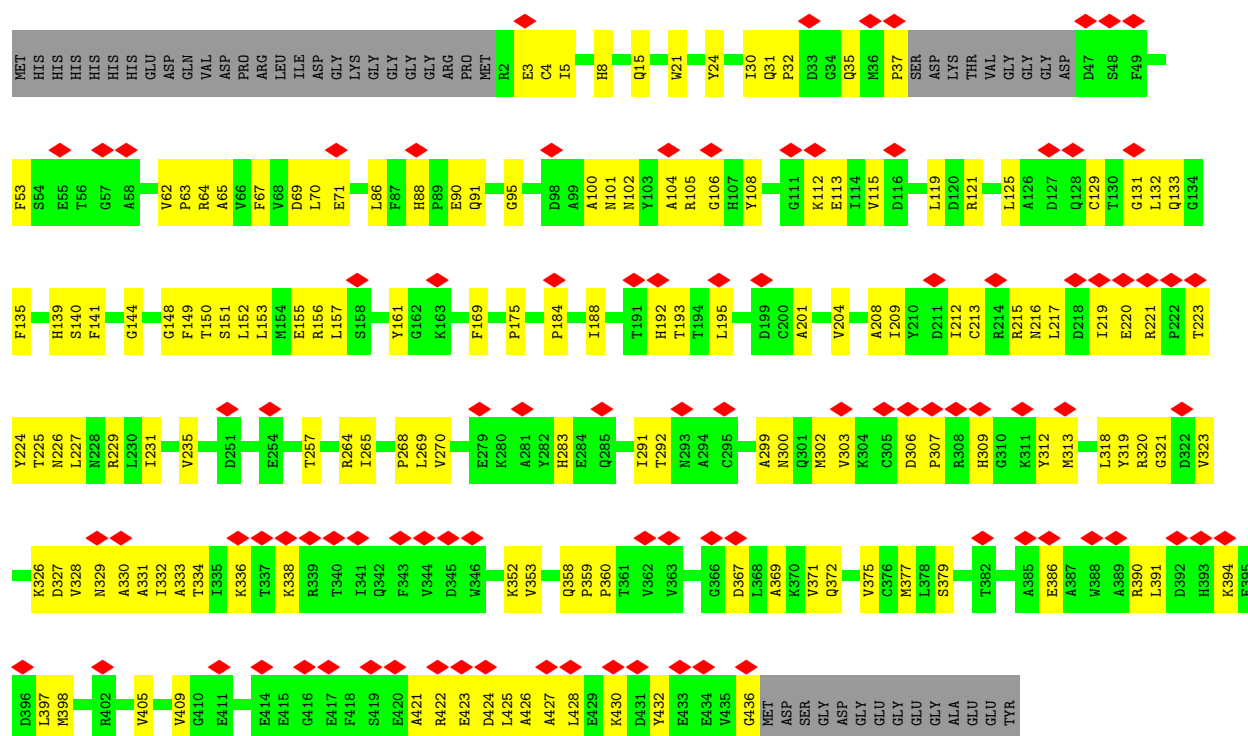




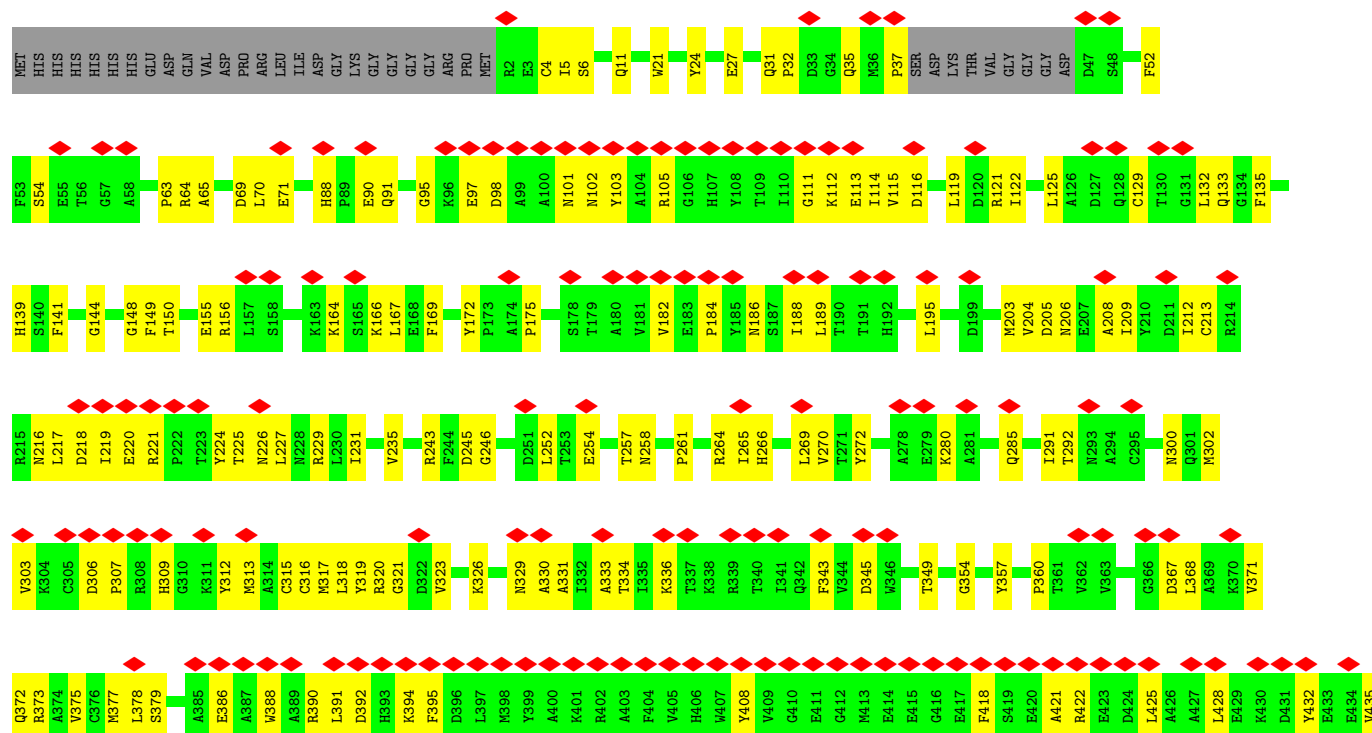
• Molecule 1: Tubulin alpha-1 chain

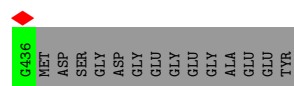


• Molecule 1: Tubulin alpha-1 chain

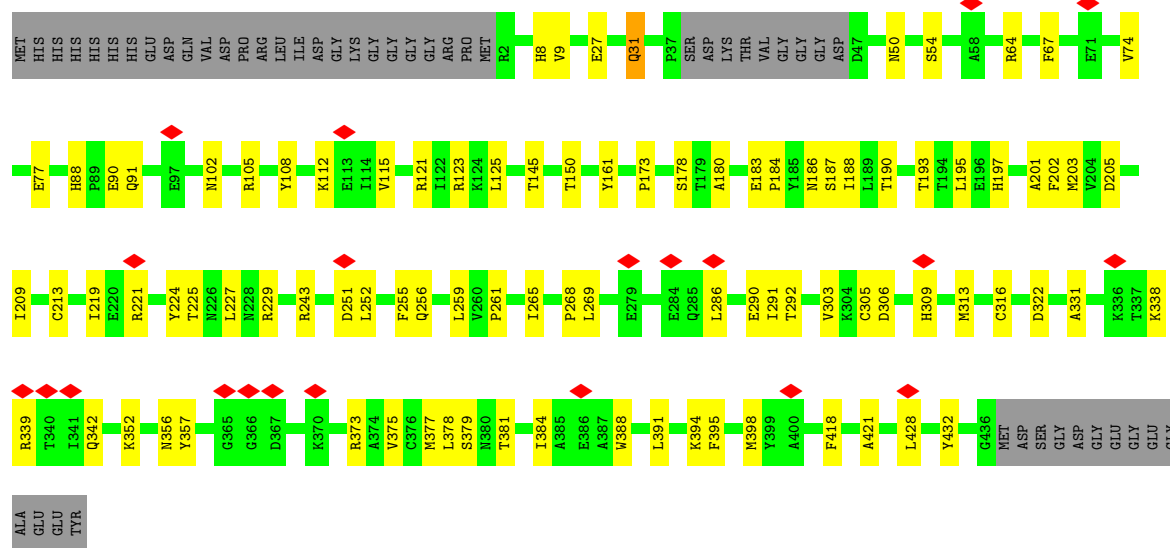


• Molecule 1: Tubulin alpha-1 chain

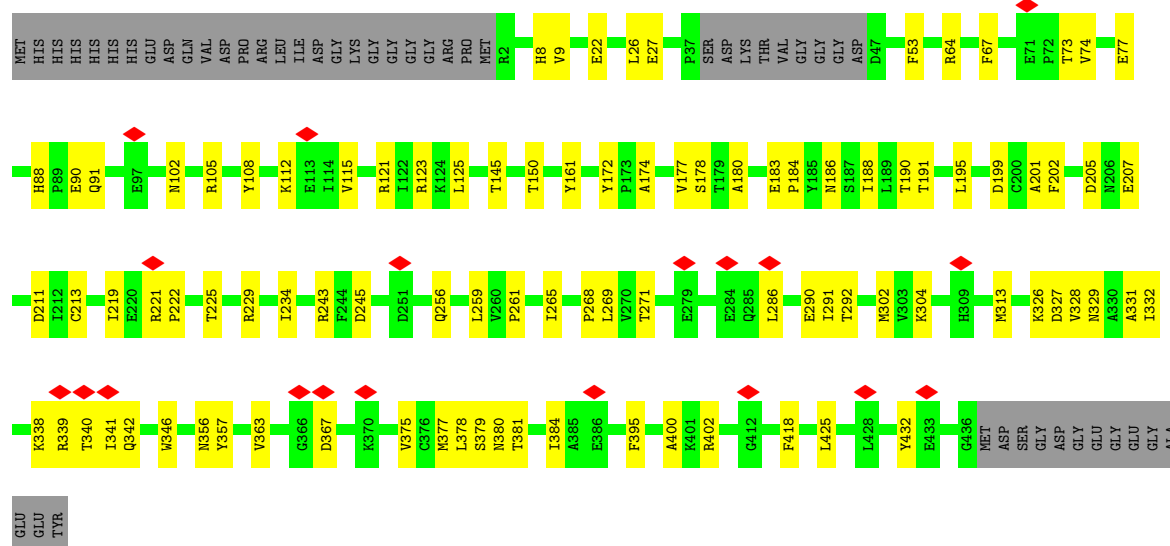




- Molecule 1: Tubulin alpha-1 chain

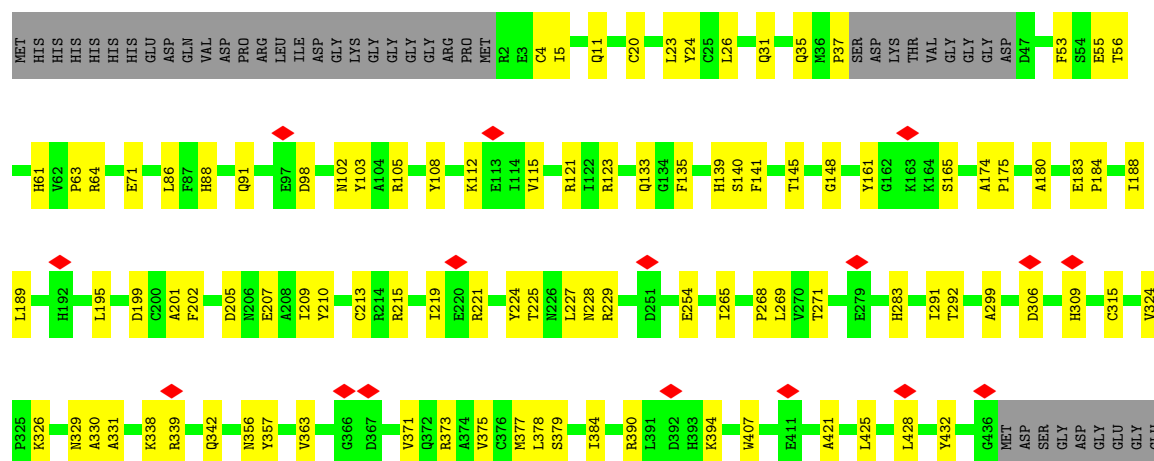


- Molecule 1: Tubulin alpha-1 chain

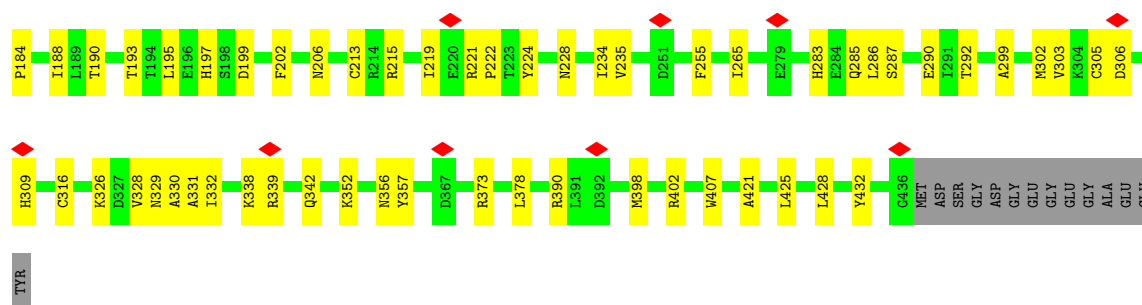


- Molecule 1: Tubulin alpha-1 chain



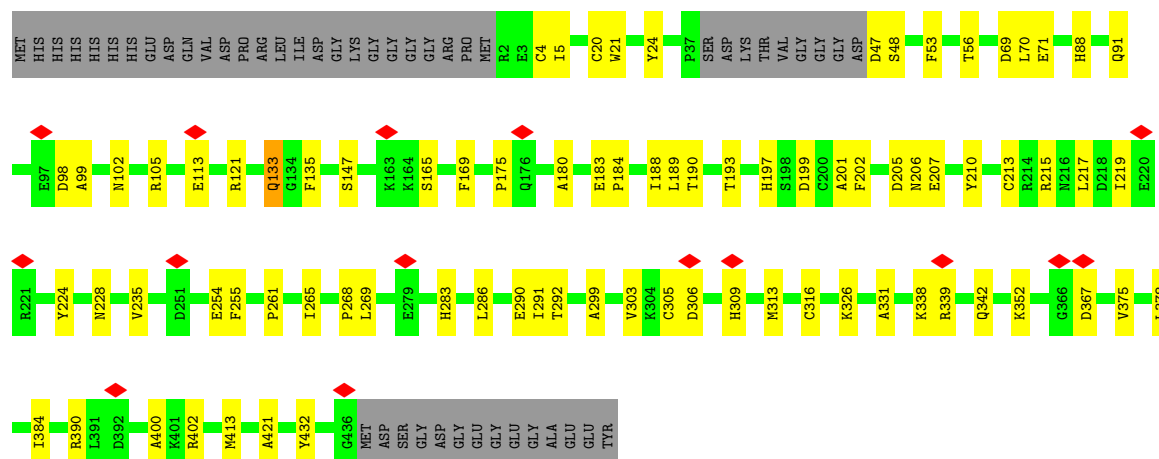






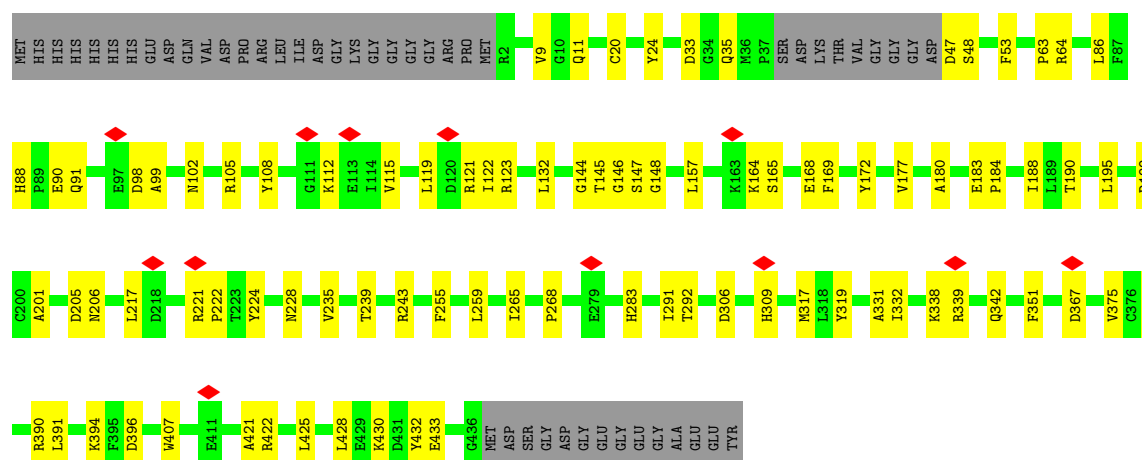
- Molecule 1: Tubulin alpha-1 chain

Chain 3E: 72% 17% 10%



- Molecule 1: Tubulin alpha-1 chain

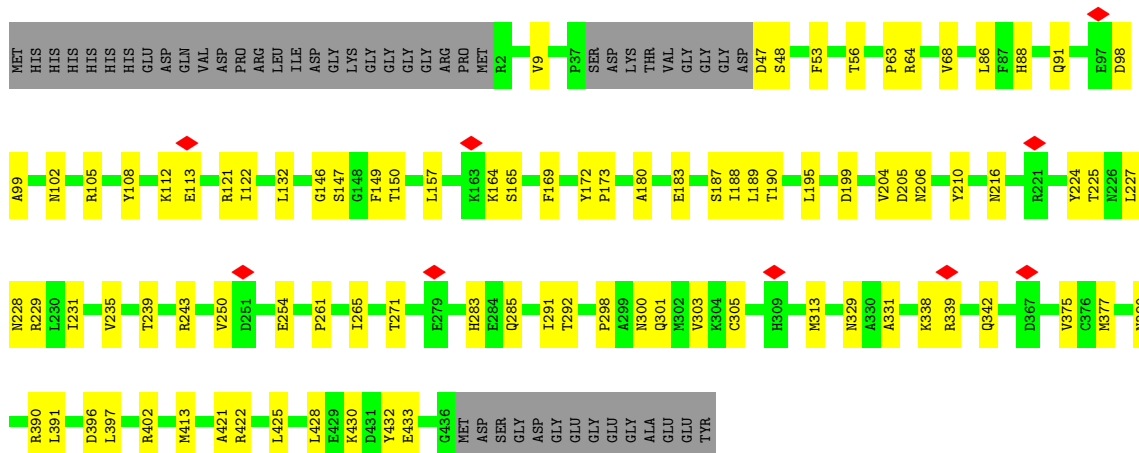
Chain 4A: 71% 19% 10%



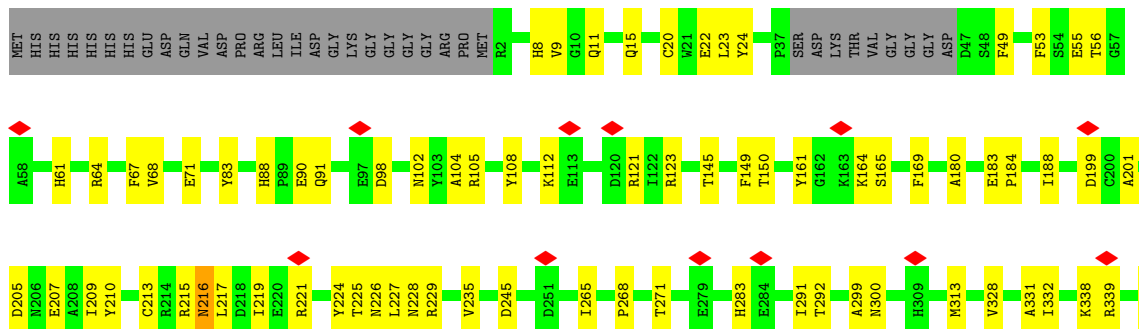
- Molecule 1: Tubulin alpha-1 chain

Chain 4C: 68% 22% 10%

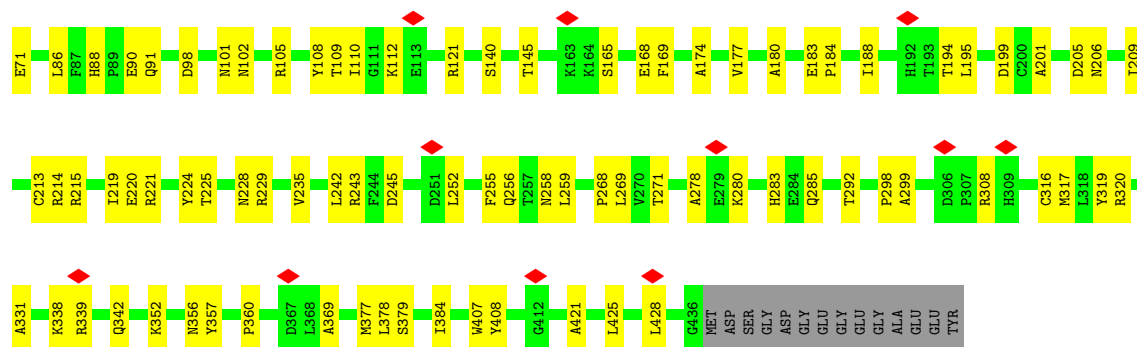
- Molecule 1: Tubulin alpha-1 chain



- Molecule 1: Tubulin alpha-1 chain

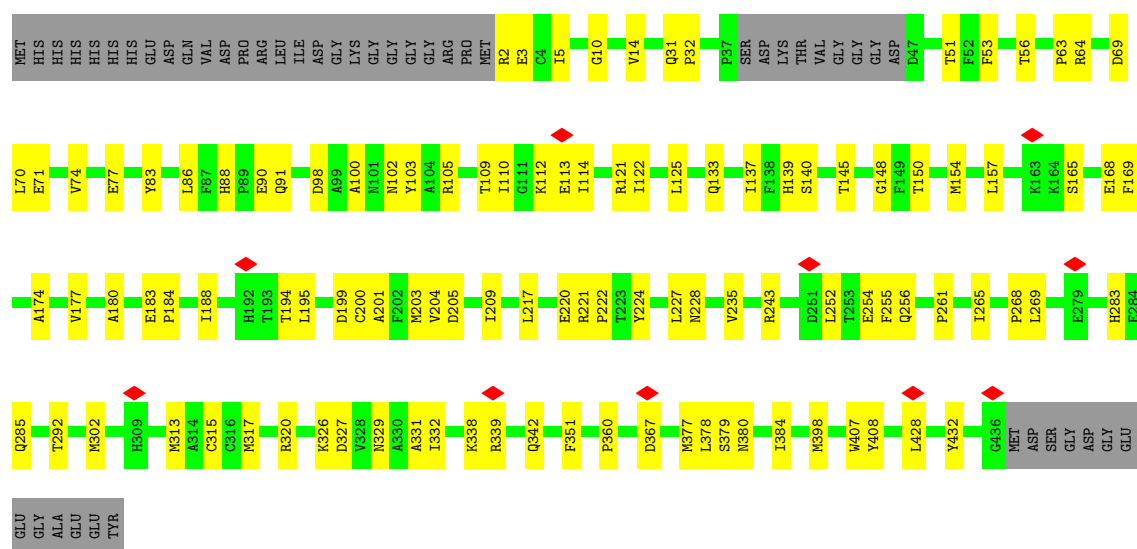






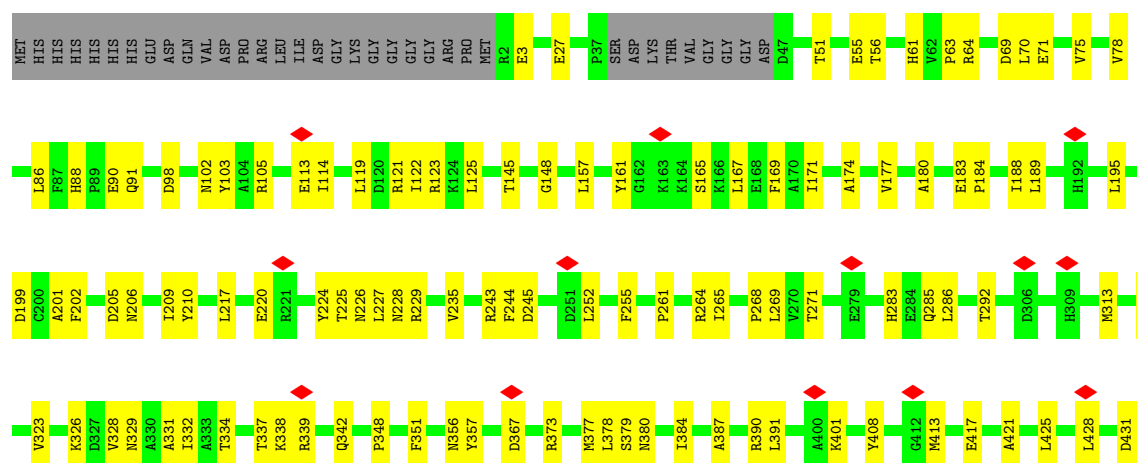
• Molecule 1: Tubulin alpha-1 chain

Chain 6C: 67% 23% 10%

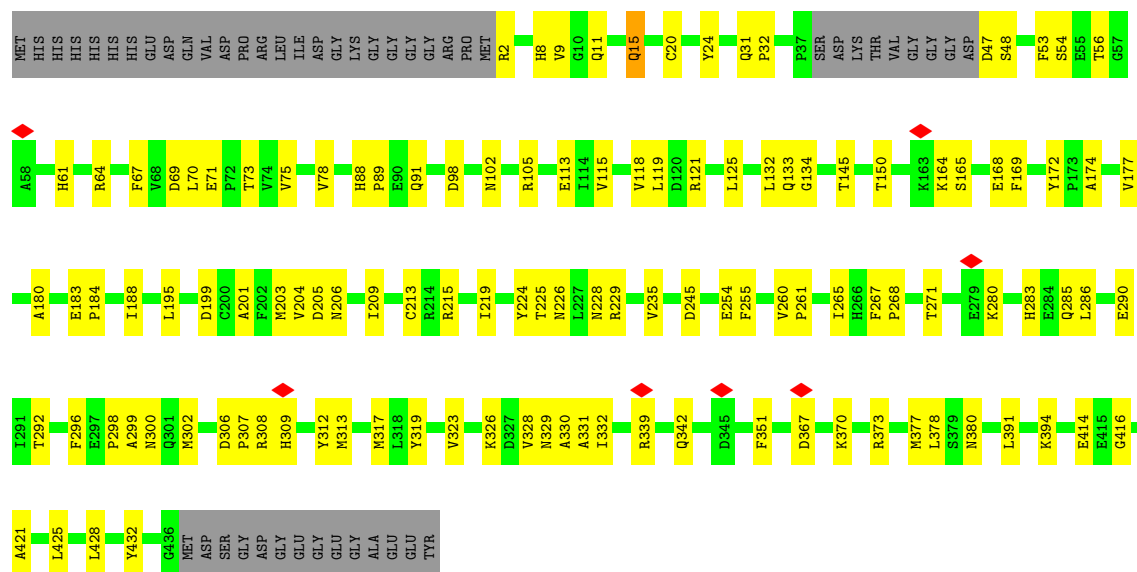


• Molecule 1: Tubulin alpha-1 chain

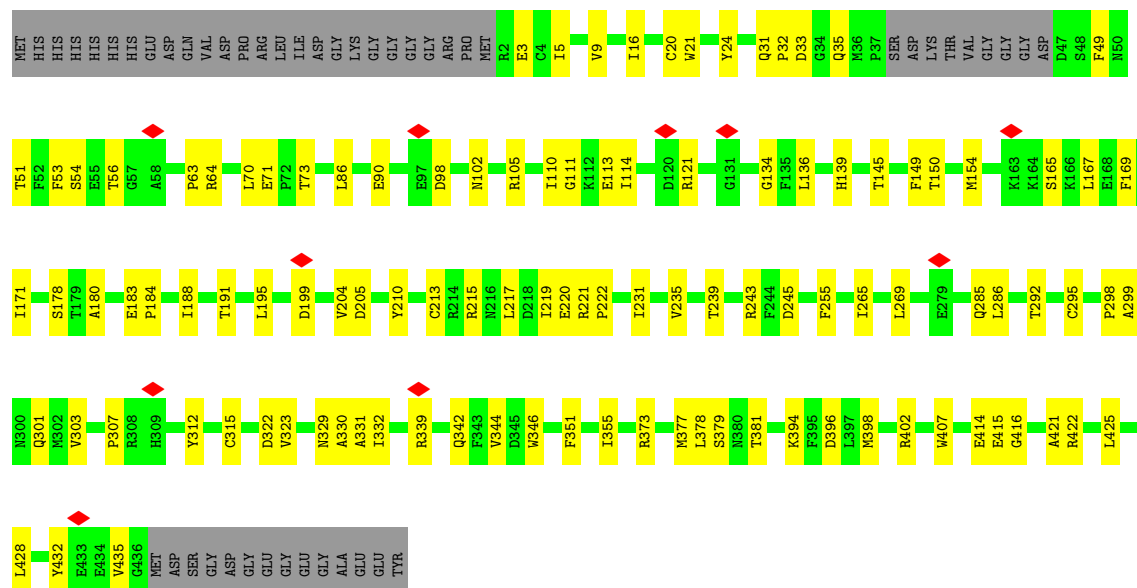
Chain 6E: 66% 23% 10%



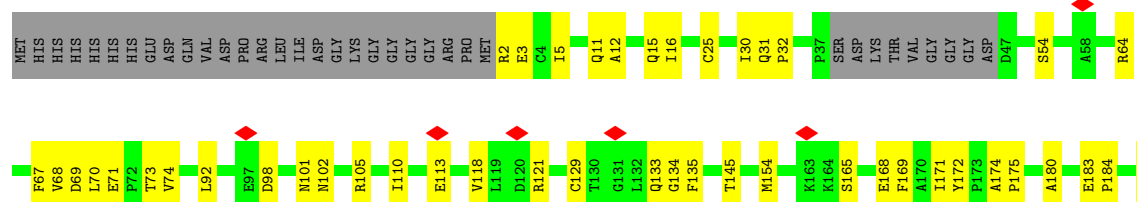




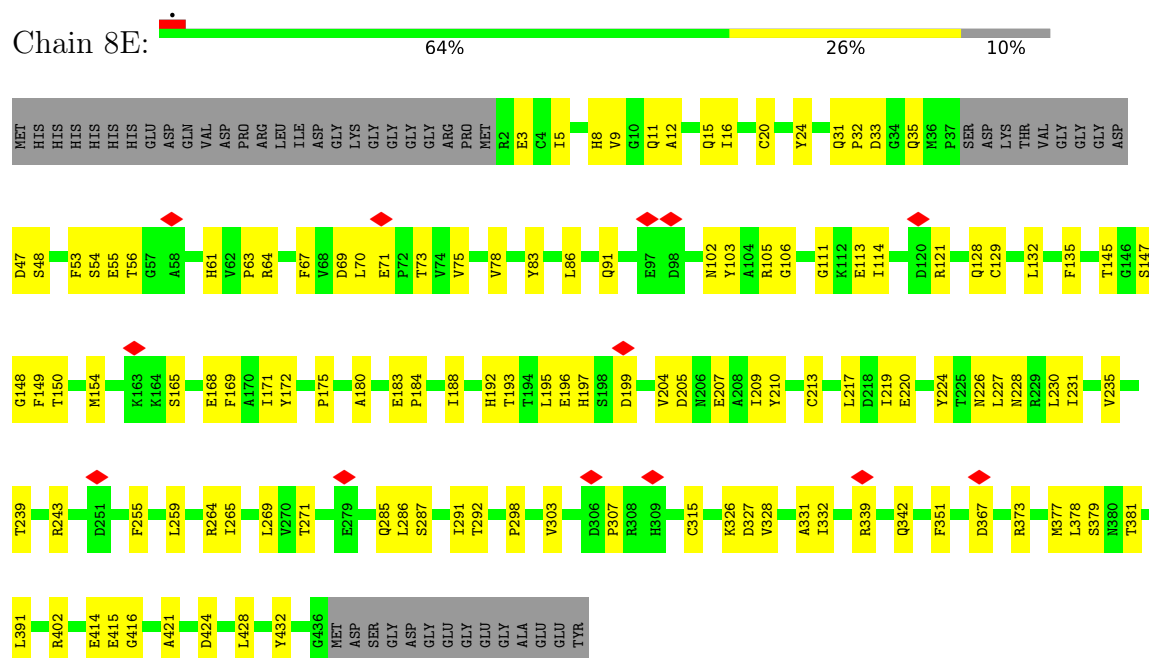
• Molecule 1: Tubulin alpha-1 chain



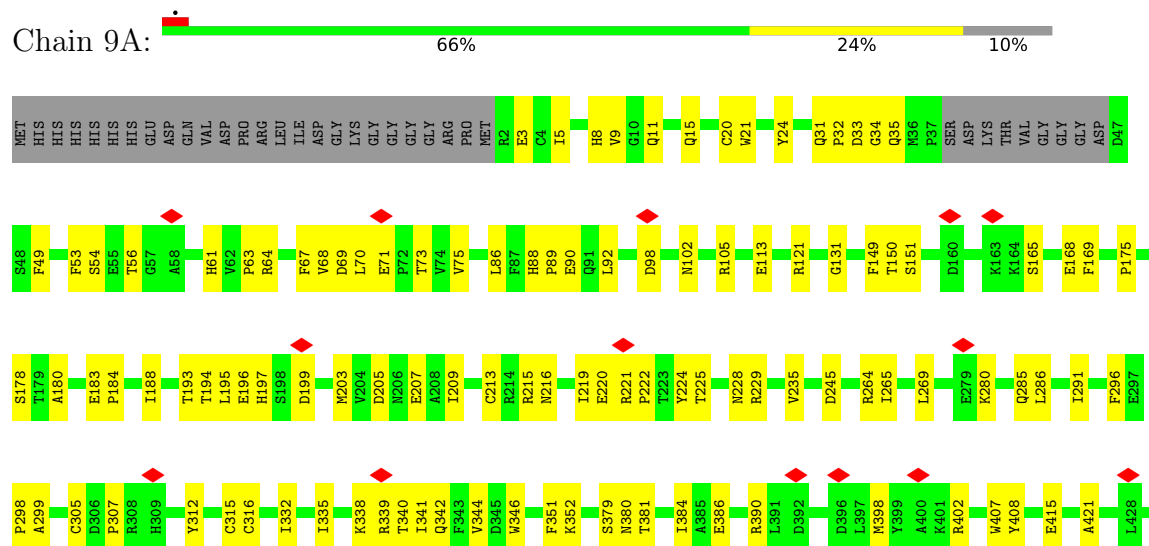
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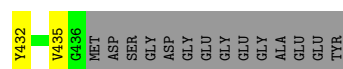


- Molecule 1: Tubulin alpha-1 chain

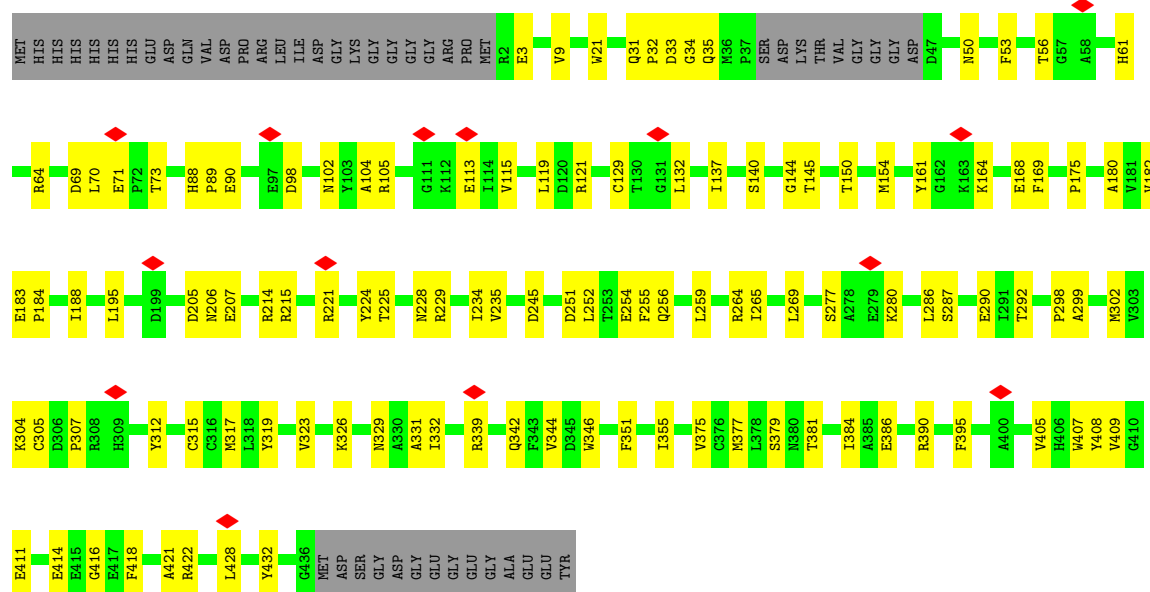


- Molecule 1: Tubulin alpha-1 chain

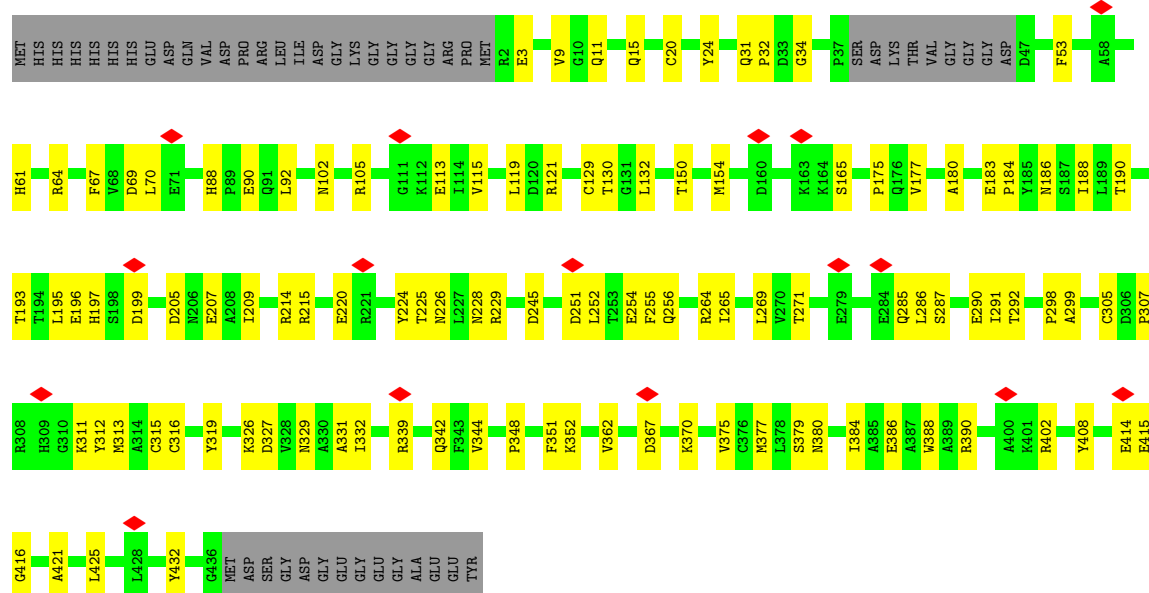




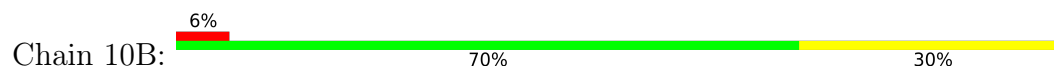
- Molecule 1: Tubulin alpha-1 chain

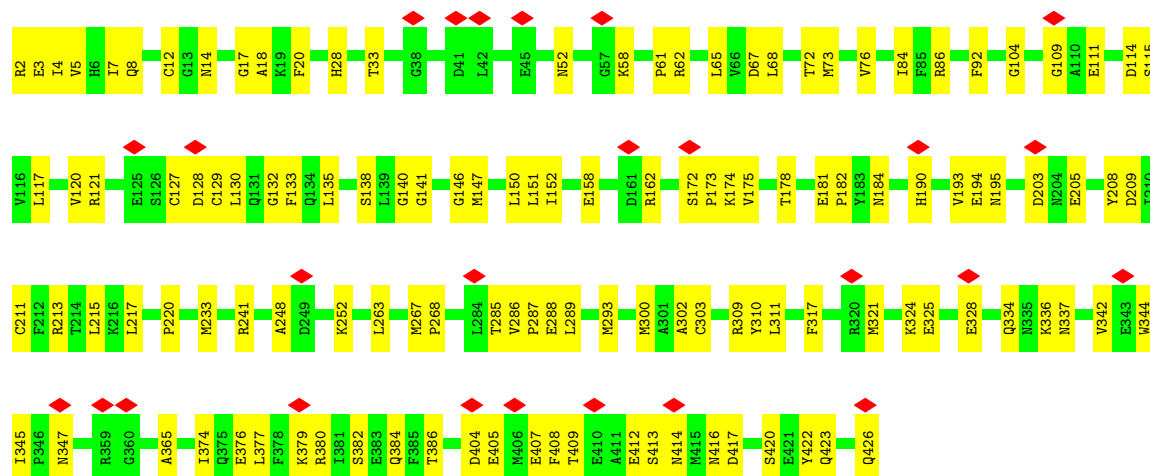


- Molecule 1: Tubulin alpha-1 chain

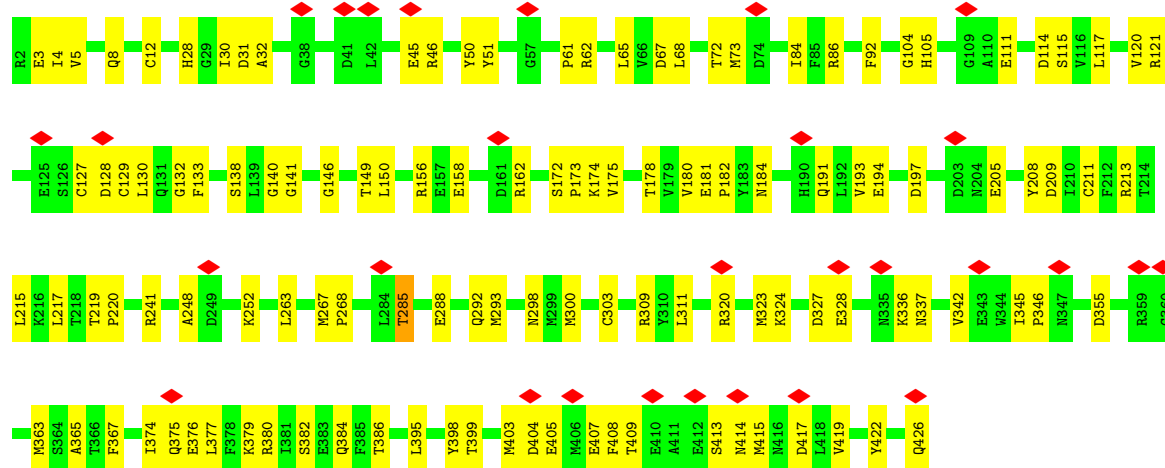
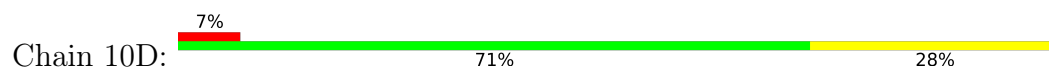


- Molecule 2: Tubulin beta-1 chain

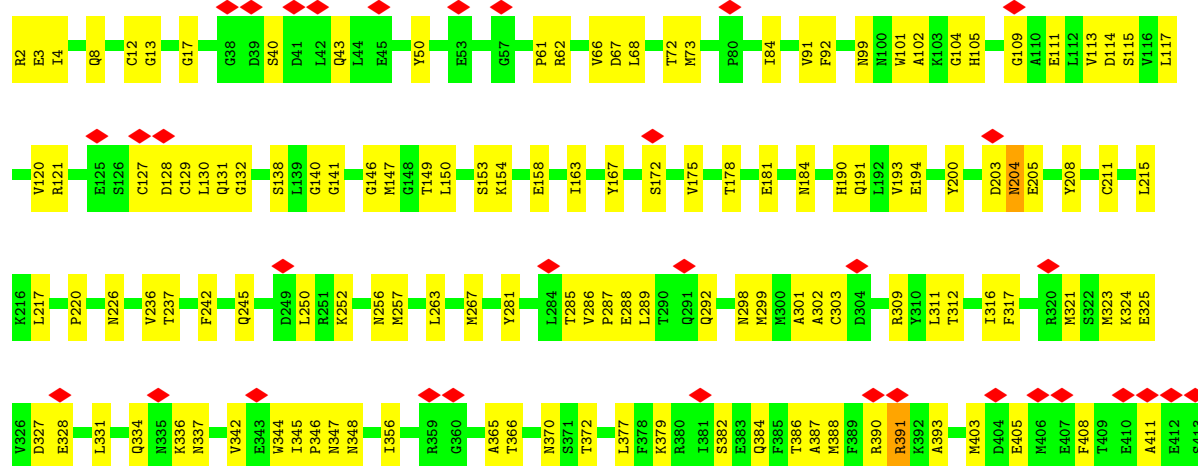


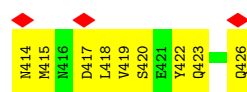


• Molecule 2: Tubulin beta-1 chain

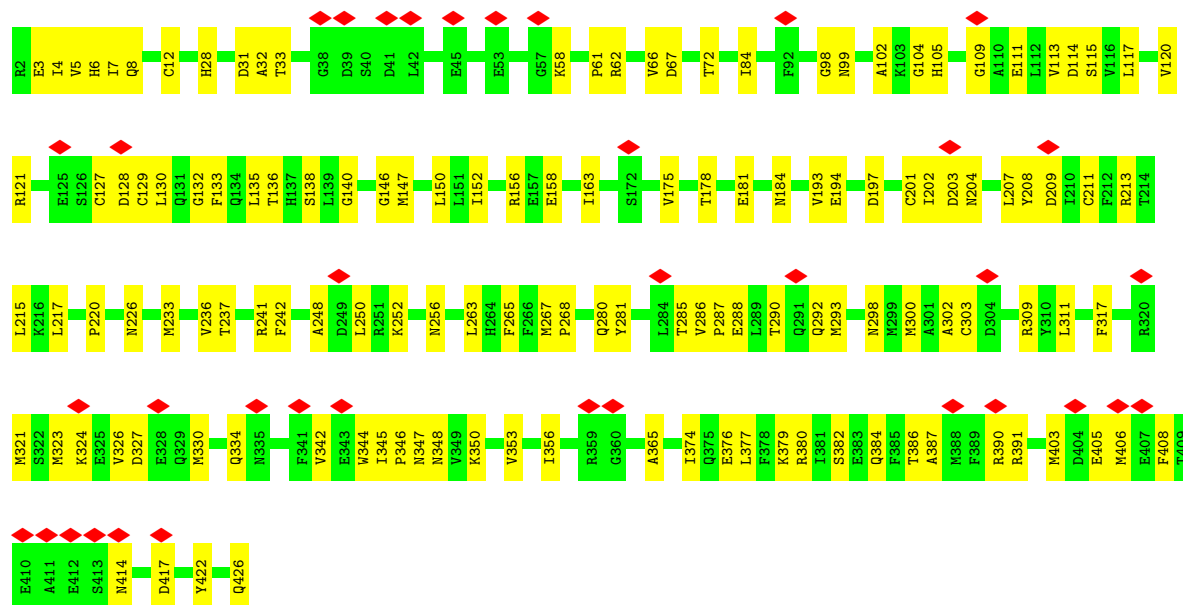
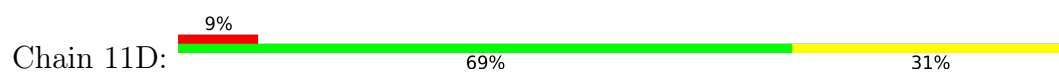


• Molecule 2: Tubulin beta-1 chain

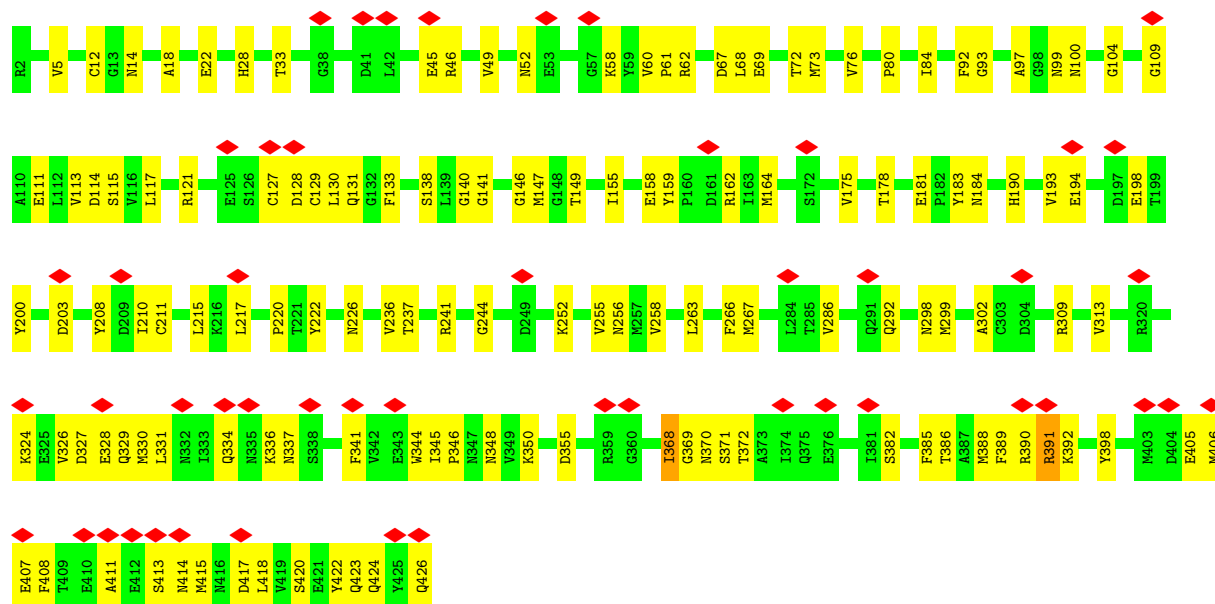




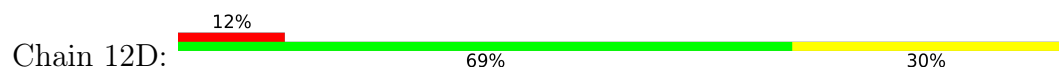
- Molecule 2: Tubulin beta-1 chain

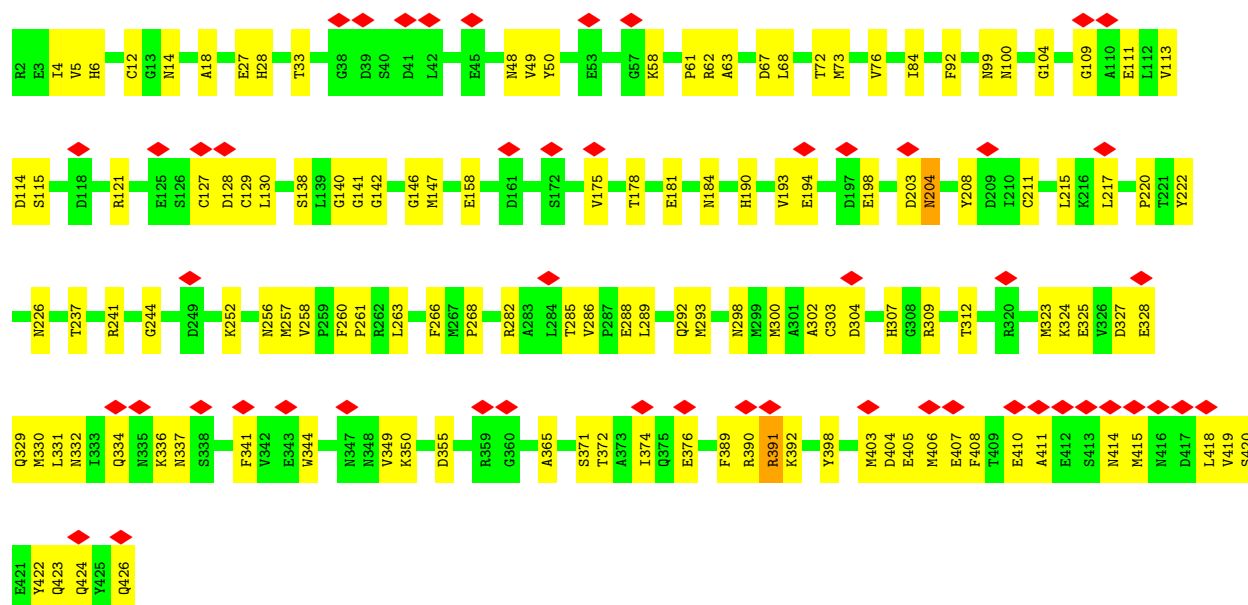


- Molecule 2: Tubulin beta-1 chain

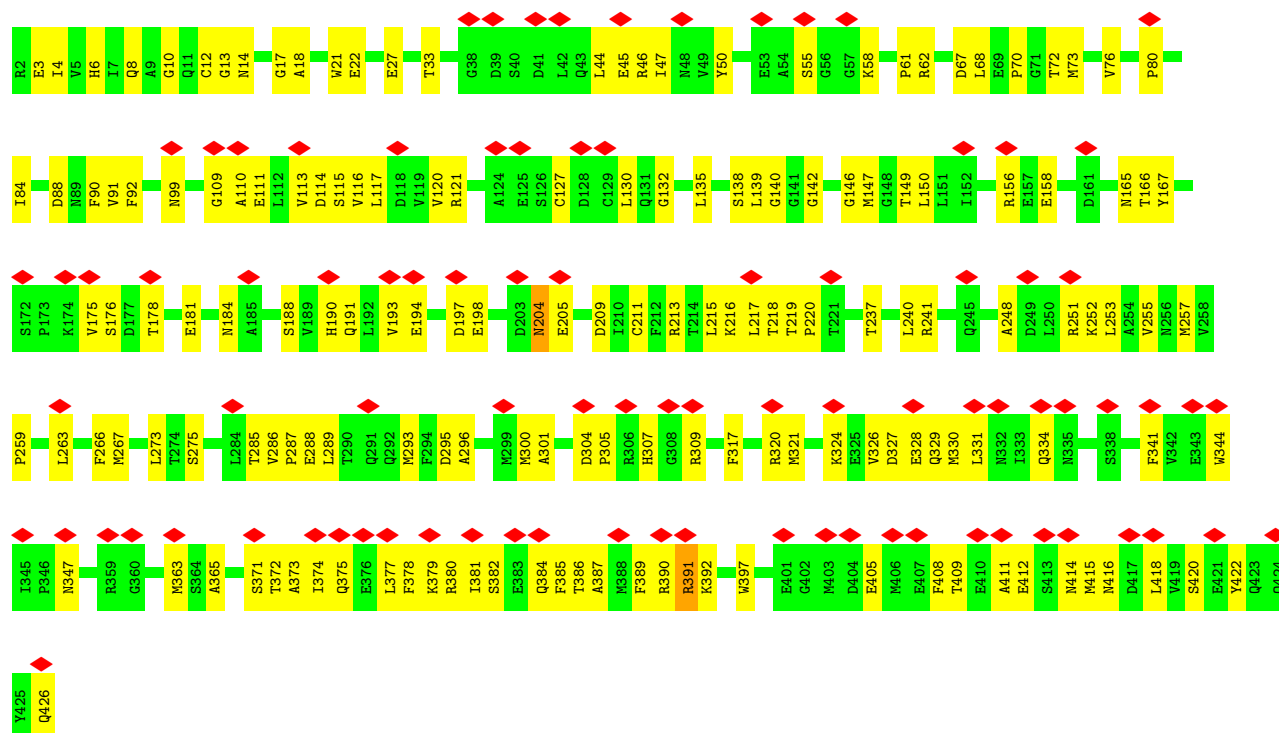


- Molecule 2: Tubulin beta-1 chain

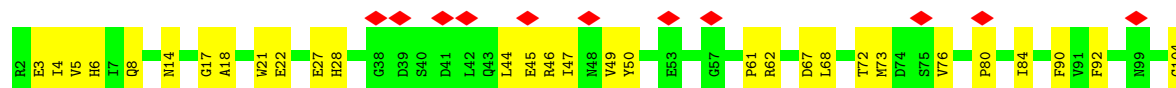


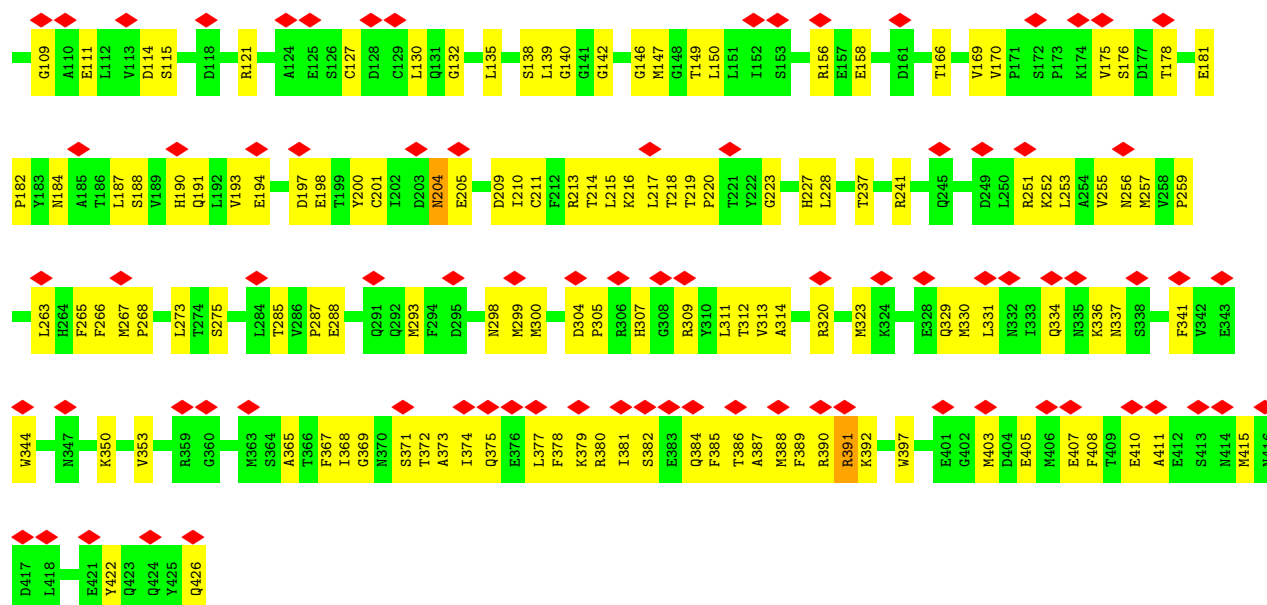


• Molecule 2: Tubulin beta-1 chain

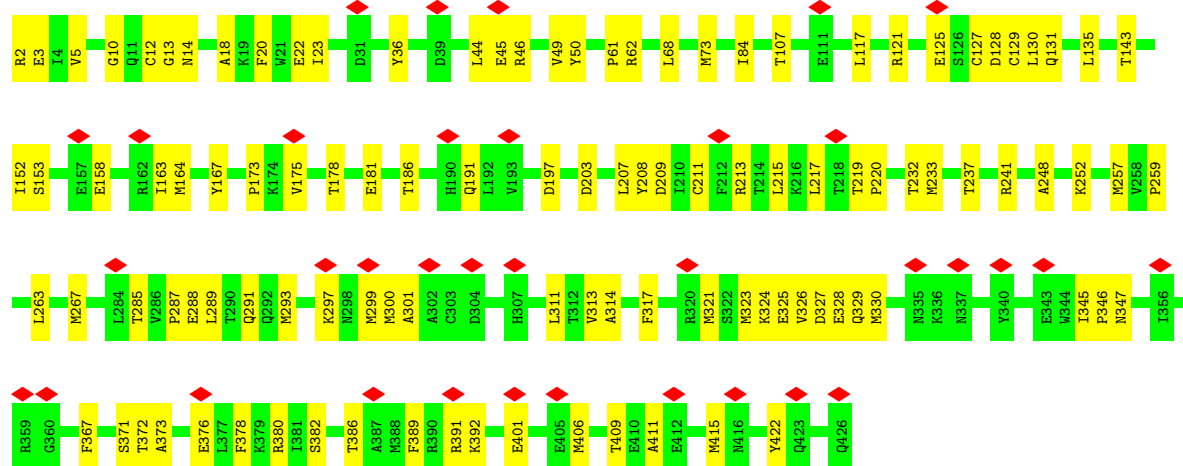
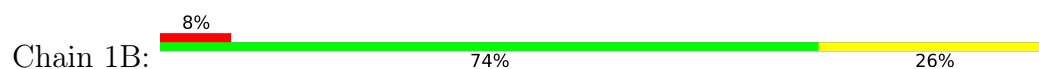


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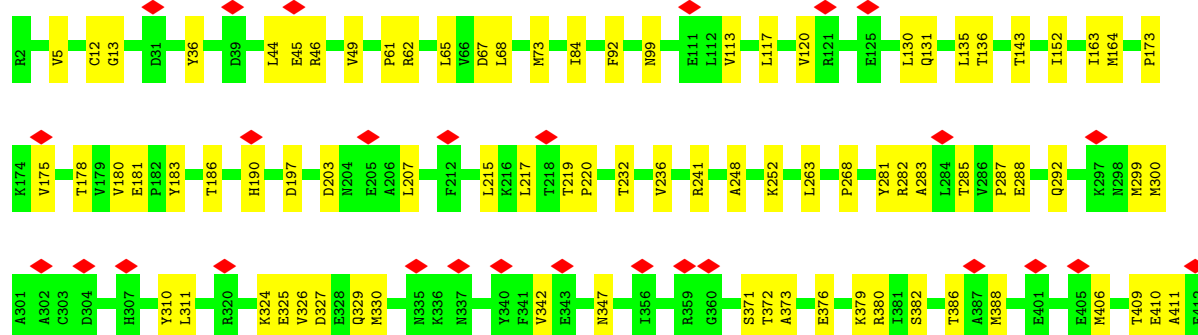
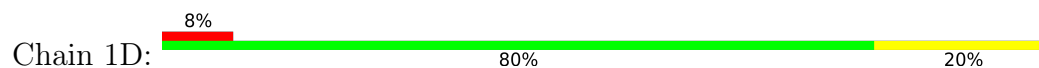


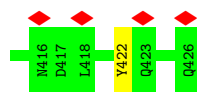


• Molecule 2: Tubulin beta-1 chain

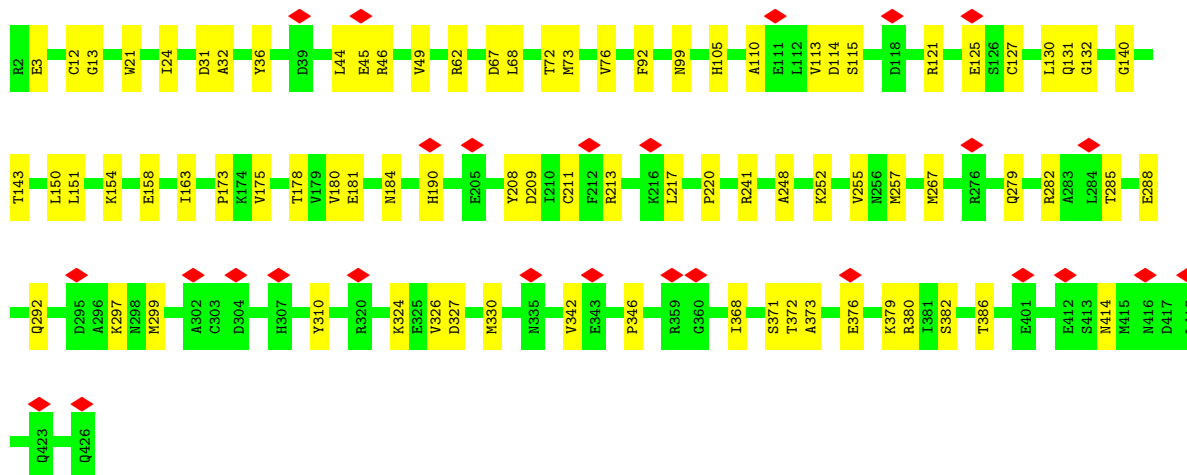
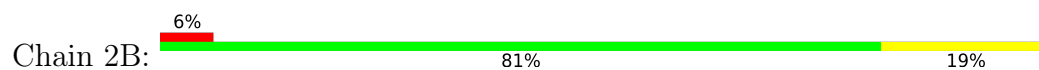


• Molecule 2: Tubulin beta-1 chain

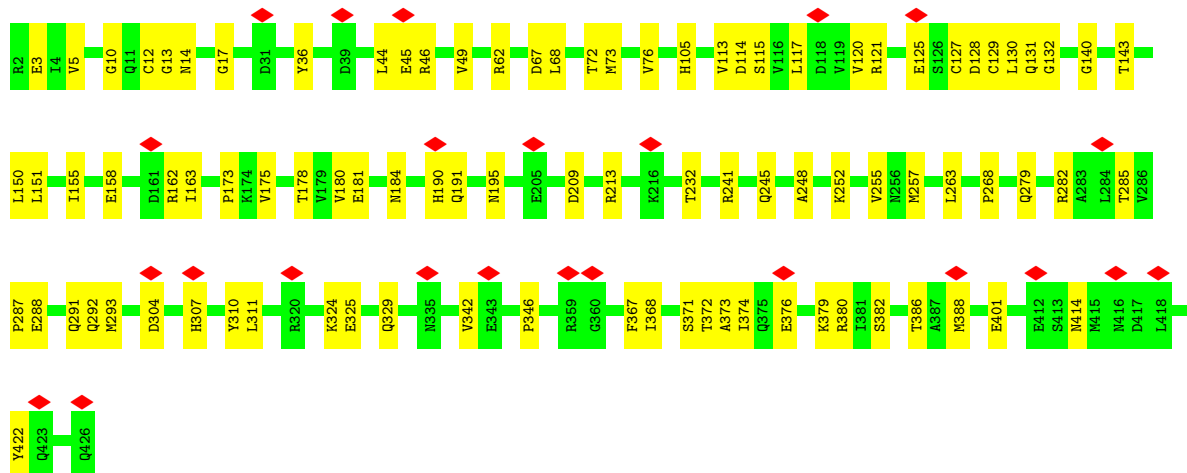
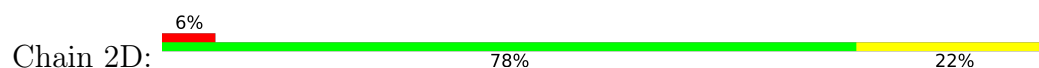




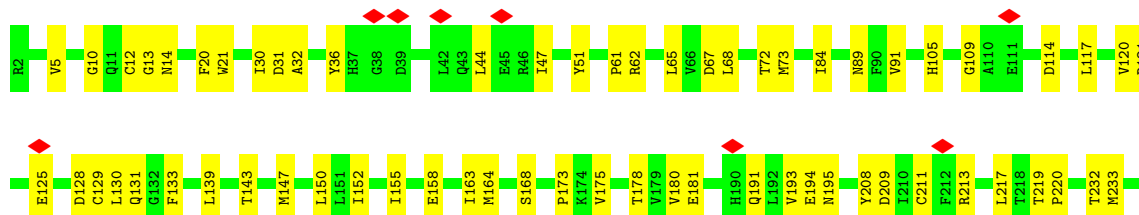
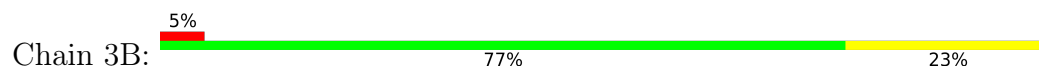
- Molecule 2: Tubulin beta-1 chain

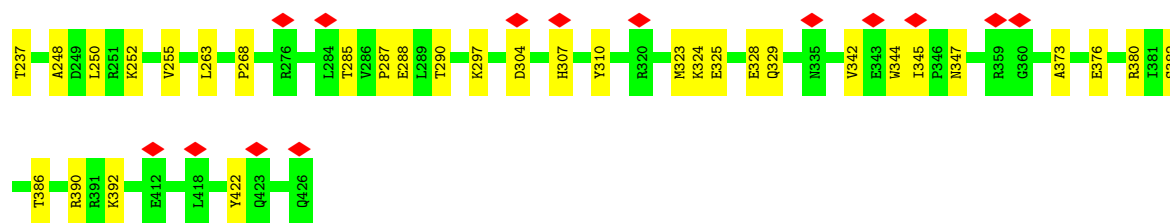


- Molecule 2: Tubulin beta-1 chain

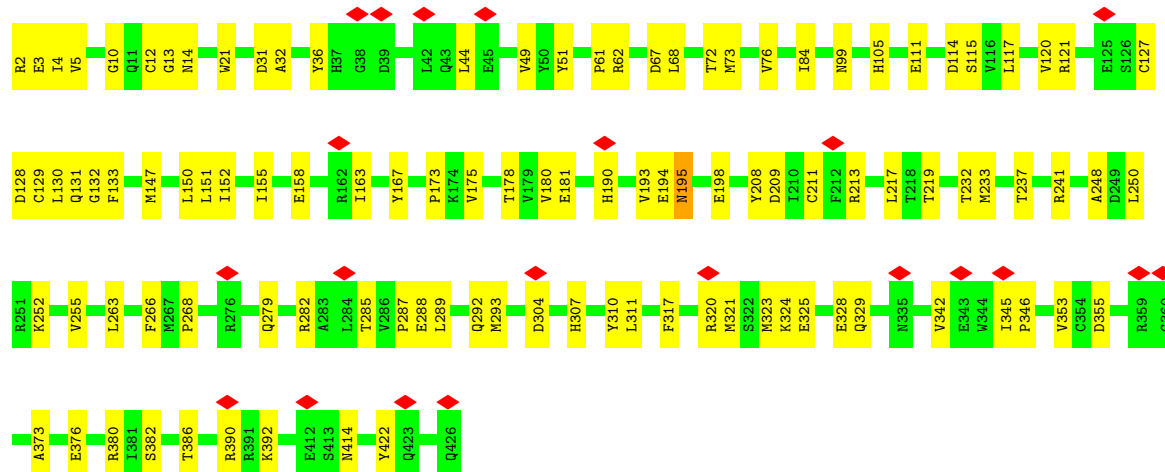
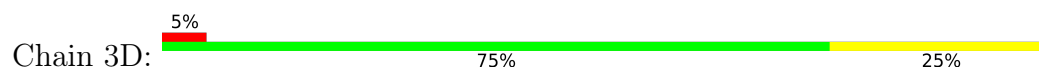


- Molecule 2: Tubulin beta-1 chain

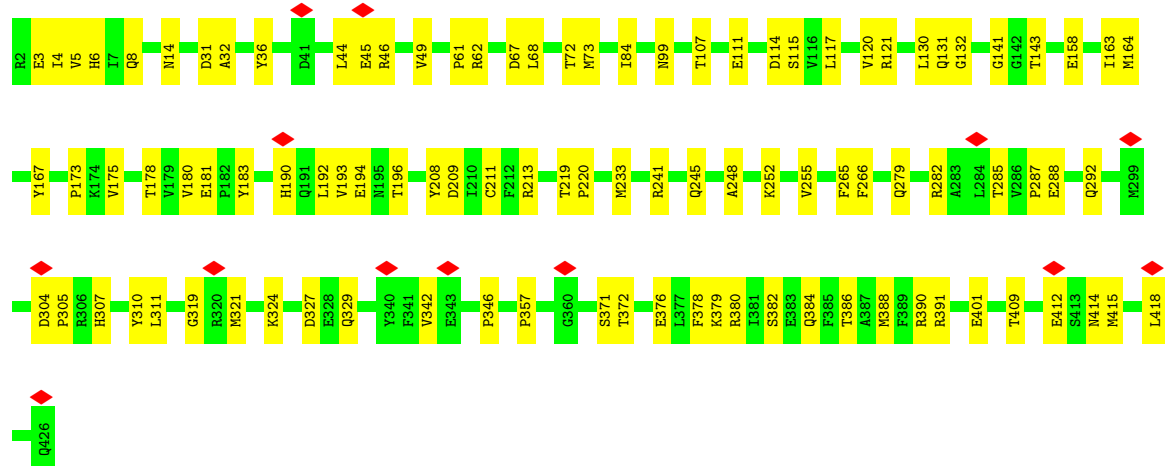
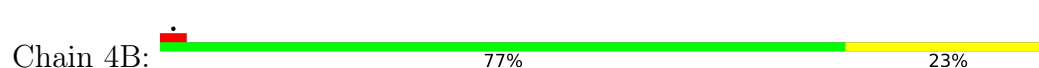




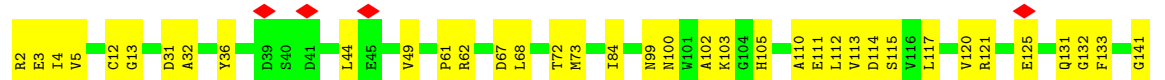
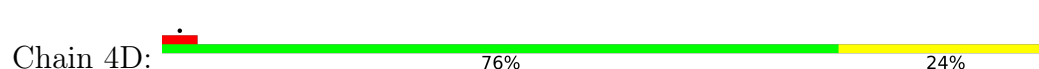
• Molecule 2: Tubulin beta-1 chain

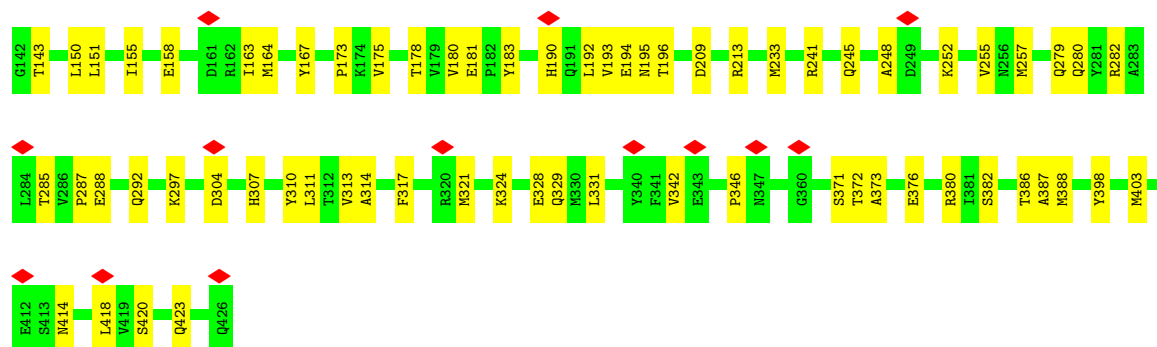


• Molecule 2: Tubulin beta-1 chain

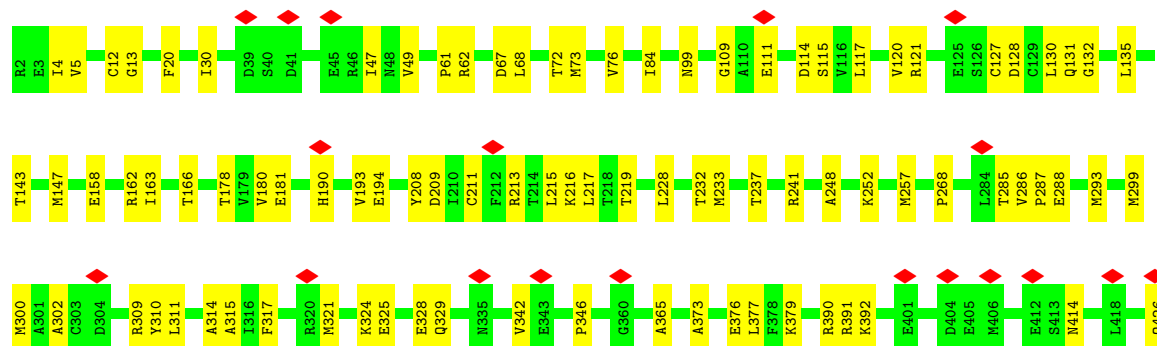
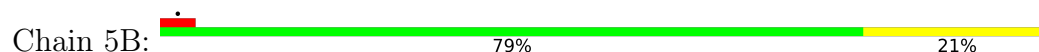


• Molecule 2: Tubulin beta-1 chain

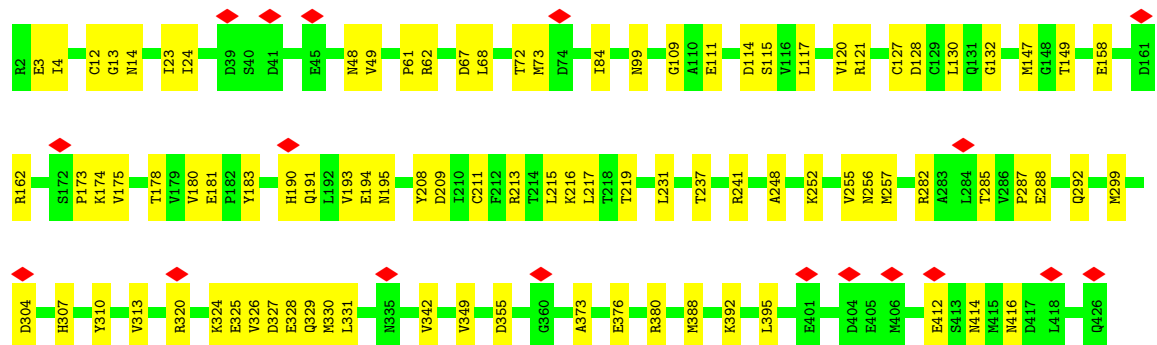
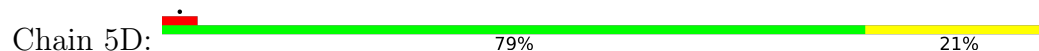




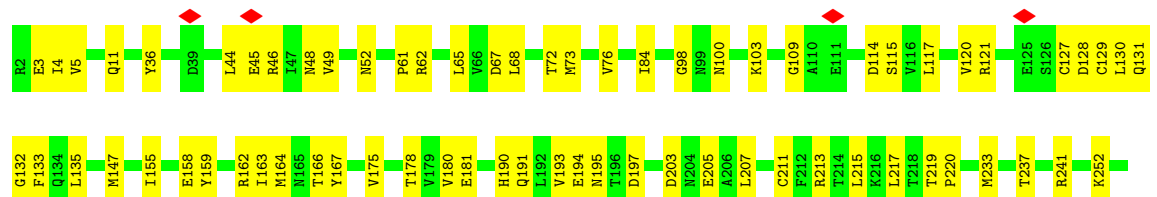
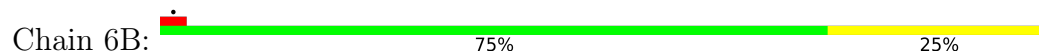
• Molecule 2: Tubulin beta-1 chain

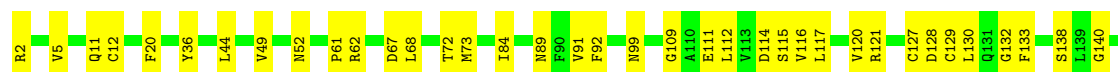


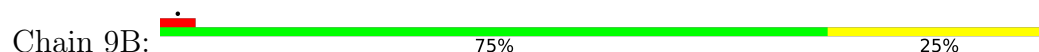
• Molecule 2: Tubulin beta-1 chain

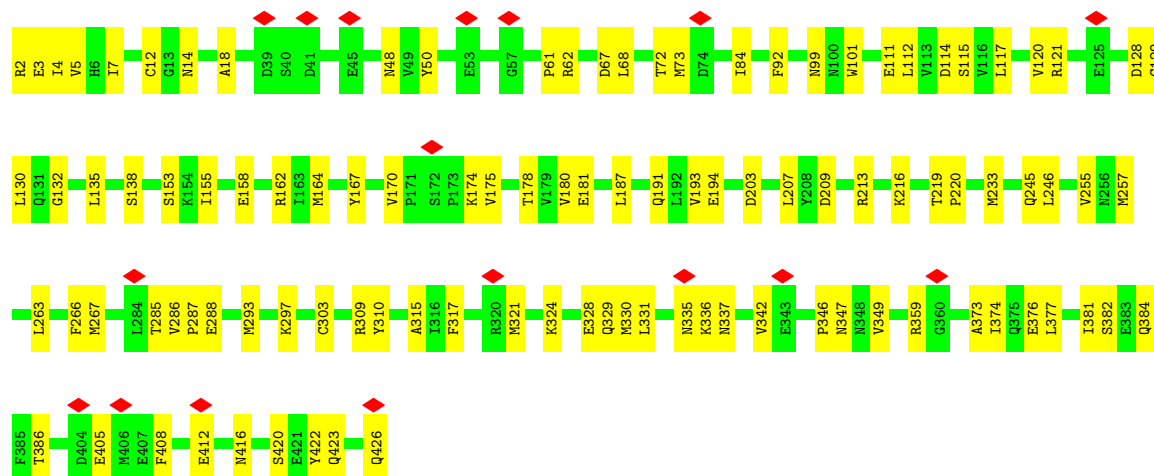


• Molecule 2: Tubulin beta-1 chain

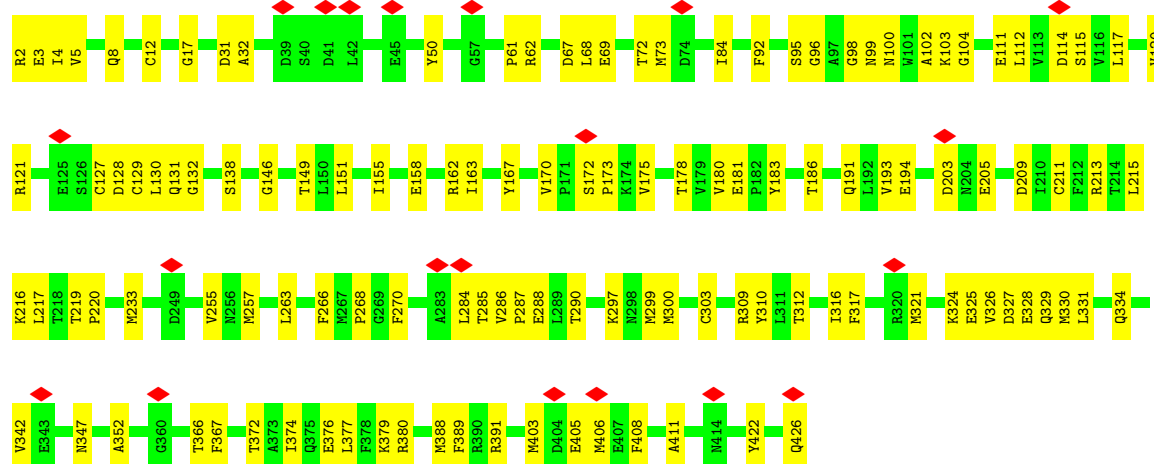
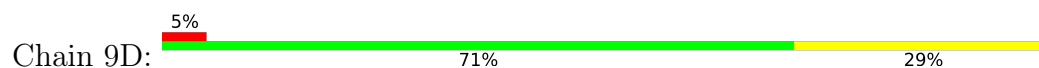








• Molecule 2: Tubulin beta-1 chain



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 39594                                   | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF                         | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 32                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 4.806                                   | Depositor |
| Minimum map value                    | -3.037                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.233                                   | Depositor |
| Recommended contour level            | 0.582                                   | Depositor |
| Map size (Å)                         | 431.984, 431.984, 431.984               | wwPDB     |
| Map dimensions                       | 392, 392, 392                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.102, 1.102, 1.102                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, GDP

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   | 10A   | 0.34         | 1/3419 (0.0%) | 0.50        | 2/4643 (0.0%) |
| 1   | 10C   | 0.24         | 0/3419        | 0.45        | 0/4643        |
| 1   | 10E   | 0.27         | 1/3419 (0.0%) | 0.47        | 1/4643 (0.0%) |
| 1   | 11A   | 0.23         | 0/3419        | 0.48        | 0/4643        |
| 1   | 11C   | 0.27         | 0/3419        | 0.50        | 0/4643        |
| 1   | 11E   | 0.23         | 0/3419        | 0.46        | 0/4643        |
| 1   | 12A   | 0.23         | 0/3419        | 0.49        | 0/4643        |
| 1   | 12C   | 0.25         | 0/3419        | 0.52        | 1/4643 (0.0%) |
| 1   | 12E   | 0.23         | 0/3419        | 0.50        | 1/4643 (0.0%) |
| 1   | 13A   | 0.25         | 0/3419        | 0.52        | 0/4643        |
| 1   | 13C   | 0.27         | 0/3419        | 0.53        | 1/4643 (0.0%) |
| 1   | 13E   | 0.24         | 0/3419        | 0.47        | 0/4643        |
| 1   | 1A    | 0.20         | 0/3419        | 0.39        | 0/4643        |
| 1   | 1C    | 0.21         | 0/3419        | 0.40        | 0/4643        |
| 1   | 1E    | 0.21         | 0/3419        | 0.39        | 0/4643        |
| 1   | 2A    | 0.20         | 0/3419        | 0.37        | 0/4643        |
| 1   | 2C    | 0.19         | 0/3419        | 0.36        | 0/4643        |
| 1   | 2E    | 0.21         | 0/3419        | 0.38        | 0/4643        |
| 1   | 3A    | 0.19         | 0/3419        | 0.37        | 0/4643        |
| 1   | 3C    | 0.20         | 0/3419        | 0.37        | 0/4643        |
| 1   | 3E    | 0.20         | 0/3419        | 0.36        | 0/4643        |
| 1   | 4A    | 0.20         | 0/3419        | 0.37        | 0/4643        |
| 1   | 4C    | 0.20         | 0/3419        | 0.36        | 0/4643        |
| 1   | 4E    | 0.20         | 0/3419        | 0.37        | 0/4643        |
| 1   | 5A    | 0.21         | 0/3419        | 0.38        | 0/4643        |
| 1   | 5C    | 0.21         | 0/3419        | 0.40        | 1/4643 (0.0%) |
| 1   | 5E    | 0.21         | 0/3419        | 0.40        | 0/4643        |
| 1   | 6A    | 0.22         | 0/3419        | 0.40        | 1/4643 (0.0%) |
| 1   | 6C    | 0.23         | 0/3419        | 0.42        | 0/4643        |
| 1   | 6E    | 0.21         | 0/3419        | 0.42        | 0/4643        |
| 1   | 7A    | 0.26         | 0/3419        | 0.46        | 1/4643 (0.0%) |
| 1   | 7C    | 0.26         | 0/3419        | 0.46        | 0/4643        |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 1   | 7E    | 0.25         | 0/3419          | 0.47        | 1/4643 (0.0%)    |
| 1   | 8A    | 0.24         | 0/3419          | 0.45        | 0/4643           |
| 1   | 8C    | 0.25         | 0/3419          | 0.47        | 0/4643           |
| 1   | 8E    | 0.23         | 0/3419          | 0.44        | 0/4643           |
| 1   | 9A    | 0.22         | 0/3419          | 0.45        | 0/4643           |
| 1   | 9C    | 0.23         | 0/3419          | 0.46        | 0/4643           |
| 1   | 9E    | 0.21         | 0/3419          | 0.44        | 0/4643           |
| 2   | 10B   | 0.24         | 0/3417          | 0.46        | 0/4627           |
| 2   | 10D   | 0.24         | 0/3417          | 0.47        | 2/4627 (0.0%)    |
| 2   | 11B   | 0.26         | 0/3417          | 0.48        | 0/4627           |
| 2   | 11D   | 0.23         | 0/3417          | 0.47        | 0/4627           |
| 2   | 12B   | 0.27         | 0/3417          | 0.55        | 2/4627 (0.0%)    |
| 2   | 12D   | 0.26         | 0/3417          | 0.49        | 0/4627           |
| 2   | 13B   | 0.26         | 0/3417          | 0.52        | 0/4627           |
| 2   | 13D   | 0.25         | 0/3417          | 0.52        | 0/4627           |
| 2   | 1B    | 0.21         | 0/3417          | 0.42        | 0/4627           |
| 2   | 1D    | 0.21         | 0/3417          | 0.42        | 0/4627           |
| 2   | 2B    | 0.22         | 0/3417          | 0.38        | 0/4627           |
| 2   | 2D    | 0.21         | 0/3417          | 0.39        | 0/4627           |
| 2   | 3B    | 0.21         | 0/3417          | 0.39        | 0/4627           |
| 2   | 3D    | 0.21         | 0/3417          | 0.39        | 0/4627           |
| 2   | 4B    | 0.22         | 0/3417          | 0.40        | 0/4627           |
| 2   | 4D    | 0.26         | 0/3417          | 0.42        | 0/4627           |
| 2   | 5B    | 0.22         | 0/3417          | 0.41        | 0/4627           |
| 2   | 5D    | 0.22         | 0/3417          | 0.41        | 0/4627           |
| 2   | 6B    | 0.24         | 0/3417          | 0.45        | 0/4627           |
| 2   | 6D    | 0.23         | 0/3417          | 0.43        | 0/4627           |
| 2   | 7B    | 0.27         | 0/3417          | 0.48        | 1/4627 (0.0%)    |
| 2   | 7D    | 0.26         | 0/3417          | 0.45        | 0/4627           |
| 2   | 8B    | 0.24         | 0/3417          | 0.46        | 2/4627 (0.0%)    |
| 2   | 8D    | 0.25         | 0/3417          | 0.47        | 0/4627           |
| 2   | 9B    | 0.24         | 0/3417          | 0.47        | 0/4627           |
| 2   | 9D    | 0.23         | 0/3417          | 0.43        | 0/4627           |
| All | All   | 0.23         | 2/222183 (0.0%) | 0.44        | 17/301379 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | 12B   | 0                   | 1                   |

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

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 10A   | 359 | PRO  | CA-C  | 10.00 | 1.61        | 1.52     |
| 1   | 10E   | 359 | PRO  | CA-C  | 6.25  | 1.57        | 1.52     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | 10A   | 360 | PRO  | CA-N-CD  | -7.21 | 101.90      | 112.00   |
| 1   | 10E   | 360 | PRO  | CA-N-CD  | -6.68 | 102.64      | 112.00   |
| 1   | 7A    | 15  | GLN  | CA-CB-CG | 6.43  | 126.95      | 114.10   |
| 1   | 7E    | 15  | GLN  | CA-CB-CG | 6.39  | 126.88      | 114.10   |
| 2   | 12B   | 368 | ILE  | CA-C-N   | -6.30 | 117.36      | 121.65   |
| 2   | 12B   | 368 | ILE  | C-N-CA   | -6.30 | 117.36      | 121.65   |
| 1   | 5C    | 15  | GLN  | CA-CB-CG | 6.26  | 126.61      | 114.10   |
| 1   | 12C   | 31  | GLN  | CA-CB-CG | 6.05  | 126.19      | 114.10   |
| 1   | 10A   | 359 | PRO  | O-C-N    | 5.58  | 128.04      | 121.46   |
| 1   | 13C   | 15  | GLN  | CA-CB-CG | 5.47  | 125.04      | 114.10   |
| 1   | 12E   | 298 | PRO  | CA-N-CD  | -5.38 | 104.47      | 112.00   |
| 1   | 6A    | 15  | GLN  | CA-CB-CG | 5.11  | 124.31      | 114.10   |
| 2   | 8B    | 285 | THR  | CA-C-N   | 5.11  | 123.46      | 120.24   |
| 2   | 8B    | 285 | THR  | C-N-CA   | 5.11  | 123.46      | 120.24   |
| 2   | 7B    | 324 | LYS  | CG-CD-CE | -5.05 | 99.68       | 111.30   |
| 2   | 10D   | 285 | THR  | CA-C-N   | 5.05  | 123.42      | 120.24   |
| 2   | 10D   | 285 | THR  | C-N-CA   | 5.05  | 123.42      | 120.24   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | 12B   | 60  | VAL  | Peptide |
| 2   | 4D    | 3   | GLU  | Peptide |

## 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   | 10A   | 3342  | 0        | 3257     | 76      | 0            |
| 1   | 10C   | 3342  | 0        | 3257     | 85      | 0            |
| 1   | 10E   | 3342  | 0        | 3257     | 84      | 0            |
| 1   | 11A   | 3342  | 0        | 3257     | 73      | 0            |
| 1   | 11C   | 3342  | 0        | 3257     | 102     | 0            |
| 1   | 11E   | 3342  | 0        | 3257     | 89      | 0            |
| 1   | 12A   | 3342  | 0        | 3257     | 96      | 0            |
| 1   | 12C   | 3342  | 0        | 3257     | 87      | 0            |
| 1   | 12E   | 3342  | 0        | 3257     | 90      | 0            |
| 1   | 13A   | 3342  | 0        | 3258     | 129     | 0            |
| 1   | 13C   | 3342  | 0        | 3257     | 117     | 0            |
| 1   | 13E   | 3342  | 0        | 3258     | 114     | 0            |
| 1   | 1A    | 3342  | 0        | 3257     | 65      | 0            |
| 1   | 1C    | 3342  | 0        | 3257     | 69      | 0            |
| 1   | 1E    | 3342  | 0        | 3257     | 62      | 0            |
| 1   | 2A    | 3342  | 0        | 3256     | 64      | 0            |
| 1   | 2C    | 3342  | 0        | 3256     | 64      | 0            |
| 1   | 2E    | 3342  | 0        | 3256     | 63      | 0            |
| 1   | 3A    | 3342  | 0        | 3256     | 71      | 0            |
| 1   | 3C    | 3342  | 0        | 3256     | 76      | 0            |
| 1   | 3E    | 3342  | 0        | 3256     | 54      | 0            |
| 1   | 4A    | 3342  | 0        | 3256     | 58      | 0            |
| 1   | 4C    | 3342  | 0        | 3256     | 77      | 0            |
| 1   | 4E    | 3342  | 0        | 3256     | 57      | 0            |
| 1   | 5A    | 3342  | 0        | 3257     | 64      | 0            |
| 1   | 5C    | 3342  | 0        | 3257     | 56      | 0            |
| 1   | 5E    | 3342  | 0        | 3257     | 73      | 0            |
| 1   | 6A    | 3342  | 0        | 3257     | 69      | 0            |
| 1   | 6C    | 3342  | 0        | 3257     | 85      | 0            |
| 1   | 6E    | 3342  | 0        | 3257     | 80      | 0            |
| 1   | 7A    | 3342  | 0        | 3257     | 95      | 0            |
| 1   | 7C    | 3342  | 0        | 3257     | 94      | 0            |
| 1   | 7E    | 3342  | 0        | 3257     | 87      | 0            |
| 1   | 8A    | 3342  | 0        | 3257     | 81      | 0            |
| 1   | 8C    | 3342  | 0        | 3256     | 80      | 0            |
| 1   | 8E    | 3342  | 0        | 3257     | 87      | 0            |
| 1   | 9A    | 3342  | 0        | 3257     | 85      | 0            |
| 1   | 9C    | 3342  | 0        | 3257     | 83      | 0            |
| 1   | 9E    | 3342  | 0        | 3257     | 74      | 0            |
| 2   | 10B   | 3343  | 0        | 3230     | 92      | 0            |
| 2   | 10D   | 3343  | 0        | 3230     | 96      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 11B   | 3343  | 0        | 3230     | 111     | 0            |
| 2   | 11D   | 3343  | 0        | 3230     | 99      | 0            |
| 2   | 12B   | 3343  | 0        | 3230     | 119     | 0            |
| 2   | 12D   | 3343  | 0        | 3230     | 104     | 0            |
| 2   | 13B   | 3343  | 0        | 3230     | 126     | 0            |
| 2   | 13D   | 3343  | 0        | 3230     | 129     | 0            |
| 2   | 1B    | 3343  | 0        | 3230     | 79      | 0            |
| 2   | 1D    | 3343  | 0        | 3230     | 62      | 0            |
| 2   | 2B    | 3343  | 0        | 3230     | 59      | 0            |
| 2   | 2D    | 3343  | 0        | 3230     | 64      | 0            |
| 2   | 3B    | 3343  | 0        | 3230     | 70      | 0            |
| 2   | 3D    | 3343  | 0        | 3230     | 79      | 0            |
| 2   | 4B    | 3343  | 0        | 3230     | 71      | 0            |
| 2   | 4D    | 3343  | 0        | 3230     | 71      | 0            |
| 2   | 5B    | 3343  | 0        | 3230     | 68      | 0            |
| 2   | 5D    | 3343  | 0        | 3230     | 69      | 0            |
| 2   | 6B    | 3343  | 0        | 3230     | 78      | 0            |
| 2   | 6D    | 3343  | 0        | 3230     | 79      | 0            |
| 2   | 7B    | 3343  | 0        | 3230     | 77      | 0            |
| 2   | 7D    | 3343  | 0        | 3230     | 84      | 0            |
| 2   | 8B    | 3343  | 0        | 3230     | 93      | 0            |
| 2   | 8D    | 3343  | 0        | 3230     | 90      | 0            |
| 2   | 9B    | 3343  | 0        | 3230     | 83      | 0            |
| 2   | 9D    | 3343  | 0        | 3230     | 89      | 0            |
| 3   | 10A   | 32    | 0        | 12       | 2       | 0            |
| 3   | 10C   | 32    | 0        | 12       | 1       | 0            |
| 3   | 10E   | 32    | 0        | 12       | 2       | 0            |
| 3   | 11A   | 32    | 0        | 12       | 5       | 0            |
| 3   | 11C   | 32    | 0        | 12       | 1       | 0            |
| 3   | 11E   | 32    | 0        | 12       | 1       | 0            |
| 3   | 12A   | 32    | 0        | 12       | 1       | 0            |
| 3   | 12C   | 32    | 0        | 12       | 2       | 0            |
| 3   | 12E   | 32    | 0        | 12       | 1       | 0            |
| 3   | 13A   | 32    | 0        | 12       | 1       | 0            |
| 3   | 13C   | 32    | 0        | 12       | 2       | 0            |
| 3   | 13E   | 32    | 0        | 12       | 1       | 0            |
| 3   | 1A    | 32    | 0        | 12       | 1       | 0            |
| 3   | 1C    | 32    | 0        | 12       | 1       | 0            |
| 3   | 1E    | 32    | 0        | 12       | 1       | 0            |
| 3   | 2A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2E    | 32    | 0        | 12       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 3A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3E    | 32    | 0        | 12       | 1       | 0            |
| 3   | 4A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4E    | 32    | 0        | 12       | 1       | 0            |
| 3   | 5A    | 32    | 0        | 12       | 3       | 0            |
| 3   | 5C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 5E    | 32    | 0        | 12       | 4       | 0            |
| 3   | 6A    | 32    | 0        | 12       | 4       | 0            |
| 3   | 6C    | 32    | 0        | 12       | 3       | 0            |
| 3   | 6E    | 32    | 0        | 12       | 3       | 0            |
| 3   | 7A    | 32    | 0        | 12       | 5       | 0            |
| 3   | 7C    | 32    | 0        | 12       | 4       | 0            |
| 3   | 7E    | 32    | 0        | 12       | 6       | 0            |
| 3   | 8A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 8C    | 32    | 0        | 12       | 3       | 0            |
| 3   | 8E    | 32    | 0        | 12       | 5       | 0            |
| 3   | 9A    | 32    | 0        | 12       | 1       | 0            |
| 3   | 9C    | 32    | 0        | 12       | 3       | 0            |
| 3   | 9E    | 32    | 0        | 12       | 0       | 0            |
| 4   | 10A   | 1     | 0        | 0        | 0       | 0            |
| 4   | 10C   | 1     | 0        | 0        | 0       | 0            |
| 4   | 10E   | 1     | 0        | 0        | 0       | 0            |
| 4   | 11A   | 1     | 0        | 0        | 0       | 0            |
| 4   | 11C   | 1     | 0        | 0        | 0       | 0            |
| 4   | 11E   | 1     | 0        | 0        | 0       | 0            |
| 4   | 12A   | 1     | 0        | 0        | 0       | 0            |
| 4   | 12C   | 1     | 0        | 0        | 0       | 0            |
| 4   | 12E   | 1     | 0        | 0        | 0       | 0            |
| 4   | 13A   | 1     | 0        | 0        | 0       | 0            |
| 4   | 13C   | 1     | 0        | 0        | 0       | 0            |
| 4   | 13E   | 1     | 0        | 0        | 0       | 0            |
| 4   | 1A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3E    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | 4A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 5A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 5C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 5E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 6A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 6C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 6E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 7A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 7C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 7E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 8A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 8C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 8E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 9A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 9C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 9E    | 1     | 0        | 0        | 0       | 0            |
| 5   | 10B   | 28    | 0        | 12       | 1       | 0            |
| 5   | 10D   | 28    | 0        | 12       | 1       | 0            |
| 5   | 11B   | 28    | 0        | 12       | 2       | 0            |
| 5   | 11D   | 28    | 0        | 12       | 1       | 0            |
| 5   | 12B   | 28    | 0        | 12       | 2       | 0            |
| 5   | 12D   | 28    | 0        | 12       | 3       | 0            |
| 5   | 13B   | 28    | 0        | 12       | 0       | 0            |
| 5   | 13D   | 28    | 0        | 12       | 0       | 0            |
| 5   | 1B    | 28    | 0        | 12       | 0       | 0            |
| 5   | 1D    | 28    | 0        | 12       | 0       | 0            |
| 5   | 2B    | 28    | 0        | 12       | 0       | 0            |
| 5   | 2D    | 28    | 0        | 12       | 1       | 0            |
| 5   | 3B    | 28    | 0        | 12       | 0       | 0            |
| 5   | 3D    | 28    | 0        | 12       | 0       | 0            |
| 5   | 4B    | 28    | 0        | 12       | 1       | 0            |
| 5   | 4D    | 28    | 0        | 12       | 1       | 0            |
| 5   | 5B    | 28    | 0        | 12       | 0       | 0            |
| 5   | 5D    | 28    | 0        | 12       | 0       | 0            |
| 5   | 6B    | 28    | 0        | 12       | 1       | 0            |
| 5   | 6D    | 28    | 0        | 12       | 0       | 0            |
| 5   | 7B    | 28    | 0        | 12       | 0       | 0            |
| 5   | 7D    | 28    | 0        | 12       | 0       | 0            |
| 5   | 8B    | 28    | 0        | 12       | 1       | 0            |
| 5   | 8D    | 28    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5   | 9B    | 28     | 0        | 12       | 0       | 0            |
| 5   | 9D    | 28     | 0        | 12       | 0       | 0            |
| All | All   | 219271 | 0        | 211775   | 4999    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (4999) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11C:302:MET:HG3  | 1:11C:303:VAL:HG23 | 1.45                     | 0.98              |
| 1:13C:216:ASN:ND2  | 1:13C:300:ASN:OD1  | 2.02                     | 0.92              |
| 1:1E:102:ASN:HD22  | 1:1E:105:ARG:HD3   | 1.35                     | 0.89              |
| 1:6E:71:GLU:HB2    | 1:6E:98:ASP:HB3    | 1.54                     | 0.88              |
| 2:9D:61:PRO:HD3    | 2:9D:84:ILE:HG22   | 1.56                     | 0.88              |
| 1:13C:421:ALA:O    | 1:13C:425:LEU:N    | 2.07                     | 0.87              |
| 1:7A:54:SER:OG     | 1:7A:64:ARG:NH1    | 2.07                     | 0.87              |
| 1:3C:102:ASN:HD22  | 1:3C:105:ARG:HD3   | 1.39                     | 0.86              |
| 1:7C:222:PRO:HD2   | 2:7D:324:LYS:HD3   | 1.57                     | 0.86              |
| 1:3E:102:ASN:HD22  | 1:3E:105:ARG:HD3   | 1.39                     | 0.86              |
| 1:2A:221:ARG:HA    | 2:2B:324:LYS:HE2   | 1.56                     | 0.86              |
| 1:7E:180:ALA:HB3   | 1:7E:183:GLU:HG3   | 1.58                     | 0.86              |
| 1:8A:71:GLU:HB2    | 1:8A:98:ASP:HB3    | 1.56                     | 0.86              |
| 1:10C:3:GLU:HB3    | 1:10C:64:ARG:HH12  | 1.40                     | 0.86              |
| 1:7A:175:PRO:O     | 1:7A:394:LYS:NZ    | 2.08                     | 0.85              |
| 2:13D:67:ASP:OD2   | 2:13D:72:THR:OG1   | 1.94                     | 0.85              |
| 1:7A:180:ALA:HB3   | 1:7A:183:GLU:HG3   | 1.58                     | 0.85              |
| 2:13D:3:GLU:HB3    | 2:13D:62:ARG:HH22  | 1.42                     | 0.85              |
| 2:12B:67:ASP:OD2   | 2:12B:72:THR:OG1   | 1.94                     | 0.84              |
| 2:6B:220:PRO:HD2   | 1:6C:326:LYS:HD3   | 1.58                     | 0.84              |
| 2:9B:61:PRO:HD3    | 2:9B:84:ILE:HG22   | 1.60                     | 0.84              |
| 1:6C:71:GLU:HB2    | 1:6C:98:ASP:HB3    | 1.57                     | 0.84              |
| 2:8B:12:CYS:HG     | 2:8B:138:SER:HG    | 1.18                     | 0.84              |
| 1:2C:102:ASN:HD22  | 1:2C:105:ARG:HD3   | 1.41                     | 0.83              |
| 1:2E:102:ASN:HD22  | 1:2E:105:ARG:HD3   | 1.40                     | 0.83              |
| 1:12A:182:VAL:HG12 | 2:12B:256:ASN:HD21 | 1.43                     | 0.83              |
| 2:5B:211:CYS:HB2   | 2:5B:217:LEU:HD12  | 1.59                     | 0.83              |
| 1:6A:71:GLU:HB2    | 1:6A:98:ASP:HB3    | 1.59                     | 0.83              |
| 1:13A:421:ALA:O    | 1:13A:425:LEU:N    | 2.11                     | 0.83              |
| 2:11D:61:PRO:HD3   | 2:11D:84:ILE:HG22  | 1.61                     | 0.83              |
| 1:12C:64:ARG:NH2   | 1:12C:128:GLN:OE1  | 2.10                     | 0.83              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7E:102:ASN:HB2   | 1:7E:105:ARG:HB2   | 1.61                     | 0.82              |
| 1:8E:402:ARG:HH22  | 1:8E:415:GLU:HB3   | 1.44                     | 0.82              |
| 1:7E:54:SER:OG     | 1:7E:64:ARG:NH1    | 2.12                     | 0.82              |
| 1:13C:320:ARG:HG3  | 1:13C:360:PRO:HG3  | 1.61                     | 0.82              |
| 2:5D:3:GLU:HB3     | 2:5D:62:ARG:HH12   | 1.41                     | 0.82              |
| 1:12C:213:CYS:HB2  | 1:12C:219:ILE:HD11 | 1.62                     | 0.81              |
| 2:11B:117:LEU:HD11 | 2:11B:154:LYS:HZ1  | 1.42                     | 0.81              |
| 2:11D:252:LYS:O    | 2:11D:256:ASN:ND2  | 2.13                     | 0.81              |
| 1:13E:209:ILE:HG21 | 1:13E:227:LEU:HG   | 1.63                     | 0.81              |
| 2:1B:257:MET:HE3   | 2:1B:314:ALA:HB2   | 1.62                     | 0.81              |
| 2:7D:67:ASP:OD2    | 2:7D:72:THR:OG1    | 1.99                     | 0.81              |
| 2:12B:411:ALA:O    | 2:12B:415:MET:N    | 2.13                     | 0.81              |
| 1:7C:175:PRO:O     | 1:7C:394:LYS:NZ    | 2.13                     | 0.81              |
| 2:9B:287:PRO:HA    | 2:9B:329:GLN:HE22  | 1.46                     | 0.81              |
| 1:4A:102:ASN:HD22  | 1:4A:105:ARG:HD3   | 1.46                     | 0.80              |
| 1:12A:421:ALA:O    | 1:12A:425:LEU:N    | 2.13                     | 0.80              |
| 2:12B:292:GLN:HE22 | 2:12B:298:ASN:HD22 | 1.30                     | 0.80              |
| 2:11B:292:GLN:HE22 | 2:11B:298:ASN:HD22 | 1.28                     | 0.80              |
| 1:13A:100:ALA:HB2  | 2:13B:251:ARG:HG2  | 1.63                     | 0.80              |
| 1:13C:139:HIS:CD2  | 1:13C:150:THR:HG21 | 2.17                     | 0.80              |
| 1:5A:221:ARG:HA    | 2:5B:324:LYS:HE2   | 1.64                     | 0.80              |
| 2:4D:317:PHE:HB3   | 2:4D:321:MET:HE1   | 1.64                     | 0.80              |
| 2:5B:302:ALA:HB3   | 2:5B:377:LEU:HD21  | 1.64                     | 0.80              |
| 2:12D:67:ASP:OD2   | 2:12D:72:THR:OG1   | 1.97                     | 0.80              |
| 1:4A:98:ASP:OD1    | 1:4A:99:ALA:N      | 2.16                     | 0.79              |
| 2:6D:67:ASP:OD2    | 2:6D:72:THR:OG1    | 1.99                     | 0.79              |
| 1:13E:101:ASN:HA   | 1:13E:144:GLY:H    | 1.46                     | 0.79              |
| 1:13E:216:ASN:ND2  | 1:13E:300:ASN:OD1  | 2.14                     | 0.79              |
| 1:1E:252:LEU:O     | 1:1E:256:GLN:NE2   | 2.15                     | 0.79              |
| 1:12C:421:ALA:O    | 1:12C:425:LEU:N    | 2.14                     | 0.79              |
| 2:13B:3:GLU:HB3    | 2:13B:62:ARG:HH22  | 1.46                     | 0.79              |
| 1:7A:206:ASN:ND2   | 3:7A:500:GTP:O2'   | 2.16                     | 0.79              |
| 2:10B:61:PRO:HD3   | 2:10B:84:ILE:HG22  | 1.64                     | 0.79              |
| 2:7B:67:ASP:OD2    | 2:7B:72:THR:OG1    | 1.98                     | 0.79              |
| 2:7D:5:VAL:HG12    | 2:7D:62:ARG:HD2    | 1.64                     | 0.79              |
| 2:10B:67:ASP:OD2   | 2:10B:72:THR:OG1   | 2.01                     | 0.78              |
| 1:4E:98:ASP:OD1    | 1:4E:99:ALA:N      | 2.16                     | 0.78              |
| 2:2B:267:MET:HE2   | 2:2B:299:MET:HE2   | 1.65                     | 0.78              |
| 2:9B:130:LEU:HG    | 2:9B:162:ARG:HH12  | 1.47                     | 0.78              |
| 1:11C:215:ARG:NH2  | 1:11C:299:ALA:O    | 2.15                     | 0.78              |
| 1:1E:191:THR:HG21  | 1:1E:425:LEU:HD21  | 1.66                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:8C:286:LEU:O     | 1:8C:373:ARG:NH1   | 2.16                     | 0.78              |
| 2:11B:61:PRO:HD3   | 2:11B:84:ILE:HG22  | 1.65                     | 0.78              |
| 1:4E:108:TYR:O     | 1:4E:112:LYS:NZ    | 2.17                     | 0.78              |
| 2:6D:287:PRO:HG3   | 2:6D:329:GLN:HE22  | 1.47                     | 0.78              |
| 2:9B:67:ASP:OD2    | 2:9B:72:THR:OG1    | 2.02                     | 0.78              |
| 2:1B:220:PRO:HD2   | 1:1C:326:LYS:HD3   | 1.64                     | 0.78              |
| 2:2D:282:ARG:NH2   | 2:2D:292:GLN:OE1   | 2.16                     | 0.78              |
| 2:11D:292:GLN:HE22 | 2:11D:298:ASN:HD22 | 1.30                     | 0.78              |
| 1:8C:3:GLU:HG3     | 1:8C:129:CYS:HA    | 1.66                     | 0.78              |
| 1:4C:102:ASN:HD22  | 1:4C:105:ARG:HD3   | 1.48                     | 0.77              |
| 1:9A:102:ASN:HB2   | 1:9A:105:ARG:HB2   | 1.66                     | 0.77              |
| 1:13E:317:MET:HE2  | 1:13E:319:TYR:CZ   | 2.18                     | 0.77              |
| 1:10A:221:ARG:HA   | 2:10B:324:LYS:HD3  | 1.66                     | 0.77              |
| 2:3D:67:ASP:HB2    | 2:3D:73:MET:HE3    | 1.66                     | 0.77              |
| 2:6B:3:GLU:OE1     | 2:6B:3:GLU:N       | 2.18                     | 0.77              |
| 2:2D:209:ASP:OD1   | 2:2D:213:ARG:NH2   | 2.16                     | 0.77              |
| 2:11D:67:ASP:OD2   | 2:11D:72:THR:OG1   | 2.03                     | 0.76              |
| 1:4A:221:ARG:HA    | 2:4B:324:LYS:HE2   | 1.67                     | 0.76              |
| 2:4B:67:ASP:OD2    | 2:4B:72:THR:OG1    | 2.02                     | 0.76              |
| 1:4E:102:ASN:HD22  | 1:4E:105:ARG:HD3   | 1.50                     | 0.76              |
| 2:9B:213:ARG:O     | 2:9B:216:LYS:NZ    | 2.18                     | 0.76              |
| 2:9D:67:ASP:OD2    | 2:9D:72:THR:OG1    | 2.03                     | 0.76              |
| 2:12D:389:PHE:O    | 2:12D:392:LYS:NZ   | 2.17                     | 0.76              |
| 2:6B:211:CYS:HB2   | 2:6B:217:LEU:HD12  | 1.68                     | 0.76              |
| 2:12B:203:ASP:OD2  | 2:12B:302:ALA:N    | 2.17                     | 0.76              |
| 1:13A:269:LEU:HG   | 1:13A:303:VAL:HG21 | 1.66                     | 0.76              |
| 1:7A:145:THR:OG1   | 3:7A:500:GTP:O3B   | 2.03                     | 0.76              |
| 2:13B:67:ASP:OD2   | 2:13B:72:THR:OG1   | 2.02                     | 0.76              |
| 2:7B:220:PRO:HD2   | 1:7C:326:LYS:HD2   | 1.67                     | 0.76              |
| 1:10A:3:GLU:HB3    | 1:10A:64:ARG:HH12  | 1.49                     | 0.76              |
| 2:11D:12:CYS:SG    | 2:11D:138:SER:OG   | 2.43                     | 0.76              |
| 1:12C:91:GLN:HA    | 1:12C:121:ARG:HH12 | 1.50                     | 0.76              |
| 1:13E:213:CYS:HB3  | 1:13E:219:ILE:HD11 | 1.68                     | 0.76              |
| 2:10B:190:HIS:NE2  | 2:10B:414:ASN:OD1  | 2.16                     | 0.76              |
| 1:2C:20:CYS:HB3    | 1:2C:24:TYR:HE2    | 1.51                     | 0.76              |
| 1:8E:64:ARG:HH21   | 1:8E:128:GLN:HE22  | 1.34                     | 0.76              |
| 2:10D:61:PRO:HD3   | 2:10D:84:ILE:HG22  | 1.66                     | 0.76              |
| 1:10A:214:ARG:HH22 | 2:10B:328:GLU:HG3  | 1.51                     | 0.75              |
| 1:9C:221:ARG:HA    | 2:9D:324:LYS:HD3   | 1.69                     | 0.75              |
| 1:6C:102:ASN:HD22  | 1:6C:408:TYR:HE1   | 1.31                     | 0.75              |
| 2:8B:67:ASP:OD2    | 2:8B:72:THR:OG1    | 2.04                     | 0.75              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:8E:15:GLN:HG3   | 3:8E:500:GTP:C6    | 2.21                     | 0.75              |
| 1:12A:31:GLN:OE1  | 1:12A:32:PRO:HD2   | 1.85                     | 0.75              |
| 2:12D:331:LEU:HA  | 2:12D:334:GLN:HB2  | 1.68                     | 0.75              |
| 2:7D:293:MET:HE2  | 2:7D:365:ALA:HB1   | 1.68                     | 0.75              |
| 2:11D:242:PHE:HB3 | 2:11D:356:ILE:HD12 | 1.68                     | 0.75              |
| 1:13C:426:ALA:O   | 1:13C:430:LYS:N    | 2.18                     | 0.75              |
| 2:1B:324:LYS:HG3  | 2:1B:325:GLU:N     | 2.01                     | 0.75              |
| 2:9D:213:ARG:O    | 2:9D:216:LYS:NZ    | 2.20                     | 0.75              |
| 2:4D:5:VAL:HG12   | 2:4D:62:ARG:HD3    | 1.67                     | 0.75              |
| 2:13D:323:MET:HE1 | 2:13D:353:VAL:HG21 | 1.69                     | 0.75              |
| 2:5D:67:ASP:OD2   | 2:5D:72:THR:OG1    | 2.04                     | 0.75              |
| 1:6A:102:ASN:HD22 | 1:6A:408:TYR:HE1   | 1.34                     | 0.75              |
| 1:12C:3:GLU:OE2   | 1:12C:64:ARG:NE    | 2.19                     | 0.75              |
| 2:4D:49:VAL:HG11  | 2:4D:241:ARG:HG2   | 1.69                     | 0.75              |
| 1:6E:102:ASN:HD22 | 1:6E:408:TYR:HE1   | 1.33                     | 0.75              |
| 2:7B:12:CYS:HG    | 2:7B:138:SER:HG    | 1.25                     | 0.75              |
| 2:12B:405:GLU:HA  | 2:12B:408:PHE:CD1  | 2.22                     | 0.74              |
| 2:13D:336:LYS:NZ  | 2:13D:337:ASN:OD1  | 2.15                     | 0.74              |
| 1:12E:421:ALA:O   | 1:12E:425:LEU:N    | 2.19                     | 0.74              |
| 2:13D:405:GLU:HA  | 2:13D:408:PHE:CD1  | 2.23                     | 0.74              |
| 2:9B:12:CYS:SG    | 2:9B:138:SER:OG    | 2.44                     | 0.74              |
| 2:10B:109:GLY:HA2 | 2:10B:147:MET:HE1  | 1.68                     | 0.74              |
| 1:12E:215:ARG:NH2 | 1:12E:299:ALA:O    | 2.19                     | 0.74              |
| 2:2D:175:VAL:HG13 | 1:2E:329:ASN:HD22  | 1.52                     | 0.74              |
| 1:11A:35:GLN:HE22 | 1:11A:37:PRO:HG3   | 1.52                     | 0.74              |
| 1:13A:104:ALA:HB3 | 1:13A:105:ARG:NH2  | 2.02                     | 0.74              |
| 1:13C:424:ASP:O   | 1:13C:428:LEU:N    | 2.16                     | 0.74              |
| 1:5C:20:CYS:HB3   | 1:5C:24:TYR:HE2    | 1.52                     | 0.74              |
| 2:11B:252:LYS:O   | 2:11B:256:ASN:ND2  | 2.19                     | 0.74              |
| 1:12E:91:GLN:HA   | 1:12E:121:ARG:HH22 | 1.52                     | 0.74              |
| 1:6E:226:ASN:ND2  | 1:6E:367:ASP:OD2   | 2.20                     | 0.74              |
| 2:11B:12:CYS:SG   | 2:11B:138:SER:OG   | 2.45                     | 0.74              |
| 2:11B:67:ASP:OD2  | 2:11B:72:THR:OG1   | 2.05                     | 0.74              |
| 1:6E:88:HIS:CD2   | 1:7E:283:HIS:HB3   | 2.22                     | 0.74              |
| 1:8C:73:THR:HG23  | 2:8D:2:ARG:HH22    | 1.51                     | 0.74              |
| 1:10E:63:PRO:HD3  | 1:10E:86:LEU:HG    | 1.68                     | 0.74              |
| 2:2B:67:ASP:OD2   | 2:2B:72:THR:OG1    | 2.05                     | 0.74              |
| 2:13B:263:LEU:HG  | 2:13B:422:TYR:CE1  | 2.23                     | 0.74              |
| 2:5B:109:GLY:HA3  | 2:5B:147:MET:HE1   | 1.68                     | 0.74              |
| 2:8B:61:PRO:HD3   | 2:8B:84:ILE:HG22   | 1.70                     | 0.74              |
| 2:9B:263:LEU:HG   | 2:9B:422:TYR:HE1   | 1.51                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2B:67:ASP:HB2    | 2:2B:73:MET:HE3    | 1.69                     | 0.73              |
| 2:2D:67:ASP:HB2    | 2:2D:73:MET:HE3    | 1.68                     | 0.73              |
| 2:12B:413:SER:O    | 2:12B:417:ASP:N    | 2.18                     | 0.73              |
| 2:11B:263:LEU:HG   | 2:11B:422:TYR:HE1  | 1.52                     | 0.73              |
| 2:4D:67:ASP:OD2    | 2:4D:72:THR:OG1    | 2.06                     | 0.73              |
| 2:12B:109:GLY:HA2  | 2:12B:147:MET:HE1  | 1.69                     | 0.73              |
| 1:13C:102:ASN:HB2  | 1:13C:105:ARG:HG2  | 1.70                     | 0.73              |
| 2:6B:67:ASP:OD2    | 2:6B:72:THR:OG1    | 2.05                     | 0.73              |
| 2:10D:12:CYS:SG    | 2:10D:138:SER:OG   | 2.47                     | 0.73              |
| 1:12A:35:GLN:HE22  | 1:12A:37:PRO:HG3   | 1.54                     | 0.73              |
| 1:6A:88:HIS:CD2    | 1:7A:283:HIS:HB3   | 2.23                     | 0.73              |
| 2:8D:67:ASP:OD2    | 2:8D:72:THR:OG1    | 2.05                     | 0.73              |
| 1:12A:398:MET:HE1  | 2:12B:345:ILE:HA   | 1.70                     | 0.73              |
| 1:8C:11:GLN:O      | 1:8C:15:GLN:HG2    | 1.88                     | 0.73              |
| 1:11A:143:GLY:N    | 3:11A:500:GTP:O2A  | 2.22                     | 0.73              |
| 1:11E:215:ARG:NH2  | 1:11E:299:ALA:O    | 2.22                     | 0.73              |
| 2:2B:31:ASP:OD2    | 2:2B:32:ALA:N      | 2.21                     | 0.73              |
| 1:9A:71:GLU:HB2    | 1:9A:98:ASP:HB3    | 1.71                     | 0.73              |
| 2:11B:242:PHE:HB3  | 2:11B:356:ILE:HD12 | 1.71                     | 0.73              |
| 1:12E:104:ALA:HB1  | 1:12E:411:GLU:HB2  | 1.71                     | 0.73              |
| 2:12B:390:ARG:HG3  | 2:12B:391:ARG:HD3  | 1.70                     | 0.72              |
| 2:8D:248:ALA:HA    | 2:8D:252:LYS:HG2   | 1.71                     | 0.72              |
| 2:10B:263:LEU:HG   | 2:10B:422:TYR:HE1  | 1.54                     | 0.72              |
| 2:1D:263:LEU:HG    | 2:1D:422:TYR:HE1   | 1.53                     | 0.72              |
| 2:2B:282:ARG:NH2   | 2:2B:292:GLN:OE1   | 2.23                     | 0.72              |
| 1:3A:20:CYS:HB3    | 1:3A:24:TYR:HE1    | 1.52                     | 0.72              |
| 1:10C:88:HIS:HD2   | 1:10C:89:PRO:HD2   | 1.54                     | 0.72              |
| 1:12E:102:ASN:HD22 | 1:12E:105:ARG:HG3  | 1.55                     | 0.72              |
| 2:13B:190:HIS:HB2  | 2:13B:411:ALA:HB2  | 1.71                     | 0.72              |
| 1:12A:215:ARG:NH2  | 1:12A:299:ALA:O    | 2.22                     | 0.72              |
| 1:13C:397:LEU:HD21 | 2:13D:344:TRP:HA   | 1.71                     | 0.72              |
| 1:9E:226:ASN:ND2   | 1:9E:367:ASP:OD2   | 2.22                     | 0.72              |
| 1:11C:88:HIS:HD2   | 1:11C:89:PRO:HD2   | 1.53                     | 0.72              |
| 2:13B:263:LEU:HG   | 2:13B:422:TYR:HE1  | 1.54                     | 0.72              |
| 2:13D:182:PRO:HG2  | 2:13D:388:MET:HE1  | 1.72                     | 0.72              |
| 2:2D:67:ASP:OD2    | 2:2D:72:THR:OG1    | 2.08                     | 0.72              |
| 2:1B:263:LEU:HG    | 2:1B:422:TYR:HE1   | 1.53                     | 0.71              |
| 1:6C:180:ALA:HB3   | 1:6C:183:GLU:HG3   | 1.71                     | 0.71              |
| 2:11B:4:ILE:HG23   | 2:11B:50:TYR:HE1   | 1.54                     | 0.71              |
| 1:12E:35:GLN:HE22  | 1:12E:37:PRO:HG3   | 1.55                     | 0.71              |
| 1:4C:180:ALA:HB3   | 1:4C:183:GLU:HG3   | 1.71                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7B:5:VAL:HG12    | 2:7B:62:ARG:HD2    | 1.72                     | 0.71              |
| 1:8E:292:THR:HG21  | 1:8E:331:ALA:HB1   | 1.71                     | 0.71              |
| 2:6D:287:PRO:HG3   | 2:6D:329:GLN:NE2   | 2.05                     | 0.71              |
| 1:8E:145:THR:OG1   | 3:8E:500:GTP:O3B   | 2.07                     | 0.71              |
| 1:10C:221:ARG:HA   | 2:10D:324:LYS:HD3  | 1.71                     | 0.71              |
| 2:10D:263:LEU:HG   | 2:10D:422:TYR:HE1  | 1.56                     | 0.71              |
| 2:3B:248:ALA:HA    | 2:3B:252:LYS:HD3   | 1.72                     | 0.71              |
| 1:6E:217:LEU:HD21  | 1:6E:367:ASP:HB3   | 1.72                     | 0.71              |
| 1:8C:71:GLU:HB2    | 1:8C:98:ASP:HB3    | 1.72                     | 0.71              |
| 1:9C:150:THR:HG22  | 1:9C:154:MET:HE1   | 1.71                     | 0.71              |
| 1:11C:34:GLY:O     | 1:11C:61:HIS:ND1   | 2.23                     | 0.71              |
| 2:13B:4:ILE:HB     | 2:13B:50:TYR:HE1   | 1.55                     | 0.71              |
| 1:1E:213:CYS:HB3   | 1:1E:219:ILE:HD11  | 1.73                     | 0.71              |
| 2:5B:67:ASP:OD2    | 2:5B:72:THR:OG1    | 2.09                     | 0.71              |
| 1:11A:63:PRO:HD3   | 1:11A:86:LEU:HG    | 1.71                     | 0.71              |
| 2:7B:178:THR:HB    | 2:7B:181:GLU:HG3   | 1.72                     | 0.71              |
| 2:9B:4:ILE:HG13    | 2:9B:132:GLY:O     | 1.90                     | 0.71              |
| 2:10D:67:ASP:OD2   | 2:10D:72:THR:OG1   | 2.07                     | 0.71              |
| 2:13B:331:LEU:HA   | 2:13B:334:GLN:HB2  | 1.73                     | 0.71              |
| 1:1A:213:CYS:HB3   | 1:1A:219:ILE:HD11  | 1.73                     | 0.71              |
| 1:13C:358:GLN:NE2  | 1:13C:359:PRO:O    | 2.23                     | 0.71              |
| 1:4C:317:MET:HE1   | 1:4C:377:MET:HG2   | 1.73                     | 0.71              |
| 1:5A:398:MET:HE1   | 2:5B:346:PRO:HD2   | 1.73                     | 0.71              |
| 2:5B:193:VAL:HG13  | 2:5B:194:GLU:HG3   | 1.72                     | 0.71              |
| 1:11C:213:CYS:HB2  | 1:11C:219:ILE:HD11 | 1.72                     | 0.71              |
| 2:13D:263:LEU:HG   | 2:13D:422:TYR:CE1  | 2.26                     | 0.71              |
| 2:13D:389:PHE:O    | 2:13D:392:LYS:NZ   | 2.21                     | 0.70              |
| 1:13E:226:ASN:ND2  | 1:13E:367:ASP:OD2  | 2.24                     | 0.70              |
| 1:6C:109:THR:HG23  | 1:6C:110:ILE:HG12  | 1.72                     | 0.70              |
| 2:9B:412:GLU:OE2   | 2:9B:416:ASN:ND2   | 2.24                     | 0.70              |
| 2:11B:211:CYS:HB2  | 2:11B:217:LEU:HD12 | 1.72                     | 0.70              |
| 1:7C:91:GLN:HG2    | 1:7C:121:ARG:HH22  | 1.55                     | 0.70              |
| 1:9A:102:ASN:HD22  | 1:9A:408:TYR:HE1   | 1.38                     | 0.70              |
| 2:10B:73:MET:HE1   | 2:10B:92:PHE:CD2   | 2.26                     | 0.70              |
| 2:10D:175:VAL:HG22 | 1:10E:329:ASN:HD21 | 1.55                     | 0.70              |
| 1:1A:252:LEU:O     | 1:1A:256:GLN:NE2   | 2.24                     | 0.70              |
| 1:13E:175:PRO:HA   | 1:13E:394:LYS:HE3  | 1.72                     | 0.70              |
| 1:6C:88:HIS:CD2    | 1:7C:283:HIS:HB3   | 2.25                     | 0.70              |
| 1:9A:402:ARG:HH22  | 1:9A:415:GLU:HB3   | 1.56                     | 0.70              |
| 2:11B:117:LEU:HD11 | 2:11B:154:LYS:NZ   | 2.06                     | 0.70              |
| 1:11E:226:ASN:ND2  | 1:11E:367:ASP:OD2  | 2.25                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:372:THR:HG21 | 2:12B:426:GLN:HA   | 1.73                     | 0.70              |
| 1:13A:112:LYS:HA   | 1:13A:115:VAL:HG12 | 1.72                     | 0.70              |
| 2:11D:193:VAL:HG13 | 2:11D:194:GLU:HG3  | 1.74                     | 0.70              |
| 2:11D:226:ASN:OD1  | 5:11D:600:GDP:N1   | 2.20                     | 0.70              |
| 2:5B:257:MET:HE1   | 2:5B:314:ALA:HB2   | 1.73                     | 0.70              |
| 1:11E:88:HIS:HD2   | 1:11E:89:PRO:HD2   | 1.55                     | 0.70              |
| 1:13A:100:ALA:HB1  | 2:13B:255:VAL:HG11 | 1.74                     | 0.70              |
| 1:13E:269:LEU:HG   | 1:13E:303:VAL:HG21 | 1.73                     | 0.70              |
| 2:6B:285:THR:HG23  | 2:6B:287:PRO:HD2   | 1.73                     | 0.70              |
| 2:12D:405:GLU:HA   | 2:12D:408:PHE:CD1  | 2.27                     | 0.70              |
| 1:2A:102:ASN:HD22  | 1:2A:408:TYR:HE1   | 1.37                     | 0.70              |
| 1:6E:292:THR:HG21  | 1:6E:331:ALA:HB1   | 1.74                     | 0.70              |
| 1:7E:2:ARG:HB2     | 1:7E:133:GLN:HE22  | 1.56                     | 0.70              |
| 1:11E:213:CYS:HB2  | 1:11E:219:ILE:HD11 | 1.74                     | 0.70              |
| 2:12D:263:LEU:HG   | 2:12D:422:TYR:HE1  | 1.55                     | 0.70              |
| 2:13B:140:GLY:O    | 2:13B:184:ASN:ND2  | 2.24                     | 0.70              |
| 2:12B:14:ASN:O     | 2:12B:18:ALA:N     | 2.23                     | 0.70              |
| 2:12D:237:THR:OG1  | 2:12D:241:ARG:NH1  | 2.24                     | 0.70              |
| 2:4B:178:THR:HB    | 2:4B:181:GLU:HG3   | 1.72                     | 0.70              |
| 2:5B:99:ASN:ND2    | 1:5C:254:GLU:OE2   | 2.25                     | 0.70              |
| 2:11D:263:LEU:HG   | 2:11D:422:TYR:HE1  | 1.57                     | 0.69              |
| 1:4A:317:MET:HE1   | 1:4A:377:MET:HG2   | 1.71                     | 0.69              |
| 2:5D:252:LYS:O     | 2:5D:256:ASN:ND2   | 2.25                     | 0.69              |
| 1:7E:15:GLN:HG3    | 3:7E:500:GTP:C6    | 2.26                     | 0.69              |
| 1:9C:3:GLU:HG3     | 1:9C:129:CYS:HA    | 1.72                     | 0.69              |
| 2:11D:109:GLY:HA2  | 2:11D:147:MET:HE1  | 1.74                     | 0.69              |
| 1:11E:35:GLN:HE22  | 1:11E:37:PRO:HG3   | 1.58                     | 0.69              |
| 1:13A:213:CYS:HA   | 1:13A:217:LEU:HD13 | 1.74                     | 0.69              |
| 1:5C:286:LEU:O     | 1:5C:373:ARG:NH1   | 2.23                     | 0.69              |
| 1:6C:255:PHE:HZ    | 1:6C:378:LEU:HD22  | 1.56                     | 0.69              |
| 1:6C:292:THR:HG21  | 1:6C:331:ALA:HB1   | 1.73                     | 0.69              |
| 2:6D:285:THR:HG23  | 2:6D:287:PRO:HD2   | 1.75                     | 0.69              |
| 2:9D:67:ASP:HB2    | 2:9D:73:MET:HE3    | 1.72                     | 0.69              |
| 2:1D:220:PRO:HD2   | 1:1E:326:LYS:HD3   | 1.75                     | 0.69              |
| 2:2B:175:VAL:HG13  | 1:2C:329:ASN:HD22  | 1.57                     | 0.69              |
| 1:5A:180:ALA:HB3   | 1:5A:183:GLU:HG3   | 1.73                     | 0.69              |
| 1:12E:209:ILE:HG23 | 1:12E:230:LEU:HD22 | 1.74                     | 0.69              |
| 2:13B:61:PRO:HG3   | 2:13B:84:ILE:HG22  | 1.74                     | 0.69              |
| 1:3A:221:ARG:HA    | 2:3B:324:LYS:HE3   | 1.74                     | 0.69              |
| 2:7B:293:MET:HE2   | 2:7B:365:ALA:HB1   | 1.74                     | 0.69              |
| 2:8D:257:MET:HE3   | 2:8D:314:ALA:HB2   | 1.73                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11A:215:ARG:NH2  | 1:11A:299:ALA:O    | 2.24                     | 0.69              |
| 2:13B:405:GLU:HA   | 2:13B:408:PHE:CD1  | 2.27                     | 0.69              |
| 2:3D:67:ASP:OD2    | 2:3D:72:THR:OG1    | 2.09                     | 0.69              |
| 1:4E:180:ALA:HB3   | 1:4E:183:GLU:HG3   | 1.73                     | 0.69              |
| 1:6A:109:THR:HG23  | 1:6A:110:ILE:HG12  | 1.74                     | 0.69              |
| 2:8D:61:PRO:HD3    | 2:8D:84:ILE:HG22   | 1.74                     | 0.69              |
| 2:12B:237:THR:OG1  | 2:12B:241:ARG:NH1  | 2.24                     | 0.69              |
| 1:8A:398:MET:HE1   | 2:8B:346:PRO:HD2   | 1.74                     | 0.69              |
| 2:12B:61:PRO:HD3   | 2:12B:84:ILE:HG22  | 1.75                     | 0.69              |
| 1:5E:206:ASN:ND2   | 3:5E:500:GTP:O2'   | 2.26                     | 0.69              |
| 2:7D:375:GLN:OE1   | 2:7D:379:LYS:NZ    | 2.24                     | 0.69              |
| 2:10D:130:LEU:HD21 | 2:10D:162:ARG:HH12 | 1.57                     | 0.69              |
| 1:11C:422:ARG:HA   | 1:11C:425:LEU:HB2  | 1.73                     | 0.69              |
| 1:13A:397:LEU:HD21 | 2:13B:344:TRP:HA   | 1.75                     | 0.69              |
| 1:2A:339:ARG:O     | 1:2A:342:GLN:NE2   | 2.26                     | 0.69              |
| 1:2C:339:ARG:O     | 1:2C:342:GLN:NE2   | 2.25                     | 0.69              |
| 1:8C:206:ASN:ND2   | 3:8C:500:GTP:O2'   | 2.26                     | 0.69              |
| 1:10C:90:GLU:OE2   | 1:11C:280:LYS:NZ   | 2.18                     | 0.69              |
| 1:11C:63:PRO:HD3   | 1:11C:86:LEU:HG    | 1.74                     | 0.69              |
| 2:3D:10:GLY:O      | 2:3D:14:ASN:ND2    | 2.26                     | 0.69              |
| 2:7D:213:ARG:O     | 2:7D:216:LYS:NZ    | 2.24                     | 0.69              |
| 1:8A:54:SER:OG     | 1:8A:64:ARG:NH2    | 2.26                     | 0.69              |
| 1:9E:188:ILE:HG22  | 1:9E:421:ALA:HB1   | 1.75                     | 0.69              |
| 2:3D:232:THR:HG21  | 2:3D:268:PRO:HB3   | 1.74                     | 0.69              |
| 2:8B:178:THR:HB    | 2:8B:181:GLU:HG3   | 1.75                     | 0.69              |
| 2:13B:389:PHE:O    | 2:13B:392:LYS:NZ   | 2.24                     | 0.68              |
| 1:7A:15:GLN:HG3    | 3:7A:500:GTP:C6    | 2.28                     | 0.68              |
| 1:10A:63:PRO:HD3   | 1:10A:86:LEU:HG    | 1.75                     | 0.68              |
| 2:13B:237:THR:OG1  | 2:13B:241:ARG:NH2  | 2.25                     | 0.68              |
| 2:9D:263:LEU:HG    | 2:9D:422:TYR:HE1   | 1.58                     | 0.68              |
| 2:11B:175:VAL:HG22 | 1:11C:329:ASN:HD21 | 1.58                     | 0.68              |
| 2:13D:140:GLY:O    | 2:13D:184:ASN:ND2  | 2.26                     | 0.68              |
| 2:3B:178:THR:HB    | 2:3B:181:GLU:HG3   | 1.75                     | 0.68              |
| 2:4D:178:THR:HB    | 2:4D:181:GLU:HG3   | 1.75                     | 0.68              |
| 1:8E:188:ILE:HG22  | 1:8E:421:ALA:HB1   | 1.76                     | 0.68              |
| 1:10C:213:CYS:HB2  | 1:10C:219:ILE:HD11 | 1.76                     | 0.68              |
| 2:13B:142:GLY:O    | 2:13B:146:GLY:N    | 2.16                     | 0.68              |
| 2:1B:219:THR:HA    | 1:1C:326:LYS:HE2   | 1.74                     | 0.68              |
| 2:1D:388:MET:HE2   | 1:1E:348:PRO:HD2   | 1.74                     | 0.68              |
| 2:9B:73:MET:HA     | 2:9B:73:MET:HE3    | 1.76                     | 0.68              |
| 1:12E:395:PHE:O    | 1:12E:399:TYR:N    | 2.19                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13A:63:PRO:HD3   | 1:13A:86:LEU:HG    | 1.76                     | 0.68              |
| 1:13A:358:GLN:NE2  | 1:13A:359:PRO:O    | 2.25                     | 0.68              |
| 2:8B:12:CYS:SG     | 2:8B:138:SER:OG    | 2.38                     | 0.68              |
| 2:13D:14:ASN:O     | 2:13D:18:ALA:N     | 2.26                     | 0.68              |
| 1:10A:102:ASN:HB2  | 1:10A:105:ARG:HB2  | 1.76                     | 0.68              |
| 2:13D:90:PHE:HB3   | 2:13D:92:PHE:HE2   | 1.57                     | 0.68              |
| 2:11B:245:GLN:HB2  | 2:11B:323:MET:HE3  | 1.76                     | 0.68              |
| 2:1B:49:VAL:HG11   | 2:1B:241:ARG:HG2   | 1.76                     | 0.68              |
| 1:5A:20:CYS:HB3    | 1:5A:24:TYR:HE2    | 1.57                     | 0.68              |
| 1:5C:195:LEU:HD12  | 1:5C:428:LEU:HD22  | 1.76                     | 0.68              |
| 1:5E:108:TYR:O     | 1:5E:112:LYS:NZ    | 2.24                     | 0.68              |
| 1:12C:35:GLN:HE22  | 1:12C:37:PRO:HG3   | 1.58                     | 0.68              |
| 1:13E:111:GLY:HA2  | 1:13E:149:PHE:CE1  | 2.28                     | 0.68              |
| 1:4C:11:GLN:NE2    | 2:4D:245:GLN:O     | 2.27                     | 0.68              |
| 1:11E:63:PRO:HD3   | 1:11E:86:LEU:HG    | 1.75                     | 0.68              |
| 1:12A:139:HIS:CD2  | 1:12A:150:THR:HG21 | 2.29                     | 0.68              |
| 2:12B:175:VAL:HG22 | 1:12C:329:ASN:HD21 | 1.58                     | 0.68              |
| 1:13A:101:ASN:HA   | 1:13A:144:GLY:H    | 1.59                     | 0.68              |
| 2:7B:61:PRO:HD3    | 2:7B:84:ILE:HG22   | 1.76                     | 0.68              |
| 2:10B:193:VAL:HG13 | 2:10B:194:GLU:HG3  | 1.75                     | 0.67              |
| 1:11C:270:VAL:H    | 1:11C:302:MET:CE   | 2.06                     | 0.67              |
| 1:12E:226:ASN:ND2  | 1:12E:367:ASP:OD2  | 2.27                     | 0.67              |
| 2:7B:213:ARG:O     | 2:7B:216:LYS:NZ    | 2.26                     | 0.67              |
| 1:10A:144:GLY:N    | 3:10A:500:GTP:O3G  | 2.27                     | 0.67              |
| 1:12A:106:GLY:HA3  | 1:12A:148:GLY:HA3  | 1.76                     | 0.67              |
| 1:1E:108:TYR:HA    | 1:1E:112:LYS:NZ    | 2.09                     | 0.67              |
| 2:6D:218:THR:O     | 1:6E:326:LYS:NZ    | 2.26                     | 0.67              |
| 1:11E:224:TYR:O    | 1:11E:228:ASN:ND2  | 2.28                     | 0.67              |
| 1:6A:180:ALA:HB3   | 1:6A:183:GLU:HG3   | 1.75                     | 0.67              |
| 1:9A:215:ARG:NH2   | 1:9A:299:ALA:O     | 2.24                     | 0.67              |
| 1:13A:226:ASN:ND2  | 1:13A:367:ASP:OD2  | 2.27                     | 0.67              |
| 1:13C:333:ALA:HA   | 1:13C:336:LYS:HB2  | 1.77                     | 0.67              |
| 1:4A:180:ALA:HB3   | 1:4A:183:GLU:HG3   | 1.74                     | 0.67              |
| 2:6B:252:LYS:O     | 2:6B:256:ASN:ND2   | 2.27                     | 0.67              |
| 1:12E:139:HIS:CD2  | 1:12E:150:THR:HG21 | 2.28                     | 0.67              |
| 2:1B:18:ALA:O      | 2:1B:22:GLU:HG3    | 1.94                     | 0.67              |
| 1:8E:102:ASN:HB2   | 1:8E:105:ARG:HB2   | 1.75                     | 0.67              |
| 2:11B:109:GLY:HA2  | 2:11B:147:MET:HE1  | 1.74                     | 0.67              |
| 1:13C:269:LEU:HG   | 1:13C:303:VAL:HG21 | 1.76                     | 0.67              |
| 2:6D:3:GLU:HG2     | 2:6D:62:ARG:HH22   | 1.60                     | 0.67              |
| 1:7A:71:GLU:HB2    | 1:7A:98:ASP:HB3    | 1.74                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:10A:89:PRO:HG2   | 1:11A:280:LYS:HD2  | 1.76                     | 0.67              |
| 1:11A:422:ARG:HA   | 1:11A:425:LEU:HB2  | 1.75                     | 0.67              |
| 1:11C:35:GLN:HE22  | 1:11C:37:PRO:HG3   | 1.59                     | 0.67              |
| 2:13D:263:LEU:HG   | 2:13D:422:TYR:HE1  | 1.58                     | 0.67              |
| 1:1C:180:ALA:HB3   | 1:1C:183:GLU:HG3   | 1.77                     | 0.67              |
| 2:4B:248:ALA:HA    | 2:4B:252:LYS:HD3   | 1.76                     | 0.67              |
| 1:5E:71:GLU:HB2    | 1:5E:98:ASP:HB3    | 1.75                     | 0.67              |
| 2:12D:407:GLU:HA   | 2:12D:410:GLU:HB2  | 1.77                     | 0.67              |
| 2:1B:209:ASP:OD1   | 2:1B:213:ARG:NH1   | 2.27                     | 0.67              |
| 1:4A:11:GLN:NE2    | 2:4B:245:GLN:O     | 2.28                     | 0.67              |
| 1:8A:145:THR:OG1   | 3:8A:500:GTP:O3B   | 2.12                     | 0.67              |
| 2:11D:293:MET:HE1  | 2:11D:365:ALA:HB1  | 1.76                     | 0.67              |
| 1:5C:180:ALA:HB3   | 1:5C:183:GLU:HG3   | 1.76                     | 0.67              |
| 2:7B:12:CYS:SG     | 2:7B:138:SER:OG    | 2.42                     | 0.67              |
| 1:9A:5:ILE:HG12    | 1:9A:64:ARG:HG2    | 1.75                     | 0.67              |
| 1:13A:91:GLN:HA    | 1:13A:121:ARG:NH1  | 2.10                     | 0.67              |
| 2:13D:334:GLN:HA   | 2:13D:341:PHE:CZ   | 2.30                     | 0.67              |
| 1:2A:71:GLU:OE2    | 1:2A:73:THR:OG1    | 2.11                     | 0.67              |
| 2:2B:178:THR:HB    | 2:2B:181:GLU:HG3   | 1.76                     | 0.67              |
| 1:12E:106:GLY:HA3  | 1:12E:148:GLY:HA3  | 1.77                     | 0.66              |
| 2:3B:10:GLY:O      | 2:3B:14:ASN:ND2    | 2.28                     | 0.66              |
| 2:4B:282:ARG:NH2   | 2:4B:292:GLN:OE1   | 2.29                     | 0.66              |
| 1:8A:204:VAL:HG11  | 1:8A:231:ILE:HD11  | 1.77                     | 0.66              |
| 2:8B:263:LEU:HG    | 2:8B:422:TYR:HE1   | 1.58                     | 0.66              |
| 1:8E:169:PHE:CE2   | 1:8E:235:VAL:HG22  | 2.30                     | 0.66              |
| 1:13E:195:LEU:HD21 | 1:13E:264:ARG:HG2  | 1.77                     | 0.66              |
| 2:2D:382:SER:O     | 2:2D:386:THR:OG1   | 2.13                     | 0.66              |
| 1:7E:206:ASN:OD1   | 3:7E:500:GTP:O2'   | 2.14                     | 0.66              |
| 2:8B:237:THR:O     | 2:8B:241:ARG:NH1   | 2.29                     | 0.66              |
| 1:10E:91:GLN:HA    | 1:10E:121:ARG:NH1  | 2.10                     | 0.66              |
| 1:13C:104:ALA:HB3  | 1:13C:105:ARG:NH2  | 2.10                     | 0.66              |
| 1:13C:209:ILE:HG21 | 1:13C:227:LEU:HG   | 1.78                     | 0.66              |
| 2:1B:324:LYS:O     | 2:1B:328:GLU:HG2   | 1.95                     | 0.66              |
| 1:2A:180:ALA:HB3   | 1:2A:183:GLU:HG3   | 1.77                     | 0.66              |
| 1:4E:292:THR:HG21  | 1:4E:331:ALA:HB1   | 1.77                     | 0.66              |
| 1:10C:286:LEU:HB3  | 1:10C:291:ILE:HD11 | 1.78                     | 0.66              |
| 1:11C:286:LEU:O    | 1:11C:373:ARG:NH1  | 2.29                     | 0.66              |
| 2:11D:99:ASN:ND2   | 1:11E:254:GLU:OE2  | 2.27                     | 0.66              |
| 1:11E:313:MET:SD   | 1:11E:313:MET:N    | 2.68                     | 0.66              |
| 1:12C:286:LEU:O    | 1:12C:373:ARG:NH1  | 2.28                     | 0.66              |
| 2:12D:256:ASN:HB2  | 2:12D:350:LYS:NZ   | 2.09                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:10A:213:CYS:HB2  | 1:10A:219:ILE:HD11 | 1.78                     | 0.66              |
| 1:11C:175:PRO:HB3  | 1:11C:390:ARG:CZ   | 2.25                     | 0.66              |
| 1:1A:339:ARG:O     | 1:1A:342:GLN:NE2   | 2.28                     | 0.66              |
| 1:2E:339:ARG:O     | 1:2E:342:GLN:NE2   | 2.29                     | 0.66              |
| 1:7E:292:THR:HG21  | 1:7E:331:ALA:HB1   | 1.77                     | 0.66              |
| 1:10C:226:ASN:ND2  | 1:10C:367:ASP:OD2  | 2.29                     | 0.66              |
| 2:12D:414:ASN:O    | 2:12D:418:LEU:N    | 2.24                     | 0.66              |
| 1:4A:206:ASN:OD1   | 3:4A:500:GTP:O2'   | 2.13                     | 0.66              |
| 1:5E:180:ALA:HB3   | 1:5E:183:GLU:HG3   | 1.78                     | 0.66              |
| 1:7A:11:GLN:O      | 1:7A:15:GLN:HG2    | 1.95                     | 0.66              |
| 1:7C:91:GLN:HA     | 1:7C:121:ARG:HH12  | 1.60                     | 0.66              |
| 1:7E:11:GLN:O      | 1:7E:15:GLN:HG2    | 1.95                     | 0.66              |
| 1:8C:180:ALA:HB3   | 1:8C:183:GLU:HG3   | 1.78                     | 0.66              |
| 1:8E:213:CYS:HB2   | 1:8E:219:ILE:HD11  | 1.76                     | 0.66              |
| 1:11A:213:CYS:HB2  | 1:11A:219:ILE:HD11 | 1.77                     | 0.66              |
| 1:11C:295:CYS:HB3  | 1:11C:377:MET:HG2  | 1.78                     | 0.66              |
| 2:12B:331:LEU:HA   | 2:12B:334:GLN:HB2  | 1.78                     | 0.66              |
| 1:1C:292:THR:HG21  | 1:1C:331:ALA:HB1   | 1.77                     | 0.66              |
| 1:1E:2:ARG:HD3     | 1:1E:242:LEU:HD22  | 1.78                     | 0.66              |
| 1:3A:339:ARG:O     | 1:3A:342:GLN:NE2   | 2.28                     | 0.66              |
| 1:6A:221:ARG:HA    | 2:6B:324:LYS:HE2   | 1.77                     | 0.66              |
| 1:7C:226:ASN:ND2   | 1:7C:367:ASP:OD1   | 2.29                     | 0.66              |
| 2:8B:382:SER:O     | 2:8B:386:THR:HG23  | 1.96                     | 0.66              |
| 1:8C:172:TYR:HB3   | 1:8C:205:ASP:OD1   | 1.95                     | 0.66              |
| 1:13A:164:LYS:O    | 1:13A:166:LYS:NZ   | 2.29                     | 0.66              |
| 2:1D:324:LYS:HG3   | 2:1D:325:GLU:N     | 2.10                     | 0.66              |
| 2:4B:49:VAL:HG11   | 2:4B:241:ARG:HG2   | 1.78                     | 0.66              |
| 1:9A:398:MET:HE1   | 2:9B:346:PRO:HD2   | 1.77                     | 0.66              |
| 2:12D:293:MET:HE1  | 2:12D:365:ALA:HB1  | 1.78                     | 0.66              |
| 2:5D:175:VAL:HG13  | 1:5E:329:ASN:HD22  | 1.60                     | 0.66              |
| 1:5E:226:ASN:ND2   | 1:5E:367:ASP:OD2   | 2.28                     | 0.66              |
| 1:7C:292:THR:HG21  | 1:7C:331:ALA:HB1   | 1.77                     | 0.66              |
| 2:10B:4:ILE:HG13   | 2:10B:132:GLY:O    | 1.95                     | 0.66              |
| 2:10D:193:VAL:HG13 | 2:10D:194:GLU:HG3  | 1.78                     | 0.66              |
| 1:5A:108:TYR:O     | 1:5A:112:LYS:NZ    | 2.29                     | 0.66              |
| 1:7A:3:GLU:OE1     | 1:7A:64:ARG:NH2    | 2.29                     | 0.66              |
| 1:7A:226:ASN:ND2   | 1:7A:367:ASP:OD1   | 2.29                     | 0.66              |
| 1:11C:421:ALA:O    | 1:11C:425:LEU:N    | 2.28                     | 0.65              |
| 2:13D:387:ALA:O    | 2:13D:391:ARG:NH2  | 2.27                     | 0.65              |
| 2:8B:286:VAL:HG12  | 2:8B:329:GLN:HE22  | 1.60                     | 0.65              |
| 1:8C:169:PHE:CE2   | 1:8C:235:VAL:HG22  | 2.31                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:13D:331:LEU:HA   | 2:13D:334:GLN:HB2  | 1.78                     | 0.65              |
| 1:13E:320:ARG:HG3  | 1:13E:360:PRO:HG3  | 1.78                     | 0.65              |
| 2:2D:178:THR:HB    | 2:2D:181:GLU:HG3   | 1.78                     | 0.65              |
| 1:6C:221:ARG:HA    | 2:6D:324:LYS:HD3   | 1.78                     | 0.65              |
| 1:9C:88:HIS:HD2    | 1:9C:89:PRO:HD2    | 1.60                     | 0.65              |
| 1:10E:26:LEU:HD12  | 1:10E:363:VAL:HG12 | 1.78                     | 0.65              |
| 1:7E:71:GLU:HB2    | 1:7E:98:ASP:HB3    | 1.76                     | 0.65              |
| 1:8C:402:ARG:HH22  | 1:8C:415:GLU:HB2   | 1.60                     | 0.65              |
| 1:8C:404:PHE:HE2   | 2:8D:256:ASN:HA    | 1.59                     | 0.65              |
| 2:8D:412:GLU:OE1   | 2:8D:416:ASN:ND2   | 2.28                     | 0.65              |
| 1:9C:145:THR:OG1   | 3:9C:500:GTP:O3B   | 2.14                     | 0.65              |
| 2:10B:175:VAL:HG22 | 1:10C:329:ASN:HD21 | 1.62                     | 0.65              |
| 1:10E:35:GLN:HE22  | 1:10E:37:PRO:HG3   | 1.61                     | 0.65              |
| 1:10E:91:GLN:HA    | 1:10E:121:ARG:HH12 | 1.61                     | 0.65              |
| 2:11D:211:CYS:HB2  | 2:11D:217:LEU:HD12 | 1.79                     | 0.65              |
| 1:11E:31:GLN:HG2   | 1:11E:32:PRO:HD2   | 1.77                     | 0.65              |
| 2:2B:376:GLU:HA    | 2:2B:379:LYS:HE2   | 1.77                     | 0.65              |
| 1:6C:398:MET:HE1   | 2:6D:345:ILE:HA    | 1.79                     | 0.65              |
| 2:7D:109:GLY:HA3   | 2:7D:147:MET:HE1   | 1.78                     | 0.65              |
| 1:8E:5:ILE:HG12    | 1:8E:64:ARG:HG2    | 1.79                     | 0.65              |
| 1:10A:26:LEU:HD12  | 1:10A:363:VAL:HG12 | 1.78                     | 0.65              |
| 1:12E:112:LYS:HA   | 1:12E:115:VAL:HG12 | 1.78                     | 0.65              |
| 2:5D:193:VAL:HG13  | 2:5D:194:GLU:HG3   | 1.78                     | 0.65              |
| 1:6C:32:PRO:HB3    | 1:6C:83:TYR:CE1    | 2.31                     | 0.65              |
| 1:10E:213:CYS:HB2  | 1:10E:219:ILE:HD11 | 1.76                     | 0.65              |
| 2:11D:267:MET:HE1  | 2:11D:303:CYS:HB2  | 1.79                     | 0.65              |
| 2:13D:237:THR:OG1  | 2:13D:241:ARG:NH1  | 2.30                     | 0.65              |
| 1:8E:180:ALA:HB3   | 1:8E:183:GLU:HG3   | 1.78                     | 0.65              |
| 1:13A:103:TYR:O    | 1:13A:148:GLY:HA3  | 1.97                     | 0.65              |
| 1:13A:209:ILE:HG21 | 1:13A:227:LEU:HG   | 1.78                     | 0.65              |
| 1:13C:226:ASN:ND2  | 1:13C:367:ASP:OD2  | 2.30                     | 0.65              |
| 2:13D:309:ARG:N    | 2:13D:372:THR:OG1  | 2.30                     | 0.65              |
| 1:1C:339:ARG:O     | 1:1C:342:GLN:NE2   | 2.29                     | 0.65              |
| 1:7A:292:THR:HG21  | 1:7A:331:ALA:HB1   | 1.79                     | 0.65              |
| 2:9D:388:MET:HE1   | 1:9E:348:PRO:HD2   | 1.79                     | 0.65              |
| 1:9E:175:PRO:HB3   | 1:9E:390:ARG:CZ    | 2.26                     | 0.65              |
| 2:8D:178:THR:HB    | 2:8D:181:GLU:HG3   | 1.78                     | 0.65              |
| 1:8E:169:PHE:HE2   | 1:8E:235:VAL:HG22  | 1.61                     | 0.65              |
| 1:10C:145:THR:OG1  | 3:10C:500:GTP:O3B  | 2.11                     | 0.65              |
| 1:13A:184:PRO:HG2  | 1:13A:398:MET:HE1  | 1.79                     | 0.65              |
| 1:1A:180:ALA:HB3   | 1:1A:183:GLU:HG3   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:6A:252:LEU:O    | 1:6A:256:GLN:NE2   | 2.30                     | 0.65              |
| 2:6B:49:VAL:HG11  | 2:6B:241:ARG:HG2   | 1.79                     | 0.65              |
| 2:6B:128:ASP:OD1  | 2:6B:129:CYS:N     | 2.29                     | 0.65              |
| 1:6E:180:ALA:HB3  | 1:6E:183:GLU:HG3   | 1.79                     | 0.65              |
| 1:10A:16:ILE:HD11 | 1:10A:171:ILE:HD11 | 1.79                     | 0.65              |
| 2:6B:117:LEU:HA   | 2:6B:120:VAL:HG22  | 1.79                     | 0.65              |
| 2:12B:121:ARG:NH2 | 2:12B:158:GLU:OE2  | 2.29                     | 0.64              |
| 2:12D:121:ARG:NH2 | 2:12D:158:GLU:OE2  | 2.29                     | 0.64              |
| 1:1A:292:THR:HG21 | 1:1A:331:ALA:HB1   | 1.79                     | 0.64              |
| 2:1D:49:VAL:HG11  | 2:1D:241:ARG:HG2   | 1.78                     | 0.64              |
| 2:6B:193:VAL:HG13 | 2:6B:194:GLU:HG3   | 1.79                     | 0.64              |
| 2:13D:142:GLY:O   | 2:13D:146:GLY:N    | 2.25                     | 0.64              |
| 1:13E:91:GLN:HA   | 1:13E:121:ARG:NH1  | 2.13                     | 0.64              |
| 1:2C:145:THR:OG1  | 3:2C:500:GTP:O3B   | 2.15                     | 0.64              |
| 1:2C:269:LEU:HD11 | 1:2C:384:ILE:HB    | 1.79                     | 0.64              |
| 1:4C:292:THR:HG21 | 1:4C:331:ALA:HB1   | 1.79                     | 0.64              |
| 1:5A:88:HIS:CD2   | 1:6A:283:HIS:HB3   | 2.31                     | 0.64              |
| 1:8A:180:ALA:HB3  | 1:8A:183:GLU:HG3   | 1.79                     | 0.64              |
| 2:9D:99:ASN:ND2   | 1:9E:254:GLU:OE2   | 2.30                     | 0.64              |
| 2:10D:320:ARG:NH1 | 2:10D:355:ASP:OD1  | 2.31                     | 0.64              |
| 1:13A:208:ALA:HB1 | 1:13A:302:MET:HA   | 1.79                     | 0.64              |
| 1:2A:371:VAL:HG12 | 1:2A:373:ARG:H     | 1.61                     | 0.64              |
| 1:3E:292:THR:HG21 | 1:3E:331:ALA:HB1   | 1.79                     | 0.64              |
| 2:5B:213:ARG:O    | 2:5B:216:LYS:NZ    | 2.29                     | 0.64              |
| 2:9B:5:VAL:HG12   | 2:9B:62:ARG:HG2    | 1.80                     | 0.64              |
| 1:12C:377:MET:HE1 | 1:12C:379:SER:HB3  | 1.80                     | 0.64              |
| 2:2B:3:GLU:HG2    | 2:2B:62:ARG:HH22   | 1.63                     | 0.64              |
| 2:3D:178:THR:HB   | 2:3D:181:GLU:HG3   | 1.78                     | 0.64              |
| 2:10B:12:CYS:SG   | 2:10B:138:SER:OG   | 2.43                     | 0.64              |
| 1:11E:306:ASP:OD2 | 1:11E:309:HIS:ND1  | 2.30                     | 0.64              |
| 2:13B:114:ASP:OD1 | 2:13B:115:SER:N    | 2.29                     | 0.64              |
| 2:13B:248:ALA:HA  | 2:13B:252:LYS:HD2  | 1.80                     | 0.64              |
| 1:5A:213:CYS:HB3  | 1:5A:219:ILE:HD11  | 1.79                     | 0.64              |
| 1:8C:195:LEU:HD12 | 1:8C:428:LEU:HD22  | 1.80                     | 0.64              |
| 2:9D:211:CYS:HB2  | 2:9D:217:LEU:HD12  | 1.78                     | 0.64              |
| 2:13B:378:PHE:O   | 2:13B:382:SER:N    | 2.26                     | 0.64              |
| 1:13C:213:CYS:HB3 | 1:13C:219:ILE:HD11 | 1.80                     | 0.64              |
| 1:2A:71:GLU:HB2   | 1:2A:98:ASP:HB3    | 1.79                     | 0.64              |
| 2:6D:61:PRO:HD3   | 2:6D:84:ILE:HG22   | 1.77                     | 0.64              |
| 2:8D:220:PRO:HD2  | 1:8E:326:LYS:HD3   | 1.77                     | 0.64              |
| 1:13A:319:TYR:HB3 | 1:13A:323:VAL:HG21 | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13A:424:ASP:O    | 1:13A:428:LEU:N    | 2.25                     | 0.64              |
| 1:13C:35:GLN:HE22  | 1:13C:37:PRO:HG3   | 1.62                     | 0.64              |
| 1:13C:69:ASP:OD1   | 1:13C:70:LEU:N     | 2.31                     | 0.64              |
| 1:13C:112:LYS:HA   | 1:13C:115:VAL:HG12 | 1.78                     | 0.64              |
| 1:7C:55:GLU:OE1    | 1:7C:61:HIS:NE2    | 2.31                     | 0.64              |
| 2:7D:193:VAL:HG13  | 2:7D:194:GLU:HG3   | 1.80                     | 0.64              |
| 2:10D:220:PRO:HD2  | 1:10E:326:LYS:HD3  | 1.78                     | 0.64              |
| 2:11B:226:ASN:OD1  | 5:11B:600:GDP:N1   | 2.25                     | 0.64              |
| 2:1B:121:ARG:O     | 2:1B:125:GLU:HG2   | 1.98                     | 0.64              |
| 1:2A:269:LEU:HD11  | 1:2A:384:ILE:HB    | 1.80                     | 0.64              |
| 1:3A:213:CYS:HB3   | 1:3A:219:ILE:HD11  | 1.78                     | 0.64              |
| 2:9B:287:PRO:HG3   | 2:9B:329:GLN:OE1   | 1.98                     | 0.64              |
| 2:13D:61:PRO:HG3   | 2:13D:84:ILE:HG22  | 1.80                     | 0.64              |
| 1:5E:123:ARG:NE    | 1:5E:161:TYR:OH    | 2.30                     | 0.64              |
| 1:7C:88:HIS:HD2    | 1:7C:89:PRO:HD2    | 1.61                     | 0.64              |
| 1:11C:31:GLN:HG2   | 1:11C:32:PRO:HD2   | 1.78                     | 0.64              |
| 1:2E:180:ALA:HB3   | 1:2E:183:GLU:HG3   | 1.79                     | 0.64              |
| 1:5A:104:ALA:HB2   | 1:5A:413:MET:HE2   | 1.79                     | 0.64              |
| 2:5B:130:LEU:HD12  | 2:5B:162:ARG:HD2   | 1.80                     | 0.64              |
| 2:5D:109:GLY:HA3   | 2:5D:147:MET:HE1   | 1.78                     | 0.64              |
| 1:6C:255:PHE:CZ    | 1:6C:378:LEU:HD22  | 2.33                     | 0.64              |
| 1:13E:422:ARG:HA   | 1:13E:425:LEU:HB2  | 1.80                     | 0.63              |
| 2:3D:49:VAL:HG11   | 2:3D:241:ARG:HG2   | 1.80                     | 0.63              |
| 2:6B:109:GLY:HA3   | 2:6B:147:MET:HE1   | 1.80                     | 0.63              |
| 2:10B:8:GLN:OE1    | 2:10B:17:GLY:HA3   | 1.98                     | 0.63              |
| 1:11A:34:GLY:O     | 1:11A:61:HIS:ND1   | 2.29                     | 0.63              |
| 1:12C:213:CYS:SG   | 1:12C:222:PRO:HG3  | 2.39                     | 0.63              |
| 1:1C:213:CYS:HB3   | 1:1C:219:ILE:HD11  | 1.79                     | 0.63              |
| 2:3B:213:ARG:NH1   | 2:3B:297:LYS:HD2   | 2.13                     | 0.63              |
| 2:5B:117:LEU:HA    | 2:5B:120:VAL:HG22  | 1.78                     | 0.63              |
| 2:6B:98:GLY:HA2    | 1:6C:254:GLU:HB3   | 1.79                     | 0.63              |
| 1:8C:102:ASN:HB3   | 1:8C:105:ARG:H     | 1.63                     | 0.63              |
| 1:12E:224:TYR:O    | 1:12E:228:ASN:ND2  | 2.31                     | 0.63              |
| 2:13D:190:HIS:HB2  | 2:13D:411:ALA:HB2  | 1.79                     | 0.63              |
| 2:6B:298:ASN:O     | 2:6B:298:ASN:ND2   | 2.30                     | 0.63              |
| 2:8D:193:VAL:HG13  | 2:8D:194:GLU:HG3   | 1.79                     | 0.63              |
| 2:9D:178:THR:HB    | 2:9D:181:GLU:HG3   | 1.80                     | 0.63              |
| 2:12B:67:ASP:HB3   | 2:12B:92:PHE:HB3   | 1.81                     | 0.63              |
| 2:12D:203:ASP:OD2  | 2:12D:302:ALA:N    | 2.19                     | 0.63              |
| 2:13D:4:ILE:HB     | 2:13D:50:TYR:HE1   | 1.64                     | 0.63              |
| 1:13E:102:ASN:HD22 | 1:13E:105:ARG:HD3  | 1.63                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3E:20:CYS:HB3    | 1:3E:24:TYR:HE1    | 1.63                     | 0.63              |
| 2:10D:382:SER:O    | 2:10D:386:THR:OG1  | 2.15                     | 0.63              |
| 1:13A:213:CYS:HB3  | 1:13A:219:ILE:HD11 | 1.81                     | 0.63              |
| 2:13B:73:MET:HA    | 2:13B:76:VAL:HG12  | 1.81                     | 0.63              |
| 1:13C:195:LEU:HD21 | 1:13C:264:ARG:HG2  | 1.80                     | 0.63              |
| 1:13E:31:GLN:HG3   | 1:13E:35:GLN:HE21  | 1.63                     | 0.63              |
| 1:7A:313:MET:HB3   | 1:7A:380:ASN:O     | 1.98                     | 0.63              |
| 2:7B:98:GLY:HA2    | 1:7C:254:GLU:HG2   | 1.81                     | 0.63              |
| 2:7D:178:THR:HB    | 2:7D:181:GLU:HG3   | 1.80                     | 0.63              |
| 2:10D:173:PRO:HG3  | 2:10D:380:ARG:HD3  | 1.80                     | 0.63              |
| 1:10E:204:VAL:HG11 | 1:10E:231:ILE:HD11 | 1.80                     | 0.63              |
| 1:12A:112:LYS:HA   | 1:12A:115:VAL:HG12 | 1.79                     | 0.63              |
| 2:12B:334:GLN:HA   | 2:12B:341:PHE:CZ   | 2.33                     | 0.63              |
| 1:13A:75:VAL:O     | 1:13A:78:VAL:HG22  | 1.98                     | 0.63              |
| 2:13B:55:SER:H     | 1:1E:285:GLN:HG2   | 1.61                     | 0.63              |
| 2:13B:121:ARG:NH2  | 2:13B:158:GLU:OE2  | 2.29                     | 0.63              |
| 1:1E:180:ALA:HB3   | 1:1E:183:GLU:HG3   | 1.81                     | 0.63              |
| 2:3D:248:ALA:HA    | 2:3D:252:LYS:HD3   | 1.80                     | 0.63              |
| 1:4E:91:GLN:HA     | 1:4E:121:ARG:HH12  | 1.62                     | 0.63              |
| 1:5E:102:ASN:HB2   | 1:5E:105:ARG:HB2   | 1.80                     | 0.63              |
| 1:7C:252:LEU:O     | 1:7C:256:GLN:NE2   | 2.32                     | 0.63              |
| 1:9E:215:ARG:NH2   | 1:9E:299:ALA:O     | 2.25                     | 0.63              |
| 2:11B:388:MET:HE3  | 2:11B:393:ALA:HB3  | 1.81                     | 0.63              |
| 2:12B:334:GLN:HA   | 2:12B:341:PHE:CE2  | 2.34                     | 0.63              |
| 1:12C:54:SER:OG    | 1:12C:64:ARG:NH2   | 2.32                     | 0.63              |
| 1:13A:200:CYS:HB2  | 1:13A:256:GLN:HE22 | 1.63                     | 0.63              |
| 1:13A:261:PRO:HG2  | 1:13A:265:ILE:HD12 | 1.81                     | 0.63              |
| 1:13E:113:GLU:HG2  | 1:13E:114:ILE:HG13 | 1.81                     | 0.63              |
| 1:1A:221:ARG:CA    | 2:1B:324:LYS:HZ1   | 2.12                     | 0.63              |
| 2:3B:173:PRO:HD2   | 2:3B:380:ARG:HH21  | 1.64                     | 0.63              |
| 1:5E:88:HIS:CD2    | 1:6E:283:HIS:HB3   | 2.32                     | 0.63              |
| 1:10A:224:TYR:O    | 1:10A:228:ASN:ND2  | 2.32                     | 0.63              |
| 2:13B:67:ASP:OD1   | 2:13B:68:LEU:N     | 2.27                     | 0.63              |
| 1:1E:292:THR:HG21  | 1:1E:331:ALA:HB1   | 1.78                     | 0.63              |
| 1:2A:306:ASP:OD2   | 1:2A:309:HIS:ND1   | 2.32                     | 0.63              |
| 1:7A:188:ILE:HG22  | 1:7A:421:ALA:HB1   | 1.80                     | 0.63              |
| 1:7E:226:ASN:ND2   | 1:7E:367:ASP:OD1   | 2.32                     | 0.63              |
| 1:10C:30:ILE:HD11  | 1:10C:61:HIS:HB2   | 1.81                     | 0.63              |
| 1:11C:224:TYR:O    | 1:11C:228:ASN:ND2  | 2.32                     | 0.63              |
| 1:12E:213:CYS:HB3  | 1:12E:219:ILE:HD11 | 1.80                     | 0.63              |
| 1:4A:98:ASP:OD1    | 1:4A:145:THR:OG1   | 2.14                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6A:317:MET:HE1   | 1:6A:377:MET:HG2   | 1.79                     | 0.63              |
| 1:9E:180:ALA:HB3   | 1:9E:183:GLU:HG3   | 1.81                     | 0.63              |
| 1:9E:402:ARG:HH22  | 1:9E:415:GLU:HB3   | 1.64                     | 0.63              |
| 1:10C:214:ARG:HH22 | 2:10D:328:GLU:HG3  | 1.63                     | 0.62              |
| 1:13C:423:GLU:O    | 1:13C:427:ALA:N    | 2.23                     | 0.62              |
| 1:1C:199:ASP:HB3   | 1:1C:256:GLN:HE22  | 1.64                     | 0.62              |
| 1:4C:91:GLN:HA     | 1:4C:121:ARG:HH12  | 1.64                     | 0.62              |
| 2:5D:191:GLN:HE21  | 2:5D:195:ASN:HD22  | 1.47                     | 0.62              |
| 2:6B:190:HIS:NE2   | 2:6B:414:ASN:OD1   | 2.32                     | 0.62              |
| 1:11C:398:MET:HE1  | 2:11D:345:ILE:HD13 | 1.81                     | 0.62              |
| 1:1E:339:ARG:O     | 1:1E:342:GLN:NE2   | 2.32                     | 0.62              |
| 1:2C:180:ALA:HB3   | 1:2C:183:GLU:HG3   | 1.80                     | 0.62              |
| 2:3B:121:ARG:NH2   | 2:3B:158:GLU:OE2   | 2.31                     | 0.62              |
| 2:4D:190:HIS:NE2   | 2:4D:414:ASN:OD1   | 2.32                     | 0.62              |
| 2:6B:237:THR:O     | 2:6B:241:ARG:NH1   | 2.33                     | 0.62              |
| 2:8B:193:VAL:HG13  | 2:8B:194:GLU:HG3   | 1.79                     | 0.62              |
| 1:9C:53:PHE:O      | 1:9C:64:ARG:NH1    | 2.32                     | 0.62              |
| 1:12A:213:CYS:HB3  | 1:12A:219:ILE:HD11 | 1.81                     | 0.62              |
| 2:13D:121:ARG:NH2  | 2:13D:158:GLU:OE2  | 2.30                     | 0.62              |
| 1:13E:35:GLN:HE22  | 1:13E:37:PRO:HG3   | 1.64                     | 0.62              |
| 1:13E:70:LEU:HA    | 1:13E:95:GLY:HA3   | 1.80                     | 0.62              |
| 1:1A:108:TYR:HA    | 1:1A:112:LYS:NZ    | 2.14                     | 0.62              |
| 2:2D:3:GLU:OE2     | 2:2D:62:ARG:NH2    | 2.32                     | 0.62              |
| 2:3D:3:GLU:OE1     | 2:3D:3:GLU:N       | 2.31                     | 0.62              |
| 2:6D:326:VAL:HG11  | 2:6D:351:THR:HG21  | 1.81                     | 0.62              |
| 1:9C:88:HIS:NE2    | 1:9C:90:GLU:OE1    | 2.32                     | 0.62              |
| 1:10C:63:PRO:HD3   | 1:10C:86:LEU:HG    | 1.81                     | 0.62              |
| 2:10D:121:ARG:NH2  | 2:10D:158:GLU:OE2  | 2.32                     | 0.62              |
| 2:13B:390:ARG:HG3  | 2:13B:391:ARG:HD3  | 1.79                     | 0.62              |
| 1:3C:339:ARG:O     | 1:3C:342:GLN:NE2   | 2.32                     | 0.62              |
| 1:3E:339:ARG:O     | 1:3E:342:GLN:NE2   | 2.32                     | 0.62              |
| 2:4D:248:ALA:HA    | 2:4D:252:LYS:HD3   | 1.81                     | 0.62              |
| 1:5E:88:HIS:HB3    | 1:5E:90:GLU:OE2    | 1.99                     | 0.62              |
| 2:7D:61:PRO:HD3    | 2:7D:84:ILE:HG22   | 1.82                     | 0.62              |
| 1:8C:16:ILE:HD11   | 1:8C:171:ILE:HD11  | 1.80                     | 0.62              |
| 1:9E:150:THR:HG22  | 1:9E:154:MET:HE1   | 1.80                     | 0.62              |
| 2:12D:390:ARG:HG3  | 2:12D:391:ARG:HD3  | 1.82                     | 0.62              |
| 1:13E:69:ASP:OD1   | 1:13E:70:LEU:N     | 2.32                     | 0.62              |
| 1:6A:292:THR:HG21  | 1:6A:331:ALA:HB1   | 1.81                     | 0.62              |
| 2:6B:287:PRO:HG3   | 2:6B:329:GLN:NE2   | 2.14                     | 0.62              |
| 2:7D:12:CYS:SG     | 2:7D:138:SER:OG    | 2.43                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:8A:188:ILE:HG22 | 1:8A:421:ALA:HB1   | 1.79                     | 0.62              |
| 2:8B:220:PRO:HD2  | 1:8C:326:LYS:HD3   | 1.79                     | 0.62              |
| 2:9B:128:ASP:OD1  | 2:9B:129:CYS:N     | 2.32                     | 0.62              |
| 2:11B:309:ARG:NH1 | 2:11B:426:GLN:OXT  | 2.32                     | 0.62              |
| 1:12E:90:GLU:O    | 1:12E:121:ARG:NH1  | 2.30                     | 0.62              |
| 1:13C:169:PHE:CE1 | 1:13C:235:VAL:HG22 | 2.34                     | 0.62              |
| 1:2A:213:CYS:HB3  | 1:2A:219:ILE:HD11  | 1.81                     | 0.62              |
| 2:2D:49:VAL:HG11  | 2:2D:241:ARG:HG2   | 1.81                     | 0.62              |
| 1:4C:195:LEU:HD12 | 1:4C:428:LEU:HD22  | 1.81                     | 0.62              |
| 1:7C:145:THR:OG1  | 3:7C:500:GTP:O3B   | 2.17                     | 0.62              |
| 1:9A:188:ILE:HG22 | 1:9A:421:ALA:HB1   | 1.81                     | 0.62              |
| 2:10D:211:CYS:HB2 | 2:10D:217:LEU:HD12 | 1.82                     | 0.62              |
| 1:11C:88:HIS:CD2  | 1:11C:89:PRO:HD2   | 2.35                     | 0.62              |
| 2:11D:220:PRO:HD2 | 1:11E:326:LYS:HD3  | 1.80                     | 0.62              |
| 1:5C:88:HIS:CE1   | 1:6C:283:HIS:HB3   | 2.34                     | 0.62              |
| 1:10A:180:ALA:HB3 | 1:10A:183:GLU:HG3  | 1.80                     | 0.62              |
| 2:12B:12:CYS:SG   | 2:12B:138:SER:OG   | 2.57                     | 0.62              |
| 1:13C:104:ALA:HB1 | 1:13C:108:TYR:HD2  | 1.65                     | 0.62              |
| 1:1E:108:TYR:HA   | 1:1E:112:LYS:HZ3   | 1.64                     | 0.62              |
| 1:2C:221:ARG:HA   | 2:2D:324:LYS:NZ    | 2.14                     | 0.62              |
| 1:3C:98:ASP:OD1   | 1:3C:99:ALA:N      | 2.33                     | 0.62              |
| 1:5A:226:ASN:ND2  | 1:5A:367:ASP:OD2   | 2.33                     | 0.62              |
| 1:5C:102:ASN:HB2  | 1:5C:105:ARG:HB2   | 1.82                     | 0.62              |
| 2:9B:14:ASN:O     | 2:9B:18:ALA:N      | 2.33                     | 0.62              |
| 1:2A:102:ASN:HB2  | 1:2A:105:ARG:HB2   | 1.81                     | 0.62              |
| 1:7E:132:LEU:HD23 | 1:7E:164:LYS:HD3   | 1.81                     | 0.62              |
| 1:8A:213:CYS:HB2  | 1:8A:219:ILE:HD11  | 1.80                     | 0.62              |
| 1:9A:88:HIS:HD2   | 1:9A:89:PRO:HD2    | 1.64                     | 0.62              |
| 1:10C:69:ASP:OD1  | 1:10C:70:LEU:N     | 2.33                     | 0.62              |
| 1:12A:424:ASP:O   | 1:12A:428:LEU:N    | 2.26                     | 0.62              |
| 2:13D:67:ASP:OD1  | 2:13D:68:LEU:N     | 2.31                     | 0.62              |
| 2:4B:99:ASN:ND2   | 1:4C:254:GLU:OE2   | 2.33                     | 0.62              |
| 1:5A:216:ASN:HD22 | 1:5A:216:ASN:N     | 1.97                     | 0.62              |
| 1:6C:5:ILE:HG12   | 1:6C:64:ARG:HG2    | 1.82                     | 0.62              |
| 1:6E:123:ARG:NE   | 1:6E:161:TYR:OH    | 2.32                     | 0.62              |
| 1:13A:333:ALA:HA  | 1:13A:336:LYS:HB2  | 1.81                     | 0.61              |
| 1:13C:424:ASP:HA  | 1:13C:427:ALA:HB3  | 1.82                     | 0.61              |
| 1:13C:428:LEU:HG  | 1:13C:432:TYR:HE2  | 1.64                     | 0.61              |
| 2:2D:10:GLY:O     | 2:2D:14:ASN:ND2    | 2.27                     | 0.61              |
| 2:5D:282:ARG:NH2  | 2:5D:292:GLN:OE1   | 2.32                     | 0.61              |
| 1:8A:402:ARG:HH22 | 1:8A:415:GLU:HB3   | 1.63                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:285:THR:HG23  | 2:8B:287:PRO:HD2   | 1.82                     | 0.61              |
| 2:13B:309:ARG:N    | 2:13B:372:THR:OG1  | 2.29                     | 0.61              |
| 2:13D:407:GLU:HA   | 2:13D:410:GLU:HB2  | 1.82                     | 0.61              |
| 1:3A:69:ASP:OD1    | 1:3A:70:LEU:N      | 2.33                     | 0.61              |
| 1:3C:180:ALA:HB3   | 1:3C:183:GLU:HG3   | 1.82                     | 0.61              |
| 1:3E:180:ALA:HB3   | 1:3E:183:GLU:HG3   | 1.82                     | 0.61              |
| 2:6D:175:VAL:HG22  | 1:6E:329:ASN:HD21  | 1.65                     | 0.61              |
| 2:7D:67:ASP:HB2    | 2:7D:73:MET:HE3    | 1.81                     | 0.61              |
| 1:8C:188:ILE:HG22  | 1:8C:421:ALA:HB1   | 1.80                     | 0.61              |
| 1:9A:175:PRO:HD2   | 1:9A:207:GLU:OE1   | 2.00                     | 0.61              |
| 2:10B:263:LEU:HG   | 2:10B:422:TYR:CE1  | 2.35                     | 0.61              |
| 1:10E:88:HIS:CD2   | 1:10E:90:GLU:HG3   | 2.35                     | 0.61              |
| 1:11A:421:ALA:O    | 1:11A:425:LEU:N    | 2.33                     | 0.61              |
| 1:11C:286:LEU:HA   | 1:11C:290:GLU:OE1  | 2.01                     | 0.61              |
| 2:12B:140:GLY:O    | 2:12B:184:ASN:ND2  | 2.33                     | 0.61              |
| 1:13C:432:TYR:O    | 1:13C:436:GLY:N    | 2.29                     | 0.61              |
| 2:1B:389:PHE:O     | 2:1B:392:LYS:NZ    | 2.26                     | 0.61              |
| 1:4C:339:ARG:O     | 1:4C:342:GLN:NE2   | 2.33                     | 0.61              |
| 2:12D:334:GLN:HA   | 2:12D:341:PHE:CE2  | 2.35                     | 0.61              |
| 1:13E:139:HIS:CD2  | 1:13E:150:THR:HG21 | 2.35                     | 0.61              |
| 1:2E:261:PRO:HG3   | 1:2E:313:MET:SD    | 2.40                     | 0.61              |
| 1:4E:216:ASN:ND2   | 1:4E:300:ASN:OD1   | 2.33                     | 0.61              |
| 2:8B:263:LEU:HG    | 2:8B:422:TYR:CE1   | 2.36                     | 0.61              |
| 2:8B:388:MET:HE1   | 1:8C:348:PRO:HD2   | 1.82                     | 0.61              |
| 1:8E:226:ASN:ND2   | 1:8E:367:ASP:OD2   | 2.33                     | 0.61              |
| 1:11E:422:ARG:HA   | 1:11E:425:LEU:HB2  | 1.81                     | 0.61              |
| 1:4C:98:ASP:OD1    | 1:4C:99:ALA:N      | 2.33                     | 0.61              |
| 1:5A:339:ARG:O     | 1:5A:342:GLN:NE2   | 2.34                     | 0.61              |
| 2:6D:293:MET:HE2   | 2:6D:365:ALA:HB1   | 1.80                     | 0.61              |
| 2:8B:237:THR:HG22  | 2:8B:250:LEU:HD21  | 1.82                     | 0.61              |
| 2:12D:292:GLN:HE22 | 2:12D:298:ASN:HD22 | 1.48                     | 0.61              |
| 1:13A:169:PHE:CE1  | 1:13A:235:VAL:HG22 | 2.35                     | 0.61              |
| 2:13B:109:GLY:HA2  | 2:13B:147:MET:HE1  | 1.83                     | 0.61              |
| 2:13B:215:LEU:HB3  | 2:13B:217:LEU:HG   | 1.82                     | 0.61              |
| 1:13C:104:ALA:O    | 1:13C:108:TYR:N    | 2.30                     | 0.61              |
| 2:2B:213:ARG:CZ    | 2:2B:297:LYS:HD2   | 2.30                     | 0.61              |
| 2:4B:382:SER:O     | 2:4B:386:THR:OG1   | 2.15                     | 0.61              |
| 2:5D:173:PRO:HD2   | 2:5D:380:ARG:HH21  | 1.65                     | 0.61              |
| 2:7D:325:GLU:O     | 2:7D:329:GLN:HG2   | 2.01                     | 0.61              |
| 1:7E:213:CYS:HB3   | 1:7E:219:ILE:HD11  | 1.82                     | 0.61              |
| 1:8A:121:ARG:HB3   | 1:8A:121:ARG:NH1   | 2.16                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11C:306:ASP:OD2  | 1:11C:309:HIS:ND1  | 2.33                     | 0.61              |
| 2:13B:334:GLN:HA   | 2:13B:341:PHE:CZ   | 2.36                     | 0.61              |
| 1:13C:208:ALA:HB1  | 1:13C:302:MET:HA   | 1.80                     | 0.61              |
| 2:1B:121:ARG:NH1   | 2:1B:158:GLU:OE1   | 2.34                     | 0.61              |
| 2:1B:121:ARG:NH2   | 2:1B:158:GLU:OE2   | 2.33                     | 0.61              |
| 2:1D:263:LEU:HG    | 2:1D:422:TYR:CE1   | 2.35                     | 0.61              |
| 1:2A:56:THR:HA     | 1:3A:285:GLN:HB2   | 1.83                     | 0.61              |
| 2:2B:68:LEU:HD12   | 2:2B:143:THR:HG23  | 1.82                     | 0.61              |
| 1:8A:213:CYS:HA    | 1:8A:217:LEU:HB2   | 1.82                     | 0.61              |
| 1:8C:222:PRO:HD2   | 2:8D:324:LYS:HD3   | 1.82                     | 0.61              |
| 1:11A:3:GLU:OE2    | 1:11A:131:GLY:N    | 2.30                     | 0.61              |
| 1:13A:35:GLN:HE22  | 1:13A:37:PRO:HG3   | 1.64                     | 0.61              |
| 2:13D:378:PHE:O    | 2:13D:382:SER:N    | 2.25                     | 0.61              |
| 2:3B:232:THR:HG21  | 2:3B:268:PRO:HB3   | 1.81                     | 0.61              |
| 1:4A:339:ARG:O     | 1:4A:342:GLN:NE2   | 2.33                     | 0.61              |
| 1:6C:217:LEU:HD21  | 1:6C:367:ASP:HB3   | 1.83                     | 0.61              |
| 1:13C:352:LYS:NZ   | 1:13C:353:VAL:O    | 2.32                     | 0.61              |
| 1:13E:54:SER:OG    | 1:13E:64:ARG:NH1   | 2.31                     | 0.61              |
| 1:2A:145:THR:OG1   | 3:2A:500:GTP:O3B   | 2.14                     | 0.61              |
| 1:2E:145:THR:OG1   | 3:2E:500:GTP:O3B   | 2.16                     | 0.61              |
| 1:3C:213:CYS:HB3   | 1:3C:219:ILE:HD11  | 1.83                     | 0.61              |
| 1:8C:54:SER:OG     | 1:8C:64:ARG:NH2    | 2.34                     | 0.61              |
| 1:11A:102:ASN:HB2  | 1:11A:105:ARG:HB2  | 1.82                     | 0.61              |
| 1:12A:209:ILE:HG21 | 1:12A:227:LEU:HG   | 1.83                     | 0.61              |
| 2:13B:10:GLY:O     | 2:13B:14:ASN:ND2   | 2.33                     | 0.61              |
| 2:5B:130:LEU:HD11  | 2:5B:162:ARG:HH11  | 1.65                     | 0.61              |
| 2:5D:208:TYR:HA    | 2:5D:211:CYS:SG    | 2.40                     | 0.61              |
| 2:10D:178:THR:HB   | 2:10D:181:GLU:HG3  | 1.83                     | 0.60              |
| 2:4B:114:ASP:OD2   | 2:4B:115:SER:N     | 2.34                     | 0.60              |
| 2:6B:5:VAL:HG12    | 2:6B:62:ARG:HD2    | 1.83                     | 0.60              |
| 2:7B:211:CYS:HB2   | 2:7B:217:LEU:HD12  | 1.83                     | 0.60              |
| 2:9B:178:THR:HB    | 2:9B:181:GLU:HG3   | 1.82                     | 0.60              |
| 2:9B:263:LEU:HG    | 2:9B:422:TYR:CE1   | 2.35                     | 0.60              |
| 2:10B:220:PRO:HD2  | 1:10C:326:LYS:HD3  | 1.82                     | 0.60              |
| 1:13A:195:LEU:HD12 | 1:13A:428:LEU:HD22 | 1.82                     | 0.60              |
| 1:1C:74:VAL:HA     | 1:1C:77:GLU:OE2    | 2.00                     | 0.60              |
| 1:7C:101:ASN:OD1   | 2:7D:252:LYS:NZ    | 2.34                     | 0.60              |
| 1:9A:3:GLU:OE2     | 1:9A:131:GLY:N     | 2.33                     | 0.60              |
| 2:10D:128:ASP:OD1  | 2:10D:129:CYS:N    | 2.34                     | 0.60              |
| 1:10E:377:MET:HE1  | 1:10E:379:SER:HB3  | 1.83                     | 0.60              |
| 1:11C:3:GLU:OE2    | 1:11C:131:GLY:N    | 2.31                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11C:203:MET:O    | 1:11C:302:MET:SD   | 2.60                     | 0.60              |
| 1:13A:104:ALA:HB1  | 1:13A:108:TYR:HD2  | 1.66                     | 0.60              |
| 2:13D:156:ARG:NH2  | 2:13D:197:ASP:OD1  | 2.33                     | 0.60              |
| 2:13D:380:ARG:O    | 2:13D:384:GLN:HG3  | 2.00                     | 0.60              |
| 1:1C:202:PHE:HE1   | 1:1C:378:LEU:HD23  | 1.66                     | 0.60              |
| 1:3A:180:ALA:HB3   | 1:3A:183:GLU:HG3   | 1.83                     | 0.60              |
| 1:4E:195:LEU:HD12  | 1:4E:428:LEU:HD22  | 1.83                     | 0.60              |
| 1:4E:250:VAL:HG23  | 1:4E:254:GLU:HG2   | 1.83                     | 0.60              |
| 1:6A:214:ARG:HH12  | 2:6B:324:LYS:HD3   | 1.66                     | 0.60              |
| 2:6D:190:HIS:NE2   | 2:6D:414:ASN:OD1   | 2.34                     | 0.60              |
| 2:7B:117:LEU:HA    | 2:7B:120:VAL:HG22  | 1.83                     | 0.60              |
| 1:8A:49:PHE:HD2    | 1:8A:53:PHE:HB2    | 1.66                     | 0.60              |
| 1:8E:3:GLU:HB2     | 1:8E:132:LEU:HA    | 1.83                     | 0.60              |
| 1:8E:55:GLU:OE1    | 1:8E:61:HIS:NE2    | 2.35                     | 0.60              |
| 1:8E:71:GLU:OE2    | 1:8E:73:THR:OG1    | 2.16                     | 0.60              |
| 2:12B:215:LEU:HB3  | 2:12B:217:LEU:HG   | 1.84                     | 0.60              |
| 1:3C:20:CYS:HB3    | 1:3C:24:TYR:HE1    | 1.66                     | 0.60              |
| 2:4D:99:ASN:ND2    | 1:4E:254:GLU:OE2   | 2.34                     | 0.60              |
| 2:5D:99:ASN:ND2    | 1:5E:254:GLU:OE2   | 2.33                     | 0.60              |
| 2:6D:237:THR:O     | 2:6D:241:ARG:NH1   | 2.34                     | 0.60              |
| 2:7B:232:THR:HG21  | 2:7B:268:PRO:HB3   | 1.84                     | 0.60              |
| 2:8D:121:ARG:NH2   | 2:8D:158:GLU:OE2   | 2.34                     | 0.60              |
| 1:10C:209:ILE:HG21 | 1:10C:227:LEU:HG   | 1.81                     | 0.60              |
| 2:11D:163:ILE:HG21 | 2:11D:250:LEU:HD22 | 1.82                     | 0.60              |
| 1:12C:26:LEU:HD12  | 1:12C:363:VAL:HG12 | 1.83                     | 0.60              |
| 2:2D:285:THR:HB    | 2:2D:287:PRO:HD2   | 1.84                     | 0.60              |
| 1:5E:20:CYS:HB3    | 1:5E:24:TYR:HE2    | 1.66                     | 0.60              |
| 2:6B:237:THR:OG1   | 2:6B:241:ARG:NH1   | 2.35                     | 0.60              |
| 2:10B:121:ARG:NH2  | 2:10B:158:GLU:OE2  | 2.34                     | 0.60              |
| 2:11B:4:ILE:HG13   | 2:11B:132:GLY:O    | 2.02                     | 0.60              |
| 2:11B:203:ASP:OD2  | 2:11B:302:ALA:N    | 2.23                     | 0.60              |
| 2:12D:12:CYS:SG    | 2:12D:138:SER:OG   | 2.59                     | 0.60              |
| 1:12E:209:ILE:HD13 | 1:12E:302:MET:SD   | 2.40                     | 0.60              |
| 2:13B:127:CYS:SG   | 2:13B:130:LEU:HB3  | 2.42                     | 0.60              |
| 1:1E:195:LEU:HD12  | 1:1E:428:LEU:HD22  | 1.82                     | 0.60              |
| 2:2B:49:VAL:HG11   | 2:2B:241:ARG:HG2   | 1.84                     | 0.60              |
| 2:2D:121:ARG:NH1   | 2:2D:158:GLU:OE1   | 2.35                     | 0.60              |
| 1:2E:213:CYS:HB3   | 1:2E:219:ILE:HD11  | 1.83                     | 0.60              |
| 2:4D:285:THR:HB    | 2:4D:287:PRO:HD2   | 1.82                     | 0.60              |
| 1:5A:102:ASN:HB2   | 1:5A:105:ARG:HB2   | 1.82                     | 0.60              |
| 2:6B:213:ARG:HH11  | 2:6B:297:LYS:HE3   | 1.66                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:7C:188:ILE:HG22  | 1:7C:421:ALA:HB1  | 1.82                     | 0.60              |
| 1:8A:114:ILE:HB    | 1:8A:149:PHE:HZ   | 1.66                     | 0.60              |
| 1:8C:145:THR:OG1   | 3:8C:500:GTP:O3B  | 2.19                     | 0.60              |
| 1:9A:90:GLU:OE2    | 1:9A:121:ARG:NH2  | 2.33                     | 0.60              |
| 1:12A:142:GLY:O    | 1:12A:186:ASN:ND2 | 2.33                     | 0.60              |
| 1:12A:313:MET:N    | 1:12A:313:MET:SD  | 2.74                     | 0.60              |
| 2:2D:376:GLU:HA    | 2:2D:379:LYS:HG2  | 1.83                     | 0.60              |
| 2:5B:67:ASP:OD1    | 2:5B:68:LEU:N     | 2.34                     | 0.60              |
| 2:5D:121:ARG:NH2   | 2:5D:158:GLU:OE2  | 2.33                     | 0.60              |
| 2:6D:117:LEU:HA    | 2:6D:120:VAL:HG22 | 1.84                     | 0.60              |
| 2:6D:121:ARG:NH2   | 2:6D:158:GLU:OE2  | 2.34                     | 0.60              |
| 1:7A:339:ARG:O     | 1:7A:342:GLN:NE2  | 2.34                     | 0.60              |
| 1:8C:169:PHE:HE2   | 1:8C:235:VAL:HG22 | 1.66                     | 0.60              |
| 2:11B:193:VAL:HG13 | 2:11B:194:GLU:HG3 | 1.84                     | 0.60              |
| 1:1A:286:LEU:HA    | 1:1A:290:GLU:OE2  | 2.02                     | 0.60              |
| 2:1B:10:GLY:O      | 2:1B:14:ASN:ND2   | 2.33                     | 0.60              |
| 2:1D:113:VAL:HG22  | 2:1D:117:LEU:HD13 | 1.84                     | 0.60              |
| 2:1D:175:VAL:HG22  | 1:1E:329:ASN:HD21 | 1.67                     | 0.60              |
| 1:3C:108:TYR:O     | 1:3C:112:LYS:NZ   | 2.31                     | 0.60              |
| 1:4E:88:HIS:CD2    | 1:5E:283:HIS:HB3  | 2.36                     | 0.60              |
| 1:5C:213:CYS:HB3   | 1:5C:219:ILE:HD11 | 1.84                     | 0.60              |
| 2:5D:237:THR:O     | 2:5D:241:ARG:NH1  | 2.35                     | 0.60              |
| 2:7B:203:ASP:O     | 2:7B:207:LEU:HD23 | 2.02                     | 0.60              |
| 1:11A:221:ARG:HA   | 2:11B:324:LYS:HD3 | 1.83                     | 0.60              |
| 2:12D:226:ASN:ND2  | 5:12D:600:GDP:O6  | 2.32                     | 0.60              |
| 1:13C:140:SER:OG   | 3:13C:500:GTP:O2A | 2.20                     | 0.60              |
| 2:13D:267:MET:HE2  | 2:13D:299:MET:HE2 | 1.84                     | 0.60              |
| 2:1B:211:CYS:HB2   | 2:1B:217:LEU:HD12 | 1.84                     | 0.60              |
| 2:2B:121:ARG:NH2   | 2:2B:158:GLU:OE2  | 2.33                     | 0.60              |
| 1:5A:292:THR:HG21  | 1:5A:331:ALA:HB1  | 1.84                     | 0.60              |
| 1:6A:271:THR:HG22  | 1:6A:377:MET:HE3  | 1.84                     | 0.60              |
| 2:6B:121:ARG:NH2   | 2:6B:158:GLU:OE2  | 2.34                     | 0.60              |
| 1:7C:140:SER:OG    | 3:7C:500:GTP:O2A  | 2.19                     | 0.60              |
| 2:11D:121:ARG:NH2  | 2:11D:158:GLU:OE2 | 2.34                     | 0.60              |
| 1:12A:397:LEU:HD21 | 2:12B:344:TRP:HA  | 1.84                     | 0.60              |
| 2:13D:127:CYS:SG   | 2:13D:130:LEU:HB3 | 2.42                     | 0.60              |
| 1:1A:74:VAL:HA     | 1:1A:77:GLU:OE2   | 2.02                     | 0.60              |
| 1:3A:306:ASP:OD2   | 1:3A:309:HIS:ND1  | 2.35                     | 0.60              |
| 2:3B:65:LEU:HB2    | 2:3B:73:MET:HE1   | 1.83                     | 0.60              |
| 1:3C:195:LEU:HD12  | 1:3C:428:LEU:HD22 | 1.84                     | 0.60              |
| 2:4D:121:ARG:NH2   | 2:4D:158:GLU:OE2  | 2.34                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:5B:121:ARG:NH2   | 2:5B:158:GLU:OE2   | 2.34                     | 0.60              |
| 1:7C:339:ARG:O     | 1:7C:342:GLN:NE2   | 2.34                     | 0.60              |
| 2:9D:263:LEU:HG    | 2:9D:422:TYR:CE1   | 2.37                     | 0.60              |
| 2:10B:382:SER:O    | 2:10B:386:THR:OG1  | 2.16                     | 0.59              |
| 2:10D:405:GLU:HA   | 2:10D:408:PHE:HD1  | 1.66                     | 0.59              |
| 1:10E:132:LEU:HD23 | 1:10E:164:LYS:NZ   | 2.17                     | 0.59              |
| 1:12A:422:ARG:HA   | 1:12A:425:LEU:HB2  | 1.84                     | 0.59              |
| 1:13A:422:ARG:HA   | 1:13A:425:LEU:HB2  | 1.84                     | 0.59              |
| 2:13D:200:TYR:HE2  | 2:13D:368:ILE:HD13 | 1.67                     | 0.59              |
| 2:13D:268:PRO:HG2  | 2:13D:300:MET:HB3  | 1.84                     | 0.59              |
| 1:2C:213:CYS:HB3   | 1:2C:219:ILE:HD11  | 1.83                     | 0.59              |
| 1:2E:211:ASP:OD2   | 1:2E:304:LYS:NZ    | 2.34                     | 0.59              |
| 2:4D:209:ASP:OD1   | 2:4D:213:ARG:NH1   | 2.34                     | 0.59              |
| 1:11C:119:LEU:HD23 | 1:11C:122:ILE:HD12 | 1.83                     | 0.59              |
| 2:12D:61:PRO:HD3   | 2:12D:84:ILE:HG22  | 1.83                     | 0.59              |
| 1:3C:91:GLN:HG2    | 1:3C:121:ARG:HH22  | 1.66                     | 0.59              |
| 2:6B:67:ASP:OD1    | 2:6B:68:LEU:N      | 2.34                     | 0.59              |
| 2:10B:20:PHE:HD1   | 2:10B:233:MET:HE3  | 1.67                     | 0.59              |
| 2:11B:4:ILE:HG23   | 2:11B:50:TYR:CE1   | 2.36                     | 0.59              |
| 1:13A:371:VAL:HG22 | 1:13A:373:ARG:H    | 1.67                     | 0.59              |
| 2:13B:405:GLU:HA   | 2:13B:408:PHE:HD1  | 1.66                     | 0.59              |
| 2:1B:263:LEU:HG    | 2:1B:422:TYR:CE1   | 2.37                     | 0.59              |
| 2:3D:121:ARG:NH2   | 2:3D:158:GLU:OE2   | 2.34                     | 0.59              |
| 1:3E:188:ILE:HG22  | 1:3E:421:ALA:HB1   | 1.84                     | 0.59              |
| 1:4C:313:MET:HB2   | 1:4C:380:ASN:O     | 2.02                     | 0.59              |
| 2:5D:190:HIS:NE2   | 2:5D:414:ASN:OD1   | 2.35                     | 0.59              |
| 2:10B:405:GLU:HA   | 2:10B:408:PHE:HD1  | 1.68                     | 0.59              |
| 2:10D:86:ARG:NH1   | 2:11D:281:TYR:O    | 2.35                     | 0.59              |
| 2:11B:220:PRO:HD2  | 1:11C:326:LYS:HD3  | 1.83                     | 0.59              |
| 2:13B:14:ASN:O     | 2:13B:18:ALA:N     | 2.35                     | 0.59              |
| 1:2E:371:VAL:HG12  | 1:2E:373:ARG:H     | 1.66                     | 0.59              |
| 1:3A:292:THR:HG21  | 1:3A:331:ALA:HB1   | 1.84                     | 0.59              |
| 2:5D:117:LEU:HA    | 2:5D:120:VAL:HG22  | 1.83                     | 0.59              |
| 1:6A:339:ARG:O     | 1:6A:342:GLN:NE2   | 2.35                     | 0.59              |
| 2:6D:293:MET:HG2   | 2:6D:367:PHE:HB2   | 1.85                     | 0.59              |
| 2:7D:73:MET:HG3    | 2:7D:92:PHE:CD1    | 2.37                     | 0.59              |
| 1:8A:221:ARG:HA    | 2:8B:324:LYS:HE3   | 1.85                     | 0.59              |
| 2:8D:128:ASP:OD1   | 2:8D:129:CYS:N     | 2.35                     | 0.59              |
| 1:10A:215:ARG:NH2  | 1:10A:299:ALA:O    | 2.34                     | 0.59              |
| 2:10B:128:ASP:OD1  | 2:10B:129:CYS:N    | 2.35                     | 0.59              |
| 2:11B:121:ARG:NH2  | 2:11B:158:GLU:OE2  | 2.35                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:405:GLU:HA   | 2:12B:408:PHE:HD1  | 1.68                     | 0.59              |
| 1:12C:213:CYS:HA   | 1:12C:217:LEU:HD13 | 1.84                     | 0.59              |
| 2:12D:190:HIS:HB2  | 2:12D:411:ALA:HB2  | 1.84                     | 0.59              |
| 2:12D:334:GLN:HA   | 2:12D:341:PHE:CZ   | 2.38                     | 0.59              |
| 1:2C:195:LEU:HD12  | 1:2C:428:LEU:HD22  | 1.84                     | 0.59              |
| 1:4A:91:GLN:HA     | 1:4A:121:ARG:HH12  | 1.67                     | 0.59              |
| 2:4B:6:HIS:CE1     | 2:4B:8:GLN:HE21    | 2.20                     | 0.59              |
| 1:4E:132:LEU:HB3   | 1:4E:164:LYS:HE2   | 1.84                     | 0.59              |
| 1:6C:222:PRO:HD2   | 2:6D:324:LYS:HD2   | 1.83                     | 0.59              |
| 1:7A:203:MET:N     | 1:7A:203:MET:SD    | 2.76                     | 0.59              |
| 2:7B:67:ASP:HB2    | 2:7B:73:MET:HE3    | 1.85                     | 0.59              |
| 1:10A:204:VAL:HG11 | 1:10A:231:ILE:HD11 | 1.85                     | 0.59              |
| 1:10C:55:GLU:OE2   | 1:10C:61:HIS:NE2   | 2.35                     | 0.59              |
| 2:13B:204:ASN:ND2  | 2:13B:204:ASN:O    | 2.35                     | 0.59              |
| 1:13C:63:PRO:HD3   | 1:13C:86:LEU:HG    | 1.85                     | 0.59              |
| 1:13E:371:VAL:HG22 | 1:13E:373:ARG:H    | 1.67                     | 0.59              |
| 1:1C:291:ILE:HD12  | 1:1C:375:VAL:HG23  | 1.84                     | 0.59              |
| 2:2B:382:SER:O     | 2:2B:386:THR:OG1   | 2.17                     | 0.59              |
| 2:9D:121:ARG:NH2   | 2:9D:158:GLU:OE2   | 2.35                     | 0.59              |
| 1:10A:175:PRO:HD2  | 1:10A:207:GLU:OE2  | 2.03                     | 0.59              |
| 1:10C:102:ASN:HD22 | 1:10C:105:ARG:HD2  | 1.68                     | 0.59              |
| 2:10D:376:GLU:HA   | 2:10D:379:LYS:HE3  | 1.84                     | 0.59              |
| 2:11B:263:LEU:HG   | 2:11B:422:TYR:CE1  | 2.35                     | 0.59              |
| 2:11B:267:MET:HE3  | 2:11B:301:ALA:HB3  | 1.83                     | 0.59              |
| 1:11C:270:VAL:H    | 1:11C:302:MET:HE3  | 1.65                     | 0.59              |
| 1:2A:292:THR:HG21  | 1:2A:331:ALA:HB1   | 1.83                     | 0.59              |
| 1:4A:88:HIS:HB3    | 1:4A:90:GLU:OE1    | 2.03                     | 0.59              |
| 1:4C:55:GLU:OE2    | 1:4C:61:HIS:NE2    | 2.36                     | 0.59              |
| 1:4C:175:PRO:HB3   | 1:4C:390:ARG:HD3   | 1.85                     | 0.59              |
| 2:4D:193:VAL:HG22  | 2:4D:418:LEU:HD21  | 1.84                     | 0.59              |
| 2:7B:237:THR:O     | 2:7B:241:ARG:NH1   | 2.35                     | 0.59              |
| 1:10C:20:CYS:HB3   | 1:10C:24:TYR:HE1   | 1.68                     | 0.59              |
| 2:12B:423:GLN:HG3  | 2:12B:424:GLN:N    | 2.18                     | 0.59              |
| 2:12D:14:ASN:O     | 2:12D:18:ALA:N     | 2.35                     | 0.59              |
| 1:13C:213:CYS:HA   | 1:13C:217:LEU:HD13 | 1.84                     | 0.59              |
| 2:3B:209:ASP:OD1   | 2:3B:213:ARG:NH1   | 2.33                     | 0.59              |
| 2:4B:121:ARG:NH2   | 2:4B:158:GLU:OE2   | 2.35                     | 0.59              |
| 2:4D:121:ARG:O     | 2:4D:125:GLU:HG2   | 2.03                     | 0.59              |
| 1:7E:271:THR:OG1   | 1:7E:300:ASN:OD1   | 2.21                     | 0.59              |
| 1:8E:8:HIS:HD1     | 1:8E:67:PHE:HE1    | 1.51                     | 0.59              |
| 1:8E:195:LEU:HD12  | 1:8E:428:LEU:HD22  | 1.84                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9C:175:PRO:HB3   | 1:9C:390:ARG:CZ    | 2.32                     | 0.59              |
| 1:10C:30:ILE:HD13  | 1:10C:53:PHE:HE2   | 1.66                     | 0.59              |
| 2:11D:323:MET:HA   | 2:11D:323:MET:HE3  | 1.85                     | 0.59              |
| 1:13C:192:HIS:HB2  | 1:13C:421:ALA:HB2  | 1.85                     | 0.59              |
| 1:3A:215:ARG:HH22  | 1:3A:299:ALA:HB1   | 1.67                     | 0.59              |
| 1:4E:339:ARG:O     | 1:4E:342:GLN:NE2   | 2.35                     | 0.59              |
| 1:12C:169:PHE:HE2  | 1:12C:235:VAL:HG22 | 1.67                     | 0.59              |
| 1:13E:208:ALA:HB1  | 1:13E:302:MET:HA   | 1.84                     | 0.59              |
| 1:1A:108:TYR:HA    | 1:1A:112:LYS:HZ1   | 1.66                     | 0.59              |
| 1:1C:27:GLU:OE1    | 1:1C:243:ARG:NH2   | 2.36                     | 0.59              |
| 2:1D:68:LEU:HD12   | 2:1D:143:THR:HG23  | 1.85                     | 0.59              |
| 2:2D:311:LEU:HD23  | 2:2D:342:VAL:HG21  | 1.85                     | 0.59              |
| 1:2E:175:PRO:HB3   | 1:2E:390:ARG:HD3   | 1.85                     | 0.59              |
| 2:5B:293:MET:HE3   | 2:5B:365:ALA:HB1   | 1.83                     | 0.59              |
| 2:7D:49:VAL:HG11   | 2:7D:241:ARG:HG2   | 1.85                     | 0.59              |
| 2:8D:382:SER:O     | 2:8D:386:THR:OG1   | 2.15                     | 0.59              |
| 1:9A:63:PRO:HD3    | 1:9A:86:LEU:HG     | 1.85                     | 0.59              |
| 1:12A:221:ARG:HA   | 2:12B:324:LYS:HD3  | 1.85                     | 0.58              |
| 1:12A:297:GLU:OE1  | 1:12A:300:ASN:ND2  | 2.35                     | 0.58              |
| 2:12D:67:ASP:HB3   | 2:12D:92:PHE:HB3   | 1.85                     | 0.58              |
| 1:13A:204:VAL:HG11 | 1:13A:231:ILE:HD11 | 1.84                     | 0.58              |
| 2:13B:12:CYS:SG    | 2:13B:138:SER:OG   | 2.60                     | 0.58              |
| 2:1B:178:THR:HB    | 2:1B:181:GLU:HG3   | 1.85                     | 0.58              |
| 2:3B:208:TYR:HA    | 2:3B:211:CYS:SG    | 2.44                     | 0.58              |
| 1:3C:202:PHE:HE1   | 1:3C:378:LEU:HD23  | 1.68                     | 0.58              |
| 1:5C:205:ASP:OD1   | 1:5C:206:ASN:N     | 2.35                     | 0.58              |
| 2:5D:178:THR:HB    | 2:5D:181:GLU:HG3   | 1.85                     | 0.58              |
| 1:6C:145:THR:OG1   | 3:6C:500:GTP:O3B   | 2.20                     | 0.58              |
| 2:7D:121:ARG:NH2   | 2:7D:158:GLU:OE2   | 2.36                     | 0.58              |
| 2:7D:128:ASP:OD1   | 2:7D:129:CYS:N     | 2.36                     | 0.58              |
| 1:8E:224:TYR:O     | 1:8E:228:ASN:ND2   | 2.35                     | 0.58              |
| 1:10C:300:ASN:O    | 1:10C:300:ASN:ND2  | 2.35                     | 0.58              |
| 2:12B:49:VAL:HG11  | 2:12B:241:ARG:HG2  | 1.85                     | 0.58              |
| 1:12C:79:ARG:HE    | 1:12C:92:LEU:HD21  | 1.67                     | 0.58              |
| 2:12D:198:GLU:HG3  | 2:12D:266:PHE:HE2  | 1.68                     | 0.58              |
| 2:12D:237:THR:O    | 2:12D:241:ARG:NH1  | 2.36                     | 0.58              |
| 2:12D:420:SER:HA   | 2:12D:423:GLN:HG2  | 1.85                     | 0.58              |
| 2:13D:215:LEU:HB3  | 2:13D:217:LEU:HG   | 1.83                     | 0.58              |
| 1:3A:98:ASP:OD1    | 1:3A:99:ALA:N      | 2.36                     | 0.58              |
| 1:3A:291:ILE:HD12  | 1:3A:375:VAL:HG23  | 1.85                     | 0.58              |
| 2:3B:121:ARG:NH1   | 2:3B:158:GLU:OE1   | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:4E:188:ILE:HG22  | 1:4E:421:ALA:HB1   | 1.84                     | 0.58              |
| 1:5A:22:GLU:OE1    | 1:5A:83:TYR:OH     | 2.15                     | 0.58              |
| 2:7D:208:TYR:HA    | 2:7D:211:CYS:SG    | 2.43                     | 0.58              |
| 2:8D:285:THR:O     | 2:8D:288:GLU:HG2   | 2.03                     | 0.58              |
| 2:8D:293:MET:HE2   | 2:8D:365:ALA:HB1   | 1.85                     | 0.58              |
| 2:12D:220:PRO:HD2  | 1:12E:326:LYS:HD3  | 1.84                     | 0.58              |
| 1:13A:70:LEU:HA    | 1:13A:95:GLY:HA3   | 1.84                     | 0.58              |
| 2:13B:371:SER:OG   | 2:13B:372:THR:N    | 2.34                     | 0.58              |
| 2:13D:114:ASP:OD1  | 2:13D:115:SER:N    | 2.35                     | 0.58              |
| 2:4D:209:ASP:OD2   | 2:4D:213:ARG:NH2   | 2.37                     | 0.58              |
| 2:6B:287:PRO:HG3   | 2:6B:329:GLN:HE22  | 1.68                     | 0.58              |
| 1:7A:324:VAL:HG12  | 1:7A:326:LYS:H     | 1.68                     | 0.58              |
| 1:8A:339:ARG:O     | 1:8A:342:GLN:NE2   | 2.36                     | 0.58              |
| 1:9A:180:ALA:HB3   | 1:9A:183:GLU:HG3   | 1.85                     | 0.58              |
| 2:11D:175:VAL:HG22 | 1:11E:329:ASN:HD21 | 1.69                     | 0.58              |
| 2:11D:267:MET:HE3  | 2:11D:374:ILE:HD13 | 1.86                     | 0.58              |
| 2:11D:376:GLU:O    | 2:11D:380:ARG:NH1  | 2.36                     | 0.58              |
| 2:1B:186:THR:HG22  | 2:1B:411:ALA:HB1   | 1.86                     | 0.58              |
| 2:3D:61:PRO:HD3    | 2:3D:84:ILE:HG22   | 1.85                     | 0.58              |
| 1:5E:292:THR:HG21  | 1:5E:331:ALA:HB1   | 1.85                     | 0.58              |
| 2:6B:213:ARG:NH1   | 2:6B:297:LYS:HE3   | 2.19                     | 0.58              |
| 1:7E:313:MET:HB3   | 1:7E:380:ASN:O     | 2.03                     | 0.58              |
| 1:8E:213:CYS:HA    | 1:8E:217:LEU:HB2   | 1.85                     | 0.58              |
| 2:9D:215:LEU:HD22  | 2:9D:217:LEU:HG    | 1.84                     | 0.58              |
| 2:10B:203:ASP:OD2  | 2:10B:302:ALA:N    | 2.25                     | 0.58              |
| 2:10B:215:LEU:HD22 | 2:10B:217:LEU:HG   | 1.86                     | 0.58              |
| 1:10E:213:CYS:SG   | 1:10E:222:PRO:HG3  | 2.43                     | 0.58              |
| 1:12C:422:ARG:HA   | 1:12C:425:LEU:HB2  | 1.85                     | 0.58              |
| 2:12D:204:ASN:HD22 | 2:12D:204:ASN:C    | 2.11                     | 0.58              |
| 1:13C:422:ARG:HA   | 1:13C:425:LEU:HB2  | 1.86                     | 0.58              |
| 1:13E:292:THR:HG21 | 1:13E:331:ALA:HB1  | 1.86                     | 0.58              |
| 2:3D:3:GLU:CG      | 2:3D:62:ARG:HH12   | 2.15                     | 0.58              |
| 1:4A:88:HIS:CD2    | 1:5A:283:HIS:HB3   | 2.37                     | 0.58              |
| 2:5B:237:THR:O     | 2:5B:241:ARG:NH1   | 2.36                     | 0.58              |
| 2:6D:178:THR:HB    | 2:6D:181:GLU:HG3   | 1.86                     | 0.58              |
| 2:7D:127:CYS:SG    | 2:7D:130:LEU:HD23  | 2.44                     | 0.58              |
| 2:8D:209:ASP:OD1   | 2:8D:213:ARG:NH1   | 2.35                     | 0.58              |
| 1:9C:344:VAL:HG11  | 1:9C:346:TRP:CE2   | 2.39                     | 0.58              |
| 2:9D:186:THR:HG22  | 2:9D:411:ALA:HB1   | 1.86                     | 0.58              |
| 1:10C:292:THR:HG21 | 1:10C:331:ALA:HB1  | 1.84                     | 0.58              |
| 1:10E:286:LEU:O    | 1:10E:373:ARG:NH2  | 2.33                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11A:295:CYS:HB3  | 1:11A:377:MET:HG2  | 1.84                     | 0.58              |
| 1:11C:121:ARG:HB3  | 1:11C:121:ARG:NH1  | 2.17                     | 0.58              |
| 2:12B:52:ASN:HB3   | 2:12B:62:ARG:NH1   | 2.18                     | 0.58              |
| 1:13C:91:GLN:HA    | 1:13C:121:ARG:NH1  | 2.18                     | 0.58              |
| 1:13E:169:PHE:CE1  | 1:13E:235:VAL:HG22 | 2.38                     | 0.58              |
| 1:1C:102:ASN:HD22  | 1:1C:105:ARG:HD3   | 1.69                     | 0.58              |
| 2:3D:99:ASN:ND2    | 1:3E:254:GLU:OE1   | 2.37                     | 0.58              |
| 2:3D:121:ARG:NH1   | 2:3D:158:GLU:OE1   | 2.36                     | 0.58              |
| 2:3D:237:THR:HG22  | 2:3D:250:LEU:HD21  | 1.85                     | 0.58              |
| 2:5D:14:ASN:ND2    | 2:5D:73:MET:HE1    | 2.18                     | 0.58              |
| 1:7A:175:PRO:HD2   | 1:7A:207:GLU:OE1   | 2.03                     | 0.58              |
| 2:7D:175:VAL:HG13  | 1:7E:329:ASN:HD22  | 1.68                     | 0.58              |
| 2:8B:216:LYS:O     | 2:8B:216:LYS:HG2   | 2.04                     | 0.58              |
| 2:8D:107:THR:OG1   | 2:8D:401:GLU:OE1   | 2.22                     | 0.58              |
| 2:10B:52:ASN:OD1   | 2:10B:62:ARG:NH2   | 2.35                     | 0.58              |
| 1:12A:113:GLU:OE1  | 1:12A:113:GLU:N    | 2.37                     | 0.58              |
| 2:12D:215:LEU:HB3  | 2:12D:217:LEU:HG   | 1.86                     | 0.58              |
| 2:12D:244:GLY:HA2  | 2:12D:355:ASP:HB2  | 1.86                     | 0.58              |
| 2:13B:90:PHE:HB3   | 2:13B:92:PHE:HE2   | 1.69                     | 0.58              |
| 2:13B:109:GLY:HA3  | 2:13B:150:LEU:HD21 | 1.85                     | 0.58              |
| 1:13C:100:ALA:HB2  | 2:13D:251:ARG:HG2  | 1.84                     | 0.58              |
| 2:2B:121:ARG:NH1   | 2:2B:158:GLU:OE1   | 2.36                     | 0.58              |
| 2:3D:193:VAL:HG13  | 2:3D:194:GLU:HG3   | 1.86                     | 0.58              |
| 1:6E:390:ARG:HD2   | 1:6E:391:LEU:HD22  | 1.85                     | 0.58              |
| 1:7A:174:ALA:HB3   | 1:7A:177:VAL:O     | 2.04                     | 0.58              |
| 2:7B:128:ASP:OD1   | 2:7B:129:CYS:N     | 2.35                     | 0.58              |
| 2:7B:387:ALA:HA    | 2:7B:390:ARG:HD2   | 1.85                     | 0.58              |
| 2:7D:237:THR:O     | 2:7D:241:ARG:NH1   | 2.37                     | 0.58              |
| 1:7E:195:LEU:HD12  | 1:7E:428:LEU:HD22  | 1.86                     | 0.58              |
| 2:9B:121:ARG:NH2   | 2:9B:158:GLU:OE2   | 2.37                     | 0.58              |
| 1:10C:180:ALA:HB3  | 1:10C:183:GLU:HG3  | 1.85                     | 0.58              |
| 1:11A:136:LEU:HD22 | 1:11A:169:PHE:HE2  | 1.69                     | 0.58              |
| 1:12E:377:MET:HE1  | 1:12E:379:SER:HB3  | 1.86                     | 0.58              |
| 1:13A:178:SER:O    | 2:13B:347:ASN:ND2  | 2.31                     | 0.58              |
| 1:2C:202:PHE:HE1   | 1:2C:378:LEU:HD23  | 1.69                     | 0.58              |
| 2:3D:173:PRO:HD2   | 2:3D:380:ARG:HH21  | 1.69                     | 0.58              |
| 2:9B:175:VAL:HG13  | 1:9C:329:ASN:ND2   | 2.19                     | 0.58              |
| 1:9C:71:GLU:HB2    | 1:9C:98:ASP:OD1    | 2.04                     | 0.58              |
| 2:10B:172:SER:HB2  | 2:10B:205:GLU:HG3  | 1.86                     | 0.58              |
| 1:11C:8:HIS:CE1    | 1:11C:138:PHE:HD2  | 2.22                     | 0.58              |
| 1:12A:16:ILE:HD11  | 1:12A:171:ILE:HD11 | 1.86                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:7A:174:ALA:HB1  | 1:7A:207:GLU:OE1   | 2.04                     | 0.58              |
| 1:7C:213:CYS:HB3  | 1:7C:219:ILE:HD11  | 1.86                     | 0.58              |
| 2:8D:285:THR:HG23 | 2:8D:287:PRO:HD2   | 1.84                     | 0.58              |
| 1:9A:175:PRO:HB3  | 1:9A:390:ARG:CZ    | 2.33                     | 0.58              |
| 2:9B:117:LEU:HA   | 2:9B:120:VAL:HG22  | 1.86                     | 0.58              |
| 1:9C:180:ALA:HB3  | 1:9C:183:GLU:HG3   | 1.85                     | 0.58              |
| 2:9D:128:ASP:OD1  | 2:9D:129:CYS:N     | 2.36                     | 0.58              |
| 2:9D:257:MET:HE1  | 2:9D:266:PHE:CE2   | 2.38                     | 0.58              |
| 2:10D:293:MET:HE2 | 2:10D:365:ALA:HB1  | 1.85                     | 0.58              |
| 1:10E:145:THR:OG1 | 3:10E:500:GTP:O3B  | 2.10                     | 0.58              |
| 2:12B:198:GLU:HG3 | 2:12B:266:PHE:HE2  | 1.67                     | 0.58              |
| 3:13C:500:GTP:O1G | 2:13D:252:LYS:NZ   | 2.37                     | 0.58              |
| 1:5E:339:ARG:O    | 1:5E:342:GLN:NE2   | 2.36                     | 0.58              |
| 2:6B:61:PRO:HD3   | 2:6B:84:ILE:HG22   | 1.85                     | 0.58              |
| 1:6E:90:GLU:OE1   | 1:7E:280:LYS:HD2   | 2.03                     | 0.58              |
| 1:8C:292:THR:HG21 | 1:8C:331:ALA:HB1   | 1.86                     | 0.58              |
| 1:12C:11:GLN:O    | 1:12C:15:GLN:HG2   | 2.03                     | 0.57              |
| 1:1E:74:VAL:HA    | 1:1E:77:GLU:OE2    | 2.03                     | 0.57              |
| 2:2B:178:THR:HG22 | 2:2B:180:VAL:H     | 1.69                     | 0.57              |
| 1:5A:145:THR:OG1  | 3:5A:500:GTP:O3B   | 2.22                     | 0.57              |
| 2:5B:68:LEU:HD12  | 2:5B:143:THR:HG23  | 1.86                     | 0.57              |
| 1:5C:140:SER:OG   | 3:5C:500:GTP:O2A   | 2.21                     | 0.57              |
| 2:8B:285:THR:O    | 2:8B:288:GLU:HG2   | 2.04                     | 0.57              |
| 1:8C:339:ARG:O    | 1:8C:342:GLN:NE2   | 2.37                     | 0.57              |
| 2:10D:4:ILE:HG13  | 2:10D:132:GLY:O    | 2.04                     | 0.57              |
| 2:11D:248:ALA:HA  | 2:11D:252:LYS:HD3  | 1.86                     | 0.57              |
| 2:12B:104:GLY:HA3 | 2:12B:146:GLY:HA3  | 1.85                     | 0.57              |
| 1:12C:224:TYR:O   | 1:12C:228:ASN:ND2  | 2.36                     | 0.57              |
| 1:12C:333:ALA:HA  | 1:12C:336:LYS:HB2  | 1.85                     | 0.57              |
| 2:13D:3:GLU:HB3   | 2:13D:62:ARG:NH2   | 2.17                     | 0.57              |
| 1:13E:319:TYR:N   | 1:13E:354:GLY:O    | 2.36                     | 0.57              |
| 1:1C:221:ARG:HA   | 2:1D:324:LYS:HE3   | 1.84                     | 0.57              |
| 1:2A:26:LEU:HD22  | 1:2A:363:VAL:HG12  | 1.86                     | 0.57              |
| 1:2E:292:THR:HG21 | 1:2E:331:ALA:HB1   | 1.86                     | 0.57              |
| 2:4B:117:LEU:HA   | 2:4B:120:VAL:HG22  | 1.84                     | 0.57              |
| 1:5A:11:GLN:O     | 1:5A:15:GLN:HG2    | 2.03                     | 0.57              |
| 2:6D:310:TYR:O    | 2:6D:342:VAL:HG23  | 2.05                     | 0.57              |
| 2:7D:203:ASP:O    | 2:7D:207:LEU:HD23  | 2.04                     | 0.57              |
| 1:12A:34:GLY:O    | 1:12A:61:HIS:ND1   | 2.33                     | 0.57              |
| 1:12C:169:PHE:CE2 | 1:12C:235:VAL:HG22 | 2.40                     | 0.57              |
| 2:12D:423:GLN:HG3 | 2:12D:424:GLN:N    | 2.19                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:13B:45:GLU:O     | 2:13B:46:ARG:NH1   | 2.37                     | 0.57              |
| 1:13E:204:VAL:HG11 | 1:13E:231:ILE:HD11 | 1.85                     | 0.57              |
| 1:1C:259:LEU:HD21  | 1:1C:380:ASN:HB2   | 1.87                     | 0.57              |
| 1:3C:69:ASP:OD1    | 1:3C:70:LEU:N      | 2.37                     | 0.57              |
| 2:5D:121:ARG:NH1   | 2:5D:158:GLU:OE1   | 2.37                     | 0.57              |
| 2:5D:211:CYS:HB2   | 2:5D:217:LEU:HD12  | 1.87                     | 0.57              |
| 1:5E:11:GLN:O      | 1:5E:15:GLN:HG2    | 2.03                     | 0.57              |
| 1:6A:2:ARG:HD3     | 1:6A:242:LEU:HD22  | 1.85                     | 0.57              |
| 2:7B:190:HIS:NE2   | 2:7B:414:ASN:OD1   | 2.37                     | 0.57              |
| 2:7B:237:THR:HG22  | 2:7B:250:LEU:HD21  | 1.87                     | 0.57              |
| 1:7E:102:ASN:HD22  | 1:7E:105:ARG:HD2   | 1.68                     | 0.57              |
| 1:9E:3:GLU:HG3     | 1:9E:129:CYS:HA    | 1.85                     | 0.57              |
| 1:11A:401:LYS:HG2  | 2:11B:344:TRP:CH2  | 2.39                     | 0.57              |
| 2:12B:114:ASP:OD1  | 2:12B:115:SER:N    | 2.37                     | 0.57              |
| 2:13D:371:SER:OG   | 2:13D:372:THR:N    | 2.37                     | 0.57              |
| 1:1E:269:LEU:HD11  | 1:1E:384:ILE:HB    | 1.86                     | 0.57              |
| 1:2C:371:VAL:HG12  | 1:2C:373:ARG:H     | 1.69                     | 0.57              |
| 2:3B:193:VAL:HG13  | 2:3B:194:GLU:HG3   | 1.86                     | 0.57              |
| 1:5A:123:ARG:NE    | 1:5A:161:TYR:OH    | 2.37                     | 0.57              |
| 2:5D:285:THR:HB    | 2:5D:287:PRO:HD2   | 1.87                     | 0.57              |
| 1:5E:145:THR:OG1   | 3:5E:500:GTP:O3B   | 2.18                     | 0.57              |
| 2:7B:36:TYR:CZ     | 2:7B:44:LEU:HD21   | 2.39                     | 0.57              |
| 2:7B:121:ARG:NH2   | 2:7B:158:GLU:OE2   | 2.37                     | 0.57              |
| 2:8B:209:ASP:OD2   | 2:8B:213:ARG:NH2   | 2.38                     | 0.57              |
| 1:10E:112:LYS:HA   | 1:10E:115:VAL:HG12 | 1.85                     | 0.57              |
| 2:11B:311:LEU:HD23 | 2:11B:342:VAL:HG21 | 1.87                     | 0.57              |
| 1:11C:106:GLY:HA3  | 1:11C:148:GLY:HA3  | 1.86                     | 0.57              |
| 2:11D:128:ASP:OD1  | 2:11D:129:CYS:N    | 2.37                     | 0.57              |
| 1:11E:106:GLY:HA3  | 1:11E:148:GLY:HA3  | 1.85                     | 0.57              |
| 1:12A:226:ASN:ND2  | 1:12A:367:ASP:OD2  | 2.38                     | 0.57              |
| 2:1B:248:ALA:HA    | 2:1B:252:LYS:HD3   | 1.85                     | 0.57              |
| 1:1C:123:ARG:HA    | 1:1C:123:ARG:HE    | 1.68                     | 0.57              |
| 2:3D:117:LEU:HA    | 2:3D:120:VAL:HG22  | 1.86                     | 0.57              |
| 1:5E:271:THR:OG1   | 1:5E:300:ASN:OD1   | 2.22                     | 0.57              |
| 2:6B:167:TYR:CE1   | 2:6B:233:MET:HG2   | 2.40                     | 0.57              |
| 1:7C:178:SER:OG    | 2:7D:347:ASN:OD1   | 2.14                     | 0.57              |
| 1:7E:188:ILE:HG22  | 1:7E:421:ALA:HB1   | 1.85                     | 0.57              |
| 1:8E:54:SER:OG     | 1:8E:64:ARG:NH2    | 2.37                     | 0.57              |
| 1:8E:56:THR:HA     | 1:9E:285:GLN:HB2   | 1.86                     | 0.57              |
| 1:9E:195:LEU:HB3   | 1:9E:196:GLU:OE1   | 2.04                     | 0.57              |
| 2:11D:376:GLU:HA   | 2:11D:379:LYS:HG2  | 1.87                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:198:GLU:HG3  | 2:12B:266:PHE:CE2  | 2.40                     | 0.57              |
| 1:12E:113:GLU:N    | 1:12E:113:GLU:OE1  | 2.38                     | 0.57              |
| 1:13A:113:GLU:OE1  | 1:13A:113:GLU:N    | 2.37                     | 0.57              |
| 1:1A:261:PRO:HG3   | 1:1A:313:MET:SD    | 2.44                     | 0.57              |
| 1:1A:269:LEU:HD11  | 1:1A:384:ILE:HB    | 1.86                     | 0.57              |
| 2:2B:190:HIS:NE2   | 2:2B:414:ASN:OD1   | 2.37                     | 0.57              |
| 2:2D:121:ARG:NH2   | 2:2D:158:GLU:OE2   | 2.36                     | 0.57              |
| 1:4A:292:THR:HG21  | 1:4A:331:ALA:HB1   | 1.86                     | 0.57              |
| 2:5B:311:LEU:HD23  | 2:5B:342:VAL:HG21  | 1.86                     | 0.57              |
| 1:6E:206:ASN:ND2   | 3:6E:500:GTP:O2'   | 2.38                     | 0.57              |
| 1:7A:132:LEU:HD23  | 1:7A:164:LYS:HD3   | 1.87                     | 0.57              |
| 2:7D:219:THR:HG22  | 1:7E:326:LYS:HE2   | 1.85                     | 0.57              |
| 2:11B:327:ASP:OD1  | 2:11B:328:GLU:N    | 2.38                     | 0.57              |
| 2:12B:309:ARG:NH1  | 2:12B:426:GLN:OXT  | 2.38                     | 0.57              |
| 2:12D:114:ASP:OD1  | 2:12D:115:SER:N    | 2.38                     | 0.57              |
| 1:13A:31:GLN:CG    | 1:13A:32:PRO:HD2   | 2.35                     | 0.57              |
| 1:1C:234:ILE:HD11  | 1:1C:302:MET:HE1   | 1.87                     | 0.57              |
| 1:3C:206:ASN:OD1   | 3:3C:500:GTP:O2'   | 2.23                     | 0.57              |
| 1:8E:64:ARG:HH21   | 1:8E:128:GLN:NE2   | 2.00                     | 0.57              |
| 1:9C:175:PRO:HD2   | 1:9C:207:GLU:OE2   | 2.05                     | 0.57              |
| 2:10B:344:TRP:O    | 2:10B:345:ILE:HD13 | 2.05                     | 0.57              |
| 1:10E:209:ILE:HG23 | 1:10E:230:LEU:HD22 | 1.86                     | 0.57              |
| 1:10E:255:PHE:CZ   | 1:10E:378:LEU:HD22 | 2.39                     | 0.57              |
| 2:12B:130:LEU:HD21 | 2:12B:162:ARG:HH12 | 1.68                     | 0.57              |
| 2:12B:183:TYR:HE1  | 2:12B:388:MET:HG2  | 1.68                     | 0.57              |
| 2:13B:198:GLU:HB2  | 2:13B:266:PHE:CE2  | 2.39                     | 0.57              |
| 1:13C:106:GLY:HA3  | 1:13C:148:GLY:HA3  | 1.87                     | 0.57              |
| 1:1A:221:ARG:HA    | 2:1B:324:LYS:HZ1   | 1.70                     | 0.57              |
| 2:1B:406:MET:O     | 2:1B:409:THR:OG1   | 2.16                     | 0.57              |
| 1:1C:108:TYR:HA    | 1:1C:112:LYS:NZ    | 2.20                     | 0.57              |
| 2:2B:73:MET:HG3    | 2:2B:92:PHE:HD1    | 1.68                     | 0.57              |
| 1:3C:112:LYS:HA    | 1:3C:115:VAL:HG12  | 1.87                     | 0.57              |
| 2:4B:14:ASN:ND2    | 2:4B:73:MET:HE1    | 2.20                     | 0.57              |
| 1:8C:101:ASN:HD21  | 2:8D:252:LYS:HE3   | 1.69                     | 0.57              |
| 2:9B:257:MET:HE1   | 2:9B:266:PHE:CE1   | 2.40                     | 0.57              |
| 2:9D:328:GLU:O     | 2:9D:331:LEU:HG    | 2.04                     | 0.57              |
| 2:11B:117:LEU:HA   | 2:11B:120:VAL:HG22 | 1.87                     | 0.57              |
| 1:12A:230:LEU:HD23 | 1:12A:302:MET:HE1  | 1.87                     | 0.57              |
| 1:13E:129:CYS:SG   | 1:13E:132:LEU:HB2  | 2.44                     | 0.57              |
| 1:1C:225:THR:O     | 1:1C:229:ARG:HG3   | 2.05                     | 0.57              |
| 1:2A:188:ILE:HG23  | 1:2A:425:LEU:HD12  | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:6D:209:ASP:OD1   | 2:6D:213:ARG:NH2   | 2.37                     | 0.57              |
| 2:7B:178:THR:HG22  | 2:7B:180:VAL:H     | 1.68                     | 0.57              |
| 2:7B:208:TYR:HA    | 2:7B:211:CYS:SG    | 2.45                     | 0.57              |
| 1:7C:203:MET:HE1   | 1:7C:267:PHE:HB3   | 1.87                     | 0.57              |
| 2:10B:285:THR:O    | 2:10B:288:GLU:HG2  | 2.05                     | 0.57              |
| 1:10C:255:PHE:CZ   | 1:10C:378:LEU:HD22 | 2.40                     | 0.57              |
| 2:11B:414:ASN:O    | 2:11B:418:LEU:N    | 2.37                     | 0.57              |
| 1:12C:313:MET:N    | 1:12C:313:MET:SD   | 2.76                     | 0.57              |
| 2:12D:28:HIS:NE2   | 2:12D:241:ARG:HD2  | 2.20                     | 0.57              |
| 2:13D:193:VAL:HG13 | 2:13D:194:GLU:HG3  | 1.86                     | 0.57              |
| 2:2D:117:LEU:HA    | 2:2D:120:VAL:HG22  | 1.85                     | 0.57              |
| 1:3E:291:ILE:HD12  | 1:3E:375:VAL:HG23  | 1.85                     | 0.57              |
| 1:5E:56:THR:HA     | 1:6E:285:GLN:HB2   | 1.87                     | 0.57              |
| 1:6A:102:ASN:HB2   | 1:6A:105:ARG:HB2   | 1.86                     | 0.57              |
| 1:6C:140:SER:OG    | 3:6C:500:GTP:O2A   | 2.22                     | 0.57              |
| 1:6E:269:LEU:HD11  | 1:6E:384:ILE:HB    | 1.87                     | 0.57              |
| 2:8D:316:ILE:HG22  | 2:8D:352:ALA:HB3   | 1.86                     | 0.57              |
| 2:9B:285:THR:OG1   | 2:9B:287:PRO:HD2   | 2.05                     | 0.57              |
| 1:9E:69:ASP:OD1    | 1:9E:70:LEU:N      | 2.36                     | 0.57              |
| 2:13B:380:ARG:O    | 2:13B:384:GLN:HG3  | 2.03                     | 0.56              |
| 1:1A:88:HIS:CD2    | 1:2A:283:HIS:HB3   | 2.40                     | 0.56              |
| 2:3B:237:THR:HG22  | 2:3B:250:LEU:HD21  | 1.87                     | 0.56              |
| 1:3C:123:ARG:NE    | 1:3C:161:TYR:OH    | 2.38                     | 0.56              |
| 1:3C:188:ILE:HG22  | 1:3C:421:ALA:HB1   | 1.87                     | 0.56              |
| 2:4D:382:SER:O     | 2:4D:386:THR:HG23  | 2.05                     | 0.56              |
| 1:6A:108:TYR:HA    | 1:6A:112:LYS:NZ    | 2.19                     | 0.56              |
| 1:7C:71:GLU:HB2    | 1:7C:98:ASP:HB3    | 1.87                     | 0.56              |
| 1:7C:221:ARG:HA    | 2:7D:324:LYS:HD3   | 1.87                     | 0.56              |
| 2:8D:4:ILE:HG12    | 2:8D:131:GLN:NE2   | 2.20                     | 0.56              |
| 2:10D:268:PRO:HG2  | 2:10D:300:MET:HB3  | 1.87                     | 0.56              |
| 2:11D:309:ARG:NH1  | 2:11D:426:GLN:OXT  | 2.38                     | 0.56              |
| 1:12A:11:GLN:HB3   | 3:12A:500:GTP:O2B  | 2.05                     | 0.56              |
| 1:12A:182:VAL:HG12 | 2:12B:256:ASN:ND2  | 2.17                     | 0.56              |
| 1:1A:112:LYS:HA    | 1:1A:115:VAL:HG12  | 1.87                     | 0.56              |
| 2:1D:282:ARG:NH2   | 2:1D:292:GLN:OE1   | 2.38                     | 0.56              |
| 2:2D:5:VAL:HG12    | 2:2D:62:ARG:HD3    | 1.87                     | 0.56              |
| 1:2E:306:ASP:OD2   | 1:2E:309:HIS:ND1   | 2.39                     | 0.56              |
| 1:5A:313:MET:HB2   | 1:5A:380:ASN:O     | 2.05                     | 0.56              |
| 1:9A:221:ARG:HA    | 2:9B:324:LYS:HE3   | 1.87                     | 0.56              |
| 1:9C:188:ILE:HG22  | 1:9C:421:ALA:HB1   | 1.87                     | 0.56              |
| 1:9E:67:PHE:HB2    | 1:9E:92:LEU:HD12   | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10B:14:ASN:O     | 2:10B:18:ALA:N     | 2.37                     | 0.56              |
| 1:11C:213:CYS:SG   | 1:11C:222:PRO:HG3  | 2.45                     | 0.56              |
| 2:11D:178:THR:HB   | 2:11D:181:GLU:HG3  | 1.86                     | 0.56              |
| 1:11E:88:HIS:CD2   | 1:11E:89:PRO:HD2   | 2.39                     | 0.56              |
| 1:12C:112:LYS:HA   | 1:12C:115:VAL:HG12 | 1.88                     | 0.56              |
| 1:12C:424:ASP:O    | 1:12C:428:LEU:N    | 2.32                     | 0.56              |
| 2:12D:257:MET:HE1  | 2:12D:266:PHE:CE2  | 2.41                     | 0.56              |
| 2:12D:404:ASP:HB3  | 2:12D:406:MET:HE1  | 1.86                     | 0.56              |
| 2:13B:289:LEU:O    | 2:13B:293:MET:N    | 2.37                     | 0.56              |
| 2:13D:257:MET:O    | 2:13D:312:THR:OG1  | 2.23                     | 0.56              |
| 1:1A:102:ASN:HD22  | 1:1A:105:ARG:HD3   | 1.70                     | 0.56              |
| 1:1C:221:ARG:HA    | 2:1D:324:LYS:CE    | 2.34                     | 0.56              |
| 1:2A:188:ILE:HG22  | 1:2A:421:ALA:HB1   | 1.86                     | 0.56              |
| 1:2C:91:GLN:HG3    | 1:2C:121:ARG:HH22  | 1.71                     | 0.56              |
| 2:4D:173:PRO:HD2   | 2:4D:380:ARG:HH21  | 1.70                     | 0.56              |
| 2:5B:285:THR:HB    | 2:5B:287:PRO:HD2   | 1.88                     | 0.56              |
| 2:5D:209:ASP:OD1   | 2:5D:213:ARG:NH1   | 2.37                     | 0.56              |
| 2:6D:219:THR:HG22  | 1:6E:326:LYS:HZ3   | 1.70                     | 0.56              |
| 1:7C:56:THR:HA     | 1:8C:285:GLN:HB2   | 1.86                     | 0.56              |
| 1:7C:180:ALA:HB3   | 1:7C:183:GLU:HG3   | 1.87                     | 0.56              |
| 1:7E:145:THR:OG1   | 3:7E:500:GTP:O3B   | 2.23                     | 0.56              |
| 2:9D:193:VAL:HG13  | 2:9D:194:GLU:HG3   | 1.86                     | 0.56              |
| 2:9D:270:PHE:HD1   | 2:9D:366:THR:HG22  | 1.70                     | 0.56              |
| 1:10C:251:ASP:O    | 1:10C:255:PHE:N    | 2.39                     | 0.56              |
| 1:12C:113:GLU:N    | 1:12C:113:GLU:OE1  | 2.39                     | 0.56              |
| 1:12C:142:GLY:O    | 1:12C:186:ASN:ND2  | 2.38                     | 0.56              |
| 1:12E:424:ASP:O    | 1:12E:428:LEU:N    | 2.33                     | 0.56              |
| 2:13B:165:ASN:HB3  | 2:13B:167:TYR:HE2  | 1.70                     | 0.56              |
| 2:13D:45:GLU:O     | 2:13D:46:ARG:NH1   | 2.38                     | 0.56              |
| 1:13E:186:ASN:OD1  | 1:13E:408:TYR:OH   | 2.18                     | 0.56              |
| 2:1B:325:GLU:O     | 2:1B:329:GLN:HG2   | 2.05                     | 0.56              |
| 1:1C:191:THR:HG21  | 1:1C:425:LEU:HD21  | 1.86                     | 0.56              |
| 2:1D:99:ASN:ND2    | 1:1E:254:GLU:OE2   | 2.39                     | 0.56              |
| 1:3A:88:HIS:CD2    | 1:4A:283:HIS:HB3   | 2.41                     | 0.56              |
| 1:3C:306:ASP:OD2   | 1:3C:309:HIS:ND1   | 2.38                     | 0.56              |
| 1:3C:398:MET:HG2   | 2:3D:345:ILE:HD13  | 1.87                     | 0.56              |
| 1:3E:69:ASP:OD1    | 1:3E:70:LEU:N      | 2.38                     | 0.56              |
| 1:8A:31:GLN:OE1    | 1:8A:32:PRO:HD2    | 2.06                     | 0.56              |
| 2:12B:210:ILE:HG22 | 2:12B:215:LEU:HD23 | 1.88                     | 0.56              |
| 2:12D:211:CYS:HB2  | 2:12D:217:LEU:HD12 | 1.87                     | 0.56              |
| 1:2E:202:PHE:HE1   | 1:2E:378:LEU:HD23  | 1.70                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:188:ILE:HG22  | 1:3A:421:ALA:HB1   | 1.87                     | 0.56              |
| 1:5C:339:ARG:O     | 1:5C:342:GLN:NE2   | 2.39                     | 0.56              |
| 1:7E:31:GLN:CG     | 1:7E:32:PRO:HD2    | 2.36                     | 0.56              |
| 1:8C:101:ASN:ND2   | 2:8D:252:LYS:HE3   | 2.20                     | 0.56              |
| 1:11C:221:ARG:HA   | 2:11D:324:LYS:HD3  | 1.87                     | 0.56              |
| 1:12E:195:LEU:HD21 | 1:12E:264:ARG:HG2  | 1.87                     | 0.56              |
| 1:13E:317:MET:HE2  | 1:13E:319:TYR:CE2  | 2.41                     | 0.56              |
| 1:1E:225:THR:O     | 1:1E:229:ARG:HG3   | 2.06                     | 0.56              |
| 1:2A:202:PHE:HE1   | 1:2A:378:LEU:HD23  | 1.70                     | 0.56              |
| 1:4A:195:LEU:HD12  | 1:4A:428:LEU:HD22  | 1.86                     | 0.56              |
| 1:5E:53:PHE:O      | 1:5E:64:ARG:NH1    | 2.32                     | 0.56              |
| 2:7B:67:ASP:OD1    | 2:7B:68:LEU:N      | 2.39                     | 0.56              |
| 1:9C:132:LEU:HD23  | 1:9C:164:LYS:HD2   | 1.87                     | 0.56              |
| 2:9D:4:ILE:HG13    | 2:9D:132:GLY:O     | 2.05                     | 0.56              |
| 2:9D:285:THR:O     | 2:9D:288:GLU:HG2   | 2.05                     | 0.56              |
| 1:10C:26:LEU:HD12  | 1:10C:363:VAL:HG12 | 1.87                     | 0.56              |
| 2:11B:8:GLN:O      | 2:11B:66:VAL:HG12  | 2.06                     | 0.56              |
| 1:11C:205:ASP:HB2  | 1:11C:303:VAL:HG22 | 1.87                     | 0.56              |
| 1:12A:204:VAL:HG11 | 1:12A:231:ILE:HD11 | 1.88                     | 0.56              |
| 2:12B:263:LEU:HG   | 2:12B:422:TYR:CE1  | 2.40                     | 0.56              |
| 2:12D:193:VAL:HG13 | 2:12D:194:GLU:HG3  | 1.88                     | 0.56              |
| 2:12D:256:ASN:HB2  | 2:12D:350:LYS:HZ3  | 1.69                     | 0.56              |
| 2:13D:28:HIS:NE2   | 2:13D:241:ARG:HD2  | 2.20                     | 0.56              |
| 2:13D:90:PHE:HB3   | 2:13D:92:PHE:CE2   | 2.38                     | 0.56              |
| 1:1A:27:GLU:OE1    | 1:1A:243:ARG:NH2   | 2.38                     | 0.56              |
| 1:1C:269:LEU:HD11  | 1:1C:384:ILE:HB    | 1.87                     | 0.56              |
| 1:2E:91:GLN:HA     | 1:2E:121:ARG:HH12  | 1.71                     | 0.56              |
| 1:5E:224:TYR:O     | 1:5E:228:ASN:ND2   | 2.39                     | 0.56              |
| 1:6A:205:ASP:OD1   | 1:6A:206:ASN:N     | 2.38                     | 0.56              |
| 2:6D:12:CYS:SG     | 2:6D:138:SER:OG    | 2.50                     | 0.56              |
| 1:7A:91:GLN:HG2    | 1:7A:121:ARG:HH22  | 1.69                     | 0.56              |
| 1:7C:53:PHE:O      | 1:7C:64:ARG:NH1    | 2.38                     | 0.56              |
| 1:8A:5:ILE:HG12    | 1:8A:64:ARG:HG2    | 1.87                     | 0.56              |
| 2:8D:67:ASP:OD1    | 2:8D:68:LEU:N      | 2.38                     | 0.56              |
| 1:10C:102:ASN:HB2  | 1:10C:105:ARG:HB2  | 1.88                     | 0.56              |
| 2:10D:303:CYS:SG   | 2:10D:377:LEU:HG   | 2.46                     | 0.56              |
| 1:11C:399:TYR:OH   | 1:11C:415:GLU:HG2  | 2.06                     | 0.56              |
| 2:11D:136:THR:HB   | 2:11D:233:MET:HE1  | 1.87                     | 0.56              |
| 2:12D:140:GLY:O    | 2:12D:184:ASN:ND2  | 2.38                     | 0.56              |
| 1:13A:140:SER:OG   | 3:13A:500:GTP:O2A  | 2.24                     | 0.56              |
| 1:2C:26:LEU:HD12   | 1:2C:363:VAL:HG12  | 1.88                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:6D:382:SER:O     | 2:6D:386:THR:HG23  | 2.06                     | 0.56              |
| 2:8B:74:ASP:OD1    | 2:8B:75:SER:N      | 2.38                     | 0.56              |
| 2:8D:293:MET:HE1   | 2:8D:315:ALA:HB1   | 1.87                     | 0.56              |
| 2:9B:285:THR:O     | 2:9B:288:GLU:HG2   | 2.05                     | 0.56              |
| 2:9B:382:SER:O     | 2:9B:386:THR:HG23  | 2.05                     | 0.56              |
| 1:11A:398:MET:HE1  | 2:11B:344:TRP:O    | 2.06                     | 0.56              |
| 1:12A:26:LEU:HD12  | 1:12A:363:VAL:HG12 | 1.86                     | 0.56              |
| 2:13B:211:CYS:HB2  | 2:13B:217:LEU:HD12 | 1.87                     | 0.56              |
| 1:13C:195:LEU:HD12 | 1:13C:428:LEU:HD22 | 1.86                     | 0.56              |
| 2:1B:3:GLU:HG2     | 2:1B:49:VAL:HA     | 1.88                     | 0.56              |
| 1:1C:88:HIS:HB3    | 1:1C:90:GLU:OE1    | 2.06                     | 0.56              |
| 2:2B:45:GLU:O      | 2:2B:46:ARG:NH1    | 2.39                     | 0.56              |
| 2:2B:121:ARG:O     | 2:2B:125:GLU:HG2   | 2.06                     | 0.56              |
| 1:3A:189:LEU:HD21  | 1:3A:413:MET:HE1   | 1.88                     | 0.56              |
| 1:3C:224:TYR:O     | 1:3C:228:ASN:ND2   | 2.38                     | 0.56              |
| 1:6A:91:GLN:HG2    | 1:6A:121:ARG:HH22  | 1.70                     | 0.56              |
| 1:6E:174:ALA:HB3   | 1:6E:177:VAL:O     | 2.06                     | 0.56              |
| 2:8B:51:TYR:O      | 2:8B:62:ARG:NH2    | 2.39                     | 0.56              |
| 2:9B:67:ASP:OD1    | 2:9B:68:LEU:N      | 2.39                     | 0.56              |
| 2:9B:303:CYS:SG    | 2:9B:377:LEU:HG    | 2.46                     | 0.56              |
| 2:11D:175:VAL:HG13 | 1:11E:329:ASN:ND2  | 2.20                     | 0.56              |
| 1:13A:182:VAL:HG12 | 1:13A:185:TYR:HB2  | 1.86                     | 0.56              |
| 1:13C:31:GLN:CG    | 1:13C:32:PRO:HD2   | 2.36                     | 0.56              |
| 2:1D:186:THR:HG22  | 2:1D:411:ALA:HB1   | 1.88                     | 0.56              |
| 2:2B:114:ASP:OD2   | 2:2B:115:SER:N     | 2.38                     | 0.56              |
| 2:2D:248:ALA:HA    | 2:2D:252:LYS:HD3   | 1.87                     | 0.56              |
| 1:5C:145:THR:OG1   | 3:5C:500:GTP:O3B   | 2.24                     | 0.56              |
| 2:5D:4:ILE:HG13    | 2:5D:132:GLY:O     | 2.06                     | 0.56              |
| 2:6B:178:THR:HB    | 2:6B:181:GLU:HG3   | 1.88                     | 0.56              |
| 1:9E:251:ASP:O     | 1:9E:255:PHE:N     | 2.39                     | 0.56              |
| 2:10B:182:PRO:HG3  | 2:10B:384:GLN:HG3  | 1.88                     | 0.55              |
| 1:11E:286:LEU:O    | 1:11E:373:ARG:NH1  | 2.39                     | 0.55              |
| 2:12B:226:ASN:ND2  | 5:12B:600:GDP:O6   | 2.36                     | 0.55              |
| 1:12C:69:ASP:OD1   | 1:12C:70:LEU:N     | 2.37                     | 0.55              |
| 2:12D:415:MET:O    | 2:12D:419:VAL:N    | 2.29                     | 0.55              |
| 2:13D:211:CYS:HB2  | 2:13D:217:LEU:HD12 | 1.88                     | 0.55              |
| 1:13E:101:ASN:HA   | 1:13E:144:GLY:N    | 2.19                     | 0.55              |
| 1:3A:20:CYS:HB3    | 1:3A:24:TYR:CE1    | 2.39                     | 0.55              |
| 1:5E:91:GLN:HA     | 1:5E:121:ARG:HH12  | 1.71                     | 0.55              |
| 1:6C:205:ASP:O     | 1:6C:209:ILE:HG12  | 2.05                     | 0.55              |
| 2:8D:303:CYS:SG    | 2:8D:377:LEU:HG    | 2.46                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:8E:114:ILE:HB    | 1:8E:149:PHE:HZ    | 1.70                     | 0.55              |
| 1:9E:292:THR:HG21  | 1:9E:331:ALA:HB1   | 1.88                     | 0.55              |
| 1:10A:196:GLU:N    | 1:10A:196:GLU:OE2  | 2.39                     | 0.55              |
| 1:11E:113:GLU:OE1  | 1:11E:113:GLU:N    | 2.39                     | 0.55              |
| 1:12C:215:ARG:NH2  | 1:12C:299:ALA:O    | 2.33                     | 0.55              |
| 1:13A:107:HIS:HA   | 1:13A:152:LEU:HD13 | 1.87                     | 0.55              |
| 1:13E:70:LEU:HB3   | 1:13E:97:GLU:O     | 2.06                     | 0.55              |
| 1:3A:223:THR:OG1   | 2:3B:323:MET:HE1   | 2.06                     | 0.55              |
| 1:3A:407:TRP:CG    | 2:3B:255:VAL:HG23  | 2.41                     | 0.55              |
| 2:5B:121:ARG:NH1   | 2:5B:158:GLU:OE1   | 2.39                     | 0.55              |
| 1:5C:188:ILE:HG23  | 1:5C:425:LEU:HD12  | 1.87                     | 0.55              |
| 1:6A:145:THR:OG1   | 3:6A:500:GTP:O3B   | 2.20                     | 0.55              |
| 1:7A:394:LYS:HG3   | 2:7B:346:PRO:HG3   | 1.87                     | 0.55              |
| 2:7D:209:ASP:OD1   | 2:7D:213:ARG:NH1   | 2.39                     | 0.55              |
| 1:11E:174:ALA:HB1  | 1:11E:207:GLU:OE1  | 2.07                     | 0.55              |
| 2:12B:193:VAL:HG13 | 2:12B:194:GLU:HG3  | 1.88                     | 0.55              |
| 2:12D:336:LYS:HD2  | 2:12D:337:ASN:OD1  | 2.07                     | 0.55              |
| 2:13B:3:GLU:HB3    | 2:13B:62:ARG:NH2   | 2.20                     | 0.55              |
| 2:13B:411:ALA:O    | 2:13B:415:MET:HG3  | 2.07                     | 0.55              |
| 1:13C:101:ASN:HA   | 1:13C:144:GLY:H    | 1.72                     | 0.55              |
| 1:1A:225:THR:O     | 1:1A:229:ARG:HG3   | 2.06                     | 0.55              |
| 2:1D:173:PRO:HD2   | 2:1D:380:ARG:HH21  | 1.72                     | 0.55              |
| 1:3E:306:ASP:OD2   | 1:3E:309:HIS:ND1   | 2.39                     | 0.55              |
| 1:4A:63:PRO:HD3    | 1:4A:86:LEU:HG     | 1.87                     | 0.55              |
| 2:4D:282:ARG:NH2   | 2:4D:292:GLN:OE1   | 2.39                     | 0.55              |
| 1:5E:188:ILE:HG22  | 1:5E:421:ALA:HB1   | 1.87                     | 0.55              |
| 1:5E:195:LEU:HD12  | 1:5E:428:LEU:HD22  | 1.88                     | 0.55              |
| 2:6D:249:ASP:H     | 2:6D:252:LYS:HD3   | 1.71                     | 0.55              |
| 2:7B:49:VAL:HG11   | 2:7B:241:ARG:HG2   | 1.87                     | 0.55              |
| 1:7C:332:ILE:HD12  | 1:7C:351:PHE:CE2   | 2.41                     | 0.55              |
| 2:7D:285:THR:O     | 2:7D:288:GLU:HG2   | 2.06                     | 0.55              |
| 1:9C:69:ASP:OD1    | 1:9C:70:LEU:N      | 2.38                     | 0.55              |
| 2:9D:98:GLY:HA2    | 1:9E:254:GLU:HB2   | 1.88                     | 0.55              |
| 2:11B:128:ASP:OD1  | 2:11B:129:CYS:N    | 2.39                     | 0.55              |
| 1:13A:336:LYS:HD3  | 1:13A:343:PHE:CZ   | 2.41                     | 0.55              |
| 1:1A:188:ILE:HG22  | 1:1A:421:ALA:HB1   | 1.87                     | 0.55              |
| 1:1C:112:LYS:HA    | 1:1C:115:VAL:HG12  | 1.88                     | 0.55              |
| 1:1E:91:GLN:HA     | 1:1E:121:ARG:HH12  | 1.72                     | 0.55              |
| 1:5A:20:CYS:HB3    | 1:5A:24:TYR:CE2    | 2.41                     | 0.55              |
| 2:5D:127:CYS:SG    | 2:5D:130:LEU:HD23  | 2.46                     | 0.55              |
| 2:6D:213:ARG:HH21  | 2:6D:297:LYS:HG3   | 1.70                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6E:145:THR:OG1   | 3:6E:500:GTP:O3B   | 2.22                     | 0.55              |
| 1:8E:111:GLY:HA2   | 1:8E:149:PHE:CE2   | 2.41                     | 0.55              |
| 2:10D:73:MET:HE1   | 2:10D:92:PHE:HB3   | 1.89                     | 0.55              |
| 2:10D:263:LEU:HG   | 2:10D:422:TYR:CE1  | 2.38                     | 0.55              |
| 2:10D:292:GLN:HE22 | 2:10D:298:ASN:HD22 | 1.53                     | 0.55              |
| 1:10E:174:ALA:HB1  | 1:10E:207:GLU:OE1  | 2.07                     | 0.55              |
| 1:12A:69:ASP:OD1   | 1:12A:70:LEU:N     | 2.39                     | 0.55              |
| 2:12B:336:LYS:HD2  | 2:12B:337:ASN:OD1  | 2.07                     | 0.55              |
| 2:12D:178:THR:HB   | 2:12D:181:GLU:HG3  | 1.88                     | 0.55              |
| 1:12E:422:ARG:HA   | 1:12E:425:LEU:HB2  | 1.89                     | 0.55              |
| 2:13D:204:ASN:ND2  | 2:13D:204:ASN:O    | 2.39                     | 0.55              |
| 1:13E:317:MET:HE3  | 1:13E:375:VAL:HG11 | 1.88                     | 0.55              |
| 1:3A:222:PRO:HD2   | 2:3B:324:LYS:HE2   | 1.87                     | 0.55              |
| 1:5A:53:PHE:O      | 1:5A:64:ARG:NH1    | 2.32                     | 0.55              |
| 2:8B:121:ARG:NH2   | 2:8B:158:GLU:OE2   | 2.39                     | 0.55              |
| 1:8C:113:GLU:N     | 1:8C:113:GLU:OE2   | 2.39                     | 0.55              |
| 1:10E:129:CYS:HB2  | 1:10E:132:LEU:HB2  | 1.89                     | 0.55              |
| 2:11B:387:ALA:HB1  | 2:11B:391:ARG:HH21 | 1.72                     | 0.55              |
| 1:11C:313:MET:SD   | 1:11C:313:MET:N    | 2.80                     | 0.55              |
| 2:12B:178:THR:HB   | 2:12B:181:GLU:HG3  | 1.89                     | 0.55              |
| 2:12D:263:LEU:HG   | 2:12D:422:TYR:CE1  | 2.39                     | 0.55              |
| 2:13B:44:LEU:HD13  | 2:13B:47:ILE:HG21  | 1.89                     | 0.55              |
| 2:13B:88:ASP:OD1   | 1:1E:280:LYS:HD2   | 2.06                     | 0.55              |
| 2:13B:111:GLU:OE1  | 2:13B:111:GLU:N    | 2.40                     | 0.55              |
| 1:13C:390:ARG:O    | 1:13C:394:LYS:HG3  | 2.07                     | 0.55              |
| 2:1D:285:THR:HG23  | 2:1D:287:PRO:HD2   | 1.89                     | 0.55              |
| 1:9A:224:TYR:O     | 1:9A:228:ASN:ND2   | 2.40                     | 0.55              |
| 2:9D:67:ASP:OD1    | 2:9D:68:LEU:N      | 2.38                     | 0.55              |
| 1:10A:69:ASP:OD1   | 1:10A:70:LEU:N     | 2.40                     | 0.55              |
| 2:12B:28:HIS:CE1   | 2:12B:241:ARG:HD2  | 2.41                     | 0.55              |
| 1:12C:11:GLN:HB3   | 3:12C:500:GTP:O2B  | 2.06                     | 0.55              |
| 1:13C:101:ASN:HD21 | 2:13D:252:LYS:HE3  | 1.70                     | 0.55              |
| 1:13E:213:CYS:HA   | 1:13E:217:LEU:HD13 | 1.87                     | 0.55              |
| 1:13E:225:THR:O    | 1:13E:229:ARG:HG3  | 2.07                     | 0.55              |
| 1:1A:203:MET:HE1   | 1:1A:388:TRP:HE1   | 1.70                     | 0.55              |
| 1:1E:88:HIS:CD2    | 1:2E:283:HIS:HB3   | 2.41                     | 0.55              |
| 2:2D:288:GLU:O     | 2:2D:291:GLN:NE2   | 2.40                     | 0.55              |
| 1:3C:292:THR:HG21  | 1:3C:331:ALA:HB1   | 1.88                     | 0.55              |
| 1:3E:175:PRO:HB3   | 1:3E:390:ARG:HD3   | 1.88                     | 0.55              |
| 1:3E:205:ASP:OD1   | 1:3E:206:ASN:N     | 2.40                     | 0.55              |
| 2:4B:61:PRO:HD3    | 2:4B:84:ILE:HG22   | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7A:261:PRO:HG3   | 1:7A:313:MET:SD    | 2.47                     | 0.55              |
| 1:7C:214:ARG:HH12  | 2:7D:324:LYS:HD2   | 1.72                     | 0.55              |
| 1:7C:228:ASN:OD1   | 3:7C:500:GTP:N2    | 2.25                     | 0.55              |
| 1:8C:204:VAL:HG23  | 1:8C:302:MET:HG2   | 1.88                     | 0.55              |
| 2:8D:209:ASP:OD2   | 2:8D:213:ARG:NH2   | 2.40                     | 0.55              |
| 1:10C:205:ASP:HB2  | 1:10C:303:VAL:HG22 | 1.87                     | 0.55              |
| 2:10D:149:THR:OG1  | 2:10D:191:GLN:HG3  | 2.06                     | 0.55              |
| 1:12A:195:LEU:HD12 | 1:12A:428:LEU:HD22 | 1.89                     | 0.55              |
| 1:13A:381:THR:HG23 | 1:13A:383:ALA:H    | 1.71                     | 0.55              |
| 2:13B:209:ASP:OD2  | 2:13B:213:ARG:NH2  | 2.36                     | 0.55              |
| 1:1A:395:PHE:HZ    | 1:1A:418:PHE:HB3   | 1.71                     | 0.55              |
| 1:1C:91:GLN:HA     | 1:1C:121:ARG:HH12  | 1.71                     | 0.55              |
| 2:1D:325:GLU:O     | 2:1D:329:GLN:HG2   | 2.07                     | 0.55              |
| 1:3A:112:LYS:HA    | 1:3A:115:VAL:HG12  | 1.89                     | 0.55              |
| 1:4E:189:LEU:HD21  | 1:4E:413:MET:HE1   | 1.88                     | 0.55              |
| 2:6D:208:TYR:HA    | 2:6D:211:CYS:SG    | 2.46                     | 0.55              |
| 2:6D:213:ARG:O     | 2:6D:216:LYS:NZ    | 2.37                     | 0.55              |
| 2:10B:140:GLY:O    | 2:10B:184:ASN:ND2  | 2.40                     | 0.55              |
| 1:10C:175:PRO:HD2  | 1:10C:207:GLU:OE2  | 2.07                     | 0.55              |
| 1:11A:142:GLY:O    | 1:11A:186:ASN:ND2  | 2.40                     | 0.55              |
| 2:11B:316:ILE:HB   | 2:11B:366:THR:HB   | 1.88                     | 0.55              |
| 1:11C:113:GLU:N    | 1:11C:113:GLU:OE2  | 2.40                     | 0.55              |
| 2:11D:263:LEU:HG   | 2:11D:422:TYR:CE1  | 2.41                     | 0.55              |
| 1:12E:11:GLN:HB3   | 3:12E:500:GTP:O2B  | 2.06                     | 0.55              |
| 1:13A:30:ILE:HD11  | 1:13A:61:HIS:HB2   | 1.87                     | 0.55              |
| 1:13A:69:ASP:OD1   | 1:13A:70:LEU:N     | 2.40                     | 0.55              |
| 1:13C:100:ALA:HB1  | 2:13D:255:VAL:HG11 | 1.87                     | 0.55              |
| 2:2B:248:ALA:HA    | 2:2B:252:LYS:HD3   | 1.87                     | 0.55              |
| 2:4D:387:ALA:C     | 2:4D:388:MET:HE2   | 2.31                     | 0.55              |
| 1:5C:71:GLU:HB2    | 1:5C:98:ASP:HB3    | 1.88                     | 0.55              |
| 1:7E:54:SER:HG     | 1:7E:64:ARG:HH12   | 1.52                     | 0.55              |
| 1:8A:33:ASP:HB2    | 1:8A:35:GLN:OE1    | 2.07                     | 0.55              |
| 1:8A:220:GLU:N     | 1:8A:220:GLU:OE1   | 2.36                     | 0.55              |
| 2:10D:28:HIS:NE2   | 2:10D:241:ARG:HD2  | 2.22                     | 0.55              |
| 1:11A:377:MET:HE1  | 1:11A:379:SER:HB3  | 1.89                     | 0.55              |
| 1:11C:175:PRO:HD2  | 1:11C:207:GLU:OE1  | 2.05                     | 0.55              |
| 1:11E:295:CYS:HB3  | 1:11E:377:MET:HG2  | 1.89                     | 0.55              |
| 1:12C:332:ILE:O    | 1:12C:336:LYS:HG2  | 2.07                     | 0.55              |
| 1:12E:169:PHE:CE2  | 1:12E:235:VAL:HG12 | 2.41                     | 0.55              |
| 1:13A:27:GLU:OE1   | 1:13A:243:ARG:NH1  | 2.38                     | 0.55              |
| 2:13B:220:PRO:HD2  | 1:13C:326:LYS:HD3  | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:184:PRO:O     | 1:1A:188:ILE:HG12  | 2.07                     | 0.55              |
| 1:3A:102:ASN:HD22  | 1:3A:105:ARG:HD3   | 1.71                     | 0.55              |
| 1:4E:56:THR:HG23   | 1:5E:285:GLN:HB2   | 1.89                     | 0.55              |
| 2:5B:131:GLN:O     | 2:5B:163:ILE:HG22  | 2.05                     | 0.55              |
| 1:5C:215:ARG:HH22  | 1:5C:299:ALA:HB1   | 1.71                     | 0.55              |
| 2:5D:209:ASP:OD2   | 2:5D:213:ARG:NH2   | 2.38                     | 0.55              |
| 1:6E:271:THR:HG22  | 1:6E:377:MET:HE3   | 1.89                     | 0.55              |
| 1:6E:313:MET:HB2   | 1:6E:380:ASN:O     | 2.07                     | 0.55              |
| 1:10C:175:PRO:HB3  | 1:10C:390:ARG:CZ   | 2.37                     | 0.54              |
| 1:11C:265:ILE:HG23 | 1:11C:432:TYR:CZ   | 2.42                     | 0.54              |
| 1:11E:216:ASN:ND2  | 1:11E:300:ASN:OD1  | 2.41                     | 0.54              |
| 2:12B:382:SER:O    | 2:12B:386:THR:OG1  | 2.17                     | 0.54              |
| 1:12E:26:LEU:HD12  | 1:12E:363:VAL:HG12 | 1.89                     | 0.54              |
| 1:13A:390:ARG:O    | 1:13A:394:LYS:HG3  | 2.08                     | 0.54              |
| 2:1D:178:THR:HG22  | 2:1D:180:VAL:H     | 1.72                     | 0.54              |
| 2:2B:173:PRO:HD2   | 2:2B:380:ARG:HH21  | 1.72                     | 0.54              |
| 2:2D:130:LEU:HD12  | 2:2D:162:ARG:HD2   | 1.89                     | 0.54              |
| 2:3D:310:TYR:O     | 2:3D:342:VAL:HG23  | 2.07                     | 0.54              |
| 2:4B:190:HIS:NE2   | 2:4B:414:ASN:OD1   | 2.40                     | 0.54              |
| 1:7C:102:ASN:HD22  | 1:7C:105:ARG:HG3   | 1.72                     | 0.54              |
| 1:7C:132:LEU:HD23  | 1:7C:164:LYS:HD3   | 1.89                     | 0.54              |
| 2:8D:257:MET:CE    | 2:8D:314:ALA:HB2   | 2.37                     | 0.54              |
| 2:8D:257:MET:HE1   | 2:8D:313:VAL:O     | 2.06                     | 0.54              |
| 1:13C:149:PHE:O    | 1:13C:153:LEU:N    | 2.29                     | 0.54              |
| 2:3B:131:GLN:O     | 2:3B:163:ILE:HG22  | 2.07                     | 0.54              |
| 1:4A:188:ILE:HG22  | 1:4A:421:ALA:HB1   | 1.88                     | 0.54              |
| 1:4C:371:VAL:HG12  | 1:4C:373:ARG:H     | 1.72                     | 0.54              |
| 2:8D:117:LEU:HA    | 2:8D:120:VAL:HG22  | 1.89                     | 0.54              |
| 2:10D:111:GLU:OE1  | 2:10D:111:GLU:N    | 2.40                     | 0.54              |
| 1:11C:3:GLU:OE2    | 1:11C:130:THR:N    | 2.39                     | 0.54              |
| 2:13B:304:ASP:HB2  | 2:13B:307:HIS:CE1  | 2.43                     | 0.54              |
| 1:13C:427:ALA:HA   | 1:13C:430:LYS:HB3  | 1.89                     | 0.54              |
| 2:13D:390:ARG:HG3  | 2:13D:391:ARG:HD3  | 1.88                     | 0.54              |
| 2:1B:371:SER:OG    | 2:1B:372:THR:N     | 2.39                     | 0.54              |
| 2:1D:5:VAL:HG12    | 2:1D:62:ARG:HD3    | 1.88                     | 0.54              |
| 1:1E:261:PRO:HG3   | 1:1E:313:MET:SD    | 2.47                     | 0.54              |
| 1:2E:209:ILE:HG21  | 1:2E:227:LEU:HG    | 1.89                     | 0.54              |
| 1:2E:291:ILE:HD12  | 1:2E:375:VAL:HG23  | 1.90                     | 0.54              |
| 1:4E:224:TYR:O     | 1:4E:228:ASN:ND2   | 2.40                     | 0.54              |
| 2:6B:175:VAL:HG22  | 1:6C:329:ASN:HD21  | 1.71                     | 0.54              |
| 2:6B:309:ARG:NH1   | 2:6B:426:GLN:OXT   | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7B:45:GLU:C      | 2:7B:46:ARG:HD2    | 2.33                     | 0.54              |
| 2:7D:372:THR:HG21  | 2:7D:426:GLN:HA    | 1.89                     | 0.54              |
| 1:8C:70:LEU:HD11   | 1:8C:110:ILE:HG22  | 1.90                     | 0.54              |
| 1:9C:31:GLN:OE1    | 1:9C:32:PRO:HD2    | 2.07                     | 0.54              |
| 1:10E:56:THR:HA    | 1:11E:285:GLN:HB2  | 1.90                     | 0.54              |
| 1:10E:102:ASN:HD22 | 1:10E:105:ARG:HG3  | 1.72                     | 0.54              |
| 2:11D:4:ILE:HG13   | 2:11D:132:GLY:O    | 2.07                     | 0.54              |
| 2:12B:390:ARG:HG3  | 2:12B:391:ARG:CD   | 2.38                     | 0.54              |
| 2:12D:111:GLU:OE1  | 2:12D:111:GLU:N    | 2.40                     | 0.54              |
| 1:13E:313:MET:N    | 1:13E:313:MET:SD   | 2.80                     | 0.54              |
| 2:2D:191:GLN:HE21  | 2:2D:195:ASN:ND2   | 2.06                     | 0.54              |
| 2:4D:102:ALA:HB2   | 2:4D:403:MET:HE2   | 1.89                     | 0.54              |
| 2:5B:178:THR:HB    | 2:5B:181:GLU:HG3   | 1.89                     | 0.54              |
| 2:6B:147:MET:HE2   | 2:6B:147:MET:HA    | 1.88                     | 0.54              |
| 1:7C:224:TYR:O     | 1:7C:228:ASN:ND2   | 2.41                     | 0.54              |
| 1:7E:261:PRO:HG3   | 1:7E:313:MET:SD    | 2.47                     | 0.54              |
| 1:8A:169:PHE:CE2   | 1:8A:235:VAL:HG22  | 2.43                     | 0.54              |
| 2:8B:45:GLU:C      | 2:8B:46:ARG:HD2    | 2.32                     | 0.54              |
| 1:11C:56:THR:HA    | 1:12C:285:GLN:HB2  | 1.90                     | 0.54              |
| 1:11E:3:GLU:HB3    | 1:11E:64:ARG:HH12  | 1.73                     | 0.54              |
| 2:12B:208:TYR:HA   | 2:12B:211:CYS:SG   | 2.47                     | 0.54              |
| 1:13A:201:ALA:O    | 1:13A:268:PRO:HD2  | 2.07                     | 0.54              |
| 2:13B:334:GLN:HA   | 2:13B:341:PHE:CE2  | 2.42                     | 0.54              |
| 2:1B:2:ARG:HB3     | 2:1B:131:GLN:NE2   | 2.22                     | 0.54              |
| 2:1D:178:THR:HB    | 2:1D:181:GLU:HG3   | 1.90                     | 0.54              |
| 1:4E:206:ASN:OD1   | 3:4E:500:GTP:O2'   | 2.26                     | 0.54              |
| 1:4E:390:ARG:HG3   | 1:4E:391:LEU:N     | 2.23                     | 0.54              |
| 1:5A:68:VAL:HG11   | 1:5A:149:PHE:HE1   | 1.73                     | 0.54              |
| 1:6A:63:PRO:HD3    | 1:6A:86:LEU:HG     | 1.89                     | 0.54              |
| 1:7C:203:MET:SD    | 1:7C:203:MET:N     | 2.80                     | 0.54              |
| 1:8E:339:ARG:O     | 1:8E:342:GLN:NE2   | 2.41                     | 0.54              |
| 1:9A:8:HIS:HE1     | 1:9A:21:TRP:HE1    | 1.54                     | 0.54              |
| 1:9C:71:GLU:OE2    | 1:9C:73:THR:OG1    | 2.25                     | 0.54              |
| 1:12E:3:GLU:OE1    | 1:12E:64:ARG:NE    | 2.41                     | 0.54              |
| 1:13E:272:TYR:HE2  | 1:13E:368:LEU:HD21 | 1.72                     | 0.54              |
| 2:2D:173:PRO:HD2   | 2:2D:380:ARG:HH21  | 1.73                     | 0.54              |
| 2:3B:191:GLN:HE21  | 2:3B:195:ASN:ND2   | 2.06                     | 0.54              |
| 1:4A:132:LEU:HB3   | 1:4A:164:LYS:HE2   | 1.89                     | 0.54              |
| 1:4C:324:VAL:HG23  | 1:4C:326:LYS:HG2   | 1.90                     | 0.54              |
| 1:5A:56:THR:HA     | 1:6A:285:GLN:HB2   | 1.88                     | 0.54              |
| 2:7B:121:ARG:NH1   | 2:7B:158:GLU:OE1   | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7C:165:SER:HA    | 1:7C:199:ASP:OD2   | 2.06                     | 0.54              |
| 1:8A:3:GLU:OE2     | 1:8A:64:ARG:NE     | 2.39                     | 0.54              |
| 1:8C:221:ARG:HA    | 2:8D:324:LYS:HE3   | 1.88                     | 0.54              |
| 2:9B:193:VAL:HG13  | 2:9B:194:GLU:HG3   | 1.89                     | 0.54              |
| 1:9C:312:TYR:O     | 1:9C:344:VAL:HG23  | 2.08                     | 0.54              |
| 1:9E:31:GLN:HG3    | 1:9E:32:PRO:HD2    | 1.88                     | 0.54              |
| 1:11A:11:GLN:HB3   | 3:11A:500:GTP:O2B  | 2.08                     | 0.54              |
| 1:12E:16:ILE:HD11  | 1:12E:171:ILE:HD11 | 1.90                     | 0.54              |
| 2:4D:4:ILE:HG13    | 2:4D:132:GLY:O     | 2.08                     | 0.54              |
| 1:6C:91:GLN:HA     | 1:6C:121:ARG:HH12  | 1.73                     | 0.54              |
| 1:6E:102:ASN:HB2   | 1:6E:105:ARG:HB2   | 1.89                     | 0.54              |
| 1:8A:195:LEU:HD12  | 1:8A:428:LEU:HD22  | 1.89                     | 0.54              |
| 1:8C:165:SER:HA    | 1:8C:199:ASP:OD2   | 2.07                     | 0.54              |
| 1:9A:339:ARG:O     | 1:9A:342:GLN:NE2   | 2.41                     | 0.54              |
| 2:10D:3:GLU:H      | 2:10D:130:LEU:HA   | 1.73                     | 0.54              |
| 2:11D:405:GLU:HA   | 2:11D:408:PHE:HD1  | 1.73                     | 0.54              |
| 2:12B:258:VAL:HG22 | 2:12B:266:PHE:HZ   | 1.71                     | 0.54              |
| 2:12B:330:MET:O    | 2:12B:334:GLN:HG3  | 2.08                     | 0.54              |
| 2:13B:176:SER:OG   | 2:13B:181:GLU:OE1  | 2.17                     | 0.54              |
| 2:1B:45:GLU:O      | 2:1B:46:ARG:NH1    | 2.41                     | 0.54              |
| 2:3D:382:SER:O     | 2:3D:386:THR:OG1   | 2.18                     | 0.54              |
| 1:3E:56:THR:HG23   | 1:4E:285:GLN:HB2   | 1.90                     | 0.54              |
| 1:4C:206:ASN:OD1   | 3:4C:500:GTP:O2'   | 2.24                     | 0.54              |
| 1:5A:215:ARG:HH22  | 1:5A:299:ALA:HB1   | 1.73                     | 0.54              |
| 1:5E:255:PHE:HZ    | 1:5E:378:LEU:HD22  | 1.73                     | 0.54              |
| 1:6A:269:LEU:HD11  | 1:6A:384:ILE:HB    | 1.90                     | 0.54              |
| 1:6C:269:LEU:HD11  | 1:6C:384:ILE:HB    | 1.90                     | 0.54              |
| 1:7A:165:SER:HA    | 1:7A:199:ASP:OD2   | 2.06                     | 0.54              |
| 2:7B:73:MET:HG3    | 2:7B:92:PHE:CD1    | 2.43                     | 0.54              |
| 2:7B:208:TYR:HE1   | 2:7B:225:LEU:HD11  | 1.72                     | 0.54              |
| 1:9A:67:PHE:HB2    | 1:9A:92:LEU:HD23   | 1.90                     | 0.54              |
| 2:10D:127:CYS:SG   | 2:10D:130:LEU:HD22 | 2.47                     | 0.54              |
| 1:11A:204:VAL:HG11 | 1:11A:231:ILE:HD11 | 1.90                     | 0.54              |
| 1:12A:399:TYR:OH   | 1:12A:415:GLU:HG2  | 2.08                     | 0.54              |
| 1:13A:129:CYS:SG   | 1:13A:132:LEU:HB2  | 2.48                     | 0.54              |
| 1:1A:221:ARG:C     | 2:1B:324:LYS:HZ1   | 2.16                     | 0.54              |
| 1:1C:395:PHE:HZ    | 1:1C:418:PHE:HB3   | 1.73                     | 0.54              |
| 1:1E:9:VAL:HG11    | 1:1E:150:THR:OG1   | 2.08                     | 0.54              |
| 2:3B:109:GLY:HA2   | 2:3B:147:MET:HE1   | 1.88                     | 0.54              |
| 2:3B:324:LYS:O     | 2:3B:328:GLU:HG2   | 2.07                     | 0.54              |
| 1:6C:174:ALA:HB3   | 1:6C:177:VAL:O     | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7C:175:PRO:HG3   | 1:7C:390:ARG:NH2   | 2.23                     | 0.54              |
| 2:8D:208:TYR:HA    | 2:8D:211:CYS:SG    | 2.48                     | 0.54              |
| 1:10E:180:ALA:HB3  | 1:10E:183:GLU:HG3  | 1.89                     | 0.54              |
| 2:11B:149:THR:OG1  | 2:11B:191:GLN:NE2  | 2.41                     | 0.54              |
| 2:11D:285:THR:O    | 2:11D:288:GLU:HG2  | 2.08                     | 0.54              |
| 2:12B:111:GLU:OE1  | 2:12B:111:GLU:N    | 2.40                     | 0.54              |
| 1:13A:104:ALA:O    | 1:13A:108:TYR:N    | 2.35                     | 0.54              |
| 2:13D:267:MET:HG3  | 2:13D:369:GLY:O    | 2.07                     | 0.54              |
| 1:13E:184:PRO:O    | 1:13E:188:ILE:HG12 | 2.08                     | 0.54              |
| 1:3C:20:CYS:HB3    | 1:3C:24:TYR:CE1    | 2.43                     | 0.54              |
| 2:6B:130:LEU:HG    | 2:6B:162:ARG:HD3   | 1.89                     | 0.54              |
| 1:6E:202:PHE:HE1   | 1:6E:378:LEU:HD23  | 1.73                     | 0.54              |
| 1:7A:102:ASN:HB3   | 1:7A:105:ARG:H     | 1.72                     | 0.54              |
| 1:7A:265:ILE:HG23  | 1:7A:432:TYR:CZ    | 2.43                     | 0.54              |
| 1:8A:16:ILE:HD11   | 1:8A:171:ILE:HD11  | 1.89                     | 0.54              |
| 1:8A:292:THR:HG21  | 1:8A:331:ALA:HB1   | 1.90                     | 0.54              |
| 1:12E:295:CYS:HB3  | 1:12E:377:MET:HG2  | 1.90                     | 0.53              |
| 1:13C:70:LEU:HA    | 1:13C:95:GLY:HA3   | 1.89                     | 0.53              |
| 1:13C:319:TYR:HB3  | 1:13C:323:VAL:HG21 | 1.91                     | 0.53              |
| 1:2E:91:GLN:HG2    | 1:2E:121:ARG:HH22  | 1.72                     | 0.53              |
| 1:2E:195:LEU:HD12  | 1:2E:428:LEU:HD22  | 1.89                     | 0.53              |
| 2:3B:219:THR:HG22  | 1:3C:326:LYS:HE2   | 1.89                     | 0.53              |
| 1:3C:407:TRP:CG    | 2:3D:255:VAL:HG23  | 2.42                     | 0.53              |
| 2:3D:285:THR:O     | 2:3D:288:GLU:HG2   | 2.08                     | 0.53              |
| 1:7E:165:SER:HA    | 1:7E:199:ASP:OD2   | 2.08                     | 0.53              |
| 1:9E:224:TYR:O     | 1:9E:228:ASN:ND2   | 2.40                     | 0.53              |
| 2:10B:111:GLU:OE1  | 2:10B:111:GLU:N    | 2.41                     | 0.53              |
| 1:10C:88:HIS:CD2   | 1:10C:89:PRO:HD2   | 2.40                     | 0.53              |
| 1:11E:265:ILE:HG23 | 1:11E:432:TYR:CZ   | 2.43                     | 0.53              |
| 1:12A:139:HIS:HE1  | 1:12A:141:PHE:CE1  | 2.26                     | 0.53              |
| 2:12D:5:VAL:HG12   | 2:12D:62:ARG:HD2   | 1.89                     | 0.53              |
| 2:12D:327:ASP:OD1  | 2:12D:328:GLU:N    | 2.41                     | 0.53              |
| 2:13D:139:LEU:HD23 | 2:13D:170:VAL:HG12 | 1.90                     | 0.53              |
| 1:3C:215:ARG:HH22  | 1:3C:299:ALA:HB1   | 1.73                     | 0.53              |
| 2:3D:311:LEU:HD23  | 2:3D:342:VAL:HG21  | 1.89                     | 0.53              |
| 1:3E:91:GLN:HA     | 1:3E:121:ARG:HH12  | 1.73                     | 0.53              |
| 2:4D:311:LEU:HD23  | 2:4D:342:VAL:HG21  | 1.91                     | 0.53              |
| 1:5A:291:ILE:HD12  | 1:5A:375:VAL:HG23  | 1.90                     | 0.53              |
| 1:6A:317:MET:HB3   | 1:6A:319:TYR:CE1   | 2.43                     | 0.53              |
| 2:6D:167:TYR:CE1   | 2:6D:233:MET:HG2   | 2.43                     | 0.53              |
| 1:7C:174:ALA:HB3   | 1:7C:177:VAL:O     | 2.09                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7D:147:MET:HE2   | 2:7D:147:MET:HA    | 1.89                     | 0.53              |
| 2:7D:382:SER:O     | 2:7D:386:THR:OG1   | 2.19                     | 0.53              |
| 1:8A:113:GLU:OE1   | 1:8A:113:GLU:N     | 2.41                     | 0.53              |
| 2:9D:334:GLN:HE22  | 2:9D:347:ASN:HA    | 1.73                     | 0.53              |
| 2:10B:268:PRO:HG2  | 2:10B:300:MET:HB3  | 1.91                     | 0.53              |
| 1:11A:265:ILE:HG23 | 1:11A:432:TYR:CZ   | 2.43                     | 0.53              |
| 2:13B:237:THR:HB   | 2:13B:240:LEU:HD12 | 1.90                     | 0.53              |
| 1:13C:113:GLU:N    | 1:13C:113:GLU:OE2  | 2.41                     | 0.53              |
| 1:13E:319:TYR:HB3  | 1:13E:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:1B:382:SER:O     | 2:1B:386:THR:HG23  | 2.08                     | 0.53              |
| 1:2A:189:LEU:HD21  | 1:2A:413:MET:HE1   | 1.88                     | 0.53              |
| 2:3B:382:SER:O     | 2:3B:386:THR:OG1   | 2.19                     | 0.53              |
| 2:4D:257:MET:HE1   | 2:4D:313:VAL:C     | 2.33                     | 0.53              |
| 2:5D:67:ASP:OD1    | 2:5D:68:LEU:N      | 2.41                     | 0.53              |
| 2:9B:4:ILE:HG23    | 2:9B:50:TYR:HE1    | 1.72                     | 0.53              |
| 2:9D:220:PRO:HD2   | 1:9E:326:LYS:HD3   | 1.89                     | 0.53              |
| 1:10C:175:PRO:HB3  | 1:10C:390:ARG:NE   | 2.23                     | 0.53              |
| 2:11B:334:GLN:HE22 | 2:11B:347:ASN:HA   | 1.73                     | 0.53              |
| 1:11C:269:LEU:HD13 | 1:11C:381:THR:HG22 | 1.91                     | 0.53              |
| 1:13C:155:GLU:HB3  | 1:13C:156:ARG:HH12 | 1.73                     | 0.53              |
| 2:13D:104:GLY:HA3  | 2:13D:146:GLY:HA3  | 1.90                     | 0.53              |
| 1:1A:91:GLN:HA     | 1:1A:121:ARG:HH12  | 1.72                     | 0.53              |
| 2:2B:209:ASP:OD2   | 2:2B:213:ARG:NH2   | 2.42                     | 0.53              |
| 1:7A:224:TYR:O     | 1:7A:228:ASN:ND2   | 2.41                     | 0.53              |
| 2:7B:209:ASP:OD2   | 2:7B:213:ARG:NH2   | 2.39                     | 0.53              |
| 1:8E:75:VAL:O      | 1:8E:78:VAL:HG22   | 2.09                     | 0.53              |
| 2:9D:3:GLU:HB3     | 2:9D:62:ARG:HH12   | 1.73                     | 0.53              |
| 2:11B:3:GLU:HB3    | 2:11B:62:ARG:HH12  | 1.73                     | 0.53              |
| 2:11D:104:GLY:HA3  | 2:11D:146:GLY:HA3  | 1.91                     | 0.53              |
| 1:12E:230:LEU:HD23 | 1:12E:302:MET:HE1  | 1.90                     | 0.53              |
| 1:13C:204:VAL:HG11 | 1:13C:231:ILE:HD11 | 1.90                     | 0.53              |
| 2:13D:111:GLU:OE1  | 2:13D:111:GLU:N    | 2.40                     | 0.53              |
| 1:1A:178:SER:OG    | 2:1B:347:ASN:OD1   | 2.18                     | 0.53              |
| 2:1B:213:ARG:CZ    | 2:1B:297:LYS:HD2   | 2.39                     | 0.53              |
| 1:1C:199:ASP:O     | 1:1C:256:GLN:NE2   | 2.41                     | 0.53              |
| 2:1D:248:ALA:HA    | 2:1D:252:LYS:HD3   | 1.90                     | 0.53              |
| 1:3E:88:HIS:CD2    | 1:4E:283:HIS:HB3   | 2.42                     | 0.53              |
| 1:4C:329:ASN:OD1   | 1:4C:330:ALA:N     | 2.42                     | 0.53              |
| 2:5B:20:PHE:HD2    | 2:5B:233:MET:HE3   | 1.74                     | 0.53              |
| 2:5B:178:THR:HG22  | 2:5B:180:VAL:H     | 1.73                     | 0.53              |
| 1:7E:224:TYR:O     | 1:7E:228:ASN:ND2   | 2.41                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:330:MET:SD    | 2:8B:349:VAL:HG11  | 2.49                     | 0.53              |
| 1:10C:213:CYS:SG   | 1:10C:222:PRO:HG3  | 2.49                     | 0.53              |
| 1:10E:88:HIS:HD2   | 1:10E:90:GLU:HG3   | 1.74                     | 0.53              |
| 1:11A:287:SER:O    | 1:11A:290:GLU:HG3  | 2.08                     | 0.53              |
| 2:11D:3:GLU:HB3    | 2:11D:62:ARG:HH12  | 1.73                     | 0.53              |
| 1:12E:31:GLN:CD    | 1:12E:32:PRO:HD2   | 2.34                     | 0.53              |
| 1:13A:184:PRO:O    | 1:13A:188:ILE:N    | 2.40                     | 0.53              |
| 1:13E:172:TYR:HB2  | 1:13E:203:MET:SD   | 2.48                     | 0.53              |
| 2:1B:289:LEU:O     | 2:1B:293:MET:HG3   | 2.09                     | 0.53              |
| 2:1B:378:PHE:HB3   | 2:1B:415:MET:HE3   | 1.91                     | 0.53              |
| 2:3B:121:ARG:O     | 2:3B:125:GLU:HG2   | 2.08                     | 0.53              |
| 1:3E:224:TYR:O     | 1:3E:228:ASN:ND2   | 2.41                     | 0.53              |
| 2:4B:5:VAL:HG12    | 2:4B:62:ARG:HD3    | 1.88                     | 0.53              |
| 1:5C:175:PRO:HD2   | 1:5C:207:GLU:OE1   | 2.08                     | 0.53              |
| 1:6E:356:ASN:OD1   | 1:6E:357:TYR:N     | 2.42                     | 0.53              |
| 1:7A:222:PRO:HD2   | 2:7B:324:LYS:HE2   | 1.90                     | 0.53              |
| 1:7C:134:GLY:HA3   | 1:7C:165:SER:O     | 2.08                     | 0.53              |
| 1:9A:121:ARG:NH1   | 1:9A:121:ARG:HB3   | 2.24                     | 0.53              |
| 1:10A:11:GLN:O     | 1:10A:15:GLN:HG2   | 2.08                     | 0.53              |
| 2:10B:336:LYS:HD2  | 2:10B:337:ASN:OD1  | 2.09                     | 0.53              |
| 1:10C:204:VAL:HG11 | 1:10C:231:ILE:HD11 | 1.91                     | 0.53              |
| 2:11B:208:TYR:HA   | 2:11B:211:CYS:SG   | 2.49                     | 0.53              |
| 2:11B:215:LEU:HB3  | 2:11B:217:LEU:HG   | 1.90                     | 0.53              |
| 1:12A:53:PHE:HD2   | 1:12A:61:HIS:HB3   | 1.73                     | 0.53              |
| 1:12E:203:MET:HE2  | 1:12E:203:MET:HA   | 1.90                     | 0.53              |
| 2:13B:156:ARG:NH2  | 2:13B:197:ASP:OD1  | 2.41                     | 0.53              |
| 2:13B:190:HIS:HB2  | 2:13B:411:ALA:CB   | 2.39                     | 0.53              |
| 1:13C:398:MET:HG2  | 2:13D:344:TRP:O    | 2.08                     | 0.53              |
| 2:13D:49:VAL:HG11  | 2:13D:241:ARG:HG2  | 1.91                     | 0.53              |
| 2:1D:371:SER:OG    | 2:1D:372:THR:N     | 2.41                     | 0.53              |
| 1:2C:324:VAL:HG23  | 1:2C:326:LYS:HG2   | 1.91                     | 0.53              |
| 2:2D:105:HIS:CD2   | 2:2D:150:LEU:HB2   | 2.44                     | 0.53              |
| 1:2E:324:VAL:HG23  | 1:2E:326:LYS:HG2   | 1.91                     | 0.53              |
| 1:6C:91:GLN:HG2    | 1:6C:121:ARG:HH22  | 1.73                     | 0.53              |
| 2:6D:376:GLU:HA    | 2:6D:379:LYS:NZ    | 2.24                     | 0.53              |
| 2:8B:373:ALA:O     | 2:8B:376:GLU:HG2   | 2.09                     | 0.53              |
| 2:8D:213:ARG:O     | 2:8D:216:LYS:NZ    | 2.33                     | 0.53              |
| 1:9E:121:ARG:HB3   | 1:9E:121:ARG:NH1   | 2.24                     | 0.53              |
| 2:10B:4:ILE:HG13   | 2:10B:132:GLY:C    | 2.33                     | 0.53              |
| 1:12C:139:HIS:CD2  | 1:12C:150:THR:HG21 | 2.44                     | 0.53              |
| 1:12C:296:PHE:CE1  | 1:12C:317:MET:HE1  | 2.44                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:251:ASP:OD2   | 1:1A:252:LEU:N     | 2.41                     | 0.53              |
| 2:1B:324:LYS:HG3   | 2:1B:325:GLU:H     | 1.73                     | 0.53              |
| 1:5C:202:PHE:HE1   | 1:5C:378:LEU:HD23  | 1.73                     | 0.53              |
| 1:6E:339:ARG:O     | 1:6E:342:GLN:NE2   | 2.41                     | 0.53              |
| 1:7A:178:SER:OG    | 2:7B:347:ASN:OD1   | 2.18                     | 0.53              |
| 2:8D:237:THR:HG22  | 2:8D:250:LEU:HD21  | 1.91                     | 0.53              |
| 1:8E:209:ILE:HG23  | 1:8E:230:LEU:HD22  | 1.91                     | 0.53              |
| 1:9E:102:ASN:OD1   | 1:9E:408:TYR:HE1   | 1.92                     | 0.53              |
| 1:10A:11:GLN:HB3   | 3:10A:500:GTP:O2B  | 2.08                     | 0.53              |
| 1:11A:313:MET:N    | 1:11A:313:MET:SD   | 2.82                     | 0.53              |
| 2:11B:257:MET:HE1  | 2:11B:370:ASN:HB2  | 1.90                     | 0.53              |
| 2:12B:389:PHE:O    | 2:12B:392:LYS:NZ   | 2.26                     | 0.53              |
| 2:13B:215:LEU:HD21 | 2:13B:273:LEU:HD22 | 1.90                     | 0.53              |
| 1:13E:119:LEU:HD23 | 1:13E:122:ILE:HD12 | 1.90                     | 0.53              |
| 1:2A:291:ILE:HD12  | 1:2A:375:VAL:HG23  | 1.90                     | 0.53              |
| 2:3D:67:ASP:OD1    | 2:3D:68:LEU:N      | 2.42                     | 0.53              |
| 1:5A:228:ASN:OD1   | 3:5A:500:GTP:N2    | 2.31                     | 0.53              |
| 1:5E:68:VAL:HG11   | 1:5E:149:PHE:HE1   | 1.74                     | 0.53              |
| 2:6B:135:LEU:HD23  | 2:6B:166:THR:HG22  | 1.89                     | 0.53              |
| 2:6B:175:VAL:HG23  | 2:6B:205:GLU:HG2   | 1.90                     | 0.53              |
| 2:7B:324:LYS:HG3   | 2:7B:325:GLU:N     | 2.22                     | 0.53              |
| 1:8C:121:ARG:HB3   | 1:8C:121:ARG:NH1   | 2.23                     | 0.53              |
| 1:9A:296:PHE:CD2   | 1:9A:335:ILE:HD13  | 2.44                     | 0.53              |
| 2:9D:117:LEU:HA    | 2:9D:120:VAL:HG22  | 1.91                     | 0.53              |
| 2:9D:286:VAL:HG22  | 2:9D:321:MET:HE3   | 1.90                     | 0.53              |
| 2:10D:336:LYS:HD2  | 2:10D:337:ASN:OD1  | 2.09                     | 0.53              |
| 1:12A:286:LEU:O    | 1:12A:373:ARG:NH1  | 2.42                     | 0.53              |
| 1:12A:377:MET:HE1  | 1:12A:379:SER:HB3  | 1.90                     | 0.53              |
| 1:12C:34:GLY:O     | 1:12C:61:HIS:ND1   | 2.37                     | 0.53              |
| 1:13C:155:GLU:HB3  | 1:13C:156:ARG:NH1  | 2.23                     | 0.53              |
| 1:13E:270:VAL:HA   | 1:13E:377:MET:O    | 2.09                     | 0.53              |
| 1:13E:386:GLU:O    | 1:13E:390:ARG:HG2  | 2.09                     | 0.53              |
| 1:2A:175:PRO:HB3   | 1:2A:390:ARG:HD3   | 1.90                     | 0.53              |
| 2:4B:3:GLU:HG2     | 2:4B:62:ARG:NH2    | 2.24                     | 0.53              |
| 2:4B:376:GLU:HA    | 2:4B:379:LYS:HE2   | 1.90                     | 0.53              |
| 1:5A:188:ILE:HG23  | 1:5A:425:LEU:HD12  | 1.91                     | 0.53              |
| 1:6A:56:THR:HA     | 1:7A:285:GLN:HB2   | 1.90                     | 0.53              |
| 1:7C:2:ARG:HB2     | 1:7C:133:GLN:HE22  | 1.73                     | 0.53              |
| 1:7E:184:PRO:O     | 1:7E:188:ILE:HG12  | 2.09                     | 0.53              |
| 1:7E:329:ASN:OD1   | 1:7E:330:ALA:N     | 2.42                     | 0.53              |
| 1:8A:63:PRO:HD3    | 1:8A:86:LEU:HG     | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:9B:130:LEU:CG    | 2:9B:162:ARG:HH12  | 2.21                     | 0.53              |
| 2:10D:140:GLY:O    | 2:10D:184:ASN:ND2  | 2.42                     | 0.52              |
| 1:10E:408:TYR:HB3  | 1:10E:413:MET:HE2  | 1.90                     | 0.52              |
| 1:11C:213:CYS:HA   | 1:11C:217:LEU:HD13 | 1.90                     | 0.52              |
| 1:11E:205:ASP:HB2  | 1:11E:303:VAL:HG22 | 1.91                     | 0.52              |
| 2:12B:237:THR:O    | 2:12B:241:ARG:NH1  | 2.42                     | 0.52              |
| 1:13C:265:ILE:HG23 | 1:13C:432:TYR:HE1  | 1.73                     | 0.52              |
| 2:1B:130:LEU:HD23  | 2:1B:130:LEU:H     | 1.74                     | 0.52              |
| 2:4D:67:ASP:OD1    | 2:4D:68:LEU:N      | 2.41                     | 0.52              |
| 1:5E:15:GLN:HG3    | 3:5E:500:GTP:C6    | 2.43                     | 0.52              |
| 1:5E:112:LYS:HA    | 1:5E:115:VAL:HG12  | 1.91                     | 0.52              |
| 2:6D:131:GLN:O     | 2:6D:163:ILE:HG22  | 2.08                     | 0.52              |
| 1:7E:339:ARG:O     | 1:7E:342:GLN:NE2   | 2.42                     | 0.52              |
| 1:8E:286:LEU:O     | 1:8E:373:ARG:NH1   | 2.42                     | 0.52              |
| 2:9D:167:TYR:CE2   | 2:9D:233:MET:HG2   | 2.45                     | 0.52              |
| 1:11A:175:PRO:HB3  | 1:11A:390:ARG:NE   | 2.24                     | 0.52              |
| 1:12C:31:GLN:OE1   | 1:12C:32:PRO:HD2   | 2.09                     | 0.52              |
| 2:12D:127:CYS:SG   | 2:12D:130:LEU:HB3  | 2.50                     | 0.52              |
| 2:12D:175:VAL:HG22 | 1:12E:329:ASN:HD21 | 1.74                     | 0.52              |
| 1:13A:88:HIS:CD2   | 2:1D:281:TYR:HB3   | 2.44                     | 0.52              |
| 2:13D:44:LEU:HD13  | 2:13D:47:ILE:HG21  | 1.91                     | 0.52              |
| 2:13D:220:PRO:HD2  | 1:13E:326:LYS:HD3  | 1.91                     | 0.52              |
| 1:13E:265:ILE:HD11 | 1:13E:435:VAL:HG21 | 1.91                     | 0.52              |
| 1:2A:261:PRO:HG3   | 1:2A:313:MET:SD    | 2.49                     | 0.52              |
| 1:5C:332:ILE:HD12  | 1:5C:351:PHE:CD2   | 2.44                     | 0.52              |
| 1:6E:27:GLU:OE1    | 1:6E:243:ARG:NH2   | 2.39                     | 0.52              |
| 1:8E:33:ASP:HB2    | 1:8E:35:GLN:OE1    | 2.09                     | 0.52              |
| 2:10B:409:THR:O    | 2:10B:413:SER:N    | 2.38                     | 0.52              |
| 1:11C:204:VAL:HG11 | 1:11C:231:ILE:HD11 | 1.91                     | 0.52              |
| 1:11E:401:LYS:NZ   | 1:11E:403:ALA:HB2  | 2.24                     | 0.52              |
| 2:12B:133:PHE:HE2  | 2:12B:155:ILE:HD12 | 1.75                     | 0.52              |
| 2:12D:334:GLN:HG2  | 2:12D:341:PHE:CZ   | 2.44                     | 0.52              |
| 1:12E:155:GLU:OE1  | 1:12E:197:HIS:NE2  | 2.42                     | 0.52              |
| 1:12E:270:VAL:O    | 1:12E:302:MET:HB3  | 2.09                     | 0.52              |
| 1:13C:386:GLU:O    | 1:13C:390:ARG:HG2  | 2.08                     | 0.52              |
| 2:4D:151:LEU:O     | 2:4D:155:ILE:HG12  | 2.09                     | 0.52              |
| 1:4E:422:ARG:O     | 1:4E:422:ARG:NH1   | 2.43                     | 0.52              |
| 1:6A:195:LEU:HD12  | 1:6A:428:LEU:HD22  | 1.91                     | 0.52              |
| 2:6B:65:LEU:HB3    | 2:6B:73:MET:HE1    | 1.92                     | 0.52              |
| 2:7B:420:SER:O     | 2:7B:423:GLN:HG3   | 2.09                     | 0.52              |
| 1:7C:328:VAL:O     | 1:7C:332:ILE:HG12  | 2.09                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7D:67:ASP:OD1    | 2:7D:68:LEU:N      | 2.42                     | 0.52              |
| 1:7E:306:ASP:OD2   | 1:7E:309:HIS:ND1   | 2.36                     | 0.52              |
| 1:8A:165:SER:HA    | 1:8A:199:ASP:OD2   | 2.09                     | 0.52              |
| 1:9C:121:ARG:HB3   | 1:9C:121:ARG:NH1   | 2.24                     | 0.52              |
| 1:10A:35:GLN:HE22  | 1:10A:37:PRO:HG3   | 1.75                     | 0.52              |
| 1:10A:332:ILE:HD12 | 1:10A:351:PHE:CE2  | 2.45                     | 0.52              |
| 2:10B:248:ALA:HA   | 2:10B:252:LYS:HD3  | 1.90                     | 0.52              |
| 1:11C:11:GLN:HB3   | 3:11C:500:GTP:O2B  | 2.10                     | 0.52              |
| 1:11E:317:MET:HE1  | 1:11E:377:MET:HB3  | 1.91                     | 0.52              |
| 1:11E:421:ALA:O    | 1:11E:425:LEU:N    | 2.38                     | 0.52              |
| 1:13A:225:THR:O    | 1:13A:229:ARG:HG3  | 2.09                     | 0.52              |
| 1:13C:330:ALA:O    | 1:13C:334:THR:N    | 2.40                     | 0.52              |
| 2:1B:61:PRO:HD3    | 2:1B:84:ILE:HG22   | 1.89                     | 0.52              |
| 1:2C:291:ILE:HD12  | 1:2C:375:VAL:HG23  | 1.91                     | 0.52              |
| 2:4B:68:LEU:HD12   | 2:4B:143:THR:HG23  | 1.91                     | 0.52              |
| 2:4B:173:PRO:HD2   | 2:4B:380:ARG:HH21  | 1.73                     | 0.52              |
| 2:4B:208:TYR:HA    | 2:4B:211:CYS:SG    | 2.49                     | 0.52              |
| 2:8B:128:ASP:OD1   | 2:8B:129:CYS:N     | 2.42                     | 0.52              |
| 1:9E:102:ASN:HD22  | 1:9E:105:ARG:HD3   | 1.74                     | 0.52              |
| 2:10B:73:MET:HE1   | 2:10B:92:PHE:HD2   | 1.70                     | 0.52              |
| 1:11C:298:PRO:HB3  | 1:11C:307:PRO:HD2  | 1.90                     | 0.52              |
| 1:11C:303:VAL:O    | 1:11C:305:CYS:N    | 2.42                     | 0.52              |
| 2:11D:114:ASP:OD1  | 2:11D:115:SER:N    | 2.43                     | 0.52              |
| 1:11E:115:VAL:HG22 | 1:11E:119:LEU:HD12 | 1.91                     | 0.52              |
| 2:12B:244:GLY:HA2  | 2:12B:355:ASP:HB2  | 1.92                     | 0.52              |
| 1:13A:408:TYR:HB3  | 1:13A:413:MET:HE1  | 1.90                     | 0.52              |
| 2:13B:375:GLN:OE1  | 2:13B:426:GLN:NE2  | 2.40                     | 0.52              |
| 2:13D:175:VAL:O    | 2:13D:175:VAL:HG12 | 2.09                     | 0.52              |
| 2:13D:256:ASN:HB2  | 2:13D:350:LYS:HZ2  | 1.74                     | 0.52              |
| 2:13D:334:GLN:HA   | 2:13D:341:PHE:CE2  | 2.44                     | 0.52              |
| 1:13E:21:TRP:CE3   | 1:13E:24:TYR:HD2   | 2.28                     | 0.52              |
| 1:13E:182:VAL:HG13 | 1:13E:186:ASN:HD21 | 1.73                     | 0.52              |
| 2:2B:310:TYR:O     | 2:2B:342:VAL:HG23  | 2.09                     | 0.52              |
| 1:2C:292:THR:HG21  | 1:2C:331:ALA:HB1   | 1.92                     | 0.52              |
| 1:5A:184:PRO:O     | 1:5A:188:ILE:HG12  | 2.10                     | 0.52              |
| 2:5B:376:GLU:HA    | 2:5B:379:LYS:HG2   | 1.91                     | 0.52              |
| 2:6B:390:ARG:NH1   | 2:6B:391:ARG:HE    | 2.07                     | 0.52              |
| 1:6C:209:ILE:HG21  | 1:6C:227:LEU:HG    | 1.91                     | 0.52              |
| 1:8E:168:GLU:C     | 1:8E:169:PHE:HD1   | 2.18                     | 0.52              |
| 1:9A:88:HIS:CE1    | 1:9A:90:GLU:HG2    | 2.44                     | 0.52              |
| 2:11B:114:ASP:OD1  | 2:11B:115:SER:N    | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2D:67:ASP:OD1    | 2:2D:68:LEU:N      | 2.43                     | 0.52              |
| 2:2D:285:THR:O     | 2:2D:288:GLU:HG2   | 2.10                     | 0.52              |
| 1:3C:88:HIS:HD2    | 1:3C:89:PRO:HD2    | 1.74                     | 0.52              |
| 1:5C:165:SER:HA    | 1:5C:199:ASP:OD2   | 2.10                     | 0.52              |
| 1:5E:255:PHE:CZ    | 1:5E:378:LEU:HD22  | 2.45                     | 0.52              |
| 1:6E:165:SER:HA    | 1:6E:199:ASP:OD2   | 2.09                     | 0.52              |
| 1:7A:169:PHE:CE1   | 1:7A:235:VAL:HG22  | 2.45                     | 0.52              |
| 2:8B:211:CYS:O     | 2:8B:217:LEU:N     | 2.40                     | 0.52              |
| 2:10B:3:GLU:H      | 2:10B:130:LEU:HA   | 1.74                     | 0.52              |
| 1:10C:285:GLN:HB2  | 1:9C:56:THR:HA     | 1.92                     | 0.52              |
| 1:10C:340:THR:HG23 | 1:10C:341:ILE:HD12 | 1.91                     | 0.52              |
| 2:10D:267:MET:HG2  | 2:10D:374:ILE:HD11 | 1.92                     | 0.52              |
| 2:11B:411:ALA:O    | 2:11B:415:MET:HG3  | 2.09                     | 0.52              |
| 1:11C:11:GLN:O     | 1:11C:15:GLN:HG2   | 2.10                     | 0.52              |
| 2:11D:208:TYR:HA   | 2:11D:211:CYS:SG   | 2.50                     | 0.52              |
| 2:11D:252:LYS:HE3  | 2:11D:350:LYS:NZ   | 2.24                     | 0.52              |
| 2:12B:371:SER:OG   | 2:12B:372:THR:N    | 2.39                     | 0.52              |
| 1:13A:102:ASN:H    | 1:13A:144:GLY:HA3  | 1.75                     | 0.52              |
| 2:13B:175:VAL:HG13 | 1:13C:329:ASN:ND2  | 2.25                     | 0.52              |
| 1:13C:139:HIS:HE1  | 1:13C:141:PHE:CE1  | 2.28                     | 0.52              |
| 1:13E:218:ASP:OD2  | 1:13E:280:LYS:HE3  | 2.10                     | 0.52              |
| 1:4A:172:TYR:HB3   | 1:4A:205:ASP:OD1   | 2.10                     | 0.52              |
| 1:5A:15:GLN:HG3    | 3:5A:500:GTP:C6    | 2.44                     | 0.52              |
| 1:6C:165:SER:HA    | 1:6C:199:ASP:OD2   | 2.08                     | 0.52              |
| 1:8E:195:LEU:HD21  | 1:8E:264:ARG:HE    | 1.74                     | 0.52              |
| 1:9A:113:GLU:N     | 1:9A:113:GLU:OE1   | 2.42                     | 0.52              |
| 2:9B:3:GLU:HG3     | 2:9B:62:ARG:HH22   | 1.75                     | 0.52              |
| 1:9C:332:ILE:HD12  | 1:9C:351:PHE:CE1   | 2.44                     | 0.52              |
| 2:11B:163:ILE:HG21 | 2:11B:250:LEU:HD22 | 1.91                     | 0.52              |
| 1:11C:332:ILE:O    | 1:11C:336:LYS:HG2  | 2.10                     | 0.52              |
| 2:11D:111:GLU:N    | 2:11D:111:GLU:OE1  | 2.43                     | 0.52              |
| 2:11D:406:MET:N    | 2:11D:406:MET:SD   | 2.82                     | 0.52              |
| 1:12A:175:PRO:HB3  | 1:12A:390:ARG:NH1  | 2.25                     | 0.52              |
| 1:12A:317:MET:HE1  | 1:12A:377:MET:HE2  | 1.92                     | 0.52              |
| 2:12B:414:ASN:HA   | 2:12B:417:ASP:HB2  | 1.92                     | 0.52              |
| 1:12E:195:LEU:HD12 | 1:12E:428:LEU:HD22 | 1.91                     | 0.52              |
| 2:2D:36:TYR:CZ     | 2:2D:44:LEU:HD21   | 2.45                     | 0.52              |
| 2:4B:131:GLN:O     | 2:4B:163:ILE:HG22  | 2.10                     | 0.52              |
| 2:4B:305:PRO:HB2   | 2:4B:310:TYR:HE1   | 1.75                     | 0.52              |
| 1:6C:224:TYR:O     | 1:6C:228:ASN:ND2   | 2.43                     | 0.52              |
| 2:7B:140:GLY:O     | 2:7B:184:ASN:ND2   | 2.43                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7D:178:THR:HG22  | 2:7D:180:VAL:H     | 1.74                     | 0.52              |
| 1:8E:20:CYS:HB3    | 1:8E:24:TYR:CE2    | 2.45                     | 0.52              |
| 1:10E:91:GLN:HG2   | 1:10E:121:ARG:HH22 | 1.74                     | 0.52              |
| 1:10E:175:PRO:HD2  | 1:10E:207:GLU:OE1  | 2.10                     | 0.52              |
| 2:11B:4:ILE:HG13   | 2:11B:132:GLY:C    | 2.35                     | 0.52              |
| 1:12C:155:GLU:HB3  | 1:12C:156:ARG:HH11 | 1.73                     | 0.52              |
| 1:13E:167:LEU:HD11 | 1:13E:252:LEU:HD11 | 1.92                     | 0.52              |
| 1:13E:306:ASP:OD2  | 1:13E:309:HIS:ND1  | 2.43                     | 0.52              |
| 1:1C:178:SER:OG    | 2:1D:347:ASN:OD1   | 2.21                     | 0.52              |
| 2:1D:311:LEU:HD12  | 2:1D:342:VAL:HG21  | 1.91                     | 0.52              |
| 2:3D:282:ARG:NH2   | 2:3D:292:GLN:OE1   | 2.41                     | 0.52              |
| 2:5B:4:ILE:HG13    | 2:5B:132:GLY:O     | 2.09                     | 0.52              |
| 1:6A:228:ASN:OD1   | 3:6A:500:GTP:N2    | 2.31                     | 0.52              |
| 1:6A:255:PHE:CZ    | 1:6A:378:LEU:HD22  | 2.45                     | 0.52              |
| 2:6B:73:MET:HA     | 2:6B:76:VAL:HG12   | 1.92                     | 0.52              |
| 1:6C:339:ARG:O     | 1:6C:342:GLN:NE2   | 2.43                     | 0.52              |
| 1:7A:102:ASN:CB    | 1:7A:105:ARG:HB2   | 2.40                     | 0.52              |
| 1:7E:134:GLY:HA3   | 1:7E:165:SER:O     | 2.10                     | 0.52              |
| 1:8A:111:GLY:HA2   | 1:8A:149:PHE:CE2   | 2.45                     | 0.52              |
| 2:8D:3:GLU:HA      | 2:8D:49:VAL:HG23   | 1.91                     | 0.52              |
| 2:8D:13:GLY:O      | 2:8D:17:GLY:N      | 2.38                     | 0.52              |
| 2:9B:328:GLU:O     | 2:9B:331:LEU:HG    | 2.09                     | 0.52              |
| 1:9C:184:PRO:O     | 1:9C:188:ILE:HG12  | 2.10                     | 0.52              |
| 1:10C:113:GLU:N    | 1:10C:113:GLU:OE2  | 2.42                     | 0.52              |
| 1:11A:394:LYS:HG3  | 2:11B:346:PRO:HG3  | 1.92                     | 0.52              |
| 1:11C:292:THR:HG21 | 1:11C:331:ALA:HB1  | 1.92                     | 0.52              |
| 1:11E:291:ILE:HD12 | 1:11E:375:VAL:HG23 | 1.91                     | 0.52              |
| 2:13B:139:LEU:HD11 | 2:13B:188:SER:OG   | 2.10                     | 0.52              |
| 2:2D:45:GLU:O      | 2:2D:46:ARG:NH1    | 2.43                     | 0.52              |
| 1:4A:306:ASP:OD2   | 1:4A:309:HIS:ND1   | 2.40                     | 0.52              |
| 2:4B:67:ASP:HB2    | 2:4B:73:MET:HE3    | 1.91                     | 0.52              |
| 1:4C:215:ARG:HH22  | 1:4C:299:ALA:HB1   | 1.75                     | 0.52              |
| 1:5E:332:ILE:HD12  | 1:5E:351:PHE:CD2   | 2.44                     | 0.52              |
| 2:6D:153:SER:HB2   | 2:6D:191:GLN:HE22  | 1.75                     | 0.52              |
| 2:6D:309:ARG:NH1   | 2:6D:426:GLN:OXT   | 2.43                     | 0.52              |
| 1:6E:255:PHE:CZ    | 1:6E:378:LEU:HD22  | 2.45                     | 0.52              |
| 1:8A:295:CYS:HB3   | 1:8A:377:MET:HG2   | 1.92                     | 0.52              |
| 1:10A:13:GLY:O     | 1:10A:17:GLY:N     | 2.37                     | 0.51              |
| 1:10A:213:CYS:SG   | 1:10A:222:PRO:HG3  | 2.50                     | 0.51              |
| 1:10E:21:TRP:HZ3   | 1:10E:53:PHE:HE1   | 1.58                     | 0.51              |
| 1:13A:121:ARG:CZ   | 1:13A:121:ARG:HB3  | 2.35                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13E:164:LYS:O   | 1:13E:166:LYS:NZ  | 2.40                     | 0.51              |
| 2:4B:311:LEU:HD23 | 2:4B:342:VAL:HG21 | 1.92                     | 0.51              |
| 2:4D:105:HIS:CD2  | 2:4D:150:LEU:HD13 | 2.44                     | 0.51              |
| 1:4E:63:PRO:HD3   | 1:4E:86:LEU:HG    | 1.91                     | 0.51              |
| 2:5B:190:HIS:NE2  | 2:5B:414:ASN:OD1  | 2.43                     | 0.51              |
| 2:6B:215:LEU:HD22 | 2:6B:217:LEU:HG   | 1.92                     | 0.51              |
| 2:7B:109:GLY:HA3  | 2:7B:147:MET:HE1  | 1.92                     | 0.51              |
| 1:7E:319:TYR:HB3  | 1:7E:323:VAL:HG21 | 1.92                     | 0.51              |
| 1:9C:339:ARG:O    | 1:9C:342:GLN:NE2  | 2.42                     | 0.51              |
| 2:9D:290:THR:HG21 | 2:9D:329:GLN:CD   | 2.35                     | 0.51              |
| 1:12E:34:GLY:O    | 1:12E:61:HIS:ND1  | 2.38                     | 0.51              |
| 1:12E:139:HIS:HE1 | 1:12E:141:PHE:CE1 | 2.29                     | 0.51              |
| 1:13E:330:ALA:O   | 1:13E:334:THR:N   | 2.40                     | 0.51              |
| 1:13E:395:PHE:HZ  | 1:13E:418:PHE:HB3 | 1.75                     | 0.51              |
| 1:1A:9:VAL:HG11   | 1:1A:150:THR:OG1  | 2.11                     | 0.51              |
| 1:1A:123:ARG:NE   | 1:1A:161:TYR:OH   | 2.40                     | 0.51              |
| 2:2B:257:MET:HE1  | 2:2B:368:ILE:HB   | 1.93                     | 0.51              |
| 2:2B:285:THR:O    | 2:2B:288:GLU:HG2  | 2.10                     | 0.51              |
| 1:2C:71:GLU:HB2   | 1:2C:98:ASP:HB3   | 1.91                     | 0.51              |
| 1:2C:112:LYS:HA   | 1:2C:115:VAL:HG12 | 1.91                     | 0.51              |
| 1:3C:329:ASN:OD1  | 1:3C:330:ALA:N    | 2.43                     | 0.51              |
| 2:5B:324:LYS:O    | 2:5B:328:GLU:HG2  | 2.10                     | 0.51              |
| 2:6B:4:ILE:HG13   | 2:6B:132:GLY:O    | 2.09                     | 0.51              |
| 1:7E:15:GLN:HG3   | 3:7E:500:GTP:N1   | 2.25                     | 0.51              |
| 2:8B:8:GLN:O      | 2:8B:66:VAL:HG12  | 2.11                     | 0.51              |
| 1:8C:210:TYR:O    | 1:8C:214:ARG:N    | 2.35                     | 0.51              |
| 1:8E:165:SER:HA   | 1:8E:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:9B:309:ARG:NH1  | 2:9B:426:GLN:OXT  | 2.43                     | 0.51              |
| 1:10A:5:ILE:O     | 1:10A:135:PHE:HA  | 2.11                     | 0.51              |
| 1:11C:175:PRO:O   | 1:11C:394:LYS:NZ  | 2.36                     | 0.51              |
| 2:13B:382:SER:O   | 2:13B:386:THR:OG1 | 2.27                     | 0.51              |
| 1:13C:318:LEU:O   | 1:13C:375:VAL:HA  | 2.11                     | 0.51              |
| 1:1C:88:HIS:CD2   | 1:2C:283:HIS:HB3  | 2.45                     | 0.51              |
| 1:2C:175:PRO:HB3  | 1:2C:390:ARG:HD3  | 1.90                     | 0.51              |
| 1:2E:188:ILE:HG23 | 1:2E:425:LEU:HD12 | 1.93                     | 0.51              |
| 2:6B:191:GLN:OE1  | 2:6B:195:ASN:ND2  | 2.43                     | 0.51              |
| 1:7A:54:SER:O     | 1:7A:61:HIS:HA    | 2.11                     | 0.51              |
| 2:7D:220:PRO:HD2  | 1:7E:326:LYS:HD2  | 1.92                     | 0.51              |
| 1:8A:322:ASP:OD1  | 1:8A:322:ASP:O    | 2.28                     | 0.51              |
| 2:8B:293:MET:HG2  | 2:8B:367:PHE:HB2  | 1.91                     | 0.51              |
| 1:9C:195:LEU:HD12 | 1:9C:428:LEU:HD22 | 1.91                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9E:225:THR:O     | 1:9E:229:ARG:HG3   | 2.11                     | 0.51              |
| 1:10A:312:TYR:O    | 1:10A:344:VAL:HG23 | 2.10                     | 0.51              |
| 2:10B:303:CYS:SG   | 2:10B:377:LEU:HG   | 2.51                     | 0.51              |
| 2:12B:220:PRO:HD2  | 1:12C:326:LYS:HD3  | 1.91                     | 0.51              |
| 2:12D:258:VAL:HG22 | 2:12D:266:PHE:HZ   | 1.75                     | 0.51              |
| 2:13B:267:MET:SD   | 2:13B:301:ALA:HB2  | 2.51                     | 0.51              |
| 1:2A:112:LYS:HA    | 1:2A:115:VAL:HG12  | 1.92                     | 0.51              |
| 1:2C:56:THR:HA     | 1:3C:285:GLN:HB2   | 1.93                     | 0.51              |
| 2:4D:121:ARG:NH1   | 2:4D:158:GLU:OE1   | 2.43                     | 0.51              |
| 1:5E:20:CYS:HB3    | 1:5E:24:TYR:CE2    | 2.44                     | 0.51              |
| 1:8C:213:CYS:SG    | 1:8C:222:PRO:HB3   | 2.50                     | 0.51              |
| 1:9C:215:ARG:NH2   | 1:9C:299:ALA:O     | 2.37                     | 0.51              |
| 1:9C:252:LEU:O     | 1:9C:256:GLN:HG2   | 2.11                     | 0.51              |
| 1:10A:286:LEU:O    | 1:10A:373:ARG:NH2  | 2.41                     | 0.51              |
| 2:11B:104:GLY:HA3  | 2:11B:146:GLY:HA3  | 1.92                     | 0.51              |
| 1:12C:175:PRO:HB3  | 1:12C:390:ARG:NE   | 2.25                     | 0.51              |
| 1:1A:195:LEU:HD12  | 1:1A:428:LEU:HD22  | 1.93                     | 0.51              |
| 2:1D:373:ALA:O     | 2:1D:376:GLU:HG2   | 2.10                     | 0.51              |
| 1:3A:222:PRO:HG2   | 2:3B:324:LYS:HD3   | 1.93                     | 0.51              |
| 1:3E:20:CYS:HB3    | 1:3E:24:TYR:CE1    | 2.45                     | 0.51              |
| 1:4A:291:ILE:HD12  | 1:4A:375:VAL:HG23  | 1.93                     | 0.51              |
| 2:6D:267:MET:HE2   | 2:6D:299:MET:SD    | 2.50                     | 0.51              |
| 2:7B:209:ASP:OD1   | 2:7B:213:ARG:NH1   | 2.43                     | 0.51              |
| 2:8D:204:ASN:ND2   | 2:8D:204:ASN:O     | 2.44                     | 0.51              |
| 2:9B:335:ASN:OD1   | 2:9B:336:LYS:N     | 2.43                     | 0.51              |
| 2:10D:104:GLY:HA3  | 2:10D:146:GLY:HA3  | 1.93                     | 0.51              |
| 2:10D:209:ASP:OD2  | 2:10D:213:ARG:NH2  | 2.41                     | 0.51              |
| 1:11C:202:PHE:HE1  | 1:11C:378:LEU:HD23 | 1.75                     | 0.51              |
| 2:12D:309:ARG:NH1  | 2:12D:426:GLN:OXT  | 2.44                     | 0.51              |
| 1:13C:115:VAL:HG23 | 1:13C:153:LEU:HD23 | 1.93                     | 0.51              |
| 1:2A:145:THR:HG1   | 3:2A:500:GTP:PG    | 2.34                     | 0.51              |
| 2:2B:36:TYR:CZ     | 2:2B:44:LEU:HD21   | 2.46                     | 0.51              |
| 1:4C:165:SER:HA    | 1:4C:199:ASP:OD2   | 2.10                     | 0.51              |
| 1:4C:222:PRO:HD2   | 2:4D:324:LYS:HD3   | 1.92                     | 0.51              |
| 1:5C:255:PHE:CZ    | 1:5C:259:LEU:HD22  | 2.46                     | 0.51              |
| 1:6E:91:GLN:HA     | 1:6E:121:ARG:HH12  | 1.76                     | 0.51              |
| 2:7B:330:MET:SD    | 2:7B:349:VAL:HG11  | 2.51                     | 0.51              |
| 1:7E:414:GLU:OE1   | 1:7E:416:GLY:N     | 2.32                     | 0.51              |
| 2:9D:287:PRO:HA    | 2:9D:290:THR:HG22  | 1.93                     | 0.51              |
| 1:10A:112:LYS:HA   | 1:10A:115:VAL:HG12 | 1.92                     | 0.51              |
| 2:10B:289:LEU:HD23 | 2:10B:365:ALA:HB2  | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:11B:67:ASP:OD1   | 2:11B:68:LEU:N     | 2.38                     | 0.51              |
| 2:12D:175:VAL:HG13 | 1:12E:329:ASN:ND2  | 2.25                     | 0.51              |
| 1:13A:220:GLU:HG2  | 1:13A:221:ARG:H    | 1.75                     | 0.51              |
| 1:4A:184:PRO:O     | 1:4A:188:ILE:HG12  | 2.10                     | 0.51              |
| 1:4A:396:ASP:OD1   | 1:4A:422:ARG:NH1   | 2.43                     | 0.51              |
| 2:4B:378:PHE:HB3   | 2:4B:415:MET:HE3   | 1.93                     | 0.51              |
| 1:5E:22:GLU:OE2    | 1:5E:83:TYR:OH     | 2.14                     | 0.51              |
| 1:7C:169:PHE:CE2   | 1:7C:235:VAL:HG22  | 2.46                     | 0.51              |
| 2:7D:36:TYR:CZ     | 2:7D:44:LEU:HD21   | 2.46                     | 0.51              |
| 1:7E:168:GLU:HG2   | 1:7E:201:ALA:HA    | 1.93                     | 0.51              |
| 1:8E:298:PRO:HB3   | 1:8E:307:PRO:HD2   | 1.92                     | 0.51              |
| 2:9D:309:ARG:NH1   | 2:9D:426:GLN:OXT   | 2.43                     | 0.51              |
| 1:10A:12:ALA:O     | 1:10A:15:GLN:HB2   | 2.11                     | 0.51              |
| 1:11A:3:GLU:HB2    | 1:11A:64:ARG:NH2   | 2.26                     | 0.51              |
| 1:12A:167:LEU:HD22 | 1:12A:202:PHE:HE2  | 1.76                     | 0.51              |
| 2:12B:127:CYS:SG   | 2:12B:130:LEU:HB3  | 2.51                     | 0.51              |
| 1:12E:298:PRO:HD2  | 1:12E:299:ALA:H    | 1.74                     | 0.51              |
| 1:13C:100:ALA:HB2  | 2:13D:251:ARG:HD3  | 1.93                     | 0.51              |
| 2:13D:309:ARG:NH1  | 2:13D:426:GLN:OXT  | 2.43                     | 0.51              |
| 2:1D:376:GLU:HA    | 2:1D:379:LYS:HG2   | 1.92                     | 0.51              |
| 1:2C:11:GLN:NE2    | 2:2D:245:GLN:O     | 2.44                     | 0.51              |
| 2:3B:344:TRP:O     | 2:3B:345:ILE:HD13  | 2.11                     | 0.51              |
| 2:3D:132:GLY:HA2   | 2:3D:163:ILE:O     | 2.11                     | 0.51              |
| 1:3E:202:PHE:HE1   | 1:3E:378:LEU:HD23  | 1.76                     | 0.51              |
| 1:4C:224:TYR:O     | 1:4C:228:ASN:ND2   | 2.43                     | 0.51              |
| 1:6C:105:ARG:HA    | 1:6C:109:THR:HG22  | 1.93                     | 0.51              |
| 2:8B:204:ASN:O     | 2:8B:204:ASN:ND2   | 2.43                     | 0.51              |
| 2:10D:375:GLN:HE21 | 2:10D:419:VAL:HG13 | 1.76                     | 0.51              |
| 2:11D:202:ILE:HD11 | 2:11D:207:LEU:HD11 | 1.93                     | 0.51              |
| 1:11E:11:GLN:O     | 1:11E:15:GLN:HG2   | 2.11                     | 0.51              |
| 2:12D:198:GLU:HG3  | 2:12D:266:PHE:CE2  | 2.44                     | 0.51              |
| 1:13A:175:PRO:HB3  | 1:13A:390:ARG:HD3  | 1.93                     | 0.51              |
| 1:1C:26:LEU:HG     | 1:1C:363:VAL:HG12  | 1.92                     | 0.51              |
| 1:3C:221:ARG:HA    | 2:3D:324:LYS:HD3   | 1.91                     | 0.51              |
| 2:3D:3:GLU:OE2     | 2:3D:127:CYS:HB2   | 2.09                     | 0.51              |
| 2:3D:12:CYS:SG     | 2:3D:13:GLY:N      | 2.83                     | 0.51              |
| 2:4D:100:ASN:HD22  | 2:4D:103:LYS:HD2   | 1.75                     | 0.51              |
| 1:6A:168:GLU:OE2   | 1:6A:194:THR:HG23  | 2.11                     | 0.51              |
| 1:6E:271:THR:HG22  | 1:6E:377:MET:HB3   | 1.93                     | 0.51              |
| 1:7A:195:LEU:HD12  | 1:7A:428:LEU:HD22  | 1.92                     | 0.51              |
| 1:8A:90:GLU:OE2    | 1:9A:280:LYS:HE3   | 2.11                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:8A:255:PHE:CZ   | 1:8A:378:LEU:HD22  | 2.45                     | 0.51              |
| 1:8A:414:GLU:OE1  | 1:8A:416:GLY:N     | 2.35                     | 0.51              |
| 2:9D:8:GLN:OE1    | 2:9D:17:GLY:HA3    | 2.10                     | 0.51              |
| 2:10B:28:HIS:NE2  | 2:10B:241:ARG:HD2  | 2.26                     | 0.51              |
| 2:10B:376:GLU:HA  | 2:10B:379:LYS:HG2  | 1.93                     | 0.51              |
| 1:10C:213:CYS:HA  | 1:10C:217:LEU:HB2  | 1.92                     | 0.51              |
| 2:11B:285:THR:O   | 2:11B:288:GLU:HG2  | 2.12                     | 0.51              |
| 1:11C:5:ILE:HG12  | 1:11C:64:ARG:HG2   | 1.92                     | 0.51              |
| 2:11D:285:THR:OG1 | 2:11D:287:PRO:HD2  | 2.11                     | 0.51              |
| 1:12A:104:ALA:HB1 | 1:12A:411:GLU:HB2  | 1.93                     | 0.51              |
| 1:12A:305:CYS:SG  | 1:12A:384:ILE:HA   | 2.51                     | 0.51              |
| 2:12B:405:GLU:HA  | 2:12B:408:PHE:CE1  | 2.46                     | 0.51              |
| 1:13C:321:GLY:HA3 | 1:13C:372:GLN:O    | 2.12                     | 0.51              |
| 1:13E:261:PRO:HG2 | 1:13E:265:ILE:HD12 | 1.93                     | 0.51              |
| 2:1D:219:THR:HA   | 1:1E:326:LYS:HE2   | 1.92                     | 0.51              |
| 2:1D:406:MET:O    | 2:1D:409:THR:OG1   | 2.19                     | 0.51              |
| 2:2D:373:ALA:O    | 2:2D:376:GLU:HG2   | 2.10                     | 0.51              |
| 1:3C:286:LEU:O    | 1:3C:373:ARG:NH1   | 2.44                     | 0.51              |
| 2:5D:178:THR:HG22 | 2:5D:180:VAL:H     | 1.75                     | 0.51              |
| 2:6B:175:VAL:HG13 | 1:6C:329:ASN:ND2   | 2.26                     | 0.51              |
| 1:7C:113:GLU:N    | 1:7C:113:GLU:OE1   | 2.44                     | 0.51              |
| 2:8B:208:TYR:HA   | 2:8B:211:CYS:SG    | 2.51                     | 0.51              |
| 1:8C:391:LEU:HD23 | 1:8C:391:LEU:O     | 2.11                     | 0.51              |
| 1:8E:113:GLU:N    | 1:8E:113:GLU:OE2   | 2.44                     | 0.51              |
| 1:10A:285:GLN:HB2 | 1:9A:56:THR:HA     | 1.93                     | 0.50              |
| 1:10C:174:ALA:HB1 | 1:10C:207:GLU:OE2  | 2.10                     | 0.50              |
| 1:11A:11:GLN:O    | 1:11A:15:GLN:HG2   | 2.11                     | 0.50              |
| 1:11A:399:TYR:OH  | 1:11A:415:GLU:HG2  | 2.10                     | 0.50              |
| 1:12C:102:ASN:HB2 | 1:12C:105:ARG:HB2  | 1.94                     | 0.50              |
| 2:13B:309:ARG:NH1 | 2:13B:426:GLN:OXT  | 2.44                     | 0.50              |
| 2:13B:381:ILE:HA  | 2:13B:384:GLN:CD   | 2.35                     | 0.50              |
| 2:13B:387:ALA:HB1 | 2:13B:391:ARG:NH2  | 2.27                     | 0.50              |
| 2:13D:300:MET:O   | 2:13D:300:MET:HG3  | 2.11                     | 0.50              |
| 1:1C:261:PRO:HG3  | 1:1C:313:MET:SD    | 2.51                     | 0.50              |
| 2:2D:131:GLN:O    | 2:2D:163:ILE:HG22  | 2.12                     | 0.50              |
| 2:3B:285:THR:O    | 2:3B:288:GLU:HG2   | 2.11                     | 0.50              |
| 2:3D:105:HIS:CD2  | 2:3D:150:LEU:HD13  | 2.47                     | 0.50              |
| 1:4A:407:TRP:CG   | 2:4B:255:VAL:HG23  | 2.46                     | 0.50              |
| 1:4C:188:ILE:HG22 | 1:4C:421:ALA:HB1   | 1.93                     | 0.50              |
| 1:5A:165:SER:HA   | 1:5A:199:ASP:OD2   | 2.10                     | 0.50              |
| 1:5A:422:ARG:O    | 1:5A:426:ALA:N     | 2.44                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:5D:412:GLU:O     | 2:5D:416:ASN:N     | 2.44                     | 0.50              |
| 1:5E:251:ASP:O     | 1:5E:255:PHE:N     | 2.44                     | 0.50              |
| 1:6A:225:THR:O     | 1:6A:229:ARG:HG3   | 2.11                     | 0.50              |
| 2:6B:36:TYR:CZ     | 2:6B:44:LEU:HD21   | 2.46                     | 0.50              |
| 2:6D:3:GLU:HB3     | 2:6D:62:ARG:HH12   | 1.76                     | 0.50              |
| 1:7A:134:GLY:HA3   | 1:7A:165:SER:O     | 2.11                     | 0.50              |
| 2:7D:140:GLY:O     | 2:7D:184:ASN:ND2   | 2.44                     | 0.50              |
| 1:8A:312:TYR:O     | 1:8A:344:VAL:HG23  | 2.12                     | 0.50              |
| 1:10C:5:ILE:O      | 1:10C:135:PHE:HA   | 2.11                     | 0.50              |
| 2:13D:109:GLY:HA3  | 2:13D:150:LEU:HD21 | 1.93                     | 0.50              |
| 1:1A:316:CYS:SG    | 1:1A:352:LYS:HB3   | 2.51                     | 0.50              |
| 1:1C:9:VAL:HG11    | 1:1C:150:THR:OG1   | 2.11                     | 0.50              |
| 2:1D:45:GLU:O      | 2:1D:46:ARG:NH1    | 2.45                     | 0.50              |
| 1:3A:175:PRO:HB3   | 1:3A:390:ARG:HD3   | 1.93                     | 0.50              |
| 2:3B:178:THR:HG22  | 2:3B:180:VAL:H     | 1.76                     | 0.50              |
| 1:5A:71:GLU:HB2    | 1:5A:98:ASP:HB3    | 1.92                     | 0.50              |
| 1:5A:91:GLN:HA     | 1:5A:121:ARG:HH12  | 1.76                     | 0.50              |
| 2:5D:49:VAL:HG11   | 2:5D:241:ARG:HG2   | 1.92                     | 0.50              |
| 2:5D:219:THR:HA    | 1:5E:326:LYS:HD3   | 1.93                     | 0.50              |
| 1:5E:313:MET:HB3   | 1:5E:380:ASN:O     | 2.11                     | 0.50              |
| 2:6D:67:ASP:OD1    | 2:6D:68:LEU:N      | 2.43                     | 0.50              |
| 2:8D:330:MET:SD    | 2:8D:349:VAL:HG11  | 2.51                     | 0.50              |
| 1:8E:69:ASP:OD1    | 1:8E:70:LEU:N      | 2.43                     | 0.50              |
| 2:10B:130:LEU:HD21 | 2:10B:162:ARG:HH12 | 1.76                     | 0.50              |
| 1:11C:255:PHE:CZ   | 1:11C:378:LEU:HD22 | 2.46                     | 0.50              |
| 2:12B:67:ASP:OD1   | 2:12B:68:LEU:N     | 2.40                     | 0.50              |
| 2:12B:334:GLN:HG2  | 2:12B:341:PHE:CZ   | 2.45                     | 0.50              |
| 1:12C:397:LEU:HD21 | 2:12D:344:TRP:HA   | 1.94                     | 0.50              |
| 1:13A:391:LEU:HA   | 1:13A:394:LYS:HD3  | 1.93                     | 0.50              |
| 2:13D:385:PHE:CZ   | 2:13D:389:PHE:HB2  | 2.45                     | 0.50              |
| 1:3A:252:LEU:O     | 1:3A:256:GLN:HG2   | 2.11                     | 0.50              |
| 2:3D:208:TYR:HA    | 2:3D:211:CYS:SG    | 2.52                     | 0.50              |
| 1:3E:215:ARG:HH22  | 1:3E:299:ALA:HB1   | 1.76                     | 0.50              |
| 1:4E:147:SER:HB2   | 1:4E:190:THR:HG21  | 1.93                     | 0.50              |
| 1:5E:291:ILE:HD12  | 1:5E:375:VAL:HG23  | 1.93                     | 0.50              |
| 2:7D:373:ALA:O     | 2:7D:376:GLU:HG2   | 2.12                     | 0.50              |
| 1:7E:91:GLN:HG2    | 1:7E:121:ARG:HH22  | 1.76                     | 0.50              |
| 1:8C:214:ARG:NH2   | 2:8D:324:LYS:HD2   | 2.27                     | 0.50              |
| 2:9B:111:GLU:OE1   | 2:9B:111:GLU:N     | 2.43                     | 0.50              |
| 1:9C:34:GLY:O      | 1:9C:61:HIS:N      | 2.44                     | 0.50              |
| 1:9C:286:LEU:HA    | 1:9C:290:GLU:OE2   | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:10A:151:SER:OG   | 1:10A:193:THR:HG21 | 2.12                     | 0.50              |
| 1:10A:169:PHE:CE2  | 1:10A:235:VAL:HG22 | 2.47                     | 0.50              |
| 2:10D:73:MET:CE    | 2:10D:92:PHE:HB3   | 2.42                     | 0.50              |
| 1:11C:251:ASP:O    | 1:11C:255:PHE:N    | 2.42                     | 0.50              |
| 2:12D:309:ARG:N    | 2:12D:372:THR:OG1  | 2.40                     | 0.50              |
| 1:13C:21:TRP:CE3   | 1:13C:24:TYR:HD2   | 2.29                     | 0.50              |
| 1:13C:30:ILE:HG21  | 1:13C:53:PHE:HE2   | 1.76                     | 0.50              |
| 1:13C:313:MET:N    | 1:13C:313:MET:SD   | 2.85                     | 0.50              |
| 2:13D:27:GLU:OE2   | 2:13D:241:ARG:NE   | 2.34                     | 0.50              |
| 1:13E:155:GLU:HB3  | 1:13E:156:ARG:HH11 | 1.75                     | 0.50              |
| 2:2D:121:ARG:O     | 2:2D:125:GLU:HG2   | 2.11                     | 0.50              |
| 2:2D:310:TYR:O     | 2:2D:342:VAL:HG23  | 2.11                     | 0.50              |
| 1:4C:336:LYS:HE3   | 1:4C:351:PHE:CE2   | 2.47                     | 0.50              |
| 1:6A:259:LEU:HD13  | 1:6A:316:CYS:SG    | 2.51                     | 0.50              |
| 1:7A:184:PRO:O     | 1:7A:188:ILE:HG12  | 2.12                     | 0.50              |
| 1:8A:191:THR:HG21  | 1:8A:425:LEU:HD11  | 1.93                     | 0.50              |
| 1:9A:75:VAL:HG13   | 1:9A:92:LEU:HD22   | 1.94                     | 0.50              |
| 2:9B:267:MET:HE3   | 2:9B:303:CYS:HB2   | 1.94                     | 0.50              |
| 1:9C:407:TRP:CD1   | 2:9D:255:VAL:HG23  | 2.47                     | 0.50              |
| 1:9E:113:GLU:OE1   | 1:9E:113:GLU:N     | 2.45                     | 0.50              |
| 1:9E:271:THR:HG22  | 1:9E:377:MET:HE3   | 1.93                     | 0.50              |
| 2:11B:111:GLU:N    | 2:11B:111:GLU:OE1  | 2.44                     | 0.50              |
| 2:11B:178:THR:HB   | 2:11B:181:GLU:HG3  | 1.94                     | 0.50              |
| 1:11C:138:PHE:HD1  | 1:11C:169:PHE:HB2  | 1.77                     | 0.50              |
| 1:11E:292:THR:HG21 | 1:11E:331:ALA:HB1  | 1.92                     | 0.50              |
| 1:13A:315:CYS:HB2  | 1:13A:379:SER:HB3  | 1.93                     | 0.50              |
| 1:13C:220:GLU:HG2  | 1:13C:221:ARG:H    | 1.75                     | 0.50              |
| 2:13D:397:TRP:CZ3  | 1:13E:257:THR:HA   | 2.47                     | 0.50              |
| 1:1C:123:ARG:NE    | 1:1C:161:TYR:OH    | 2.43                     | 0.50              |
| 1:1E:145:THR:OG1   | 3:1E:500:GTP:O3B   | 2.30                     | 0.50              |
| 1:4C:63:PRO:HD3    | 1:4C:86:LEU:HG     | 1.92                     | 0.50              |
| 2:5B:67:ASP:HB2    | 2:5B:73:MET:HE3    | 1.93                     | 0.50              |
| 2:5B:208:TYR:HA    | 2:5B:211:CYS:SG    | 2.51                     | 0.50              |
| 2:5D:67:ASP:HB2    | 2:5D:73:MET:HE3    | 1.93                     | 0.50              |
| 2:5D:109:GLY:HA3   | 2:5D:147:MET:CE    | 2.42                     | 0.50              |
| 1:6A:258:ASN:OD1   | 1:6A:352:LYS:HD3   | 2.11                     | 0.50              |
| 1:7C:255:PHE:CE1   | 1:7C:378:LEU:HD11  | 2.47                     | 0.50              |
| 1:9A:286:LEU:HD12  | 1:9A:291:ILE:HD11  | 1.94                     | 0.50              |
| 2:9B:4:ILE:CG2     | 2:9B:50:TYR:HE1    | 2.24                     | 0.50              |
| 1:9E:332:ILE:HD12  | 1:9E:351:PHE:CE2   | 2.47                     | 0.50              |
| 1:11A:306:ASP:OD2  | 1:11A:309:HIS:ND1  | 2.39                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:11B:117:LEU:HD21 | 2:11B:154:LYS:HE2  | 1.93                     | 0.50              |
| 2:11B:211:CYS:HA   | 2:11B:215:LEU:HB2  | 1.93                     | 0.50              |
| 1:11C:101:ASN:OD1  | 2:11D:252:LYS:NZ   | 2.31                     | 0.50              |
| 2:12B:159:TYR:HB3  | 2:12B:162:ARG:HD2  | 1.93                     | 0.50              |
| 2:12B:211:CYS:HB2  | 2:12B:217:LEU:HD12 | 1.93                     | 0.50              |
| 1:12C:221:ARG:HA   | 2:12D:324:LYS:HD3  | 1.94                     | 0.50              |
| 2:12D:260:PHE:HB2  | 2:12D:263:LEU:HD13 | 1.92                     | 0.50              |
| 1:12E:204:VAL:HG11 | 1:12E:231:ILE:HD11 | 1.94                     | 0.50              |
| 1:13E:195:LEU:HD12 | 1:13E:428:LEU:HD22 | 1.93                     | 0.50              |
| 2:1D:285:THR:O     | 2:1D:288:GLU:HG2   | 2.11                     | 0.50              |
| 1:2C:329:ASN:OD1   | 1:2C:330:ALA:N     | 2.45                     | 0.50              |
| 2:3B:105:HIS:CD2   | 2:3B:150:LEU:HD13  | 2.46                     | 0.50              |
| 2:3D:324:LYS:O     | 2:3D:328:GLU:HG2   | 2.11                     | 0.50              |
| 2:4B:107:THR:OG1   | 2:4B:401:GLU:OE1   | 2.27                     | 0.50              |
| 2:4D:12:CYS:SG     | 2:4D:13:GLY:N      | 2.84                     | 0.50              |
| 1:5E:202:PHE:HE1   | 1:5E:378:LEU:HD23  | 1.77                     | 0.50              |
| 1:7E:169:PHE:CE2   | 1:7E:235:VAL:HG22  | 2.47                     | 0.50              |
| 1:8A:215:ARG:NH2   | 1:8A:299:ALA:O     | 2.32                     | 0.50              |
| 2:8D:256:ASN:ND2   | 2:8D:350:LYS:HD2   | 2.26                     | 0.50              |
| 1:9C:255:PHE:CZ    | 1:9C:259:LEU:HD22  | 2.46                     | 0.50              |
| 2:10B:334:GLN:HE22 | 2:10B:347:ASN:HA   | 1.77                     | 0.50              |
| 1:12C:251:ASP:O    | 1:12C:255:PHE:N    | 2.44                     | 0.50              |
| 2:12D:67:ASP:OD1   | 2:12D:68:LEU:N     | 2.41                     | 0.50              |
| 1:13A:91:GLN:HG2   | 1:13A:121:ARG:HH22 | 1.77                     | 0.50              |
| 2:13B:390:ARG:HG3  | 2:13B:391:ARG:CD   | 2.42                     | 0.50              |
| 1:13C:428:LEU:HG   | 1:13C:432:TYR:CE2  | 2.46                     | 0.50              |
| 2:13D:156:ARG:NH1  | 2:13D:197:ASP:OD2  | 2.44                     | 0.50              |
| 1:13E:27:GLU:OE1   | 1:13E:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:1C:123:ARG:HA    | 1:1C:123:ARG:NE    | 2.26                     | 0.50              |
| 1:3A:4:CYS:SG      | 1:3A:133:GLN:HB2   | 2.52                     | 0.50              |
| 1:3A:222:PRO:HD2   | 2:3B:324:LYS:CE    | 2.42                     | 0.50              |
| 1:4A:224:TYR:O     | 1:4A:228:ASN:ND2   | 2.44                     | 0.50              |
| 2:5D:130:LEU:HD11  | 2:5D:162:ARG:HD3   | 1.94                     | 0.50              |
| 1:6C:313:MET:HB2   | 1:6C:380:ASN:O     | 2.11                     | 0.50              |
| 2:6D:116:VAL:HG23  | 2:6D:117:LEU:HD12  | 1.93                     | 0.50              |
| 2:8B:209:ASP:OD1   | 2:8B:213:ARG:NH1   | 2.45                     | 0.50              |
| 2:8B:309:ARG:NH1   | 2:8B:426:GLN:OXT   | 2.45                     | 0.50              |
| 1:8E:150:THR:O     | 1:8E:154:MET:HG3   | 2.11                     | 0.50              |
| 2:9D:316:ILE:HG22  | 2:9D:352:ALA:HB3   | 1.94                     | 0.50              |
| 2:10B:384:GLN:OE1  | 1:10C:348:PRO:HG3  | 2.11                     | 0.50              |
| 1:12A:201:ALA:O    | 1:12A:268:PRO:HD2  | 2.10                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:12A:259:LEU:HD13 | 1:12A:316:CYS:SG   | 2.52                     | 0.50              |
| 1:13C:4:CYS:SG     | 1:13C:133:GLN:HB2  | 2.52                     | 0.50              |
| 2:13D:5:VAL:HG12   | 2:13D:62:ARG:HE    | 1.76                     | 0.50              |
| 2:13D:214:THR:HG21 | 2:13D:298:ASN:ND2  | 2.26                     | 0.50              |
| 2:13D:304:ASP:HB2  | 2:13D:307:HIS:CE1  | 2.47                     | 0.50              |
| 1:13E:88:HIS:HB3   | 1:13E:90:GLU:OE1   | 2.12                     | 0.50              |
| 2:1B:259:PRO:HG3   | 2:1B:311:LEU:HD21  | 1.94                     | 0.50              |
| 2:1B:285:THR:O     | 2:1B:288:GLU:HG2   | 2.12                     | 0.50              |
| 1:2C:407:TRP:CG    | 2:2D:255:VAL:HG23  | 2.47                     | 0.50              |
| 1:3A:91:GLN:HA     | 1:3A:121:ARG:HH12  | 1.76                     | 0.50              |
| 1:5A:271:THR:HG22  | 1:5A:377:MET:HB3   | 1.94                     | 0.50              |
| 2:5B:286:VAL:HG22  | 2:5B:321:MET:HE3   | 1.92                     | 0.50              |
| 1:6A:165:SER:HA    | 1:6A:199:ASP:OD2   | 2.11                     | 0.50              |
| 2:6D:211:CYS:HB2   | 2:6D:217:LEU:HD12  | 1.94                     | 0.50              |
| 2:7D:111:GLU:OE1   | 2:7D:111:GLU:N     | 2.45                     | 0.50              |
| 1:7E:204:VAL:HG23  | 1:7E:302:MET:HG3   | 1.93                     | 0.50              |
| 2:9D:100:ASN:HD22  | 2:9D:103:LYS:HD2   | 1.77                     | 0.50              |
| 1:9E:315:CYS:HA    | 1:9E:379:SER:HA    | 1.93                     | 0.50              |
| 2:10D:130:LEU:HD23 | 2:10D:130:LEU:H    | 1.76                     | 0.50              |
| 1:11E:307:PRO:HB3  | 1:11E:312:TYR:CE1  | 2.47                     | 0.50              |
| 2:13D:198:GLU:HB2  | 2:13D:266:PHE:CE2  | 2.46                     | 0.50              |
| 1:1E:255:PHE:CE1   | 1:1E:259:LEU:HD22  | 2.47                     | 0.50              |
| 2:3B:68:LEU:HD12   | 2:3B:143:THR:HG23  | 1.94                     | 0.50              |
| 1:4C:390:ARG:HG3   | 1:4C:391:LEU:N     | 2.27                     | 0.50              |
| 1:4E:265:ILE:HG23  | 1:4E:432:TYR:CZ    | 2.47                     | 0.50              |
| 1:7A:15:GLN:HG3    | 3:7A:500:GTP:N1    | 2.26                     | 0.50              |
| 1:8E:16:ILE:HD11   | 1:8E:171:ILE:HD11  | 1.93                     | 0.50              |
| 1:9A:298:PRO:HB3   | 1:9A:307:PRO:HD2   | 1.94                     | 0.50              |
| 1:10A:90:GLU:HG2   | 1:10A:121:ARG:HH12 | 1.75                     | 0.49              |
| 2:10B:5:VAL:HG22   | 2:10B:133:PHE:CD1  | 2.46                     | 0.49              |
| 1:10C:224:TYR:O    | 1:10C:228:ASN:ND2  | 2.46                     | 0.49              |
| 1:11A:112:LYS:HA   | 1:11A:115:VAL:HG12 | 1.94                     | 0.49              |
| 1:12C:122:ILE:HD13 | 1:12C:157:LEU:HD21 | 1.94                     | 0.49              |
| 2:12D:304:ASP:HB2  | 2:12D:307:HIS:CE1  | 2.47                     | 0.49              |
| 1:13A:386:GLU:O    | 1:13A:390:ARG:HG2  | 2.11                     | 0.49              |
| 2:13B:317:PHE:HB3  | 2:13B:321:MET:HE1  | 1.93                     | 0.49              |
| 2:13D:209:ASP:OD2  | 2:13D:213:ARG:NH2  | 2.40                     | 0.49              |
| 2:1B:135:LEU:HD22  | 2:1B:152:ILE:HD11  | 1.93                     | 0.49              |
| 1:1E:102:ASN:HB2   | 1:1E:105:ARG:HB2   | 1.94                     | 0.49              |
| 1:1E:186:ASN:O     | 1:1E:190:THR:HG23  | 2.12                     | 0.49              |
| 1:3C:91:GLN:HA     | 1:3C:121:ARG:HH12  | 1.76                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:4A:317:MET:HB3  | 1:4A:319:TYR:CE1   | 2.47                     | 0.49              |
| 2:4D:175:VAL:HG22 | 1:4E:329:ASN:HD21  | 1.77                     | 0.49              |
| 1:5A:224:TYR:O    | 1:5A:228:ASN:ND2   | 2.45                     | 0.49              |
| 1:5E:228:ASN:OD1  | 3:5E:500:GTP:N2    | 2.33                     | 0.49              |
| 1:8A:298:PRO:HB3  | 1:8A:307:PRO:HD2   | 1.94                     | 0.49              |
| 1:9A:33:ASP:HB2   | 1:9A:35:GLN:OE1    | 2.12                     | 0.49              |
| 1:9C:113:GLU:N    | 1:9C:113:GLU:OE2   | 2.45                     | 0.49              |
| 1:9E:339:ARG:O    | 1:9E:342:GLN:NE2   | 2.44                     | 0.49              |
| 1:10A:220:GLU:OE1 | 1:10A:220:GLU:N    | 2.45                     | 0.49              |
| 2:10D:327:ASP:OD1 | 2:10D:328:GLU:N    | 2.45                     | 0.49              |
| 2:11D:3:GLU:HB3   | 2:11D:62:ARG:NH1   | 2.28                     | 0.49              |
| 1:11E:11:GLN:HB3  | 3:11E:500:GTP:O2B  | 2.12                     | 0.49              |
| 2:12D:390:ARG:HG3 | 2:12D:391:ARG:CD   | 2.42                     | 0.49              |
| 1:12E:305:CYS:SG  | 1:12E:384:ILE:HA   | 2.52                     | 0.49              |
| 1:13A:21:TRP:CE3  | 1:13A:24:TYR:HD2   | 2.30                     | 0.49              |
| 1:13C:175:PRO:HB3 | 1:13C:390:ARG:HD3  | 1.94                     | 0.49              |
| 2:13D:149:THR:OG1 | 2:13D:191:GLN:HG3  | 2.11                     | 0.49              |
| 1:13E:4:CYS:SG    | 1:13E:133:GLN:HB2  | 2.52                     | 0.49              |
| 2:1D:12:CYS:SG    | 2:1D:13:GLY:N      | 2.85                     | 0.49              |
| 2:4B:132:GLY:HA2  | 2:4B:163:ILE:O     | 2.12                     | 0.49              |
| 2:4D:257:MET:HE2  | 2:4D:314:ALA:HB2   | 1.94                     | 0.49              |
| 1:5C:292:THR:HG21 | 1:5C:331:ALA:HB1   | 1.94                     | 0.49              |
| 1:6E:102:ASN:OD1  | 1:6E:105:ARG:HD3   | 2.12                     | 0.49              |
| 2:8B:130:LEU:HD11 | 2:8B:133:PHE:HE1   | 1.77                     | 0.49              |
| 2:8D:203:ASP:OD2  | 2:8D:302:ALA:N     | 2.35                     | 0.49              |
| 1:9A:220:GLU:OE1  | 1:9A:220:GLU:N     | 2.44                     | 0.49              |
| 1:9C:102:ASN:HD22 | 1:9C:105:ARG:HD3   | 1.77                     | 0.49              |
| 1:10A:195:LEU:HB3 | 1:10A:196:GLU:OE2  | 2.12                     | 0.49              |
| 1:10C:91:GLN:HA   | 1:10C:121:ARG:HH12 | 1.76                     | 0.49              |
| 1:11A:113:GLU:OE1 | 1:11A:113:GLU:N    | 2.45                     | 0.49              |
| 2:11D:268:PRO:HG2 | 2:11D:300:MET:HB3  | 1.94                     | 0.49              |
| 1:11E:175:PRO:HB3 | 1:11E:390:ARG:NE   | 2.27                     | 0.49              |
| 1:12C:79:ARG:HE   | 1:12C:92:LEU:CD2   | 2.24                     | 0.49              |
| 2:12D:208:TYR:HA  | 2:12D:211:CYS:SG   | 2.52                     | 0.49              |
| 1:13A:224:TYR:O   | 1:13A:228:ASN:ND2  | 2.45                     | 0.49              |
| 1:13A:424:ASP:HA  | 1:13A:427:ALA:HB3  | 1.94                     | 0.49              |
| 2:13B:178:THR:HB  | 2:13B:181:GLU:HG3  | 1.95                     | 0.49              |
| 1:13E:220:GLU:HG2 | 1:13E:221:ARG:H    | 1.78                     | 0.49              |
| 2:1B:14:ASN:OD1   | 2:1B:73:MET:HE1    | 2.13                     | 0.49              |
| 2:2B:208:TYR:HA   | 2:2B:211:CYS:SG    | 2.51                     | 0.49              |
| 2:4D:73:MET:HA    | 2:4D:73:MET:HE3    | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5A:332:ILE:HD12  | 1:5A:351:PHE:CD2   | 2.47                     | 0.49              |
| 2:5B:310:TYR:O     | 2:5B:342:VAL:HG23  | 2.12                     | 0.49              |
| 2:5D:48:ASN:O      | 2:5D:62:ARG:NH2    | 2.45                     | 0.49              |
| 2:5D:248:ALA:HA    | 2:5D:252:LYS:HD3   | 1.94                     | 0.49              |
| 1:5E:185:TYR:HE1   | 1:5E:398:MET:HB3   | 1.76                     | 0.49              |
| 2:7B:130:LEU:HD11  | 2:7B:133:PHE:HE1   | 1.77                     | 0.49              |
| 1:9A:196:GLU:OE1   | 1:9A:196:GLU:N     | 2.46                     | 0.49              |
| 2:9D:111:GLU:OE1   | 2:9D:111:GLU:N     | 2.44                     | 0.49              |
| 1:9E:188:ILE:HG23  | 1:9E:425:LEU:HD12  | 1.95                     | 0.49              |
| 1:10C:214:ARG:HH21 | 2:10D:324:LYS:HE2  | 1.77                     | 0.49              |
| 1:11A:332:ILE:HD12 | 1:11A:351:PHE:CE2  | 2.48                     | 0.49              |
| 2:11B:66:VAL:HG23  | 2:11B:91:VAL:HB    | 1.94                     | 0.49              |
| 1:12E:154:MET:HE1  | 1:12E:168:GLU:OE1  | 2.11                     | 0.49              |
| 1:13A:4:CYS:SG     | 1:13A:133:GLN:HB2  | 2.53                     | 0.49              |
| 2:13D:73:MET:HA    | 2:13D:76:VAL:HG12  | 1.94                     | 0.49              |
| 2:13D:220:PRO:HG2  | 1:13E:326:LYS:HB3  | 1.94                     | 0.49              |
| 2:13D:228:LEU:HB3  | 2:13D:300:MET:HE1  | 1.94                     | 0.49              |
| 2:5B:373:ALA:O     | 2:5B:376:GLU:HG2   | 2.12                     | 0.49              |
| 2:6B:376:GLU:HA    | 2:6B:379:LYS:HG2   | 1.93                     | 0.49              |
| 1:7A:222:PRO:CD    | 2:7B:324:LYS:HE2   | 2.42                     | 0.49              |
| 2:7D:237:THR:HG22  | 2:7D:250:LEU:HD21  | 1.94                     | 0.49              |
| 2:7D:328:GLU:O     | 2:7D:331:LEU:HG    | 2.12                     | 0.49              |
| 1:8E:145:THR:HG1   | 3:8E:500:GTP:PG    | 2.34                     | 0.49              |
| 2:9B:209:ASP:OD2   | 2:9B:213:ARG:NH2   | 2.46                     | 0.49              |
| 1:10A:344:VAL:HG11 | 1:10A:346:TRP:CE2  | 2.47                     | 0.49              |
| 2:10B:86:ARG:NH1   | 2:11B:281:TYR:O    | 2.45                     | 0.49              |
| 1:10C:306:ASP:OD2  | 1:10C:309:HIS:ND1  | 2.40                     | 0.49              |
| 2:10D:182:PRO:HG3  | 2:10D:384:GLN:HG3  | 1.93                     | 0.49              |
| 1:11A:305:CYS:HA   | 1:11A:386:GLU:OE2  | 2.13                     | 0.49              |
| 2:11B:175:VAL:HG13 | 1:11C:329:ASN:ND2  | 2.27                     | 0.49              |
| 1:12A:135:PHE:CD2  | 1:12A:157:LEU:HD13 | 2.47                     | 0.49              |
| 2:12B:141:GLY:HA3  | 5:12B:600:GDP:O2A  | 2.13                     | 0.49              |
| 2:12B:286:VAL:HG11 | 2:12B:326:VAL:HG22 | 1.93                     | 0.49              |
| 1:13A:184:PRO:O    | 1:13A:188:ILE:HG12 | 2.13                     | 0.49              |
| 1:13C:129:CYS:SG   | 1:13C:132:LEU:HB2  | 2.52                     | 0.49              |
| 2:13D:216:LYS:HB2  | 2:13D:275:SER:OG   | 2.12                     | 0.49              |
| 2:13D:285:THR:OG1  | 2:13D:287:PRO:HD2  | 2.12                     | 0.49              |
| 2:1B:209:ASP:OD2   | 2:1B:213:ARG:NH2   | 2.44                     | 0.49              |
| 1:1C:145:THR:OG1   | 3:1C:500:GTP:O3B   | 2.27                     | 0.49              |
| 1:1E:175:PRO:HB3   | 1:1E:390:ARG:HD3   | 1.93                     | 0.49              |
| 1:2A:108:TYR:HA    | 1:2A:112:LYS:NZ    | 2.26                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:4C:394:LYS:HG2   | 2:4D:346:PRO:HG3   | 1.93                     | 0.49              |
| 2:5D:285:THR:O     | 2:5D:288:GLU:HG2   | 2.12                     | 0.49              |
| 1:6A:140:SER:OG    | 3:6A:500:GTP:O2A   | 2.29                     | 0.49              |
| 2:7B:111:GLU:OE1   | 2:7B:111:GLU:N     | 2.45                     | 0.49              |
| 1:7C:72:PRO:HD2    | 2:7D:2:ARG:HH21    | 1.76                     | 0.49              |
| 1:7C:414:GLU:OE1   | 1:7C:416:GLY:N     | 2.38                     | 0.49              |
| 2:8D:270:PHE:HD2   | 2:8D:366:THR:HG22  | 1.76                     | 0.49              |
| 2:10D:172:SER:HB2  | 2:10D:205:GLU:OE2  | 2.13                     | 0.49              |
| 2:10D:208:TYR:HA   | 2:10D:211:CYS:SG   | 2.52                     | 0.49              |
| 2:10D:215:LEU:HD23 | 2:10D:215:LEU:O    | 2.12                     | 0.49              |
| 2:10D:376:GLU:HA   | 2:10D:379:LYS:HG2  | 1.94                     | 0.49              |
| 1:11C:112:LYS:HA   | 1:11C:115:VAL:HG12 | 1.94                     | 0.49              |
| 1:11C:305:CYS:HA   | 1:11C:386:GLU:OE2  | 2.12                     | 0.49              |
| 2:11D:345:ILE:O    | 2:11D:348:ASN:ND2  | 2.46                     | 0.49              |
| 1:11E:313:MET:HB2  | 1:11E:347:CYS:SG   | 2.52                     | 0.49              |
| 2:12D:330:MET:SD   | 2:12D:349:VAL:HG11 | 2.52                     | 0.49              |
| 1:13E:112:LYS:HA   | 1:13E:115:VAL:HG12 | 1.94                     | 0.49              |
| 1:1A:291:ILE:HD12  | 1:1A:375:VAL:HG23  | 1.94                     | 0.49              |
| 2:1B:215:LEU:HB3   | 2:1B:217:LEU:HG    | 1.94                     | 0.49              |
| 2:1B:317:PHE:HB3   | 2:1B:321:MET:HE1   | 1.95                     | 0.49              |
| 1:2C:265:ILE:HG23  | 1:2C:432:TYR:CZ    | 2.48                     | 0.49              |
| 2:2D:151:LEU:O     | 2:2D:155:ILE:HG12  | 2.12                     | 0.49              |
| 1:3E:206:ASN:OD1   | 3:3E:500:GTP:O2'   | 2.31                     | 0.49              |
| 1:4C:407:TRP:CG    | 2:4D:255:VAL:HG23  | 2.47                     | 0.49              |
| 1:5A:20:CYS:O      | 1:5A:23:LEU:N      | 2.45                     | 0.49              |
| 1:5C:271:THR:HG22  | 1:5C:377:MET:HB3   | 1.94                     | 0.49              |
| 1:7A:56:THR:HG23   | 1:8A:285:GLN:HB2   | 1.93                     | 0.49              |
| 2:7B:309:ARG:NH1   | 2:7B:426:GLN:OXT   | 2.46                     | 0.49              |
| 2:7B:372:THR:HG21  | 2:7B:426:GLN:HA    | 1.95                     | 0.49              |
| 1:7C:398:MET:HE1   | 2:7D:346:PRO:HD2   | 1.95                     | 0.49              |
| 2:7D:212:PHE:CE1   | 2:7D:220:PRO:HG3   | 2.47                     | 0.49              |
| 1:8E:195:LEU:HB3   | 1:8E:196:GLU:OE2   | 2.13                     | 0.49              |
| 1:8E:204:VAL:HG11  | 1:8E:231:ILE:HD11  | 1.94                     | 0.49              |
| 1:9C:137:ILE:HB    | 1:9C:168:GLU:HB3   | 1.93                     | 0.49              |
| 2:9D:151:LEU:O     | 2:9D:155:ILE:HG12  | 2.13                     | 0.49              |
| 2:10B:285:THR:OG1  | 2:10B:287:PRO:HD2  | 2.11                     | 0.49              |
| 2:11B:236:VAL:HG23 | 2:11B:237:THR:HG23 | 1.95                     | 0.49              |
| 1:11E:223:THR:HG23 | 1:11E:225:THR:HG23 | 1.94                     | 0.49              |
| 1:13A:270:VAL:O    | 1:13A:302:MET:HB3  | 2.13                     | 0.49              |
| 2:13D:257:MET:HE1  | 2:13D:266:PHE:CZ   | 2.48                     | 0.49              |
| 1:13E:139:HIS:HE1  | 1:13E:141:PHE:CE1  | 2.30                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1E:184:PRO:O    | 1:1E:188:ILE:HG12  | 2.12                     | 0.49              |
| 1:2C:306:ASP:OD2  | 1:2C:309:HIS:ND1   | 2.46                     | 0.49              |
| 2:4B:175:VAL:HG12 | 2:4B:175:VAL:O     | 2.13                     | 0.49              |
| 1:4E:122:ILE:HD13 | 1:4E:157:LEU:HD21  | 1.94                     | 0.49              |
| 1:6C:102:ASN:HB2  | 1:6C:105:ARG:HB2   | 1.93                     | 0.49              |
| 1:6E:167:LEU:HD11 | 1:6E:252:LEU:HD11  | 1.93                     | 0.49              |
| 1:7A:101:ASN:OD1  | 2:7B:252:LYS:NZ    | 2.45                     | 0.49              |
| 2:7B:310:TYR:O    | 2:7B:342:VAL:HG23  | 2.12                     | 0.49              |
| 2:7B:388:MET:HE2  | 1:7C:348:PRO:HD2   | 1.95                     | 0.49              |
| 2:8D:263:LEU:HG   | 2:8D:422:TYR:CE2   | 2.48                     | 0.49              |
| 1:8E:184:PRO:O    | 1:8E:188:ILE:HG12  | 2.13                     | 0.49              |
| 1:9A:315:CYS:HA   | 1:9A:379:SER:HA    | 1.94                     | 0.49              |
| 2:9B:48:ASN:O     | 2:9B:62:ARG:NH2    | 2.46                     | 0.49              |
| 1:10C:220:GLU:OE1 | 1:10C:220:GLU:N    | 2.46                     | 0.49              |
| 1:10E:270:VAL:O   | 1:10E:302:MET:HB2  | 2.13                     | 0.49              |
| 1:11A:88:HIS:CE1  | 1:12A:283:HIS:HB2  | 2.47                     | 0.49              |
| 2:11B:3:GLU:HB3   | 2:11B:62:ARG:NH1   | 2.28                     | 0.49              |
| 1:11C:70:LEU:HD11 | 1:11C:110:ILE:HG21 | 1.95                     | 0.49              |
| 1:12C:69:ASP:CG   | 1:12C:71:GLU:H     | 2.20                     | 0.49              |
| 2:12D:390:ARG:HG3 | 2:12D:391:ARG:NE   | 2.28                     | 0.49              |
| 2:13B:385:PHE:CZ  | 2:13B:389:PHE:HB2  | 2.48                     | 0.49              |
| 2:1B:173:PRO:HD2  | 2:1B:380:ARG:HH21  | 1.78                     | 0.49              |
| 1:1E:112:LYS:HA   | 1:1E:115:VAL:HG12  | 1.95                     | 0.49              |
| 2:2D:190:HIS:NE2  | 2:2D:414:ASN:OD1   | 2.45                     | 0.49              |
| 2:3B:117:LEU:HA   | 2:3B:120:VAL:HG22  | 1.95                     | 0.49              |
| 2:3D:325:GLU:O    | 2:3D:329:GLN:HG2   | 2.12                     | 0.49              |
| 1:3E:213:CYS:HB3  | 1:3E:219:ILE:HD11  | 1.95                     | 0.49              |
| 1:4A:168:GLU:HG2  | 1:4A:201:ALA:HA    | 1.93                     | 0.49              |
| 1:5A:55:GLU:OE2   | 1:5A:61:HIS:NE2    | 2.46                     | 0.49              |
| 2:5B:127:CYS:SG   | 2:5B:130:LEU:HD23  | 2.53                     | 0.49              |
| 2:6B:285:THR:O    | 2:6B:288:GLU:HG2   | 2.12                     | 0.49              |
| 2:6D:173:PRO:HD2  | 2:6D:380:ARG:HH21  | 1.77                     | 0.49              |
| 1:7A:20:CYS:HB3   | 1:7A:24:TYR:CE2    | 2.48                     | 0.49              |
| 1:7A:203:MET:HE1  | 1:7A:267:PHE:HB3   | 1.94                     | 0.49              |
| 1:7C:88:HIS:CD2   | 1:7C:89:PRO:HD2    | 2.44                     | 0.49              |
| 1:7C:356:ASN:OD1  | 1:7C:357:TYR:N     | 2.46                     | 0.49              |
| 2:8B:396:HIS:CE1  | 2:8B:397:TRP:CD1   | 3.00                     | 0.49              |
| 1:9A:175:PRO:HB3  | 1:9A:390:ARG:NE    | 2.27                     | 0.49              |
| 1:9A:195:LEU:HB3  | 1:9A:196:GLU:OE1   | 2.13                     | 0.49              |
| 1:10A:175:PRO:HB3 | 1:10A:390:ARG:CZ   | 2.42                     | 0.49              |
| 2:10B:127:CYS:SG  | 2:10B:130:LEU:HD22 | 2.53                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:73:MET:N     | 2:12B:73:MET:SD    | 2.83                     | 0.49              |
| 1:12C:157:LEU:O    | 1:12C:161:TYR:HD1  | 1.95                     | 0.49              |
| 2:12D:147:MET:HE2  | 2:12D:147:MET:HA   | 1.95                     | 0.49              |
| 1:13E:333:ALA:HA   | 1:13E:336:LYS:HB2  | 1.95                     | 0.49              |
| 2:1B:12:CYS:SG     | 2:1B:13:GLY:N      | 2.85                     | 0.49              |
| 1:2A:407:TRP:CG    | 2:2B:255:VAL:HG23  | 2.48                     | 0.49              |
| 1:2E:329:ASN:OD1   | 1:2E:330:ALA:N     | 2.46                     | 0.49              |
| 1:3C:88:HIS:CD2    | 1:3C:89:PRO:HD2    | 2.47                     | 0.49              |
| 2:4D:310:TYR:O     | 2:4D:342:VAL:HG23  | 2.13                     | 0.49              |
| 2:4D:328:GLU:O     | 2:4D:331:LEU:HG    | 2.13                     | 0.49              |
| 1:7C:145:THR:HG1   | 3:7C:500:GTP:PG    | 2.36                     | 0.49              |
| 2:7D:420:SER:O     | 2:7D:423:GLN:HG3   | 2.12                     | 0.49              |
| 1:7E:118:VAL:HA    | 1:7E:121:ARG:HB2   | 1.94                     | 0.49              |
| 1:8C:395:PHE:HZ    | 1:8C:418:PHE:HB3   | 1.78                     | 0.49              |
| 1:9A:69:ASP:OD1    | 1:9A:70:LEU:N      | 2.46                     | 0.49              |
| 1:9E:184:PRO:O     | 1:9E:188:ILE:HG12  | 2.12                     | 0.49              |
| 1:10E:132:LEU:HD23 | 1:10E:164:LYS:HZ1  | 1.77                     | 0.49              |
| 1:10E:220:GLU:OE1  | 1:10E:220:GLU:N    | 2.45                     | 0.49              |
| 1:11A:290:GLU:OE2  | 1:11A:291:ILE:HG23 | 2.12                     | 0.49              |
| 2:11B:153:SER:HB2  | 2:11B:191:GLN:OE1  | 2.13                     | 0.49              |
| 1:11C:213:CYS:HA   | 1:11C:217:LEU:HB2  | 1.95                     | 0.49              |
| 1:3A:108:TYR:HA    | 1:3A:112:LYS:NZ    | 2.27                     | 0.49              |
| 1:3A:224:TYR:O     | 1:3A:228:ASN:ND2   | 2.45                     | 0.49              |
| 1:4E:239:THR:OG1   | 1:4E:243:ARG:NH1   | 2.46                     | 0.49              |
| 1:4E:261:PRO:HG3   | 1:4E:313:MET:SD    | 2.53                     | 0.49              |
| 1:7A:306:ASP:OD2   | 1:7A:309:HIS:ND1   | 2.40                     | 0.49              |
| 1:8A:20:CYS:HB3    | 1:8A:24:TYR:CE2    | 2.48                     | 0.49              |
| 1:8E:265:ILE:HG23  | 1:8E:432:TYR:CZ    | 2.47                     | 0.49              |
| 2:9B:336:LYS:HD2   | 2:9B:337:ASN:OD1   | 2.13                     | 0.49              |
| 1:10A:255:PHE:HZ   | 1:10A:378:LEU:HD22 | 1.78                     | 0.48              |
| 2:10B:5:VAL:HG12   | 2:10B:62:ARG:HD3   | 1.95                     | 0.48              |
| 1:10C:269:LEU:HD11 | 1:10C:384:ILE:HB   | 1.95                     | 0.48              |
| 1:10E:291:ILE:HD12 | 1:10E:375:VAL:HG23 | 1.94                     | 0.48              |
| 1:11A:307:PRO:HB3  | 1:11A:312:TYR:HE1  | 1.78                     | 0.48              |
| 1:11C:397:LEU:HD21 | 2:11D:344:TRP:HA   | 1.94                     | 0.48              |
| 2:11D:236:VAL:HG23 | 2:11D:237:THR:HG23 | 1.95                     | 0.48              |
| 2:12B:128:ASP:OD1  | 2:12B:129:CYS:N    | 2.41                     | 0.48              |
| 2:13B:135:LEU:HD23 | 2:13B:166:THR:HG22 | 1.95                     | 0.48              |
| 2:13B:175:VAL:HG21 | 2:13B:205:GLU:HA   | 1.95                     | 0.48              |
| 2:13D:405:GLU:HA   | 2:13D:408:PHE:HD1  | 1.73                     | 0.48              |
| 1:1A:88:HIS:HB3    | 1:1A:90:GLU:OE1    | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2D:12:CYS:SG     | 2:2D:13:GLY:N      | 2.86                     | 0.48              |
| 1:2E:269:LEU:HD11  | 1:2E:384:ILE:HB    | 1.95                     | 0.48              |
| 2:3B:5:VAL:HG22    | 2:3B:133:PHE:CD1   | 2.48                     | 0.48              |
| 1:5C:413:MET:HE3   | 1:5C:417:GLU:HG2   | 1.94                     | 0.48              |
| 2:6D:263:LEU:HG    | 2:6D:422:TYR:CE1   | 2.48                     | 0.48              |
| 2:7B:287:PRO:HB3   | 2:7B:329:GLN:OE1   | 2.13                     | 0.48              |
| 2:8B:117:LEU:HA    | 2:8B:120:VAL:HG22  | 1.95                     | 0.48              |
| 1:8E:9:VAL:HG11    | 1:8E:150:THR:OG1   | 2.13                     | 0.48              |
| 1:8E:175:PRO:HD2   | 1:8E:207:GLU:OE1   | 2.12                     | 0.48              |
| 1:9A:344:VAL:HG11  | 1:9A:346:TRP:CE2   | 2.48                     | 0.48              |
| 1:9E:252:LEU:O     | 1:9E:256:GLN:HG2   | 2.13                     | 0.48              |
| 2:10B:309:ARG:NH1  | 2:10B:426:GLN:OXT  | 2.46                     | 0.48              |
| 1:10C:209:ILE:CG2  | 1:10C:227:LEU:HG   | 2.43                     | 0.48              |
| 1:11C:138:PHE:CD1  | 1:11C:169:PHE:HB2  | 2.48                     | 0.48              |
| 1:11E:213:CYS:HA   | 1:11E:217:LEU:HD13 | 1.95                     | 0.48              |
| 1:12A:31:GLN:HB3   | 1:12A:35:GLN:HG3   | 1.95                     | 0.48              |
| 2:13D:178:THR:HB   | 2:13D:181:GLU:HG3  | 1.95                     | 0.48              |
| 1:13E:5:ILE:O      | 1:13E:135:PHE:HA   | 2.14                     | 0.48              |
| 1:1A:306:ASP:OD2   | 1:1A:309:HIS:ND1   | 2.46                     | 0.48              |
| 2:1B:287:PRO:O     | 2:1B:291:GLN:HG2   | 2.14                     | 0.48              |
| 2:1D:175:VAL:O     | 2:1D:175:VAL:HG12  | 2.13                     | 0.48              |
| 1:2E:88:HIS:HB3    | 1:2E:90:GLU:OE1    | 2.13                     | 0.48              |
| 1:2E:112:LYS:HA    | 1:2E:115:VAL:HG12  | 1.94                     | 0.48              |
| 1:3A:206:ASN:OD1   | 3:3A:500:GTP:O2'   | 2.31                     | 0.48              |
| 2:4B:121:ARG:NH1   | 2:4B:158:GLU:OE1   | 2.45                     | 0.48              |
| 2:4B:220:PRO:HD2   | 1:4C:326:LYS:HD2   | 1.95                     | 0.48              |
| 1:4E:291:ILE:HD12  | 1:4E:375:VAL:HG23  | 1.95                     | 0.48              |
| 1:5A:217:LEU:HD11  | 1:5A:367:ASP:O     | 2.14                     | 0.48              |
| 2:5B:109:GLY:HA3   | 2:5B:147:MET:CE    | 2.41                     | 0.48              |
| 1:6C:169:PHE:CE1   | 1:6C:235:VAL:HG22  | 2.49                     | 0.48              |
| 1:6C:200:CYS:HB2   | 1:6C:256:GLN:HE22  | 1.78                     | 0.48              |
| 1:6E:56:THR:HG23   | 1:7E:285:GLN:HB2   | 1.95                     | 0.48              |
| 1:7E:174:ALA:HB3   | 1:7E:177:VAL:O     | 2.13                     | 0.48              |
| 1:8C:255:PHE:CZ    | 1:8C:378:LEU:HD22  | 2.48                     | 0.48              |
| 2:8D:7:ILE:O       | 2:8D:135:LEU:HA    | 2.13                     | 0.48              |
| 1:9A:225:THR:O     | 1:9A:229:ARG:HG3   | 2.13                     | 0.48              |
| 1:9A:312:TYR:O     | 1:9A:344:VAL:HG23  | 2.13                     | 0.48              |
| 1:11E:90:GLU:HB3   | 1:11E:121:ARG:CZ   | 2.43                     | 0.48              |
| 1:11E:405:VAL:HG22 | 1:11E:409:VAL:HG23 | 1.96                     | 0.48              |
| 2:12B:263:LEU:O    | 2:12B:370:ASN:ND2  | 2.46                     | 0.48              |
| 2:12D:403:MET:SD   | 2:12D:404:ASP:N    | 2.86                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13A:156:ARG:HD2  | 1:13A:156:ARG:N    | 2.28                     | 0.48              |
| 1:13A:284:GLU:OE1  | 1:13A:284:GLU:N    | 2.46                     | 0.48              |
| 1:1C:265:ILE:HG23  | 1:1C:432:TYR:CE1   | 2.48                     | 0.48              |
| 2:1D:175:VAL:HG22  | 1:1E:329:ASN:ND2   | 2.28                     | 0.48              |
| 2:1D:382:SER:O     | 2:1D:386:THR:HG23  | 2.12                     | 0.48              |
| 1:1E:271:THR:HG22  | 1:1E:377:MET:HB3   | 1.94                     | 0.48              |
| 2:2B:140:GLY:O     | 2:2B:184:ASN:ND2   | 2.30                     | 0.48              |
| 1:2C:123:ARG:NE    | 1:2C:161:TYR:OH    | 2.44                     | 0.48              |
| 1:2C:225:THR:O     | 1:2C:229:ARG:HG3   | 2.13                     | 0.48              |
| 1:3A:169:PHE:CE2   | 1:3A:235:VAL:HG22  | 2.48                     | 0.48              |
| 1:3E:169:PHE:CE2   | 1:3E:235:VAL:HG22  | 2.48                     | 0.48              |
| 1:3E:184:PRO:O     | 1:3E:188:ILE:HG12  | 2.13                     | 0.48              |
| 1:4A:188:ILE:HG23  | 1:4A:425:LEU:HD12  | 1.94                     | 0.48              |
| 1:4A:265:ILE:HG23  | 1:4A:432:TYR:CZ    | 2.47                     | 0.48              |
| 1:4C:336:LYS:HE3   | 1:4C:351:PHE:HE2   | 1.77                     | 0.48              |
| 1:6A:213:CYS:HB3   | 1:6A:219:ILE:HD11  | 1.94                     | 0.48              |
| 1:6A:215:ARG:NH2   | 1:6A:299:ALA:HB1   | 2.28                     | 0.48              |
| 2:6B:293:MET:CE    | 2:6B:365:ALA:HB1   | 2.42                     | 0.48              |
| 2:6D:28:HIS:NE2    | 2:6D:241:ARG:HD2   | 2.28                     | 0.48              |
| 1:7A:11:GLN:HG3    | 1:7A:74:VAL:HG21   | 1.96                     | 0.48              |
| 1:8A:407:TRP:CG    | 2:8B:255:VAL:HG23  | 2.48                     | 0.48              |
| 2:8B:65:LEU:HD22   | 2:8B:73:MET:HE1    | 1.94                     | 0.48              |
| 1:9A:11:GLN:HG2    | 1:9A:15:GLN:HE22   | 1.79                     | 0.48              |
| 1:9E:265:ILE:HG23  | 1:9E:432:TYR:CZ    | 2.48                     | 0.48              |
| 1:10C:188:ILE:HG22 | 1:10C:421:ALA:HB1  | 1.94                     | 0.48              |
| 1:11C:405:VAL:HG22 | 1:11C:409:VAL:HG23 | 1.95                     | 0.48              |
| 2:12D:286:VAL:HB   | 2:12D:325:GLU:HG2  | 1.94                     | 0.48              |
| 1:13A:30:ILE:HG21  | 1:13A:53:PHE:HE2   | 1.77                     | 0.48              |
| 1:1E:259:LEU:HD13  | 1:1E:316:CYS:SG    | 2.53                     | 0.48              |
| 1:1E:265:ILE:HG23  | 1:1E:432:TYR:CZ    | 2.48                     | 0.48              |
| 1:3C:165:SER:HA    | 1:3C:199:ASP:OD2   | 2.14                     | 0.48              |
| 2:3D:73:MET:HA     | 2:3D:76:VAL:HG12   | 1.95                     | 0.48              |
| 2:3D:219:THR:HG22  | 1:3E:326:LYS:HE2   | 1.95                     | 0.48              |
| 1:4C:265:ILE:HG23  | 1:4C:432:TYR:CZ    | 2.47                     | 0.48              |
| 1:4C:286:LEU:O     | 1:4C:373:ARG:NH2   | 2.45                     | 0.48              |
| 2:6B:373:ALA:O     | 2:6B:376:GLU:HG2   | 2.13                     | 0.48              |
| 1:6C:261:PRO:HG3   | 1:6C:313:MET:HE2   | 1.95                     | 0.48              |
| 2:6D:373:ALA:O     | 2:6D:376:GLU:HG2   | 2.13                     | 0.48              |
| 1:8A:184:PRO:O     | 1:8A:188:ILE:HG12  | 2.14                     | 0.48              |
| 1:8C:220:GLU:OE1   | 1:8C:220:GLU:N     | 2.41                     | 0.48              |
| 1:9A:165:SER:HA    | 1:9A:199:ASP:OD2   | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11C:220:GLU:OE1  | 1:11C:220:GLU:N    | 2.44                     | 0.48              |
| 1:11E:142:GLY:O    | 1:11E:186:ASN:ND2  | 2.46                     | 0.48              |
| 1:12A:265:ILE:HG23 | 1:12A:432:TYR:OH   | 2.14                     | 0.48              |
| 2:12D:130:LEU:H    | 2:12D:130:LEU:HD23 | 1.78                     | 0.48              |
| 2:13B:90:PHE:HB3   | 2:13B:92:PHE:CE2   | 2.46                     | 0.48              |
| 2:13D:411:ALA:O    | 2:13D:415:MET:HG3  | 2.13                     | 0.48              |
| 2:1B:299:MET:HE3   | 2:1B:299:MET:HB2   | 1.75                     | 0.48              |
| 2:3D:175:VAL:O     | 2:3D:175:VAL:HG12  | 2.13                     | 0.48              |
| 2:4B:390:ARG:HH12  | 2:4B:391:ARG:HE    | 1.61                     | 0.48              |
| 1:5A:205:ASP:OD2   | 1:5A:207:GLU:HG2   | 2.14                     | 0.48              |
| 2:5D:213:ARG:O     | 2:5D:216:LYS:NZ    | 2.30                     | 0.48              |
| 1:8A:344:VAL:HG11  | 1:8A:346:TRP:CE2   | 2.48                     | 0.48              |
| 1:8C:12:ALA:O      | 1:8C:15:GLN:HB2    | 2.13                     | 0.48              |
| 1:9A:213:CYS:SG    | 1:9A:219:ILE:HD11  | 2.53                     | 0.48              |
| 1:9C:298:PRO:HB3   | 1:9C:307:PRO:HD2   | 1.96                     | 0.48              |
| 1:9C:414:GLU:OE1   | 1:9C:416:GLY:N     | 2.37                     | 0.48              |
| 2:9D:209:ASP:OD2   | 2:9D:213:ARG:NH2   | 2.45                     | 0.48              |
| 1:9E:269:LEU:HD11  | 1:9E:384:ILE:HB    | 1.95                     | 0.48              |
| 1:10A:214:ARG:HH21 | 2:10B:324:LYS:HE2  | 1.78                     | 0.48              |
| 1:10C:286:LEU:O    | 1:10C:373:ARG:NH2  | 2.46                     | 0.48              |
| 1:10E:332:ILE:HD12 | 1:10E:351:PHE:CE2  | 2.49                     | 0.48              |
| 2:11D:382:SER:O    | 2:11D:386:THR:OG1  | 2.17                     | 0.48              |
| 2:11D:405:GLU:HA   | 2:11D:408:PHE:CD1  | 2.49                     | 0.48              |
| 1:12C:403:ALA:HA   | 2:12D:260:PHE:HE1  | 1.77                     | 0.48              |
| 1:12E:102:ASN:OD1  | 1:12E:408:TYR:HE1  | 1.97                     | 0.48              |
| 1:13C:225:THR:O    | 1:13C:229:ARG:HG3  | 2.14                     | 0.48              |
| 2:13D:387:ALA:HA   | 2:13D:390:ARG:HD3  | 1.96                     | 0.48              |
| 1:1A:224:TYR:CD2   | 2:1B:323:MET:HE3   | 2.48                     | 0.48              |
| 1:2C:221:ARG:HA    | 2:2D:324:LYS:HZ1   | 1.79                     | 0.48              |
| 2:2D:324:LYS:HG3   | 2:2D:325:GLU:N     | 2.29                     | 0.48              |
| 2:4B:304:ASP:HB2   | 2:4B:307:HIS:CD2   | 2.48                     | 0.48              |
| 1:5C:234:ILE:HD11  | 1:5C:302:MET:HE3   | 1.95                     | 0.48              |
| 1:6A:102:ASN:OD1   | 1:6A:105:ARG:HD3   | 2.14                     | 0.48              |
| 1:6C:31:GLN:HG3    | 1:6C:32:PRO:HD2    | 1.96                     | 0.48              |
| 2:6D:285:THR:O     | 2:6D:288:GLU:HG2   | 2.13                     | 0.48              |
| 1:6E:91:GLN:HG2    | 1:6E:121:ARG:HH22  | 1.78                     | 0.48              |
| 1:7C:184:PRO:O     | 1:7C:188:ILE:HG12  | 2.14                     | 0.48              |
| 1:7E:113:GLU:OE1   | 1:7E:113:GLU:N     | 2.46                     | 0.48              |
| 1:7E:203:MET:HE1   | 1:7E:267:PHE:HB3   | 1.95                     | 0.48              |
| 1:9A:216:ASN:O     | 1:9A:280:LYS:NZ    | 2.47                     | 0.48              |
| 2:9B:167:TYR:CE1   | 2:9B:233:MET:HG2   | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:9B:420:SER:O     | 2:9B:423:GLN:HG3   | 2.13                     | 0.48              |
| 2:10B:178:THR:HB   | 2:10B:181:GLU:HG3  | 1.95                     | 0.48              |
| 2:10D:4:ILE:HG23   | 2:10D:50:TYR:HE1   | 1.78                     | 0.48              |
| 2:10D:248:ALA:HA   | 2:10D:252:LYS:HD3  | 1.94                     | 0.48              |
| 2:11B:73:MET:HE2   | 2:11B:92:PHE:HB3   | 1.95                     | 0.48              |
| 2:11B:317:PHE:HB3  | 2:11B:321:MET:SD   | 2.54                     | 0.48              |
| 1:11C:5:ILE:O      | 1:11C:135:PHE:HA   | 2.13                     | 0.48              |
| 1:11C:168:GLU:HG2  | 1:11C:201:ALA:HA   | 1.94                     | 0.48              |
| 2:11D:215:LEU:HB3  | 2:11D:217:LEU:HG   | 1.96                     | 0.48              |
| 1:11E:112:LYS:HA   | 1:11E:115:VAL:HG12 | 1.95                     | 0.48              |
| 1:12A:320:ARG:O    | 1:12A:373:ARG:HA   | 2.13                     | 0.48              |
| 1:12C:52:PHE:C     | 1:12C:53:PHE:HD1   | 2.22                     | 0.48              |
| 1:12C:135:PHE:CD2  | 1:12C:157:LEU:HD13 | 2.49                     | 0.48              |
| 1:13E:195:LEU:HA   | 1:13E:266:HIS:CE1  | 2.49                     | 0.48              |
| 2:1B:5:VAL:HG12    | 2:1B:62:ARG:HD3    | 1.96                     | 0.48              |
| 2:2D:257:MET:HE1   | 2:2D:368:ILE:HB    | 1.95                     | 0.48              |
| 2:3B:12:CYS:SG     | 2:3B:13:GLY:N      | 2.86                     | 0.48              |
| 2:3B:175:VAL:O     | 2:3B:175:VAL:HG12  | 2.14                     | 0.48              |
| 1:3C:98:ASP:OD1    | 1:3C:145:THR:OG1   | 2.28                     | 0.48              |
| 1:3E:71:GLU:HB2    | 1:3E:98:ASP:HB2    | 1.95                     | 0.48              |
| 1:4E:169:PHE:CE2   | 1:4E:235:VAL:HG22  | 2.49                     | 0.48              |
| 2:5B:325:GLU:O     | 2:5B:329:GLN:HG2   | 2.14                     | 0.48              |
| 1:6A:174:ALA:HB3   | 1:6A:177:VAL:O     | 2.14                     | 0.48              |
| 1:6E:413:MET:HE3   | 1:6E:417:GLU:HG2   | 1.95                     | 0.48              |
| 1:7A:31:GLN:CG     | 1:7A:32:PRO:HD2    | 2.43                     | 0.48              |
| 2:8B:13:GLY:O      | 2:8B:17:GLY:N      | 2.40                     | 0.48              |
| 2:8D:113:VAL:HG11  | 2:8D:150:LEU:HD22  | 1.96                     | 0.48              |
| 1:8E:53:PHE:O      | 1:8E:64:ARG:NH2    | 2.35                     | 0.48              |
| 1:9A:220:GLU:O     | 2:9B:324:LYS:HE3   | 2.14                     | 0.48              |
| 1:9C:50:ASN:O      | 1:9C:64:ARG:NH1    | 2.47                     | 0.48              |
| 1:11A:56:THR:HA    | 1:12A:285:GLN:HB2  | 1.96                     | 0.48              |
| 1:11A:213:CYS:HA   | 1:11A:217:LEU:HD13 | 1.96                     | 0.48              |
| 1:11E:34:GLY:O     | 1:11E:61:HIS:ND1   | 2.39                     | 0.48              |
| 1:12A:14:VAL:O     | 1:12A:18:ASN:N     | 2.45                     | 0.48              |
| 2:12B:222:TYR:O    | 2:12B:226:ASN:ND2  | 2.47                     | 0.48              |
| 2:12B:328:GLU:O    | 2:12B:331:LEU:HG   | 2.13                     | 0.48              |
| 2:12D:260:PHE:HB3  | 2:12D:261:PRO:HD2  | 1.95                     | 0.48              |
| 2:12D:372:THR:HG21 | 2:12D:426:GLN:HA   | 1.96                     | 0.48              |
| 1:12E:14:VAL:O     | 1:12E:18:ASN:N     | 2.44                     | 0.48              |
| 2:13B:293:MET:HE1  | 2:13B:365:ALA:HB1  | 1.95                     | 0.48              |
| 1:13C:70:LEU:HD11  | 1:13C:149:PHE:CE2  | 2.48                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13C:306:ASP:OD2  | 1:13C:309:HIS:ND1  | 2.47                     | 0.48              |
| 2:13D:135:LEU:HD23 | 2:13D:166:THR:HG22 | 1.96                     | 0.48              |
| 2:13D:381:ILE:HA   | 2:13D:384:GLN:CD   | 2.39                     | 0.48              |
| 2:1B:68:LEU:HD12   | 2:1B:143:THR:HG23  | 1.95                     | 0.48              |
| 1:1C:211:ASP:OD2   | 1:1C:304:LYS:NZ    | 2.47                     | 0.48              |
| 2:1D:135:LEU:HD23  | 2:1D:152:ILE:HD11  | 1.95                     | 0.48              |
| 1:3C:11:GLN:HB3    | 3:3C:500:GTP:O2B   | 2.13                     | 0.48              |
| 1:3C:234:ILE:HD11  | 1:3C:302:MET:HE3   | 1.96                     | 0.48              |
| 2:3D:130:LEU:HD23  | 2:3D:130:LEU:H     | 1.78                     | 0.48              |
| 1:3E:5:ILE:HB      | 1:3E:135:PHE:HD1   | 1.77                     | 0.48              |
| 1:4C:175:PRO:HD2   | 1:4C:207:GLU:OE1   | 2.14                     | 0.48              |
| 2:4D:285:THR:O     | 2:4D:288:GLU:HG2   | 2.14                     | 0.48              |
| 2:5B:248:ALA:HA    | 2:5B:252:LYS:HD3   | 1.96                     | 0.48              |
| 2:6B:3:GLU:OE2     | 2:6B:127:CYS:HB2   | 2.14                     | 0.48              |
| 2:6B:52:ASN:HB3    | 2:6B:62:ARG:NH1    | 2.27                     | 0.48              |
| 1:7C:312:TYR:O     | 1:7C:344:VAL:HG23  | 2.14                     | 0.48              |
| 2:7D:20:PHE:CD2    | 2:7D:233:MET:HE2   | 2.49                     | 0.48              |
| 2:8B:303:CYS:SG    | 2:8B:377:LEU:HG    | 2.54                     | 0.48              |
| 1:8C:220:GLU:O     | 2:8D:324:LYS:HE2   | 2.14                     | 0.48              |
| 1:9A:316:CYS:SG    | 1:9A:352:LYS:HB3   | 2.54                     | 0.48              |
| 1:9E:53:PHE:O      | 1:9E:64:ARG:NH1    | 2.45                     | 0.48              |
| 2:10B:147:MET:HE2  | 2:10B:147:MET:HA   | 1.96                     | 0.48              |
| 2:10B:211:CYS:HB2  | 2:10B:217:LEU:HD12 | 1.96                     | 0.48              |
| 1:11E:255:PHE:CZ   | 1:11E:378:LEU:HD22 | 2.49                     | 0.48              |
| 2:12B:33:THR:O     | 2:12B:58:LYS:HE3   | 2.14                     | 0.48              |
| 1:12E:265:ILE:HG23 | 1:12E:432:TYR:CZ   | 2.49                     | 0.48              |
| 1:13A:104:ALA:HB1  | 1:13A:108:TYR:CD2  | 2.47                     | 0.48              |
| 1:13A:391:LEU:HD12 | 1:13A:394:LYS:HD3  | 1.95                     | 0.48              |
| 1:1A:259:LEU:HD13  | 1:1A:316:CYS:SG    | 2.54                     | 0.48              |
| 2:2B:99:ASN:ND2    | 1:2C:254:GLU:OE2   | 2.47                     | 0.48              |
| 1:3E:4:CYS:SG      | 1:3E:133:GLN:HB2   | 2.54                     | 0.48              |
| 1:5A:430:LYS:O     | 1:5A:433:GLU:HG2   | 2.14                     | 0.48              |
| 1:6A:91:GLN:HA     | 1:6A:121:ARG:HH12  | 1.79                     | 0.48              |
| 1:6C:53:PHE:O      | 1:6C:64:ARG:NH2    | 2.46                     | 0.48              |
| 1:8E:3:GLU:HG3     | 1:8E:129:CYS:HB2   | 1.95                     | 0.48              |
| 1:8E:326:LYS:HG3   | 1:8E:327:ASP:N     | 2.29                     | 0.48              |
| 1:9A:31:GLN:CG     | 1:9A:32:PRO:HD2    | 2.43                     | 0.48              |
| 2:9B:178:THR:HG22  | 2:9B:180:VAL:H     | 1.77                     | 0.48              |
| 2:10B:7:ILE:O      | 2:10B:135:LEU:HA   | 2.14                     | 0.48              |
| 1:10C:398:MET:HE1  | 2:10D:345:ILE:HA   | 1.96                     | 0.48              |
| 1:10E:226:ASN:ND2  | 1:10E:367:ASP:OD2  | 2.47                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11C:390:ARG:HG2  | 1:11C:390:ARG:HH11 | 1.79                     | 0.48              |
| 1:12E:135:PHE:CD2  | 1:12E:157:LEU:HD13 | 2.49                     | 0.48              |
| 2:1B:373:ALA:O     | 2:1B:376:GLU:HG2   | 2.13                     | 0.48              |
| 1:2E:188:ILE:HG22  | 1:2E:421:ALA:HB1   | 1.96                     | 0.48              |
| 1:8E:192:HIS:ND1   | 1:8E:424:ASP:OD2   | 2.28                     | 0.48              |
| 1:8E:220:GLU:OE1   | 1:8E:220:GLU:N     | 2.40                     | 0.48              |
| 2:9B:73:MET:HG3    | 2:9B:92:PHE:CD1    | 2.49                     | 0.48              |
| 1:9C:224:TYR:O     | 1:9C:228:ASN:ND2   | 2.46                     | 0.48              |
| 1:11A:129:CYS:SG   | 1:11A:132:LEU:HD12 | 2.54                     | 0.47              |
| 1:11E:172:TYR:CG   | 1:11E:173:PRO:HD2  | 2.49                     | 0.47              |
| 1:11E:344:VAL:HG11 | 1:11E:346:TRP:CE2  | 2.49                     | 0.47              |
| 2:12B:327:ASP:OD1  | 2:12B:328:GLU:N    | 2.47                     | 0.47              |
| 1:13A:307:PRO:HB3  | 1:13A:312:TYR:OH   | 2.14                     | 0.47              |
| 2:13D:397:TRP:HZ3  | 1:13E:257:THR:HA   | 1.79                     | 0.47              |
| 1:1E:356:ASN:OD1   | 1:1E:357:TYR:N     | 2.47                     | 0.47              |
| 2:2D:325:GLU:O     | 2:2D:329:GLN:HG2   | 2.14                     | 0.47              |
| 1:3C:123:ARG:NE    | 1:3C:123:ARG:HA    | 2.29                     | 0.47              |
| 1:5C:20:CYS:HB3    | 1:5C:24:TYR:CE2    | 2.40                     | 0.47              |
| 2:5D:320:ARG:NH1   | 2:5D:355:ASP:OD1   | 2.47                     | 0.47              |
| 2:5D:373:ALA:O     | 2:5D:376:GLU:HG2   | 2.14                     | 0.47              |
| 2:6D:191:GLN:HE21  | 2:6D:195:ASN:ND2   | 2.12                     | 0.47              |
| 1:7E:145:THR:HG1   | 3:7E:500:GTP:PG    | 2.37                     | 0.47              |
| 1:7E:298:PRO:HG3   | 1:7E:308:ARG:NE    | 2.29                     | 0.47              |
| 1:8E:239:THR:OG1   | 1:8E:243:ARG:NH1   | 2.47                     | 0.47              |
| 1:9A:222:PRO:HD2   | 2:9B:324:LYS:HD3   | 1.95                     | 0.47              |
| 1:10E:175:PRO:HB3  | 1:10E:390:ARG:NE   | 2.28                     | 0.47              |
| 1:10E:304:LYS:HE2  | 1:10E:304:LYS:HB2  | 1.68                     | 0.47              |
| 2:11B:285:THR:HG23 | 2:11B:288:GLU:H    | 1.79                     | 0.47              |
| 2:11B:414:ASN:HA   | 2:11B:417:ASP:HB2  | 1.95                     | 0.47              |
| 2:11D:201:CYS:SG   | 2:11D:265:PHE:HD1  | 2.36                     | 0.47              |
| 1:12A:317:MET:HB3  | 1:12A:319:TYR:CE2  | 2.49                     | 0.47              |
| 2:12D:142:GLY:O    | 2:12D:146:GLY:N    | 2.43                     | 0.47              |
| 1:12E:172:TYR:HB2  | 1:12E:203:MET:SD   | 2.54                     | 0.47              |
| 2:13D:215:LEU:HD21 | 2:13D:273:LEU:HD22 | 1.96                     | 0.47              |
| 2:13D:285:THR:O    | 2:13D:288:GLU:HG3  | 2.14                     | 0.47              |
| 1:13E:188:ILE:HG13 | 1:13E:395:PHE:CG   | 2.49                     | 0.47              |
| 1:2A:93:ILE:HG22   | 1:2A:114:ILE:HD11  | 1.96                     | 0.47              |
| 1:2C:103:TYR:CE1   | 1:2C:189:LEU:HB3   | 2.49                     | 0.47              |
| 1:2C:210:TYR:HE1   | 1:2C:227:LEU:HD11  | 1.79                     | 0.47              |
| 1:2C:221:ARG:HA    | 2:2D:324:LYS:HZ2   | 1.78                     | 0.47              |
| 1:4C:271:THR:HG22  | 1:4C:377:MET:HB3   | 1.96                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:5A:91:GLN:HG2    | 1:5A:121:ARG:HH22 | 1.79                     | 0.47              |
| 1:6A:356:ASN:OD1   | 1:6A:357:TYR:N    | 2.47                     | 0.47              |
| 2:6B:257:MET:HE1   | 2:6B:314:ALA:HB2  | 1.96                     | 0.47              |
| 1:6C:168:GLU:OE2   | 1:6C:194:THR:HG23 | 2.13                     | 0.47              |
| 1:6C:398:MET:HE1   | 2:6D:345:ILE:HD13 | 1.95                     | 0.47              |
| 1:7A:319:TYR:HB3   | 1:7A:323:VAL:HG21 | 1.96                     | 0.47              |
| 2:8D:8:GLN:NE2     | 2:8D:65:LEU:HD22  | 2.29                     | 0.47              |
| 1:10A:22:GLU:OE1   | 1:10A:83:TYR:OH   | 2.26                     | 0.47              |
| 2:12D:33:THR:O     | 2:12D:58:LYS:HE3  | 2.14                     | 0.47              |
| 2:12D:330:MET:O    | 2:12D:334:GLN:HG3 | 2.14                     | 0.47              |
| 1:2C:102:ASN:HB2   | 1:2C:105:ARG:HB2  | 1.97                     | 0.47              |
| 1:2E:313:MET:HB3   | 1:2E:380:ASN:O    | 2.14                     | 0.47              |
| 1:3C:4:CYS:SG      | 1:3C:133:GLN:HB2  | 2.54                     | 0.47              |
| 1:3C:56:THR:HG23   | 1:4C:285:GLN:HB2  | 1.96                     | 0.47              |
| 2:3D:320:ARG:NH1   | 2:3D:355:ASP:OD1  | 2.47                     | 0.47              |
| 1:4C:261:PRO:HG3   | 1:4C:313:MET:HE2  | 1.96                     | 0.47              |
| 1:5C:68:VAL:CG1    | 1:5C:149:PHE:HE2  | 2.27                     | 0.47              |
| 1:5E:132:LEU:HD23  | 1:5E:164:LYS:HD3  | 1.96                     | 0.47              |
| 1:6C:103:TYR:CE2   | 1:6C:148:GLY:HA2  | 2.49                     | 0.47              |
| 2:6D:128:ASP:OD1   | 2:6D:129:CYS:N    | 2.43                     | 0.47              |
| 1:7E:88:HIS:ND1    | 1:7E:89:PRO:HD2   | 2.29                     | 0.47              |
| 2:8D:4:ILE:HG12    | 2:8D:131:GLN:HE22 | 1.79                     | 0.47              |
| 1:9E:88:HIS:NE2    | 1:9E:90:GLU:HG2   | 2.30                     | 0.47              |
| 2:10D:8:GLN:HE21   | 2:10D:65:LEU:HD22 | 1.79                     | 0.47              |
| 2:11B:286:VAL:HG22 | 2:11B:321:MET:HE3 | 1.95                     | 0.47              |
| 2:12D:222:TYR:O    | 2:12D:226:ASN:ND2 | 2.47                     | 0.47              |
| 1:12E:286:LEU:HA   | 1:12E:290:GLU:OE1 | 2.14                     | 0.47              |
| 1:13A:306:ASP:OD2  | 1:13A:309:HIS:ND1 | 2.47                     | 0.47              |
| 1:1C:172:TYR:HB3   | 1:1C:205:ASP:OD1  | 2.15                     | 0.47              |
| 1:1C:286:LEU:HA    | 1:1C:290:GLU:OE1  | 2.15                     | 0.47              |
| 2:2B:67:ASP:OD1    | 2:2B:68:LEU:N     | 2.47                     | 0.47              |
| 2:2D:72:THR:OG1    | 2:2D:73:MET:HE2   | 2.14                     | 0.47              |
| 1:3A:178:SER:OG    | 2:3B:347:ASN:OD1  | 2.18                     | 0.47              |
| 2:3D:5:VAL:HG12    | 2:3D:62:ARG:HD2   | 1.95                     | 0.47              |
| 1:4A:122:ILE:HD13  | 1:4A:157:LEU:HD21 | 1.95                     | 0.47              |
| 1:5C:56:THR:HA     | 1:6C:285:GLN:HB2  | 1.97                     | 0.47              |
| 1:5C:68:VAL:HG11   | 1:5C:149:PHE:HE2  | 1.80                     | 0.47              |
| 1:6C:220:GLU:OE1   | 1:6C:220:GLU:N    | 2.40                     | 0.47              |
| 2:6D:421:GLU:O     | 2:6D:424:GLN:HG2  | 2.14                     | 0.47              |
| 1:8E:106:GLY:HA3   | 1:8E:148:GLY:HA3  | 1.94                     | 0.47              |
| 1:9C:31:GLN:HB3    | 1:9C:35:GLN:OE1   | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10B:20:PHE:CD1   | 2:10B:233:MET:HE3  | 2.46                     | 0.47              |
| 2:11B:415:MET:O    | 2:11B:419:VAL:N    | 2.34                     | 0.47              |
| 2:11D:117:LEU:HD23 | 2:11D:117:LEU:HA   | 1.75                     | 0.47              |
| 1:11E:14:VAL:HG22  | 1:11E:67:PHE:HD1   | 1.80                     | 0.47              |
| 1:12A:155:GLU:OE1  | 1:12A:197:HIS:NE2  | 2.48                     | 0.47              |
| 2:12D:128:ASP:OD1  | 2:12D:129:CYS:N    | 2.46                     | 0.47              |
| 2:13B:414:ASN:O    | 2:13B:418:LEU:N    | 2.33                     | 0.47              |
| 1:1A:50:ASN:O      | 1:1A:64:ARG:NH1    | 2.48                     | 0.47              |
| 2:1B:127:CYS:SG    | 2:1B:130:LEU:HB3   | 2.54                     | 0.47              |
| 2:1D:268:PRO:HG2   | 2:1D:300:MET:HE3   | 1.96                     | 0.47              |
| 2:2B:376:GLU:HA    | 2:2B:379:LYS:CE    | 2.43                     | 0.47              |
| 1:2E:102:ASN:HB2   | 1:2E:105:ARG:HB2   | 1.97                     | 0.47              |
| 1:2E:265:ILE:HG23  | 1:2E:432:TYR:CZ    | 2.50                     | 0.47              |
| 2:3D:4:ILE:HG23    | 2:3D:132:GLY:O     | 2.13                     | 0.47              |
| 2:5B:49:VAL:HG11   | 2:5B:241:ARG:HG2   | 1.96                     | 0.47              |
| 1:6C:228:ASN:OD1   | 3:6C:500:GTP:N2    | 2.31                     | 0.47              |
| 1:6C:326:LYS:HG3   | 1:6C:327:ASP:N     | 2.29                     | 0.47              |
| 1:6E:334:THR:O     | 1:6E:337:THR:OG1   | 2.31                     | 0.47              |
| 1:7A:175:PRO:HG3   | 1:7A:390:ARG:NH2   | 2.29                     | 0.47              |
| 1:7A:225:THR:O     | 1:7A:229:ARG:HG3   | 2.14                     | 0.47              |
| 2:7D:99:ASN:ND2    | 1:7E:254:GLU:OE2   | 2.48                     | 0.47              |
| 1:8E:63:PRO:HD3    | 1:8E:86:LEU:HG     | 1.96                     | 0.47              |
| 2:9D:213:ARG:CZ    | 2:9D:297:LYS:HE3   | 2.44                     | 0.47              |
| 1:10A:108:TYR:HD1  | 1:10A:112:LYS:HZ1  | 1.63                     | 0.47              |
| 1:11A:101:ASN:HD21 | 2:11B:252:LYS:NZ   | 2.12                     | 0.47              |
| 2:11B:405:GLU:HA   | 2:11B:408:PHE:HD1  | 1.80                     | 0.47              |
| 2:11B:420:SER:O    | 2:11B:423:GLN:HG3  | 2.15                     | 0.47              |
| 1:11C:79:ARG:HE    | 1:11C:92:LEU:CD2   | 2.28                     | 0.47              |
| 1:11E:227:LEU:H    | 1:11E:227:LEU:HD12 | 1.79                     | 0.47              |
| 1:12A:316:CYS:O    | 1:12A:377:MET:HA   | 2.14                     | 0.47              |
| 2:12D:48:ASN:O     | 2:12D:62:ARG:NH2   | 2.47                     | 0.47              |
| 2:13B:91:VAL:HG21  | 2:13B:116:VAL:HG12 | 1.96                     | 0.47              |
| 1:13C:157:LEU:O    | 1:13C:161:TYR:HD1  | 1.97                     | 0.47              |
| 2:13D:259:PRO:HG2  | 2:13D:263:LEU:HD22 | 1.96                     | 0.47              |
| 2:13D:381:ILE:O    | 2:13D:384:GLN:HB2  | 2.14                     | 0.47              |
| 1:13E:315:CYS:HA   | 1:13E:379:SER:HA   | 1.95                     | 0.47              |
| 1:1A:394:LYS:HG2   | 2:1B:346:PRO:HG3   | 1.95                     | 0.47              |
| 2:1B:285:THR:HG23  | 2:1B:287:PRO:HD2   | 1.96                     | 0.47              |
| 1:1E:377:MET:SD    | 1:1E:379:SER:HB3   | 2.55                     | 0.47              |
| 1:2A:255:PHE:CZ    | 1:2A:378:LEU:HD22  | 2.50                     | 0.47              |
| 1:2A:303:VAL:O     | 1:2A:305:CYS:N     | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3B:373:ALA:O     | 2:3B:376:GLU:HG2   | 2.15                     | 0.47              |
| 1:3E:147:SER:HB2   | 1:3E:190:THR:HG21  | 1.96                     | 0.47              |
| 1:4A:33:ASP:HB2    | 1:4A:35:GLN:OE1    | 2.15                     | 0.47              |
| 1:4A:239:THR:OG1   | 1:4A:243:ARG:NH1   | 2.48                     | 0.47              |
| 2:4B:285:THR:O     | 2:4B:288:GLU:HG2   | 2.14                     | 0.47              |
| 2:5B:73:MET:HA     | 2:5B:76:VAL:HG12   | 1.95                     | 0.47              |
| 1:7A:88:HIS:ND1    | 1:7A:89:PRO:HD2    | 2.29                     | 0.47              |
| 2:7B:109:GLY:HA3   | 2:7B:147:MET:CE    | 2.44                     | 0.47              |
| 2:7D:114:ASP:OD1   | 2:7D:115:SER:N     | 2.47                     | 0.47              |
| 2:8B:396:HIS:NE2   | 1:8C:262:TYR:HA    | 2.29                     | 0.47              |
| 2:8D:390:ARG:O     | 2:8D:392:LYS:NZ    | 2.48                     | 0.47              |
| 1:9A:178:SER:OG    | 2:9B:347:ASN:OD1   | 2.18                     | 0.47              |
| 1:9E:165:SER:HA    | 1:9E:199:ASP:OD2   | 2.15                     | 0.47              |
| 1:10C:30:ILE:HD13  | 1:10C:53:PHE:CE2   | 2.47                     | 0.47              |
| 1:10C:31:GLN:CG    | 1:10C:32:PRO:HD2   | 2.45                     | 0.47              |
| 1:10C:115:VAL:HG22 | 1:10C:119:LEU:HD12 | 1.97                     | 0.47              |
| 1:10C:265:ILE:HG23 | 1:10C:432:TYR:CZ   | 2.50                     | 0.47              |
| 1:10C:332:ILE:O    | 1:10C:336:LYS:HG2  | 2.15                     | 0.47              |
| 1:11A:102:ASN:OD1  | 1:11A:408:TYR:HE1  | 1.98                     | 0.47              |
| 2:11B:190:HIS:ND1  | 2:11B:411:ALA:HA   | 2.29                     | 0.47              |
| 2:11B:384:GLN:OE1  | 1:11C:348:PRO:HB2  | 2.15                     | 0.47              |
| 1:11C:316:CYS:SG   | 1:11C:352:LYS:HB3  | 2.55                     | 0.47              |
| 1:12A:225:THR:O    | 1:12A:229:ARG:HG3  | 2.14                     | 0.47              |
| 2:12B:256:ASN:CB   | 2:12B:350:LYS:HZ1  | 2.27                     | 0.47              |
| 1:12C:156:ARG:N    | 1:12C:156:ARG:HD2  | 2.29                     | 0.47              |
| 2:12D:100:ASN:OD1  | 2:12D:398:TYR:HE1  | 1.98                     | 0.47              |
| 1:13A:169:PHE:HE1  | 1:13A:235:VAL:HG22 | 1.78                     | 0.47              |
| 2:13B:259:PRO:HG2  | 2:13B:263:LEU:HD22 | 1.96                     | 0.47              |
| 1:13E:265:ILE:HG23 | 1:13E:432:TYR:CE1  | 2.50                     | 0.47              |
| 2:1B:287:PRO:HG3   | 2:1B:329:GLN:CD    | 2.40                     | 0.47              |
| 2:1D:131:GLN:O     | 2:1D:163:ILE:HG22  | 2.14                     | 0.47              |
| 1:2A:165:SER:HA    | 1:2A:199:ASP:OD2   | 2.15                     | 0.47              |
| 1:2E:414:GLU:OE1   | 1:2E:416:GLY:N     | 2.42                     | 0.47              |
| 2:3B:147:MET:HE2   | 2:3B:147:MET:HB2   | 1.68                     | 0.47              |
| 1:3C:402:ARG:HH11  | 1:3C:402:ARG:HG3   | 1.79                     | 0.47              |
| 1:3E:193:THR:O     | 1:3E:197:HIS:HB2   | 2.14                     | 0.47              |
| 1:3E:286:LEU:HA    | 1:3E:290:GLU:OE1   | 2.14                     | 0.47              |
| 1:4A:394:LYS:HG2   | 2:4B:346:PRO:HG3   | 1.97                     | 0.47              |
| 2:4B:371:SER:OG    | 2:4B:372:THR:N     | 2.48                     | 0.47              |
| 1:4C:91:GLN:HG2    | 1:4C:121:ARG:HH22  | 1.80                     | 0.47              |
| 1:4C:286:LEU:HA    | 1:4C:290:GLU:OE2   | 2.15                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:4D:178:THR:HG22  | 2:4D:180:VAL:H     | 1.79                     | 0.47              |
| 1:5A:90:GLU:OE1    | 1:6A:280:LYS:HD2   | 2.15                     | 0.47              |
| 2:5D:3:GLU:HB3     | 2:5D:62:ARG:NH1    | 2.21                     | 0.47              |
| 1:5E:184:PRO:O     | 1:5E:188:ILE:HG12  | 2.15                     | 0.47              |
| 1:5E:215:ARG:HH22  | 1:5E:299:ALA:HB1   | 1.79                     | 0.47              |
| 1:5E:217:LEU:HD11  | 1:5E:367:ASP:O     | 2.15                     | 0.47              |
| 1:6A:51:THR:HG21   | 1:6A:243:ARG:HG2   | 1.97                     | 0.47              |
| 1:6A:88:HIS:ND1    | 1:6A:90:GLU:OE1    | 2.48                     | 0.47              |
| 2:6B:48:ASN:O      | 2:6B:62:ARG:NH2    | 2.48                     | 0.47              |
| 1:6C:122:ILE:HD13  | 1:6C:157:LEU:HD21  | 1.97                     | 0.47              |
| 1:6C:317:MET:SD    | 1:6C:377:MET:HG2   | 2.54                     | 0.47              |
| 2:6D:193:VAL:HG13  | 2:6D:194:GLU:HG3   | 1.97                     | 0.47              |
| 2:7B:299:MET:HE3   | 2:7B:305:PRO:HG3   | 1.96                     | 0.47              |
| 2:7B:371:SER:OG    | 2:7B:372:THR:N     | 2.47                     | 0.47              |
| 1:7E:20:CYS:HB3    | 1:7E:24:TYR:CE2    | 2.49                     | 0.47              |
| 1:8A:9:VAL:HG11    | 1:8A:150:THR:OG1   | 2.14                     | 0.47              |
| 1:8A:255:PHE:HZ    | 1:8A:378:LEU:HD22  | 1.78                     | 0.47              |
| 2:8B:127:CYS:SG    | 2:8B:130:LEU:HD22  | 2.54                     | 0.47              |
| 1:8C:68:VAL:HG22   | 1:8C:118:VAL:HG11  | 1.95                     | 0.47              |
| 1:8C:239:THR:OG1   | 1:8C:243:ARG:NH1   | 2.48                     | 0.47              |
| 2:8D:109:GLY:O     | 2:8D:113:VAL:HG13  | 2.14                     | 0.47              |
| 1:8E:11:GLN:O      | 1:8E:15:GLN:HG2    | 2.15                     | 0.47              |
| 1:8E:31:GLN:CG     | 1:8E:32:PRO:HD2    | 2.44                     | 0.47              |
| 2:9B:203:ASP:O     | 2:9B:207:LEU:HD23  | 2.15                     | 0.47              |
| 2:9B:220:PRO:HD2   | 1:9C:326:LYS:HD3   | 1.97                     | 0.47              |
| 1:9C:251:ASP:H     | 1:9C:254:GLU:HB3   | 1.79                     | 0.47              |
| 2:9D:376:GLU:HA    | 2:9D:379:LYS:HG2   | 1.96                     | 0.47              |
| 1:9E:186:ASN:O     | 1:9E:190:THR:HG23  | 2.14                     | 0.47              |
| 1:11A:144:GLY:N    | 3:11A:500:GTP:O3G  | 2.48                     | 0.47              |
| 2:11B:127:CYS:SG   | 2:11B:130:LEU:HB3  | 2.54                     | 0.47              |
| 2:11D:286:VAL:HG22 | 2:11D:321:MET:HE3  | 1.97                     | 0.47              |
| 2:11D:384:GLN:OE1  | 1:11E:348:PRO:HB2  | 2.15                     | 0.47              |
| 2:12D:282:ARG:HH11 | 2:12D:282:ARG:HG3  | 1.79                     | 0.47              |
| 1:13A:102:ASN:HB2  | 1:13A:105:ARG:HG2  | 1.97                     | 0.47              |
| 1:13A:320:ARG:HG3  | 1:13A:360:PRO:HG3  | 1.96                     | 0.47              |
| 1:13C:184:PRO:O    | 1:13C:188:ILE:HG12 | 2.15                     | 0.47              |
| 1:13E:391:LEU:HA   | 1:13E:394:LYS:HB2  | 1.97                     | 0.47              |
| 2:1B:326:VAL:O     | 2:1B:330:MET:HG2   | 2.15                     | 0.47              |
| 2:1D:310:TYR:O     | 2:1D:342:VAL:HG23  | 2.15                     | 0.47              |
| 2:2B:132:GLY:HA2   | 2:2B:163:ILE:O     | 2.15                     | 0.47              |
| 2:2D:13:GLY:O      | 2:2D:17:GLY:N      | 2.40                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2D:73:MET:HA     | 2:2D:76:VAL:HG12   | 1.97                     | 0.47              |
| 1:2E:88:HIS:CE1    | 1:3E:283:HIS:HB3   | 2.49                     | 0.47              |
| 2:3D:2:ARG:HB3     | 2:3D:131:GLN:NE2   | 2.30                     | 0.47              |
| 1:4C:134:GLY:HA3   | 1:4C:165:SER:O     | 2.15                     | 0.47              |
| 1:6A:105:ARG:HA    | 1:6A:109:THR:HG22  | 1.97                     | 0.47              |
| 1:6C:407:TRP:CG    | 2:6D:255:VAL:HG23  | 2.49                     | 0.47              |
| 1:7A:260:VAL:HG13  | 1:7A:265:ILE:O     | 2.15                     | 0.47              |
| 1:7C:189:LEU:HD23  | 1:7C:413:MET:HE1   | 1.97                     | 0.47              |
| 1:7E:228:ASN:OD1   | 3:7E:500:GTP:N2    | 2.39                     | 0.47              |
| 2:8D:219:THR:HA    | 1:8E:326:LYS:HD3   | 1.97                     | 0.47              |
| 2:9D:12:CYS:SG     | 2:9D:138:SER:HB2   | 2.55                     | 0.47              |
| 2:9D:285:THR:HG23  | 2:9D:288:GLU:H     | 1.80                     | 0.47              |
| 2:10D:114:ASP:OD1  | 2:10D:115:SER:N    | 2.48                     | 0.47              |
| 1:10E:298:PRO:HB3  | 1:10E:307:PRO:HD2  | 1.96                     | 0.47              |
| 1:11A:205:ASP:HB2  | 1:11A:303:VAL:HG22 | 1.97                     | 0.47              |
| 2:11B:328:GLU:O    | 2:11B:331:LEU:HG   | 2.15                     | 0.47              |
| 1:12A:265:ILE:HG23 | 1:12A:432:TYR:CZ   | 2.50                     | 0.47              |
| 2:12B:73:MET:HE2   | 2:12B:92:PHE:CD2   | 2.49                     | 0.47              |
| 2:12B:423:GLN:HG3  | 2:12B:424:GLN:OE1  | 2.15                     | 0.47              |
| 1:12C:209:ILE:HG21 | 1:12C:227:LEU:HG   | 1.97                     | 0.47              |
| 2:12D:323:MET:HA   | 2:12D:323:MET:HE3  | 1.97                     | 0.47              |
| 1:13C:21:TRP:CZ2   | 1:13C:65:ALA:HB2   | 2.50                     | 0.47              |
| 2:13D:190:HIS:HB2  | 2:13D:411:ALA:CB   | 2.44                     | 0.47              |
| 1:13E:156:ARG:HD2  | 1:13E:156:ARG:N    | 2.30                     | 0.47              |
| 1:2A:119:LEU:O     | 1:2A:123:ARG:HG2   | 2.15                     | 0.47              |
| 1:2C:108:TYR:HA    | 1:2C:112:LYS:NZ    | 2.29                     | 0.47              |
| 1:2C:271:THR:HG22  | 1:2C:377:MET:HB3   | 1.97                     | 0.47              |
| 2:2D:140:GLY:O     | 2:2D:184:ASN:ND2   | 2.35                     | 0.47              |
| 1:2E:165:SER:HA    | 1:2E:199:ASP:OD2   | 2.15                     | 0.47              |
| 1:3C:56:THR:HA     | 1:4C:285:GLN:HB2   | 1.96                     | 0.47              |
| 1:4A:177:VAL:HG13  | 2:4B:327:ASP:HB2   | 1.97                     | 0.47              |
| 2:4B:4:ILE:HG13    | 2:4B:132:GLY:O     | 2.15                     | 0.47              |
| 2:4B:209:ASP:CG    | 2:4B:213:ARG:HH12  | 2.21                     | 0.47              |
| 2:4D:132:GLY:HA2   | 2:4D:163:ILE:O     | 2.15                     | 0.47              |
| 1:5A:188:ILE:HG22  | 1:5A:421:ALA:HB1   | 1.96                     | 0.47              |
| 1:5A:225:THR:O     | 1:5A:229:ARG:HG3   | 2.14                     | 0.47              |
| 2:5B:5:VAL:HG12    | 2:5B:62:ARG:HD3    | 1.96                     | 0.47              |
| 1:5C:188:ILE:HG22  | 1:5C:421:ALA:HB1   | 1.97                     | 0.47              |
| 1:5E:165:SER:HA    | 1:5E:199:ASP:OD2   | 2.14                     | 0.47              |
| 1:6C:113:GLU:OE1   | 1:6C:113:GLU:N     | 2.48                     | 0.47              |
| 1:6C:200:CYS:HB2   | 1:6C:256:GLN:NE2   | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:8C:5:ILE:O       | 1:8C:135:PHE:HA    | 2.15                     | 0.47              |
| 1:8E:91:GLN:HG2    | 1:8E:121:ARG:NH2   | 2.30                     | 0.47              |
| 1:9E:255:PHE:HE1   | 1:9E:316:CYS:HG    | 1.62                     | 0.47              |
| 1:10E:215:ARG:NH2  | 1:10E:299:ALA:O    | 2.47                     | 0.47              |
| 2:11B:102:ALA:HB2  | 2:11B:403:MET:HE1  | 1.96                     | 0.47              |
| 2:11B:309:ARG:N    | 2:11B:372:THR:OG1  | 2.48                     | 0.47              |
| 2:11D:323:MET:SD   | 2:11D:353:VAL:HG11 | 2.55                     | 0.47              |
| 2:12D:257:MET:O    | 2:12D:312:THR:OG1  | 2.32                     | 0.47              |
| 2:12D:268:PRO:HG2  | 2:12D:300:MET:HG2  | 1.97                     | 0.47              |
| 1:12E:91:GLN:HE22  | 1:12E:125:LEU:HD11 | 1.80                     | 0.47              |
| 1:12E:167:LEU:HD22 | 1:12E:202:PHE:HE2  | 1.80                     | 0.47              |
| 2:13B:156:ARG:NH1  | 2:13B:197:ASP:OD2  | 2.46                     | 0.47              |
| 1:13C:148:GLY:O    | 1:13C:152:LEU:N    | 2.47                     | 0.47              |
| 2:13D:6:HIS:HD1    | 2:13D:21:TRP:NE1   | 2.13                     | 0.47              |
| 1:1A:356:ASN:OD1   | 1:1A:357:TYR:N     | 2.48                     | 0.47              |
| 1:1C:356:ASN:OD1   | 1:1C:357:TYR:N     | 2.47                     | 0.47              |
| 1:2C:165:SER:HA    | 1:2C:199:ASP:OD2   | 2.14                     | 0.47              |
| 1:3A:119:LEU:O     | 1:3A:123:ARG:HG2   | 2.15                     | 0.47              |
| 2:4B:130:LEU:HD23  | 2:4B:130:LEU:H     | 1.80                     | 0.47              |
| 1:5A:205:ASP:O     | 1:5A:209:ILE:HG12  | 2.15                     | 0.47              |
| 1:6C:90:GLU:OE2    | 1:7C:280:LYS:HD2   | 2.14                     | 0.47              |
| 2:7D:52:ASN:HB3    | 2:7D:62:ARG:NH1    | 2.29                     | 0.47              |
| 1:8C:195:LEU:HD21  | 1:8C:264:ARG:HE    | 1.80                     | 0.47              |
| 1:8E:224:TYR:HD1   | 1:8E:227:LEU:HD13  | 1.80                     | 0.47              |
| 1:9A:332:ILE:HD12  | 1:9A:351:PHE:CE2   | 2.50                     | 0.47              |
| 2:9B:330:MET:SD    | 2:9B:349:VAL:HG11  | 2.54                     | 0.47              |
| 2:10B:150:LEU:HD12 | 2:10B:151:LEU:HD12 | 1.97                     | 0.46              |
| 2:10D:5:VAL:HG22   | 2:10D:133:PHE:CD1  | 2.50                     | 0.46              |
| 1:11A:21:TRP:CZ2   | 1:11A:65:ALA:HB2   | 2.49                     | 0.46              |
| 2:11B:257:MET:O    | 2:11B:312:THR:OG1  | 2.26                     | 0.46              |
| 2:11D:127:CYS:SG   | 2:11D:130:LEU:HB3  | 2.55                     | 0.46              |
| 1:12A:317:MET:HE1  | 1:12A:377:MET:HB2  | 1.97                     | 0.46              |
| 2:12B:130:LEU:CD2  | 2:12B:162:ARG:HH12 | 2.28                     | 0.46              |
| 1:12C:88:HIS:CE1   | 1:13C:283:HIS:HB2  | 2.50                     | 0.46              |
| 2:12D:73:MET:O     | 2:12D:76:VAL:HG12  | 2.14                     | 0.46              |
| 1:13A:102:ASN:HB3  | 1:13A:105:ARG:NH1  | 2.30                     | 0.46              |
| 1:13A:394:LYS:O    | 1:13A:398:MET:HG3  | 2.14                     | 0.46              |
| 2:13B:216:LYS:HB2  | 2:13B:275:SER:OG   | 2.15                     | 0.46              |
| 1:1A:255:PHE:CZ    | 1:1A:259:LEU:HD22  | 2.50                     | 0.46              |
| 1:3A:147:SER:HB2   | 1:3A:190:THR:CG2   | 2.44                     | 0.46              |
| 2:3D:36:TYR:CZ     | 2:3D:44:LEU:HD21   | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5C:103:TYR:CE1   | 1:5C:189:LEU:HB3   | 2.50                     | 0.46              |
| 2:5D:61:PRO:HD3    | 2:5D:84:ILE:HG22   | 1.97                     | 0.46              |
| 2:5D:114:ASP:OD1   | 2:5D:115:SER:N     | 2.48                     | 0.46              |
| 1:6A:317:MET:HB3   | 1:6A:319:TYR:HE1   | 1.80                     | 0.46              |
| 2:7D:68:LEU:HD23   | 2:7D:112:LEU:HD13  | 1.96                     | 0.46              |
| 2:8D:3:GLU:HG3     | 2:8D:62:ARG:NH2    | 2.29                     | 0.46              |
| 2:8D:375:GLN:O     | 2:8D:379:LYS:HG2   | 2.15                     | 0.46              |
| 1:9A:222:PRO:HD2   | 2:9B:324:LYS:HE3   | 1.97                     | 0.46              |
| 1:9C:175:PRO:HB3   | 1:9C:390:ARG:NE    | 2.29                     | 0.46              |
| 1:9E:195:LEU:HD21  | 1:9E:264:ARG:HE    | 1.80                     | 0.46              |
| 1:9E:298:PRO:HB3   | 1:9E:307:PRO:HD2   | 1.96                     | 0.46              |
| 1:9E:312:TYR:O     | 1:9E:344:VAL:HG23  | 2.15                     | 0.46              |
| 1:9E:414:GLU:OE1   | 1:9E:416:GLY:N     | 2.42                     | 0.46              |
| 1:10A:321:GLY:HA3  | 1:10A:372:GLN:O    | 2.16                     | 0.46              |
| 2:10D:414:ASN:HA   | 2:10D:417:ASP:HB2  | 1.97                     | 0.46              |
| 1:10E:224:TYR:CD1  | 1:10E:227:LEU:HD12 | 2.50                     | 0.46              |
| 1:11A:102:ASN:HD22 | 1:11A:105:ARG:HD2  | 1.80                     | 0.46              |
| 1:11A:317:MET:HB3  | 1:11A:319:TYR:CE2  | 2.50                     | 0.46              |
| 2:11B:285:THR:OG1  | 2:11B:287:PRO:HD2  | 2.16                     | 0.46              |
| 2:11D:209:ASP:OD2  | 2:11D:213:ARG:NH2  | 2.45                     | 0.46              |
| 1:12E:225:THR:O    | 1:12E:229:ARG:HG3  | 2.15                     | 0.46              |
| 2:13B:4:ILE:HB     | 2:13B:50:TYR:CE1   | 2.42                     | 0.46              |
| 2:13B:70:PRO:HA    | 2:13B:73:MET:HE1   | 1.97                     | 0.46              |
| 2:13B:253:LEU:O    | 2:13B:257:MET:N    | 2.49                     | 0.46              |
| 1:13C:215:ARG:NH2  | 1:13C:299:ALA:O    | 2.37                     | 0.46              |
| 2:1B:131:GLN:O     | 2:1B:163:ILE:HG22  | 2.14                     | 0.46              |
| 1:1C:121:ARG:HH21  | 1:1C:125:LEU:HG    | 1.80                     | 0.46              |
| 1:1C:271:THR:HG22  | 1:1C:377:MET:HB3   | 1.97                     | 0.46              |
| 2:2B:131:GLN:O     | 2:2B:163:ILE:HG22  | 2.15                     | 0.46              |
| 1:2C:108:TYR:O     | 1:2C:112:LYS:NZ    | 2.41                     | 0.46              |
| 2:3B:20:PHE:HD1    | 2:3B:233:MET:HE3   | 1.80                     | 0.46              |
| 2:3B:61:PRO:HD3    | 2:3B:84:ILE:HG22   | 1.97                     | 0.46              |
| 1:3C:303:VAL:O     | 1:3C:305:CYS:N     | 2.48                     | 0.46              |
| 2:3D:390:ARG:O     | 2:3D:392:LYS:NZ    | 2.49                     | 0.46              |
| 1:3E:5:ILE:HB      | 1:3E:135:PHE:CD1   | 2.50                     | 0.46              |
| 1:4A:91:GLN:HG2    | 1:4A:121:ARG:HH22  | 1.81                     | 0.46              |
| 1:6A:177:VAL:HG13  | 2:6B:327:ASP:HB2   | 1.98                     | 0.46              |
| 1:6E:261:PRO:HG3   | 1:6E:313:MET:HE2   | 1.98                     | 0.46              |
| 1:7A:377:MET:SD    | 1:7A:379:SER:HB3   | 2.56                     | 0.46              |
| 1:7C:205:ASP:O     | 1:7C:209:ILE:HG12  | 2.15                     | 0.46              |
| 2:7D:117:LEU:HA    | 2:7D:120:VAL:HG22  | 1.95                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:8C:377:MET:SD   | 1:8C:379:SER:HB3  | 2.55                     | 0.46              |
| 2:8D:376:GLU:HA   | 2:8D:379:LYS:HG2  | 1.98                     | 0.46              |
| 2:9D:31:ASP:CG    | 2:9D:32:ALA:H     | 2.23                     | 0.46              |
| 1:10A:213:CYS:HA  | 1:10A:217:LEU:HB2 | 1.97                     | 0.46              |
| 1:10C:339:ARG:O   | 1:10C:342:GLN:NE2 | 2.48                     | 0.46              |
| 2:10D:67:ASP:OD1  | 2:10D:68:LEU:N    | 2.49                     | 0.46              |
| 1:10E:5:ILE:O     | 1:10E:135:PHE:HA  | 2.15                     | 0.46              |
| 1:10E:224:TYR:O   | 1:10E:228:ASN:ND2 | 2.48                     | 0.46              |
| 1:10E:295:CYS:HB3 | 1:10E:377:MET:HG2 | 1.97                     | 0.46              |
| 1:12E:201:ALA:O   | 1:12E:268:PRO:HD2 | 2.15                     | 0.46              |
| 1:13A:106:GLY:HA3 | 1:13A:149:PHE:N   | 2.30                     | 0.46              |
| 1:13A:184:PRO:HG2 | 1:13A:398:MET:CE  | 2.44                     | 0.46              |
| 1:2A:269:LEU:HD13 | 1:2A:381:THR:HG22 | 1.97                     | 0.46              |
| 2:3B:89:ASN:O     | 2:3B:91:VAL:HG23  | 2.15                     | 0.46              |
| 2:3D:2:ARG:HB3    | 2:3D:131:GLN:HE22 | 1.80                     | 0.46              |
| 2:3D:178:THR:HG22 | 2:3D:180:VAL:H    | 1.80                     | 0.46              |
| 1:4A:102:ASN:HB2  | 1:4A:105:ARG:HB2  | 1.98                     | 0.46              |
| 1:4A:112:LYS:HA   | 1:4A:115:VAL:HG12 | 1.97                     | 0.46              |
| 2:4D:114:ASP:OD1  | 2:4D:115:SER:N    | 2.49                     | 0.46              |
| 1:4E:298:PRO:HA   | 1:4E:301:GLN:HG2  | 1.98                     | 0.46              |
| 1:5E:220:GLU:OE1  | 1:5E:220:GLU:N    | 2.43                     | 0.46              |
| 1:6A:169:PHE:CE1  | 1:6A:235:VAL:HG22 | 2.51                     | 0.46              |
| 1:6A:184:PRO:O    | 1:6A:188:ILE:HG12 | 2.15                     | 0.46              |
| 2:6B:203:ASP:O    | 2:6B:207:LEU:HD23 | 2.15                     | 0.46              |
| 1:6E:122:ILE:HD13 | 1:6E:157:LEU:HD21 | 1.98                     | 0.46              |
| 1:7A:271:THR:HG22 | 1:7A:377:MET:HB3  | 1.98                     | 0.46              |
| 1:8A:178:SER:OG   | 2:8B:347:ASN:OD1  | 2.18                     | 0.46              |
| 1:8C:323:VAL:HG23 | 1:8C:355:ILE:HG23 | 1.96                     | 0.46              |
| 2:8D:245:GLN:N    | 2:8D:245:GLN:OE1  | 2.47                     | 0.46              |
| 1:8E:271:THR:HG22 | 1:8E:377:MET:HE3  | 1.98                     | 0.46              |
| 2:9D:172:SER:OG   | 2:9D:205:GLU:HB2  | 2.15                     | 0.46              |
| 1:11E:305:CYS:HA  | 1:11E:386:GLU:OE2 | 2.16                     | 0.46              |
| 2:12B:345:ILE:O   | 2:12B:348:ASN:ND2 | 2.49                     | 0.46              |
| 1:12E:251:ASP:O   | 1:12E:255:PHE:N   | 2.49                     | 0.46              |
| 1:3A:123:ARG:NE   | 1:3A:161:TYR:OH   | 2.49                     | 0.46              |
| 2:3B:21:TRP:HZ3   | 2:3B:51:TYR:HE1   | 1.64                     | 0.46              |
| 2:3B:36:TYR:CZ    | 2:3B:44:LEU:HD21  | 2.50                     | 0.46              |
| 2:3D:3:GLU:HG3    | 2:3D:62:ARG:HH12  | 1.79                     | 0.46              |
| 2:4D:131:GLN:O    | 2:4D:163:ILE:HG22 | 2.15                     | 0.46              |
| 1:5E:91:GLN:HG2   | 1:5E:121:ARG:HH22 | 1.80                     | 0.46              |
| 1:5E:329:ASN:OD1  | 1:5E:330:ALA:N    | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:6B:121:ARG:NH1   | 2:6B:158:GLU:OE1   | 2.49                     | 0.46              |
| 1:6E:70:LEU:HD12   | 1:6E:114:ILE:HD12  | 1.97                     | 0.46              |
| 1:6E:264:ARG:HG2   | 1:6E:431:ASP:OD2   | 2.15                     | 0.46              |
| 1:7C:31:GLN:CG     | 1:7C:32:PRO:HD2    | 2.45                     | 0.46              |
| 1:7C:265:ILE:HG23  | 1:7C:432:TYR:CE1   | 2.50                     | 0.46              |
| 2:7D:121:ARG:NH1   | 2:7D:158:GLU:OE1   | 2.48                     | 0.46              |
| 2:7D:153:SER:HA    | 2:7D:195:ASN:HD22  | 1.80                     | 0.46              |
| 1:7E:31:GLN:HG2    | 1:7E:32:PRO:HD2    | 1.97                     | 0.46              |
| 2:9B:7:ILE:O       | 2:9B:135:LEU:HA    | 2.15                     | 0.46              |
| 2:9B:114:ASP:OD1   | 2:9B:115:SER:N     | 2.49                     | 0.46              |
| 2:9D:130:LEU:HD23  | 2:9D:130:LEU:H     | 1.79                     | 0.46              |
| 2:9D:183:TYR:HE2   | 2:9D:388:MET:HG2   | 1.80                     | 0.46              |
| 1:9E:220:GLU:OE1   | 1:9E:220:GLU:N     | 2.48                     | 0.46              |
| 1:9E:313:MET:HG2   | 1:9E:380:ASN:O     | 2.15                     | 0.46              |
| 2:10B:208:TYR:HA   | 2:10B:211:CYS:SG   | 2.55                     | 0.46              |
| 1:10C:398:MET:CE   | 2:10D:346:PRO:HD2  | 2.46                     | 0.46              |
| 2:10D:323:MET:HA   | 2:10D:323:MET:HE3  | 1.98                     | 0.46              |
| 1:10E:213:CYS:HA   | 1:10E:217:LEU:HB2  | 1.97                     | 0.46              |
| 1:11A:220:GLU:OE1  | 1:11A:220:GLU:N    | 2.45                     | 0.46              |
| 1:11A:252:LEU:O    | 1:11A:256:GLN:HG2  | 2.14                     | 0.46              |
| 2:11B:267:MET:HE2  | 2:11B:299:MET:SD   | 2.55                     | 0.46              |
| 2:11B:336:LYS:HD2  | 2:11B:337:ASN:OD1  | 2.16                     | 0.46              |
| 2:11D:285:THR:HG23 | 2:11D:288:GLU:H    | 1.80                     | 0.46              |
| 1:11E:312:TYR:O    | 1:11E:344:VAL:HG23 | 2.15                     | 0.46              |
| 1:12C:115:VAL:HG22 | 1:12C:119:LEU:HD12 | 1.98                     | 0.46              |
| 1:12C:200:CYS:HA   | 1:12C:266:HIS:HB2  | 1.96                     | 0.46              |
| 1:13A:69:ASP:CG    | 1:13A:71:GLU:H     | 2.23                     | 0.46              |
| 2:13B:285:THR:O    | 2:13B:288:GLU:HG2  | 2.16                     | 0.46              |
| 2:13B:286:VAL:HG11 | 2:13B:326:VAL:HG22 | 1.98                     | 0.46              |
| 1:13C:5:ILE:O      | 1:13C:135:PHE:HA   | 2.15                     | 0.46              |
| 2:1B:175:VAL:O     | 2:1B:175:VAL:HG12  | 2.15                     | 0.46              |
| 1:2C:63:PRO:HD3    | 1:2C:86:LEU:CD2    | 2.46                     | 0.46              |
| 1:3A:193:THR:O     | 1:3A:197:HIS:HB2   | 2.16                     | 0.46              |
| 1:3A:407:TRP:O     | 1:3A:411:GLU:HG2   | 2.16                     | 0.46              |
| 1:6A:33:ASP:HB2    | 1:6A:35:GLN:OE1    | 2.16                     | 0.46              |
| 1:6A:188:ILE:HG22  | 1:6A:421:ALA:HB1   | 1.98                     | 0.46              |
| 1:6E:169:PHE:CE1   | 1:6E:235:VAL:HG22  | 2.51                     | 0.46              |
| 1:6E:319:TYR:HB3   | 1:6E:323:VAL:HG21  | 1.98                     | 0.46              |
| 2:8D:178:THR:HG22  | 2:8D:180:VAL:H     | 1.81                     | 0.46              |
| 2:8D:310:TYR:O     | 2:8D:342:VAL:HG23  | 2.16                     | 0.46              |
| 1:8E:5:ILE:O       | 1:8E:135:PHE:HA    | 2.16                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9A:269:LEU:HD11  | 1:9A:384:ILE:HB    | 1.97                     | 0.46              |
| 2:9B:373:ALA:O     | 2:9B:376:GLU:HG2   | 2.16                     | 0.46              |
| 1:9C:407:TRP:CG    | 2:9D:255:VAL:HG23  | 2.51                     | 0.46              |
| 2:10D:285:THR:HG23 | 2:10D:288:GLU:H    | 1.80                     | 0.46              |
| 1:10E:31:GLN:CG    | 1:10E:32:PRO:HD2   | 2.45                     | 0.46              |
| 1:10E:150:THR:HG22 | 1:10E:154:MET:HE1  | 1.98                     | 0.46              |
| 1:11C:122:ILE:HD13 | 1:11C:157:LEU:HD21 | 1.97                     | 0.46              |
| 1:12A:304:LYS:HE2  | 1:12A:304:LYS:HB2  | 1.69                     | 0.46              |
| 1:12A:317:MET:CE   | 1:12A:377:MET:HB2  | 2.46                     | 0.46              |
| 2:12B:420:SER:O    | 2:12B:423:GLN:HG2  | 2.16                     | 0.46              |
| 2:13B:397:TRP:CZ3  | 1:13C:257:THR:HA   | 2.50                     | 0.46              |
| 1:13C:292:THR:HG21 | 1:13C:331:ALA:HB1  | 1.97                     | 0.46              |
| 1:13E:11:GLN:HB3   | 3:13E:500:GTP:O2B  | 2.16                     | 0.46              |
| 1:13E:111:GLY:HA2  | 1:13E:149:PHE:HE1  | 1.74                     | 0.46              |
| 1:1E:54:SER:OG     | 1:1E:64:ARG:NH2    | 2.49                     | 0.46              |
| 1:2A:184:PRO:O     | 1:2A:188:ILE:HG12  | 2.15                     | 0.46              |
| 1:2C:394:LYS:HG2   | 2:2D:346:PRO:HG3   | 1.98                     | 0.46              |
| 1:3A:63:PRO:HD3    | 1:3A:86:LEU:HG     | 1.97                     | 0.46              |
| 2:4B:167:TYR:CE1   | 2:4B:233:MET:HG2   | 2.51                     | 0.46              |
| 1:4C:168:GLU:HG2   | 1:4C:201:ALA:HA    | 1.96                     | 0.46              |
| 1:4C:413:MET:HE3   | 1:4C:417:GLU:HG2   | 1.98                     | 0.46              |
| 1:4E:396:ASP:OD1   | 1:4E:397:LEU:N     | 2.48                     | 0.46              |
| 2:5D:174:LYS:HD3   | 2:5D:174:LYS:HA    | 1.74                     | 0.46              |
| 1:6C:221:ARG:HA    | 2:6D:324:LYS:CD    | 2.45                     | 0.46              |
| 1:7E:53:PHE:O      | 1:7E:64:ARG:NH2    | 2.49                     | 0.46              |
| 1:8A:269:LEU:HD13  | 1:8A:381:THR:HG22  | 1.98                     | 0.46              |
| 1:8A:298:PRO:HA    | 1:8A:301:GLN:HG2   | 1.97                     | 0.46              |
| 1:8E:71:GLU:HG2    | 1:8E:73:THR:H      | 1.80                     | 0.46              |
| 1:8E:210:TYR:CE1   | 1:8E:227:LEU:HD21  | 2.50                     | 0.46              |
| 1:9C:34:GLY:O      | 1:9C:61:HIS:ND1    | 2.44                     | 0.46              |
| 1:9C:265:ILE:HG23  | 1:9C:432:TYR:CZ    | 2.50                     | 0.46              |
| 2:9D:4:ILE:HG23    | 2:9D:50:TYR:HE1    | 1.80                     | 0.46              |
| 1:11E:70:LEU:HD11  | 1:11E:110:ILE:HG21 | 1.98                     | 0.46              |
| 1:12C:209:ILE:HG23 | 1:12C:230:LEU:HD22 | 1.97                     | 0.46              |
| 2:12D:268:PRO:HG2  | 2:12D:300:MET:CG   | 2.46                     | 0.46              |
| 1:12E:54:SER:CB    | 1:12E:64:ARG:HH22  | 2.29                     | 0.46              |
| 1:13C:307:PRO:HB3  | 1:13C:312:TYR:OH   | 2.15                     | 0.46              |
| 1:1A:8:HIS:HD2     | 1:1A:67:PHE:CE1    | 2.34                     | 0.46              |
| 1:1C:22:GLU:O      | 1:1C:26:LEU:HD23   | 2.14                     | 0.46              |
| 1:2A:195:LEU:HD12  | 1:2A:428:LEU:HD22  | 1.97                     | 0.46              |
| 1:2C:140:SER:OG    | 3:2C:500:GTP:O2A   | 2.34                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2E:108:TYR:HA    | 1:2E:112:LYS:NZ    | 2.31                     | 0.46              |
| 2:3B:30:ILE:HD11   | 2:3B:47:ILE:HD11   | 1.97                     | 0.46              |
| 2:4D:117:LEU:HA    | 2:4D:120:VAL:HG22  | 1.96                     | 0.46              |
| 2:5B:61:PRO:HD3    | 2:5B:84:ILE:HG22   | 1.98                     | 0.46              |
| 2:5B:135:LEU:HB3   | 2:5B:166:THR:HG22  | 1.97                     | 0.46              |
| 2:5D:304:ASP:HB2   | 2:5D:307:HIS:CD2   | 2.50                     | 0.46              |
| 1:7C:370:LYS:HB3   | 1:7C:370:LYS:HE3   | 1.76                     | 0.46              |
| 2:8B:219:THR:HA    | 1:8C:326:LYS:HD3   | 1.98                     | 0.46              |
| 2:8B:310:TYR:O     | 2:8B:342:VAL:HG23  | 2.14                     | 0.46              |
| 1:8C:69:ASP:OD2    | 1:8C:74:VAL:HG22   | 2.16                     | 0.46              |
| 1:8C:217:LEU:HD23  | 1:8C:367:ASP:OD2   | 2.16                     | 0.46              |
| 2:9D:324:LYS:HG3   | 2:9D:325:GLU:N     | 2.30                     | 0.46              |
| 2:10B:324:LYS:HG3  | 2:10B:325:GLU:N    | 2.31                     | 0.46              |
| 1:10C:169:PHE:CE2  | 1:10C:235:VAL:HG22 | 2.51                     | 0.46              |
| 2:10D:4:ILE:HG13   | 2:10D:132:GLY:C    | 2.41                     | 0.46              |
| 2:10D:309:ARG:NH1  | 2:10D:426:GLN:OXT  | 2.49                     | 0.46              |
| 1:11A:70:LEU:HD11  | 1:11A:110:ILE:HG21 | 1.98                     | 0.46              |
| 1:11C:104:ALA:HB1  | 1:11C:411:GLU:HB2  | 1.97                     | 0.46              |
| 2:11D:130:LEU:HD23 | 2:11D:130:LEU:H    | 1.80                     | 0.46              |
| 1:11E:31:GLN:CG    | 1:11E:32:PRO:HD2   | 2.45                     | 0.46              |
| 1:12A:214:ARG:NH2  | 2:12B:328:GLU:HG3  | 2.31                     | 0.46              |
| 1:12E:191:THR:OG1  | 1:12E:421:ALA:HB1  | 2.16                     | 0.46              |
| 2:13B:27:GLU:OE1   | 2:13B:241:ARG:NH1  | 2.49                     | 0.46              |
| 2:13D:139:LEU:HD11 | 2:13D:188:SER:OG   | 2.16                     | 0.46              |
| 2:1D:61:PRO:HD3    | 2:1D:84:ILE:HG22   | 1.98                     | 0.46              |
| 1:1E:269:LEU:HD13  | 1:1E:381:THR:HG22  | 1.97                     | 0.46              |
| 2:2B:105:HIS:CD2   | 2:2B:150:LEU:HD13  | 2.51                     | 0.46              |
| 1:3A:184:PRO:O     | 1:3A:188:ILE:HG12  | 2.16                     | 0.46              |
| 1:3E:189:LEU:HD21  | 1:3E:413:MET:HE1   | 1.97                     | 0.46              |
| 2:5D:12:CYS:SG     | 2:5D:13:GLY:N      | 2.89                     | 0.46              |
| 1:7C:171:ILE:HD13  | 1:7C:206:ASN:HD21  | 1.81                     | 0.46              |
| 2:7D:267:MET:HE3   | 2:7D:303:CYS:HB3   | 1.97                     | 0.46              |
| 1:7E:286:LEU:O     | 1:7E:373:ARG:NH1   | 2.49                     | 0.46              |
| 2:8B:3:GLU:HG3     | 2:8B:49:VAL:HA     | 1.98                     | 0.46              |
| 2:8B:211:CYS:HB2   | 2:8B:217:LEU:HD12  | 1.98                     | 0.46              |
| 2:8D:213:ARG:NH1   | 2:8D:297:LYS:HG3   | 2.31                     | 0.46              |
| 1:10A:188:ILE:HG22 | 1:10A:421:ALA:HB1  | 1.97                     | 0.46              |
| 2:10B:67:ASP:OD1   | 2:10B:68:LEU:N     | 2.47                     | 0.46              |
| 2:10B:420:SER:O    | 2:10B:423:GLN:HG3  | 2.16                     | 0.46              |
| 1:11C:31:GLN:CG    | 1:11C:32:PRO:HD2   | 2.45                     | 0.46              |
| 1:11C:313:MET:HB2  | 1:11C:347:CYS:SG   | 2.56                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:12A:115:VAL:HG22 | 1:12A:119:LEU:HD12 | 1.98                     | 0.46              |
| 2:13B:287:PRO:HG3  | 2:13B:329:GLN:HG3  | 1.98                     | 0.46              |
| 2:13D:187:LEU:HD22 | 2:13D:403:MET:HE1  | 1.98                     | 0.46              |
| 1:2A:118:VAL:O     | 1:2A:122:ILE:N     | 2.44                     | 0.46              |
| 1:6A:201:ALA:O     | 1:6A:268:PRO:HD2   | 2.16                     | 0.46              |
| 1:6C:100:ALA:HA    | 2:6D:252:LYS:HG2   | 1.97                     | 0.46              |
| 1:6E:119:LEU:O     | 1:6E:123:ARG:HG2   | 2.16                     | 0.46              |
| 1:7C:271:THR:HG22  | 1:7C:377:MET:HE3   | 1.98                     | 0.46              |
| 2:8B:61:PRO:HD3    | 2:8B:84:ILE:CG2    | 2.44                     | 0.46              |
| 1:8C:31:GLN:HG3    | 1:8C:32:PRO:HD2    | 1.98                     | 0.46              |
| 2:8D:131:GLN:OE1   | 2:8D:131:GLN:N     | 2.49                     | 0.46              |
| 1:9A:184:PRO:O     | 1:9A:188:ILE:HG12  | 2.16                     | 0.46              |
| 1:10C:222:PRO:HD2  | 2:10D:324:LYS:HD3  | 1.97                     | 0.46              |
| 1:10E:20:CYS:HB3   | 1:10E:24:TYR:CE2   | 2.50                     | 0.46              |
| 1:10E:91:GLN:HG2   | 1:10E:121:ARG:NH2  | 2.31                     | 0.46              |
| 1:10E:306:ASP:OD2  | 1:10E:309:HIS:ND1  | 2.39                     | 0.46              |
| 2:11D:117:LEU:HA   | 2:11D:120:VAL:HG22 | 1.98                     | 0.46              |
| 2:11D:203:ASP:OD2  | 2:11D:302:ALA:N    | 2.34                     | 0.46              |
| 2:12D:4:ILE:HB     | 2:12D:50:TYR:HE1   | 1.81                     | 0.46              |
| 1:13A:56:THR:HG23  | 2:1D:283:ALA:HA    | 1.97                     | 0.46              |
| 1:13C:151:SER:OG   | 1:13C:193:THR:HG21 | 2.15                     | 0.46              |
| 1:13C:265:ILE:HG23 | 1:13C:432:TYR:CE1  | 2.50                     | 0.46              |
| 2:1B:391:ARG:NH2   | 1:1C:346:TRP:HB3   | 2.31                     | 0.46              |
| 2:1D:36:TYR:CZ     | 2:1D:44:LEU:HD21   | 2.51                     | 0.46              |
| 1:2A:4:CYS:SG      | 1:2A:133:GLN:HB2   | 2.56                     | 0.46              |
| 1:2A:332:ILE:HD12  | 1:2A:351:PHE:CE2   | 2.51                     | 0.46              |
| 1:3A:11:GLN:HB3    | 3:3A:500:GTP:O2B   | 2.16                     | 0.46              |
| 1:3C:407:TRP:CD1   | 2:3D:255:VAL:HG23  | 2.51                     | 0.46              |
| 1:4A:255:PHE:CE1   | 1:4A:259:LEU:HD22  | 2.51                     | 0.46              |
| 1:4C:121:ARG:HH21  | 1:4C:125:LEU:HG    | 1.81                     | 0.46              |
| 1:5A:20:CYS:O      | 1:5A:24:TYR:HD2    | 1.99                     | 0.46              |
| 1:6C:209:ILE:CG2   | 1:6C:227:LEU:HG    | 2.46                     | 0.46              |
| 1:7A:145:THR:HG1   | 3:7A:500:GTP:PG    | 2.37                     | 0.46              |
| 1:7C:344:VAL:HG11  | 1:7C:346:TRP:CE2   | 2.51                     | 0.46              |
| 2:7D:323:MET:HE1   | 2:7D:353:VAL:HG21  | 1.98                     | 0.46              |
| 1:7E:260:VAL:HG13  | 1:7E:265:ILE:O     | 2.16                     | 0.46              |
| 1:8A:220:GLU:O     | 2:8B:324:LYS:HE2   | 2.16                     | 0.46              |
| 1:8E:269:LEU:HD13  | 1:8E:381:THR:HG22  | 1.97                     | 0.46              |
| 1:9A:265:ILE:HG23  | 1:9A:432:TYR:CZ    | 2.50                     | 0.46              |
| 1:9C:104:ALA:HB1   | 1:9C:411:GLU:HB2   | 1.98                     | 0.46              |
| 2:9D:285:THR:OG1   | 2:9D:287:PRO:HD2   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:10A:31:GLN:CG    | 1:10A:32:PRO:HD2   | 2.46                     | 0.45              |
| 1:10A:205:ASP:HB2  | 1:10A:303:VAL:HG22 | 1.98                     | 0.45              |
| 1:10A:210:TYR:HE1  | 1:10A:227:LEU:HD11 | 1.81                     | 0.45              |
| 2:10B:65:LEU:HD23  | 2:10B:65:LEU:HA    | 1.72                     | 0.45              |
| 2:10B:174:LYS:HB2  | 2:10B:205:GLU:OE1  | 2.15                     | 0.45              |
| 1:11A:119:LEU:HD23 | 1:11A:122:ILE:HD12 | 1.97                     | 0.45              |
| 1:11C:255:PHE:HZ   | 1:11C:378:LEU:HD22 | 1.80                     | 0.45              |
| 1:13C:88:HIS:ND1   | 1:13C:90:GLU:OE2   | 2.49                     | 0.45              |
| 1:13E:175:PRO:HB3  | 1:13E:390:ARG:HD3  | 1.98                     | 0.45              |
| 1:13E:316:CYS:HB2  | 1:13E:378:LEU:HB2  | 1.96                     | 0.45              |
| 1:2A:102:ASN:OD1   | 1:2A:105:ARG:HD3   | 2.16                     | 0.45              |
| 1:2A:329:ASN:OD1   | 1:2A:330:ALA:N     | 2.50                     | 0.45              |
| 2:2B:373:ALA:O     | 2:2B:376:GLU:HG2   | 2.16                     | 0.45              |
| 2:2D:105:HIS:HD2   | 2:2D:150:LEU:HB2   | 1.81                     | 0.45              |
| 2:2D:114:ASP:OD1   | 2:2D:115:SER:N     | 2.49                     | 0.45              |
| 2:3D:209:ASP:CG    | 2:3D:213:ARG:HH12  | 2.25                     | 0.45              |
| 1:5C:56:THR:HG23   | 1:6C:285:GLN:HB2   | 1.98                     | 0.45              |
| 1:6C:195:LEU:HD12  | 1:6C:428:LEU:HD22  | 1.98                     | 0.45              |
| 2:6D:36:TYR:CZ     | 2:6D:44:LEU:HD21   | 2.51                     | 0.45              |
| 2:7B:114:ASP:OD1   | 2:7B:115:SER:N     | 2.49                     | 0.45              |
| 1:7E:328:VAL:O     | 1:7E:332:ILE:HG12  | 2.16                     | 0.45              |
| 1:10A:115:VAL:HG22 | 1:10A:119:LEU:HD12 | 1.97                     | 0.45              |
| 2:10B:286:VAL:HG22 | 2:10B:321:MET:HE3  | 1.96                     | 0.45              |
| 2:10D:293:MET:HG2  | 2:10D:367:PHE:HB2  | 1.99                     | 0.45              |
| 2:11B:99:ASN:ND2   | 1:11C:254:GLU:OE2  | 2.49                     | 0.45              |
| 2:11D:5:VAL:HG22   | 2:11D:133:PHE:CD1  | 2.51                     | 0.45              |
| 2:11D:311:LEU:HD23 | 2:11D:342:VAL:HG21 | 1.98                     | 0.45              |
| 1:11E:5:ILE:HG12   | 1:11E:64:ARG:HG2   | 1.97                     | 0.45              |
| 1:11E:21:TRP:CZ2   | 1:11E:65:ALA:HB2   | 2.51                     | 0.45              |
| 1:12A:101:ASN:HD21 | 2:12B:252:LYS:HE3  | 1.82                     | 0.45              |
| 1:13A:182:VAL:HG12 | 1:13A:182:VAL:O    | 2.15                     | 0.45              |
| 1:13A:287:SER:HB3  | 1:13A:290:GLU:HB2  | 1.98                     | 0.45              |
| 1:13A:313:MET:N    | 1:13A:313:MET:SD   | 2.89                     | 0.45              |
| 2:13B:149:THR:OG1  | 2:13B:191:GLN:HG3  | 2.16                     | 0.45              |
| 2:13B:285:THR:HG23 | 2:13B:288:GLU:H    | 1.81                     | 0.45              |
| 1:13C:201:ALA:O    | 1:13C:268:PRO:HD2  | 2.15                     | 0.45              |
| 2:13D:375:GLN:OE1  | 2:13D:426:GLN:NE2  | 2.43                     | 0.45              |
| 1:2C:20:CYS:O      | 1:2C:23:LEU:N      | 2.49                     | 0.45              |
| 2:3B:390:ARG:O     | 2:3B:392:LYS:NZ    | 2.50                     | 0.45              |
| 1:4C:56:THR:OG1    | 1:4C:60:LYS:HB3    | 2.16                     | 0.45              |
| 2:5B:309:ARG:NH1   | 2:5B:426:GLN:OXT   | 2.49                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:5B:324:LYS:HD2   | 2:5B:325:GLU:N     | 2.31                     | 0.45              |
| 2:5B:377:LEU:HD23  | 2:5B:377:LEU:HA    | 1.76                     | 0.45              |
| 2:6D:130:LEU:HG    | 2:6D:162:ARG:HD3   | 1.97                     | 0.45              |
| 1:6E:63:PRO:HD3    | 1:6E:86:LEU:HG     | 1.98                     | 0.45              |
| 1:7A:220:GLU:OE1   | 1:7A:220:GLU:N     | 2.46                     | 0.45              |
| 1:7C:91:GLN:HA     | 1:7C:121:ARG:NH1   | 2.30                     | 0.45              |
| 2:8D:167:TYR:CD2   | 2:8D:233:MET:HE1   | 2.51                     | 0.45              |
| 1:8E:32:PRO:HB3    | 1:8E:83:TYR:CD2    | 2.51                     | 0.45              |
| 1:9C:144:GLY:N     | 3:9C:500:GTP:O3G   | 2.49                     | 0.45              |
| 1:10C:332:ILE:HD12 | 1:10C:351:PHE:CE2  | 2.52                     | 0.45              |
| 1:10E:106:GLY:HA3  | 1:10E:148:GLY:HA3  | 1.98                     | 0.45              |
| 2:11B:405:GLU:HA   | 2:11B:408:PHE:CD1  | 2.52                     | 0.45              |
| 1:12E:50:ASN:HA    | 1:12E:53:PHE:O     | 2.15                     | 0.45              |
| 1:12E:108:TYR:HE2  | 1:12E:413:MET:HB3  | 1.81                     | 0.45              |
| 1:13A:427:ALA:O    | 1:13A:431:ASP:N    | 2.45                     | 0.45              |
| 1:13C:231:ILE:O    | 1:13C:235:VAL:HG23 | 2.17                     | 0.45              |
| 2:13D:311:LEU:H    | 2:13D:371:SER:HA   | 1.81                     | 0.45              |
| 1:13E:31:GLN:HB3   | 1:13E:32:PRO:HD2   | 1.97                     | 0.45              |
| 2:1B:164:MET:O     | 2:1B:197:ASP:HB2   | 2.15                     | 0.45              |
| 1:1E:211:ASP:OD2   | 1:1E:304:LYS:NZ    | 2.49                     | 0.45              |
| 1:2E:71:GLU:HB2    | 1:2E:98:ASP:HB3    | 1.98                     | 0.45              |
| 1:3C:33:ASP:HA     | 1:3C:85:GLN:HB2    | 1.97                     | 0.45              |
| 2:4B:319:GLY:HA2   | 2:4B:357:PRO:HB3   | 1.99                     | 0.45              |
| 1:4C:53:PHE:O      | 1:4C:64:ARG:NH1    | 2.50                     | 0.45              |
| 2:4D:373:ALA:O     | 2:4D:376:GLU:HG2   | 2.16                     | 0.45              |
| 2:5B:228:LEU:HD23  | 2:5B:300:MET:HE2   | 1.98                     | 0.45              |
| 1:6E:188:ILE:HG22  | 1:6E:421:ALA:HB1   | 1.98                     | 0.45              |
| 2:7B:219:THR:HG22  | 1:7C:326:LYS:HE2   | 1.98                     | 0.45              |
| 1:7C:215:ARG:NH2   | 1:7C:299:ALA:HB1   | 2.31                     | 0.45              |
| 1:8E:414:GLU:OE1   | 1:8E:416:GLY:N     | 2.40                     | 0.45              |
| 1:9A:88:HIS:CD2    | 1:9A:89:PRO:HD2    | 2.49                     | 0.45              |
| 1:10E:188:ILE:HG22 | 1:10E:421:ALA:HB1  | 1.98                     | 0.45              |
| 1:10E:251:ASP:O    | 1:10E:255:PHE:N    | 2.44                     | 0.45              |
| 2:11B:172:SER:OG   | 2:11B:205:GLU:HB2  | 2.17                     | 0.45              |
| 2:11B:204:ASN:O    | 2:11B:204:ASN:ND2  | 2.49                     | 0.45              |
| 2:11B:382:SER:O    | 2:11B:386:THR:N    | 2.49                     | 0.45              |
| 2:11B:387:ALA:HA   | 2:11B:390:ARG:HD3  | 1.97                     | 0.45              |
| 1:11C:3:GLU:OE1    | 1:11C:3:GLU:N      | 2.49                     | 0.45              |
| 2:11D:102:ALA:HB2  | 2:11D:403:MET:HE1  | 1.97                     | 0.45              |
| 2:11D:327:ASP:OD2  | 2:11D:327:ASP:N    | 2.48                     | 0.45              |
| 2:12B:164:MET:HE2  | 2:12B:164:MET:HB2  | 1.85                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:12C:319:TYR:CD2  | 1:12C:375:VAL:HG22 | 2.52                     | 0.45              |
| 1:13C:169:PHE:HE1  | 1:13C:235:VAL:HG22 | 1.80                     | 0.45              |
| 2:13D:253:LEU:O    | 2:13D:257:MET:N    | 2.49                     | 0.45              |
| 1:1C:326:LYS:HG3   | 1:1C:327:ASP:N     | 2.31                     | 0.45              |
| 2:2D:127:CYS:SG    | 2:2D:130:LEU:HD23  | 2.56                     | 0.45              |
| 2:2D:263:LEU:HG    | 2:2D:422:TYR:CE1   | 2.51                     | 0.45              |
| 1:2E:398:MET:HE3   | 1:2E:398:MET:HB2   | 1.87                     | 0.45              |
| 1:3C:108:TYR:HA    | 1:3C:112:LYS:NZ    | 2.31                     | 0.45              |
| 2:3D:167:TYR:HD2   | 2:3D:233:MET:HE2   | 1.80                     | 0.45              |
| 2:4B:321:MET:HE2   | 2:4B:321:MET:HB3   | 1.85                     | 0.45              |
| 2:4B:376:GLU:HA    | 2:4B:379:LYS:HG2   | 1.98                     | 0.45              |
| 2:4D:36:TYR:CZ     | 2:4D:44:LEU:HD21   | 2.51                     | 0.45              |
| 2:4D:194:GLU:C     | 2:4D:195:ASN:HD22  | 2.25                     | 0.45              |
| 2:5B:114:ASP:OD1   | 2:5B:115:SER:N     | 2.49                     | 0.45              |
| 2:5B:285:THR:O     | 2:5B:288:GLU:HG2   | 2.16                     | 0.45              |
| 2:5B:391:ARG:HD3   | 2:5B:391:ARG:HA    | 1.82                     | 0.45              |
| 1:5C:20:CYS:O      | 1:5C:23:LEU:N      | 2.49                     | 0.45              |
| 1:6A:108:TYR:HA    | 1:6A:112:LYS:HZ3   | 1.81                     | 0.45              |
| 1:6C:51:THR:HG21   | 1:6C:243:ARG:HG2   | 1.99                     | 0.45              |
| 1:6C:70:LEU:HD12   | 1:6C:114:ILE:HD12  | 1.98                     | 0.45              |
| 1:7A:3:GLU:CD      | 1:7A:64:ARG:HH21   | 2.23                     | 0.45              |
| 2:7D:310:TYR:O     | 2:7D:342:VAL:HG23  | 2.16                     | 0.45              |
| 2:8B:67:ASP:O      | 2:8B:92:PHE:HA     | 2.15                     | 0.45              |
| 2:8D:3:GLU:HG3     | 2:8D:62:ARG:HH21   | 1.81                     | 0.45              |
| 2:10B:175:VAL:HG13 | 1:10C:329:ASN:ND2  | 2.31                     | 0.45              |
| 2:10D:4:ILE:CG2    | 2:10D:50:TYR:HE1   | 2.29                     | 0.45              |
| 1:11A:73:THR:HG23  | 2:11B:2:ARG:HH22   | 1.82                     | 0.45              |
| 2:11B:109:GLY:O    | 2:11B:113:VAL:HB   | 2.16                     | 0.45              |
| 1:11E:102:ASN:HB2  | 1:11E:105:ARG:HB3  | 1.99                     | 0.45              |
| 1:11E:169:PHE:HE2  | 1:11E:235:VAL:HG13 | 1.81                     | 0.45              |
| 1:11E:307:PRO:HB3  | 1:11E:312:TYR:HE1  | 1.82                     | 0.45              |
| 1:11E:399:TYR:OH   | 1:11E:415:GLU:HG2  | 2.17                     | 0.45              |
| 1:12A:209:ILE:HD13 | 1:12A:302:MET:SD   | 2.57                     | 0.45              |
| 1:12C:195:LEU:HD21 | 1:12C:264:ARG:HG2  | 1.98                     | 0.45              |
| 2:12D:49:VAL:HG11  | 2:12D:241:ARG:HG2  | 1.99                     | 0.45              |
| 1:12E:313:MET:N    | 1:12E:313:MET:SD   | 2.90                     | 0.45              |
| 1:12E:332:ILE:O    | 1:12E:336:LYS:HG2  | 2.16                     | 0.45              |
| 1:1C:108:TYR:HA    | 1:1C:112:LYS:HZ1   | 1.82                     | 0.45              |
| 1:1E:395:PHE:HZ    | 1:1E:418:PHE:HB3   | 1.82                     | 0.45              |
| 1:2C:103:TYR:CE2   | 1:2C:148:GLY:HA2   | 2.52                     | 0.45              |
| 1:3C:287:SER:N     | 1:3C:290:GLU:OE2   | 2.31                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:3E:165:SER:HA    | 1:3E:199:ASP:OD2  | 2.17                     | 0.45              |
| 1:4A:165:SER:HA    | 1:4A:199:ASP:OD2  | 2.15                     | 0.45              |
| 2:5B:390:ARG:O     | 2:5B:392:LYS:NZ   | 2.49                     | 0.45              |
| 1:7C:122:ILE:HD13  | 1:7C:157:LEU:HD21 | 1.99                     | 0.45              |
| 1:7C:195:LEU:HD12  | 1:7C:428:LEU:HD22 | 1.98                     | 0.45              |
| 1:7E:56:THR:HG23   | 1:8E:285:GLN:HB2  | 1.99                     | 0.45              |
| 1:7E:75:VAL:O      | 1:7E:78:VAL:HG22  | 2.16                     | 0.45              |
| 1:7E:370:LYS:HB3   | 1:7E:370:LYS:HE3  | 1.77                     | 0.45              |
| 1:8A:51:THR:HG21   | 1:8A:243:ARG:HG2  | 1.98                     | 0.45              |
| 1:8A:265:ILE:HG23  | 1:8A:432:TYR:CZ   | 2.51                     | 0.45              |
| 1:8A:332:ILE:HD12  | 1:8A:351:PHE:CD2  | 2.52                     | 0.45              |
| 1:8A:396:ASP:OD1   | 1:8A:422:ARG:NH1  | 2.50                     | 0.45              |
| 2:8D:132:GLY:HA2   | 2:8D:163:ILE:O    | 2.16                     | 0.45              |
| 1:8E:12:ALA:O      | 1:8E:15:GLN:HB2   | 2.16                     | 0.45              |
| 1:9C:251:ASP:O     | 1:9C:255:PHE:N    | 2.48                     | 0.45              |
| 2:10B:190:HIS:CD2  | 2:10B:414:ASN:HB2 | 2.51                     | 0.45              |
| 2:10B:412:GLU:OE2  | 2:10B:416:ASN:ND2 | 2.49                     | 0.45              |
| 2:10D:175:VAL:HG23 | 2:10D:205:GLU:OE1 | 2.17                     | 0.45              |
| 1:13C:62:VAL:HG21  | 1:13C:88:HIS:NE2  | 2.32                     | 0.45              |
| 1:1A:269:LEU:HD13  | 1:1A:381:THR:HG22 | 1.98                     | 0.45              |
| 2:1D:287:PRO:HG3   | 2:1D:329:GLN:CD   | 2.42                     | 0.45              |
| 1:2C:88:HIS:ND1    | 1:3C:283:HIS:HB3  | 2.31                     | 0.45              |
| 2:2D:232:THR:HG21  | 2:2D:268:PRO:HB3  | 1.97                     | 0.45              |
| 1:3A:329:ASN:OD1   | 1:3A:330:ALA:N    | 2.50                     | 0.45              |
| 1:3C:255:PHE:CZ    | 1:3C:378:LEU:HD22 | 2.52                     | 0.45              |
| 1:4A:102:ASN:ND2   | 1:4A:105:ARG:HD3  | 2.24                     | 0.45              |
| 2:4B:14:ASN:HD21   | 2:4B:73:MET:HE1   | 1.81                     | 0.45              |
| 2:4D:164:MET:HE3   | 2:4D:164:MET:HB3  | 1.73                     | 0.45              |
| 2:5B:12:CYS:SG     | 2:5B:13:GLY:N     | 2.89                     | 0.45              |
| 1:5C:169:PHE:CE2   | 1:5C:235:VAL:HG22 | 2.52                     | 0.45              |
| 1:5C:265:ILE:HG23  | 1:5C:432:TYR:CZ   | 2.52                     | 0.45              |
| 1:6A:55:GLU:OE1    | 1:6A:61:HIS:NE2   | 2.50                     | 0.45              |
| 1:6C:139:HIS:ND1   | 1:6C:150:THR:HG21 | 2.31                     | 0.45              |
| 2:6D:121:ARG:NH1   | 2:6D:158:GLU:OE1  | 2.50                     | 0.45              |
| 2:7D:390:ARG:O     | 2:7D:392:LYS:NZ   | 2.50                     | 0.45              |
| 1:7E:215:ARG:NH2   | 1:7E:299:ALA:HB1  | 2.32                     | 0.45              |
| 1:8A:102:ASN:HB3   | 1:8A:105:ARG:H    | 1.81                     | 0.45              |
| 2:8B:49:VAL:HG11   | 2:8B:241:ARG:HG2  | 1.99                     | 0.45              |
| 1:8C:154:MET:HE1   | 1:8C:168:GLU:HB3  | 1.98                     | 0.45              |
| 1:8E:228:ASN:OD1   | 3:8E:500:GTP:N2   | 2.43                     | 0.45              |
| 1:9E:286:LEU:HB3   | 1:9E:291:ILE:HD11 | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:10A:210:TYR:CE1  | 1:10A:227:LEU:HD21 | 2.52                     | 0.45              |
| 2:10B:117:LEU:HA   | 2:10B:120:VAL:HG22 | 1.99                     | 0.45              |
| 1:10C:21:TRP:HZ3   | 1:10C:53:PHE:HE1   | 1.65                     | 0.45              |
| 1:10E:169:PHE:CE2  | 1:10E:235:VAL:HG22 | 2.52                     | 0.45              |
| 2:11B:140:GLY:O    | 2:11B:184:ASN:ND2  | 2.49                     | 0.45              |
| 2:11D:209:ASP:CG   | 2:11D:213:ARG:HH12 | 2.23                     | 0.45              |
| 2:11D:387:ALA:HA   | 2:11D:390:ARG:HD2  | 1.97                     | 0.45              |
| 1:11E:180:ALA:HB3  | 1:11E:183:GLU:HG3  | 1.99                     | 0.45              |
| 1:12E:157:LEU:O    | 1:12E:161:TYR:HD2  | 2.00                     | 0.45              |
| 1:13A:320:ARG:O    | 1:13A:373:ARG:HA   | 2.16                     | 0.45              |
| 2:13B:22:GLU:OE2   | 2:13B:80:PRO:HG2   | 2.17                     | 0.45              |
| 1:13C:291:ILE:HD12 | 1:13C:375:VAL:HG23 | 1.97                     | 0.45              |
| 1:1A:54:SER:OG     | 1:1A:64:ARG:NH2    | 2.50                     | 0.45              |
| 1:1A:145:THR:OG1   | 3:1A:500:GTP:O3B   | 2.34                     | 0.45              |
| 2:1B:128:ASP:OD2   | 2:1B:129:CYS:N     | 2.49                     | 0.45              |
| 2:1B:324:LYS:HA    | 2:1B:327:ASP:OD2   | 2.15                     | 0.45              |
| 1:4A:9:VAL:HG12    | 1:4A:146:GLY:HA2   | 1.99                     | 0.45              |
| 1:4C:91:GLN:HA     | 1:4C:121:ARG:NH1   | 2.32                     | 0.45              |
| 1:5C:220:GLU:OE1   | 1:5C:220:GLU:N     | 2.43                     | 0.45              |
| 2:5D:191:GLN:HE21  | 2:5D:195:ASN:ND2   | 2.12                     | 0.45              |
| 2:5D:325:GLU:O     | 2:5D:329:GLN:HG2   | 2.17                     | 0.45              |
| 1:7C:407:TRP:CG    | 2:7D:255:VAL:HG23  | 2.52                     | 0.45              |
| 1:8A:64:ARG:NH1    | 1:8A:64:ARG:HB2    | 2.32                     | 0.45              |
| 1:8C:2:ARG:HG3     | 1:8C:133:GLN:HE22  | 1.81                     | 0.45              |
| 1:8C:252:LEU:HD23  | 1:8C:252:LEU:HA    | 1.79                     | 0.45              |
| 1:10E:213:CYS:HA   | 1:10E:217:LEU:HD13 | 1.98                     | 0.45              |
| 1:11C:53:PHE:HD2   | 1:11C:61:HIS:HB3   | 1.81                     | 0.45              |
| 1:11C:398:MET:HE1  | 2:11D:345:ILE:HA   | 1.99                     | 0.45              |
| 1:11E:175:PRO:HB3  | 1:11E:390:ARG:CZ   | 2.46                     | 0.45              |
| 1:12A:214:ARG:HH21 | 2:12B:328:GLU:HG3  | 1.82                     | 0.45              |
| 2:12B:45:GLU:C     | 2:12B:46:ARG:HD2   | 2.42                     | 0.45              |
| 2:12B:159:TYR:HB3  | 2:12B:162:ARG:CD   | 2.47                     | 0.45              |
| 1:12C:312:TYR:O    | 1:12C:344:VAL:HG23 | 2.15                     | 0.45              |
| 1:12E:20:CYS:HB3   | 1:12E:24:TYR:CE2   | 2.52                     | 0.45              |
| 1:12E:358:GLN:NE2  | 1:12E:359:PRO:O    | 2.50                     | 0.45              |
| 2:13D:314:ALA:N    | 2:13D:368:ILE:O    | 2.41                     | 0.45              |
| 1:1A:186:ASN:O     | 1:1A:190:THR:HG23  | 2.17                     | 0.45              |
| 1:1A:303:VAL:O     | 1:1A:305:CYS:N     | 2.49                     | 0.45              |
| 2:1B:208:TYR:HA    | 2:1B:211:CYS:SG    | 2.56                     | 0.45              |
| 1:1C:174:ALA:HB1   | 1:1C:207:GLU:OE2   | 2.17                     | 0.45              |
| 1:3A:205:ASP:OD1   | 1:3A:206:ASN:N     | 2.50                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3D:72:THR:OG1    | 2:3D:73:MET:HE2    | 2.17                     | 0.45              |
| 1:4A:147:SER:HB2   | 1:4A:190:THR:HG21  | 1.99                     | 0.45              |
| 1:5E:103:TYR:CE2   | 1:5E:189:LEU:HB3   | 2.52                     | 0.45              |
| 1:6C:338:LYS:HD3   | 1:6C:338:LYS:HA    | 1.74                     | 0.45              |
| 2:6D:248:ALA:HA    | 2:6D:252:LYS:HD3   | 1.99                     | 0.45              |
| 1:6E:387:ALA:O     | 1:6E:391:LEU:HD23  | 2.17                     | 0.45              |
| 1:7A:332:ILE:HD12  | 1:7A:351:PHE:CE2   | 2.51                     | 0.45              |
| 2:7D:309:ARG:NH1   | 2:7D:426:GLN:OXT   | 2.50                     | 0.45              |
| 2:8B:390:ARG:O     | 2:8B:392:LYS:NZ    | 2.46                     | 0.45              |
| 2:8D:19:LYS:HD3    | 2:8D:19:LYS:HA     | 1.80                     | 0.45              |
| 2:8D:309:ARG:NH1   | 2:8D:426:GLN:OXT   | 2.49                     | 0.45              |
| 1:9A:34:GLY:O      | 1:9A:61:HIS:N      | 2.49                     | 0.45              |
| 1:9A:73:THR:HG23   | 2:9B:2:ARG:HH22    | 1.82                     | 0.45              |
| 1:9A:269:LEU:HD13  | 1:9A:381:THR:HG22  | 1.98                     | 0.45              |
| 1:9A:305:CYS:HA    | 1:9A:386:GLU:OE2   | 2.17                     | 0.45              |
| 2:9D:175:VAL:HG13  | 1:9E:329:ASN:ND2   | 2.32                     | 0.45              |
| 1:10A:303:VAL:O    | 1:10A:305:CYS:N    | 2.50                     | 0.45              |
| 1:10C:394:LYS:HG2  | 2:10D:346:PRO:HG3  | 1.99                     | 0.45              |
| 1:10C:394:LYS:NZ   | 2:10D:346:PRO:HB2  | 2.32                     | 0.45              |
| 2:10D:174:LYS:HB2  | 2:10D:205:GLU:OE2  | 2.17                     | 0.45              |
| 1:10E:11:GLN:HB3   | 3:10E:500:GTP:O2B  | 2.17                     | 0.45              |
| 2:11B:105:HIS:HD2  | 2:11B:150:LEU:HD12 | 1.82                     | 0.45              |
| 1:12C:344:VAL:HG11 | 1:12C:346:TRP:CE2  | 2.52                     | 0.45              |
| 1:13A:331:ALA:O    | 1:13A:334:THR:HB   | 2.17                     | 0.45              |
| 1:13C:391:LEU:HA   | 1:13C:394:LYS:HD3  | 1.98                     | 0.45              |
| 1:13E:321:GLY:HA3  | 1:13E:372:GLN:O    | 2.17                     | 0.45              |
| 1:2E:47:ASP:HB3    | 1:2E:48:SER:H      | 1.58                     | 0.45              |
| 1:3C:175:PRO:HB3   | 1:3C:390:ARG:NH1   | 2.31                     | 0.45              |
| 2:3D:304:ASP:HB2   | 2:3D:307:HIS:CE1   | 2.51                     | 0.45              |
| 2:4D:287:PRO:HG3   | 2:4D:329:GLN:NE2   | 2.31                     | 0.45              |
| 1:6A:20:CYS:HB3    | 1:6A:24:TYR:CE2    | 2.52                     | 0.45              |
| 1:6A:224:TYR:O     | 1:6A:228:ASN:ND2   | 2.50                     | 0.45              |
| 1:6E:51:THR:HG21   | 1:6E:243:ARG:HG2   | 1.99                     | 0.45              |
| 1:6E:338:LYS:HD3   | 1:6E:338:LYS:HA    | 1.74                     | 0.45              |
| 1:7A:100:ALA:HA    | 2:7B:252:LYS:HG2   | 1.99                     | 0.45              |
| 1:7A:394:LYS:HE2   | 2:7B:346:PRO:HB2   | 1.98                     | 0.45              |
| 2:7D:190:HIS:NE2   | 2:7D:414:ASN:OD1   | 2.50                     | 0.45              |
| 1:8A:239:THR:OG1   | 1:8A:243:ARG:NH1   | 2.47                     | 0.45              |
| 1:8A:315:CYS:HA    | 1:8A:379:SER:HA    | 1.99                     | 0.45              |
| 1:8A:377:MET:HE1   | 1:8A:379:SER:HB3   | 1.99                     | 0.45              |
| 1:8C:326:LYS:HG3   | 1:8C:327:ASP:N     | 2.32                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:8C:395:PHE:HE2   | 1:8C:422:ARG:HG3   | 1.82                     | 0.45              |
| 1:9A:54:SER:OG     | 1:9A:64:ARG:NH2    | 2.50                     | 0.45              |
| 1:9C:395:PHE:HZ    | 1:9C:418:PHE:HB3   | 1.80                     | 0.45              |
| 2:9D:127:CYS:SG    | 2:9D:130:LEU:HB3   | 2.56                     | 0.45              |
| 2:9D:405:GLU:HG2   | 2:9D:406:MET:HE2   | 1.98                     | 0.45              |
| 1:10A:251:ASP:O    | 1:10A:255:PHE:N    | 2.49                     | 0.45              |
| 1:10E:201:ALA:O    | 1:10E:268:PRO:HD2  | 2.17                     | 0.45              |
| 1:10E:292:THR:HG21 | 1:10E:331:ALA:HB1  | 1.99                     | 0.45              |
| 2:11B:131:GLN:O    | 2:11B:163:ILE:HG22 | 2.17                     | 0.45              |
| 2:11B:190:HIS:HE1  | 2:11B:414:ASN:OD1  | 2.00                     | 0.45              |
| 1:11E:313:MET:SD   | 1:11E:380:ASN:O    | 2.75                     | 0.45              |
| 2:12B:22:GLU:OE2   | 2:12B:80:PRO:HG2   | 2.17                     | 0.45              |
| 2:12B:267:MET:O    | 2:12B:368:ILE:HA   | 2.16                     | 0.45              |
| 1:12C:305:CYS:SG   | 1:12C:384:ILE:HA   | 2.57                     | 0.45              |
| 1:12C:420:GLU:O    | 1:12C:424:ASP:N    | 2.35                     | 0.45              |
| 2:13B:113:VAL:HG22 | 2:13B:117:LEU:HG   | 1.99                     | 0.45              |
| 1:13E:144:GLY:O    | 1:13E:148:GLY:N    | 2.45                     | 0.45              |
| 2:1B:220:PRO:HD2   | 1:1C:326:LYS:CD    | 2.43                     | 0.45              |
| 1:1E:202:PHE:HE1   | 1:1E:378:LEU:HD23  | 1.82                     | 0.45              |
| 2:2B:220:PRO:HD2   | 1:2C:326:LYS:HD2   | 1.99                     | 0.45              |
| 1:3A:164:LYS:HB2   | 1:3A:164:LYS:HE2   | 1.76                     | 0.45              |
| 1:3A:165:SER:HA    | 1:3A:199:ASP:OD2   | 2.17                     | 0.45              |
| 1:5A:328:VAL:O     | 1:5A:332:ILE:HG12  | 2.17                     | 0.45              |
| 2:5B:111:GLU:N     | 2:5B:111:GLU:OE1   | 2.50                     | 0.45              |
| 2:6D:215:LEU:O     | 2:6D:215:LEU:HD23  | 2.17                     | 0.45              |
| 1:6E:113:GLU:OE2   | 1:6E:113:GLU:N     | 2.49                     | 0.45              |
| 1:7E:332:ILE:HD12  | 1:7E:351:PHE:CE1   | 2.52                     | 0.45              |
| 1:8C:184:PRO:O     | 1:8C:188:ILE:HG12  | 2.17                     | 0.45              |
| 2:8D:111:GLU:OE1   | 2:8D:111:GLU:N     | 2.50                     | 0.45              |
| 1:8E:255:PHE:CZ    | 1:8E:378:LEU:HD22  | 2.51                     | 0.45              |
| 1:9A:338:LYS:HB2   | 1:9A:338:LYS:HE3   | 1.64                     | 0.45              |
| 2:9D:257:MET:HG2   | 2:9D:312:THR:OG1   | 2.17                     | 0.45              |
| 1:11E:5:ILE:O      | 1:11E:135:PHE:HA   | 2.17                     | 0.44              |
| 1:11E:225:THR:O    | 1:11E:229:ARG:HG3  | 2.16                     | 0.44              |
| 1:11E:271:THR:HG22 | 1:11E:377:MET:SD   | 2.57                     | 0.44              |
| 1:12A:69:ASP:CG    | 1:12A:71:GLU:H     | 2.24                     | 0.44              |
| 2:12D:104:GLY:HA3  | 2:12D:146:GLY:HA3  | 1.98                     | 0.44              |
| 2:13B:374:ILE:O    | 2:13B:377:LEU:HB2  | 2.17                     | 0.44              |
| 1:13C:70:LEU:HD11  | 1:13C:149:PHE:HE2  | 1.82                     | 0.44              |
| 1:13E:388:TRP:O    | 1:13E:392:ASP:N    | 2.28                     | 0.44              |
| 1:1A:255:PHE:CZ    | 1:1A:378:LEU:HD22  | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1E:204:VAL:HG13  | 1:1E:302:MET:HG2   | 1.99                     | 0.44              |
| 1:2A:174:ALA:HB1   | 1:2A:207:GLU:OE2   | 2.17                     | 0.44              |
| 2:2B:130:LEU:HD23  | 2:2B:130:LEU:H     | 1.82                     | 0.44              |
| 2:3B:263:LEU:HG    | 2:3B:422:TYR:CE1   | 2.53                     | 0.44              |
| 1:4C:225:THR:O     | 1:4C:229:ARG:HG3   | 2.17                     | 0.44              |
| 1:4E:91:GLN:HG2    | 1:4E:121:ARG:HH22  | 1.82                     | 0.44              |
| 1:4E:303:VAL:O     | 1:4E:305:CYS:N     | 2.49                     | 0.44              |
| 1:6A:90:GLU:OE2    | 1:7A:280:LYS:HD2   | 2.17                     | 0.44              |
| 1:6A:407:TRP:CG    | 2:6B:255:VAL:HG23  | 2.51                     | 0.44              |
| 1:6C:184:PRO:O     | 1:6C:188:ILE:HG12  | 2.17                     | 0.44              |
| 1:6E:103:TYR:CE1   | 1:6E:148:GLY:HA2   | 2.51                     | 0.44              |
| 2:7B:68:LEU:HD23   | 2:7B:112:LEU:HD13  | 1.99                     | 0.44              |
| 1:7E:391:LEU:O     | 1:7E:394:LYS:HB2   | 2.17                     | 0.44              |
| 1:8C:5:ILE:HG12    | 1:8C:64:ARG:HG2    | 1.98                     | 0.44              |
| 1:8C:224:TYR:O     | 1:8C:228:ASN:ND2   | 2.50                     | 0.44              |
| 1:8E:102:ASN:HD22  | 1:8E:105:ARG:HD2   | 1.81                     | 0.44              |
| 1:9C:35:GLN:OE1    | 1:9C:35:GLN:N      | 2.40                     | 0.44              |
| 2:9D:149:THR:OG1   | 2:9D:191:GLN:HG3   | 2.17                     | 0.44              |
| 2:9D:389:PHE:CE1   | 2:9D:408:PHE:HD2   | 2.34                     | 0.44              |
| 1:9E:305:CYS:HA    | 1:9E:386:GLU:OE2   | 2.18                     | 0.44              |
| 2:10B:114:ASP:OD1  | 2:10B:115:SER:N    | 2.50                     | 0.44              |
| 1:10C:338:LYS:HG2  | 1:10C:340:THR:HG22 | 1.99                     | 0.44              |
| 2:10D:105:HIS:HD2  | 2:10D:150:LEU:HD23 | 1.82                     | 0.44              |
| 1:10E:210:TYR:CE1  | 1:10E:227:LEU:HD21 | 2.52                     | 0.44              |
| 1:10E:269:LEU:HD11 | 1:10E:384:ILE:HB   | 1.98                     | 0.44              |
| 1:11A:298:PRO:HB3  | 1:11A:307:PRO:HD2  | 1.98                     | 0.44              |
| 1:11C:312:TYR:O    | 1:11C:344:VAL:N    | 2.43                     | 0.44              |
| 1:11E:2:ARG:C      | 1:11E:133:GLN:HE22 | 2.25                     | 0.44              |
| 2:12B:68:LEU:HA    | 2:12B:93:GLY:H     | 1.82                     | 0.44              |
| 1:12C:265:ILE:HG23 | 1:12C:432:TYR:OH   | 2.17                     | 0.44              |
| 2:13B:220:PRO:HD2  | 1:13C:326:LYS:CD   | 2.47                     | 0.44              |
| 2:13B:305:PRO:HA   | 2:13B:373:ALA:HB2  | 1.99                     | 0.44              |
| 1:13E:21:TRP:CZ2   | 1:13E:65:ALA:HB2   | 2.52                     | 0.44              |
| 1:3A:5:ILE:HB      | 1:3A:135:PHE:HD1   | 1.81                     | 0.44              |
| 2:4B:287:PRO:HG3   | 2:4B:329:GLN:NE2   | 2.32                     | 0.44              |
| 1:5C:215:ARG:NH2   | 1:5C:299:ALA:HB1   | 2.33                     | 0.44              |
| 1:5C:222:PRO:HD2   | 2:5D:324:LYS:HD3   | 1.99                     | 0.44              |
| 2:6D:48:ASN:O      | 2:6D:62:ARG:NH2    | 2.50                     | 0.44              |
| 1:6E:205:ASP:O     | 1:6E:209:ILE:HG12  | 2.17                     | 0.44              |
| 1:6E:224:TYR:O     | 1:6E:228:ASN:ND2   | 2.50                     | 0.44              |
| 1:8A:145:THR:HG1   | 3:8A:500:GTP:PG    | 2.39                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:203:ASP:OD2   | 2:8B:302:ALA:N     | 2.26                     | 0.44              |
| 2:8B:405:GLU:O     | 2:8B:409:THR:HG23  | 2.18                     | 0.44              |
| 1:8C:228:ASN:OD1   | 3:8C:500:GTP:N2    | 2.35                     | 0.44              |
| 1:8E:315:CYS:HA    | 1:8E:379:SER:HA    | 1.99                     | 0.44              |
| 1:9E:31:GLN:HG3    | 1:9E:32:PRO:CD     | 2.48                     | 0.44              |
| 2:10D:395:LEU:O    | 2:10D:399:THR:OG1  | 2.34                     | 0.44              |
| 1:10E:184:PRO:O    | 1:10E:188:ILE:HG12 | 2.18                     | 0.44              |
| 1:12A:88:HIS:CE1   | 1:13A:283:HIS:HB2  | 2.52                     | 0.44              |
| 2:12B:117:LEU:HD23 | 2:12B:117:LEU:HA   | 1.86                     | 0.44              |
| 2:12B:309:ARG:N    | 2:12B:372:THR:OG1  | 2.49                     | 0.44              |
| 1:13A:161:TYR:HB3  | 1:13A:164:LYS:NZ   | 2.32                     | 0.44              |
| 2:13B:73:MET:N     | 2:13B:73:MET:SD    | 2.91                     | 0.44              |
| 2:13B:117:LEU:HA   | 2:13B:120:VAL:HG22 | 1.98                     | 0.44              |
| 1:13C:8:HIS:CD2    | 1:13C:67:PHE:HE1   | 2.36                     | 0.44              |
| 1:13C:223:THR:O    | 1:13C:226:ASN:N    | 2.49                     | 0.44              |
| 1:1A:193:THR:O     | 1:1A:197:HIS:HB2   | 2.17                     | 0.44              |
| 1:1A:209:ILE:CG2   | 1:1A:227:LEU:HG    | 2.46                     | 0.44              |
| 1:1E:8:HIS:HD2     | 1:1E:67:PHE:CE1    | 2.35                     | 0.44              |
| 2:2B:379:LYS:HB2   | 2:2B:379:LYS:HE3   | 1.74                     | 0.44              |
| 1:2E:119:LEU:O     | 1:2E:123:ARG:HG2   | 2.17                     | 0.44              |
| 1:3C:147:SER:HB2   | 1:3C:190:THR:CG2   | 2.47                     | 0.44              |
| 2:3D:279:GLN:H     | 2:3D:279:GLN:HG3   | 1.66                     | 0.44              |
| 1:3E:217:LEU:HD23  | 1:3E:367:ASP:OD2   | 2.17                     | 0.44              |
| 1:3E:265:ILE:HG23  | 1:3E:432:TYR:CE2   | 2.52                     | 0.44              |
| 1:4A:108:TYR:HA    | 1:4A:112:LYS:NZ    | 2.33                     | 0.44              |
| 2:4B:164:MET:HE3   | 2:4B:164:MET:HB3   | 1.81                     | 0.44              |
| 2:4B:220:PRO:HD2   | 1:4C:326:LYS:CD    | 2.47                     | 0.44              |
| 1:4C:9:VAL:HG12    | 1:4C:146:GLY:HA2   | 2.00                     | 0.44              |
| 1:4C:147:SER:HB2   | 1:4C:190:THR:HG21  | 2.00                     | 0.44              |
| 1:5C:91:GLN:HG2    | 1:5C:121:ARG:HH22  | 1.82                     | 0.44              |
| 2:5D:310:TYR:O     | 2:5D:342:VAL:HG23  | 2.17                     | 0.44              |
| 1:5E:63:PRO:HD3    | 1:5E:86:LEU:HG     | 1.99                     | 0.44              |
| 2:6D:111:GLU:N     | 2:6D:111:GLU:OE1   | 2.49                     | 0.44              |
| 2:6D:114:ASP:OD1   | 2:6D:115:SER:N     | 2.50                     | 0.44              |
| 2:6D:311:LEU:HD23  | 2:6D:342:VAL:HG21  | 1.99                     | 0.44              |
| 1:6E:225:THR:O     | 1:6E:229:ARG:HG3   | 2.17                     | 0.44              |
| 1:7A:215:ARG:NH2   | 1:7A:299:ALA:HB1   | 2.32                     | 0.44              |
| 1:7E:205:ASP:O     | 1:7E:209:ILE:HG12  | 2.16                     | 0.44              |
| 1:8A:56:THR:HA     | 1:9A:285:GLN:HB2   | 2.00                     | 0.44              |
| 2:8B:293:MET:CG    | 2:8B:367:PHE:HB2   | 2.48                     | 0.44              |
| 2:8B:359:ARG:HD3   | 2:8B:359:ARG:N     | 2.32                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10B:130:LEU:HD23 | 2:10B:130:LEU:H    | 1.82                     | 0.44              |
| 1:12A:433:GLU:HA   | 1:12A:433:GLU:OE2  | 2.16                     | 0.44              |
| 1:12C:231:ILE:O    | 1:12C:235:VAL:HG23 | 2.17                     | 0.44              |
| 1:13C:88:HIS:HB3   | 1:13C:90:GLU:CD    | 2.42                     | 0.44              |
| 1:1A:391:LEU:HD23  | 1:1A:394:LYS:HD2   | 1.98                     | 0.44              |
| 1:1C:184:PRO:O     | 1:1C:188:ILE:HG12  | 2.18                     | 0.44              |
| 1:3A:144:GLY:O     | 1:3A:148:GLY:N     | 2.47                     | 0.44              |
| 2:3B:105:HIS:HD2   | 2:3B:150:LEU:HD13  | 1.83                     | 0.44              |
| 2:3B:304:ASP:HB2   | 2:3B:307:HIS:ND1   | 2.32                     | 0.44              |
| 2:3D:31:ASP:CG     | 2:3D:32:ALA:H      | 2.25                     | 0.44              |
| 2:3D:114:ASP:OD2   | 2:3D:115:SER:N     | 2.50                     | 0.44              |
| 2:3D:198:GLU:HG3   | 2:3D:266:PHE:CE2   | 2.53                     | 0.44              |
| 2:3D:323:MET:HE1   | 2:3D:353:VAL:HG21  | 1.98                     | 0.44              |
| 1:5A:216:ASN:HD22  | 1:5A:216:ASN:H     | 1.63                     | 0.44              |
| 1:5C:103:TYR:CE2   | 1:5C:148:GLY:HA2   | 2.52                     | 0.44              |
| 1:5C:184:PRO:O     | 1:5C:188:ILE:HG12  | 2.17                     | 0.44              |
| 2:5D:128:ASP:OD1   | 2:5D:128:ASP:N     | 2.50                     | 0.44              |
| 1:5E:28:HIS:NE2    | 1:5E:243:ARG:HD2   | 2.32                     | 0.44              |
| 1:7A:119:LEU:O     | 1:7A:123:ARG:HG2   | 2.17                     | 0.44              |
| 1:7A:298:PRO:HG3   | 1:7A:308:ARG:NE    | 2.32                     | 0.44              |
| 2:7B:186:THR:HG22  | 2:7B:411:ALA:HB1   | 1.98                     | 0.44              |
| 2:7D:5:VAL:HG22    | 2:7D:133:PHE:CD1   | 2.52                     | 0.44              |
| 1:7E:255:PHE:CZ    | 1:7E:378:LEU:HD11  | 2.53                     | 0.44              |
| 1:9A:68:VAL:HG11   | 1:9A:149:PHE:HE2   | 1.82                     | 0.44              |
| 1:9A:195:LEU:HD21  | 1:9A:264:ARG:HE    | 1.82                     | 0.44              |
| 2:9B:155:ILE:HG22  | 2:9B:164:MET:HE1   | 1.99                     | 0.44              |
| 2:9D:391:ARG:HA    | 2:9D:391:ARG:HD3   | 1.74                     | 0.44              |
| 1:9E:214:ARG:NH2   | 1:9E:220:GLU:O     | 2.40                     | 0.44              |
| 1:10A:71:GLU:HB2   | 1:10A:98:ASP:HB3   | 1.99                     | 0.44              |
| 2:10D:363:MET:HE2  | 2:10D:363:MET:HB3  | 1.95                     | 0.44              |
| 1:10E:35:GLN:NE2   | 1:10E:37:PRO:HG3   | 2.31                     | 0.44              |
| 1:10E:312:TYR:O    | 1:10E:344:VAL:HG23 | 2.18                     | 0.44              |
| 1:11C:225:THR:O    | 1:11C:229:ARG:HG3  | 2.17                     | 0.44              |
| 1:13C:391:LEU:HD12 | 1:13C:394:LYS:HD3  | 1.99                     | 0.44              |
| 1:13E:254:GLU:O    | 1:13E:258:ASN:ND2  | 2.50                     | 0.44              |
| 1:1C:186:ASN:O     | 1:1C:190:THR:HG23  | 2.17                     | 0.44              |
| 1:2A:265:ILE:HG23  | 1:2A:432:TYR:CZ    | 2.53                     | 0.44              |
| 1:2A:414:GLU:OE1   | 1:2A:416:GLY:N     | 2.38                     | 0.44              |
| 2:2D:401:GLU:OE1   | 2:2D:401:GLU:N     | 2.50                     | 0.44              |
| 1:3A:5:ILE:HB      | 1:3A:135:PHE:CD1   | 2.52                     | 0.44              |
| 1:5A:332:ILE:HD12  | 1:5A:351:PHE:CE2   | 2.52                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5C:221:ARG:HA    | 2:5D:324:LYS:HE3   | 2.00                     | 0.44              |
| 1:5C:370:LYS:HE3   | 1:5C:370:LYS:HB3   | 1.75                     | 0.44              |
| 1:5E:430:LYS:O     | 1:5E:433:GLU:HG3   | 2.18                     | 0.44              |
| 1:6E:328:VAL:O     | 1:6E:332:ILE:HG12  | 2.18                     | 0.44              |
| 1:7A:213:CYS:HB3   | 1:7A:219:ILE:HD11  | 1.99                     | 0.44              |
| 1:7C:269:LEU:HD11  | 1:7C:384:ILE:HB    | 2.00                     | 0.44              |
| 1:7E:225:THR:O     | 1:7E:229:ARG:HG3   | 2.18                     | 0.44              |
| 1:8A:398:MET:CE    | 2:8B:346:PRO:HD2   | 2.46                     | 0.44              |
| 1:8E:193:THR:O     | 1:8E:197:HIS:HB2   | 2.17                     | 0.44              |
| 2:9B:310:TYR:O     | 2:9B:342:VAL:HG23  | 2.18                     | 0.44              |
| 2:9D:102:ALA:HB2   | 2:9D:403:MET:HE1   | 2.00                     | 0.44              |
| 1:9E:255:PHE:HE1   | 1:9E:316:CYS:SG    | 2.40                     | 0.44              |
| 2:10B:73:MET:O     | 2:10B:76:VAL:HG12  | 2.18                     | 0.44              |
| 2:10B:209:ASP:OD2  | 2:10B:213:ARG:NH2  | 2.47                     | 0.44              |
| 1:10C:184:PRO:O    | 1:10C:188:ILE:HG12 | 2.17                     | 0.44              |
| 1:12A:129:CYS:SG   | 1:12A:132:LEU:HB2  | 2.57                     | 0.44              |
| 2:12B:263:LEU:HG   | 2:12B:422:TYR:HE1  | 1.82                     | 0.44              |
| 1:12E:259:LEU:HD13 | 1:12E:316:CYS:SG   | 2.57                     | 0.44              |
| 1:12E:330:ALA:O    | 1:12E:334:THR:N    | 2.48                     | 0.44              |
| 1:13A:62:VAL:HG21  | 1:13A:88:HIS:NE2   | 2.33                     | 0.44              |
| 1:13A:91:GLN:HG2   | 1:13A:121:ARG:NH2  | 2.33                     | 0.44              |
| 2:13D:391:ARG:NH1  | 1:13E:345:ASP:OD2  | 2.46                     | 0.44              |
| 1:13E:6:SER:OG     | 1:13E:21:TRP:HZ2   | 2.00                     | 0.44              |
| 1:1A:123:ARG:NE    | 1:1A:123:ARG:HA    | 2.33                     | 0.44              |
| 2:1B:287:PRO:HG3   | 2:1B:329:GLN:OE1   | 2.17                     | 0.44              |
| 1:1E:174:ALA:HB1   | 1:1E:207:GLU:OE2   | 2.18                     | 0.44              |
| 1:2A:220:GLU:OE1   | 1:2A:220:GLU:N     | 2.42                     | 0.44              |
| 1:2A:255:PHE:CZ    | 1:2A:259:LEU:HD22  | 2.52                     | 0.44              |
| 1:2E:4:CYS:SG      | 1:2E:133:GLN:HB2   | 2.58                     | 0.44              |
| 1:2E:108:TYR:O     | 1:2E:112:LYS:NZ    | 2.39                     | 0.44              |
| 1:3C:169:PHE:CE2   | 1:3C:235:VAL:HG22  | 2.53                     | 0.44              |
| 1:4C:88:HIS:ND1    | 1:5C:283:HIS:HB3   | 2.32                     | 0.44              |
| 1:4C:239:THR:OG1   | 1:4C:243:ARG:NH1   | 2.51                     | 0.44              |
| 2:4D:193:VAL:HG21  | 2:4D:418:LEU:HD11  | 2.00                     | 0.44              |
| 2:5B:293:MET:CE    | 2:5B:365:ALA:HB1   | 2.48                     | 0.44              |
| 2:5D:330:MET:SD    | 2:5D:349:VAL:HG11  | 2.58                     | 0.44              |
| 1:6A:317:MET:CE    | 1:6A:377:MET:HG2   | 2.46                     | 0.44              |
| 2:6B:311:LEU:HD23  | 2:6B:342:VAL:HG21  | 1.99                     | 0.44              |
| 1:7C:303:VAL:O     | 1:7C:305:CYS:N     | 2.51                     | 0.44              |
| 1:7C:425:LEU:HD23  | 1:7C:425:LEU:HA    | 1.87                     | 0.44              |
| 1:8A:210:TYR:HA    | 1:8A:213:CYS:SG    | 2.57                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:420:SER:O     | 2:8B:423:GLN:HG3   | 2.18                     | 0.44              |
| 2:8D:131:GLN:O     | 2:8D:162:ARG:HB2   | 2.18                     | 0.44              |
| 2:9B:246:LEU:HD12  | 2:9B:246:LEU:HA    | 1.87                     | 0.44              |
| 1:9C:161:TYR:HB3   | 1:9C:164:LYS:HE3   | 2.00                     | 0.44              |
| 1:9C:225:THR:O     | 1:9C:229:ARG:HG3   | 2.18                     | 0.44              |
| 1:10A:265:ILE:HD11 | 1:10A:435:VAL:HG21 | 2.00                     | 0.44              |
| 1:11A:201:ALA:O    | 1:11A:268:PRO:HD2  | 2.17                     | 0.44              |
| 1:11A:209:ILE:HG23 | 1:11A:230:LEU:HD22 | 1.98                     | 0.44              |
| 2:12B:67:ASP:O     | 2:12B:92:PHE:HA    | 2.18                     | 0.44              |
| 1:12E:315:CYS:HA   | 1:12E:379:SER:HA   | 2.00                     | 0.44              |
| 2:13B:4:ILE:HG23   | 2:13B:132:GLY:O    | 2.18                     | 0.44              |
| 2:13B:13:GLY:O     | 2:13B:17:GLY:N     | 2.40                     | 0.44              |
| 1:13E:269:LEU:HB2  | 1:13E:379:SER:O    | 2.18                     | 0.44              |
| 2:1B:50:TYR:OH     | 2:1B:237:THR:HG21  | 2.18                     | 0.44              |
| 1:1C:269:LEU:HD13  | 1:1C:381:THR:HG22  | 1.99                     | 0.44              |
| 1:2C:205:ASP:O     | 1:2C:209:ILE:HG12  | 2.17                     | 0.44              |
| 1:3C:398:MET:SD    | 2:3D:346:PRO:HD2   | 2.58                     | 0.44              |
| 2:3D:320:ARG:HA    | 2:3D:320:ARG:HD2   | 1.70                     | 0.44              |
| 1:4C:11:GLN:HB3    | 3:4C:500:GTP:O2B   | 2.18                     | 0.44              |
| 1:4C:113:GLU:N     | 1:4C:113:GLU:OE2   | 2.51                     | 0.44              |
| 2:4D:133:PHE:HD2   | 2:4D:164:MET:SD    | 2.40                     | 0.44              |
| 1:4E:9:VAL:HG11    | 1:4E:150:THR:OG1   | 2.18                     | 0.44              |
| 1:6A:205:ASP:O     | 1:6A:209:ILE:HG12  | 2.18                     | 0.44              |
| 1:6C:3:GLU:H       | 1:6C:133:GLN:HG2   | 1.83                     | 0.44              |
| 1:6C:320:ARG:HG3   | 1:6C:360:PRO:HD3   | 1.98                     | 0.44              |
| 2:6D:257:MET:HE1   | 2:6D:314:ALA:HB3   | 2.00                     | 0.44              |
| 2:8D:328:GLU:O     | 2:8D:331:LEU:HG    | 2.16                     | 0.44              |
| 1:9A:9:VAL:HG11    | 1:9A:150:THR:OG1   | 2.18                     | 0.44              |
| 1:9A:168:GLU:OE2   | 1:9A:194:THR:HG23  | 2.16                     | 0.44              |
| 1:9A:222:PRO:HD2   | 2:9B:324:LYS:CD    | 2.47                     | 0.44              |
| 2:9B:153:SER:HB2   | 2:9B:191:GLN:NE2   | 2.32                     | 0.44              |
| 2:9B:170:VAL:HG13  | 2:9B:203:ASP:OD1   | 2.17                     | 0.44              |
| 2:9B:219:THR:HA    | 1:9C:326:LYS:HD3   | 1.98                     | 0.44              |
| 2:9B:381:ILE:O     | 2:9B:384:GLN:HB2   | 2.18                     | 0.44              |
| 2:9D:215:LEU:O     | 2:9D:215:LEU:HD23  | 2.17                     | 0.44              |
| 2:9D:219:THR:HA    | 1:9E:326:LYS:HD3   | 2.00                     | 0.44              |
| 1:10C:255:PHE:HZ   | 1:10C:378:LEU:HD22 | 1.81                     | 0.44              |
| 1:12A:8:HIS:CD2    | 1:12A:67:PHE:HE1   | 2.36                     | 0.44              |
| 2:12B:73:MET:O     | 2:12B:76:VAL:HG12  | 2.17                     | 0.44              |
| 1:12E:200:CYS:HB2  | 1:12E:256:GLN:OE1  | 2.18                     | 0.44              |
| 1:13A:105:ARG:CD   | 1:13A:411:GLU:HG3  | 2.47                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:13A:216:ASN:OD1  | 1:13A:300:ASN:ND2  | 2.51                     | 0.44              |
| 2:13B:99:ASN:HB3   | 2:13B:142:GLY:H    | 1.83                     | 0.44              |
| 1:13E:103:TYR:CD1  | 1:13E:189:LEU:HD23 | 2.53                     | 0.44              |
| 1:13E:292:THR:HB   | 1:13E:317:MET:HE1  | 2.00                     | 0.44              |
| 1:13E:336:LYS:HD3  | 1:13E:343:PHE:CZ   | 2.52                     | 0.44              |
| 1:1A:209:ILE:HG21  | 1:1A:227:LEU:HG    | 1.99                     | 0.44              |
| 1:2A:394:LYS:HG2   | 2:2B:346:PRO:HG3   | 2.00                     | 0.44              |
| 1:2E:88:HIS:ND1    | 1:3E:283:HIS:HB3   | 2.32                     | 0.44              |
| 2:3B:287:PRO:HA    | 2:3B:290:THR:HG22  | 2.00                     | 0.44              |
| 2:3D:151:LEU:O     | 2:3D:155:ILE:HG12  | 2.17                     | 0.44              |
| 1:4C:88:HIS:CE1    | 1:5C:283:HIS:HB3   | 2.52                     | 0.44              |
| 1:4C:214:ARG:HG2   | 1:4C:214:ARG:HH11  | 1.83                     | 0.44              |
| 1:5C:214:ARG:NH2   | 2:5D:324:LYS:HD2   | 2.33                     | 0.44              |
| 1:6C:265:ILE:HG23  | 1:6C:432:TYR:CZ    | 2.52                     | 0.44              |
| 1:8A:105:ARG:HG2   | 1:8A:110:ILE:HG12  | 2.00                     | 0.44              |
| 2:8B:245:GLN:OE1   | 2:8B:245:GLN:N     | 2.50                     | 0.44              |
| 1:8C:31:GLN:CG     | 1:8C:32:PRO:HD2    | 2.48                     | 0.44              |
| 1:8C:191:THR:HG21  | 1:8C:425:LEU:HD11  | 2.00                     | 0.44              |
| 1:9C:269:LEU:HD13  | 1:9C:381:THR:HG22  | 1.99                     | 0.44              |
| 1:10A:315:CYS:HA   | 1:10A:379:SER:HA   | 1.99                     | 0.44              |
| 1:10C:20:CYS:HB3   | 1:10C:24:TYR:CE1   | 2.49                     | 0.44              |
| 2:10D:51:TYR:O     | 2:10D:62:ARG:NH2   | 2.51                     | 0.44              |
| 1:10E:5:ILE:HD12   | 1:10E:132:LEU:HD11 | 1.99                     | 0.44              |
| 2:11B:130:LEU:HD23 | 2:11B:130:LEU:H    | 1.83                     | 0.44              |
| 2:11D:414:ASN:HA   | 2:11D:417:ASP:HB2  | 2.00                     | 0.44              |
| 1:11E:213:CYS:SG   | 1:11E:222:PRO:HG3  | 2.58                     | 0.44              |
| 1:11E:332:ILE:HD12 | 1:11E:351:PHE:CE2  | 2.52                     | 0.44              |
| 1:12A:269:LEU:HD13 | 1:12A:381:THR:HG22 | 2.00                     | 0.44              |
| 2:12B:130:LEU:CG   | 2:12B:162:ARG:HH12 | 2.30                     | 0.44              |
| 2:12D:73:MET:HE2   | 2:12D:92:PHE:CD2   | 2.53                     | 0.44              |
| 1:12E:31:GLN:OE1   | 1:12E:32:PRO:HD2   | 2.18                     | 0.44              |
| 1:13A:223:THR:O    | 1:13A:226:ASN:N    | 2.49                     | 0.44              |
| 1:2A:210:TYR:HE1   | 1:2A:227:LEU:HD11  | 1.83                     | 0.44              |
| 1:2A:414:GLU:OE2   | 1:2A:417:GLU:HG2   | 2.18                     | 0.44              |
| 2:2D:371:SER:OG    | 2:2D:372:THR:N     | 2.50                     | 0.44              |
| 2:3B:67:ASP:OD2    | 2:3B:72:THR:OG1    | 2.36                     | 0.44              |
| 1:4C:303:VAL:O     | 1:4C:305:CYS:N     | 2.50                     | 0.44              |
| 2:4D:213:ARG:NE    | 2:4D:297:LYS:HE3   | 2.33                     | 0.44              |
| 1:4E:91:GLN:HA     | 1:4E:121:ARG:NH1   | 2.31                     | 0.44              |
| 1:4E:165:SER:HA    | 1:4E:199:ASP:OD2   | 2.17                     | 0.44              |
| 2:6B:114:ASP:OD1   | 2:6B:115:SER:N     | 2.51                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:7A:102:ASN:HB3   | 1:7A:105:ARG:HB2  | 1.99                     | 0.44              |
| 1:7C:255:PHE:HD2   | 1:7C:256:GLN:OE1  | 2.01                     | 0.44              |
| 2:7D:172:SER:HB2   | 2:7D:205:GLU:OE1  | 2.18                     | 0.44              |
| 2:7D:211:CYS:O     | 2:7D:217:LEU:HB2  | 2.18                     | 0.44              |
| 2:7D:317:PHE:HB3   | 2:7D:321:MET:SD   | 2.58                     | 0.44              |
| 1:8C:398:MET:HE1   | 2:8D:345:ILE:HG23 | 1.99                     | 0.44              |
| 1:9C:269:LEU:HD11  | 1:9C:384:ILE:HB   | 2.00                     | 0.44              |
| 1:9C:292:THR:HG21  | 1:9C:331:ALA:HB1  | 1.99                     | 0.44              |
| 1:9C:395:PHE:HE2   | 1:9C:422:ARG:HG3  | 1.83                     | 0.44              |
| 2:9D:372:THR:HG21  | 2:9D:426:GLN:HG3  | 1.99                     | 0.44              |
| 2:10B:293:MET:CE   | 2:10B:365:ALA:HB1 | 2.48                     | 0.43              |
| 1:10E:172:TYR:CG   | 1:10E:173:PRO:HD2 | 2.53                     | 0.43              |
| 1:11A:101:ASN:HD21 | 2:11B:252:LYS:HZ1 | 1.66                     | 0.43              |
| 2:11D:303:CYS:SG   | 2:11D:377:LEU:HG  | 2.58                     | 0.43              |
| 1:11E:298:PRO:HG3  | 1:11E:308:ARG:CZ  | 2.48                     | 0.43              |
| 2:13B:193:VAL:HG13 | 2:13B:194:GLU:HG3 | 2.00                     | 0.43              |
| 2:1B:36:TYR:CZ     | 2:1B:44:LEU:HD21  | 2.53                     | 0.43              |
| 1:1C:400:ALA:O     | 1:1C:402:ARG:NH1  | 2.51                     | 0.43              |
| 1:2A:420:GLU:HA    | 1:2A:423:GLU:HB2  | 2.00                     | 0.43              |
| 2:2D:132:GLY:HA2   | 2:2D:163:ILE:O    | 2.18                     | 0.43              |
| 1:2E:63:PRO:HD3    | 1:2E:86:LEU:CD2   | 2.48                     | 0.43              |
| 2:3B:325:GLU:O     | 2:3B:329:GLN:HG2  | 2.17                     | 0.43              |
| 1:3C:222:PRO:HD2   | 2:3D:324:LYS:HD3  | 2.00                     | 0.43              |
| 2:3D:128:ASP:OD1   | 2:3D:129:CYS:N    | 2.47                     | 0.43              |
| 1:3E:400:ALA:O     | 1:3E:402:ARG:NH1  | 2.51                     | 0.43              |
| 1:4A:53:PHE:O      | 1:4A:64:ARG:NH1   | 2.51                     | 0.43              |
| 2:4D:371:SER:OG    | 2:4D:372:THR:N    | 2.51                     | 0.43              |
| 1:5A:338:LYS:HD3   | 1:5A:338:LYS:HA   | 1.72                     | 0.43              |
| 2:5D:388:MET:HE1   | 1:5E:348:PRO:HD2  | 2.00                     | 0.43              |
| 1:5E:103:TYR:CE1   | 1:5E:148:GLY:HA2  | 2.53                     | 0.43              |
| 1:6A:377:MET:SD    | 1:6A:379:SER:HB3  | 2.58                     | 0.43              |
| 1:6C:203:MET:HE2   | 1:6C:203:MET:HB2  | 1.92                     | 0.43              |
| 1:7A:102:ASN:HB2   | 1:7A:105:ARG:HB2  | 1.99                     | 0.43              |
| 2:7D:179:VAL:HG12  | 2:7D:394:PHE:HE2  | 1.83                     | 0.43              |
| 2:8B:155:ILE:HG22  | 2:8B:164:MET:HE1  | 1.99                     | 0.43              |
| 2:8B:156:ARG:HH12  | 2:8B:197:ASP:CG   | 2.23                     | 0.43              |
| 1:9C:88:HIS:CD2    | 1:9C:89:PRO:HD2   | 2.46                     | 0.43              |
| 2:9D:73:MET:HG3    | 2:9D:92:PHE:CD1   | 2.53                     | 0.43              |
| 1:10A:31:GLN:HG3   | 1:10A:32:PRO:HD2  | 2.00                     | 0.43              |
| 1:10A:338:LYS:HB2  | 1:10A:338:LYS:HE3 | 1.73                     | 0.43              |
| 2:10B:104:GLY:HA3  | 2:10B:146:GLY:HA3 | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10D:73:MET:HE1   | 2:10D:92:PHE:HD2   | 1.83                     | 0.43              |
| 1:11A:304:LYS:HB3  | 1:11A:304:LYS:HE3  | 1.75                     | 0.43              |
| 2:11B:382:SER:O    | 2:11B:386:THR:OG1  | 2.25                     | 0.43              |
| 1:12A:53:PHE:CD2   | 1:12A:61:HIS:HB3   | 2.52                     | 0.43              |
| 1:12A:63:PRO:HD3   | 1:12A:86:LEU:HG    | 2.00                     | 0.43              |
| 1:12A:358:GLN:NE2  | 1:12A:359:PRO:O    | 2.51                     | 0.43              |
| 2:12B:52:ASN:HB3   | 2:12B:62:ARG:HH12  | 1.82                     | 0.43              |
| 1:12E:129:CYS:SG   | 1:12E:132:LEU:HB2  | 2.58                     | 0.43              |
| 1:12E:298:PRO:HD2  | 1:12E:299:ALA:N    | 2.33                     | 0.43              |
| 1:13A:8:HIS:HB3    | 1:13A:13:GLY:O     | 2.18                     | 0.43              |
| 2:13B:375:GLN:C    | 2:13B:379:LYS:HE3  | 2.43                     | 0.43              |
| 2:13D:218:THR:HG23 | 2:13D:219:THR:HG23 | 2.00                     | 0.43              |
| 2:1B:107:THR:OG1   | 2:1B:401:GLU:OE1   | 2.33                     | 0.43              |
| 2:2B:21:TRP:HA     | 2:2B:24:ILE:HG22   | 1.99                     | 0.43              |
| 2:3D:285:THR:HG23  | 2:3D:287:PRO:HD2   | 2.00                     | 0.43              |
| 1:3E:255:PHE:CZ    | 1:3E:378:LEU:HD22  | 2.53                     | 0.43              |
| 1:4A:144:GLY:O     | 1:4A:148:GLY:N     | 2.43                     | 0.43              |
| 1:4C:204:VAL:HG11  | 1:4C:231:ILE:HD11  | 2.00                     | 0.43              |
| 1:5E:49:PHE:HD2    | 1:5E:53:PHE:HB2    | 1.82                     | 0.43              |
| 1:6A:188:ILE:HG23  | 1:6A:425:LEU:HD12  | 2.00                     | 0.43              |
| 1:7C:120:ASP:OD1   | 1:7C:121:ARG:N     | 2.51                     | 0.43              |
| 1:7E:286:LEU:HA    | 1:7E:290:GLU:OE1   | 2.18                     | 0.43              |
| 1:8A:286:LEU:O     | 1:8A:373:ARG:NH1   | 2.49                     | 0.43              |
| 1:8E:287:SER:O     | 1:8E:291:ILE:HG13  | 2.18                     | 0.43              |
| 1:9C:205:ASP:OD2   | 1:9C:206:ASN:N     | 2.49                     | 0.43              |
| 1:9C:277:SER:OG    | 1:9C:280:LYS:HB2   | 2.17                     | 0.43              |
| 2:10B:416:ASN:OD1  | 2:10B:417:ASP:N    | 2.51                     | 0.43              |
| 2:11B:101:TRP:NE1  | 2:11B:149:THR:HG21 | 2.33                     | 0.43              |
| 1:13A:31:GLN:HG2   | 1:13A:32:PRO:HD2   | 1.98                     | 0.43              |
| 2:13B:324:LYS:HA   | 2:13B:327:ASP:OD2  | 2.18                     | 0.43              |
| 2:13D:121:ARG:NH1  | 2:13D:158:GLU:OE1  | 2.51                     | 0.43              |
| 2:13D:201:CYS:SG   | 2:13D:265:PHE:HD1  | 2.40                     | 0.43              |
| 2:13D:293:MET:SD   | 2:13D:367:PHE:HB2  | 2.59                     | 0.43              |
| 1:3A:265:ILE:HG23  | 1:3A:432:TYR:CE2   | 2.53                     | 0.43              |
| 1:3A:286:LEU:HA    | 1:3A:290:GLU:OE1   | 2.18                     | 0.43              |
| 2:3D:289:LEU:O     | 2:3D:293:MET:HG3   | 2.19                     | 0.43              |
| 2:6B:263:LEU:HG    | 2:6B:422:TYR:CE1   | 2.53                     | 0.43              |
| 1:6C:10:GLY:O      | 1:6C:14:VAL:HG23   | 2.18                     | 0.43              |
| 1:6C:102:ASN:HD21  | 2:6D:255:VAL:HG21  | 1.83                     | 0.43              |
| 1:7C:5:ILE:O       | 1:7C:135:PHE:HA    | 2.18                     | 0.43              |
| 1:7E:47:ASP:HB3    | 1:7E:48:SER:H      | 1.57                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:9A:265:ILE:HG22 | 1:9A:380:ASN:HD21  | 1.82                     | 0.43              |
| 2:9B:405:GLU:HA   | 2:9B:408:PHE:HD1   | 1.82                     | 0.43              |
| 1:9C:33:ASP:HB2   | 1:9C:35:GLN:OE1    | 2.18                     | 0.43              |
| 2:9D:299:MET:HE1  | 2:9D:367:PHE:CD2   | 2.53                     | 0.43              |
| 2:10B:61:PRO:HD3  | 2:10B:84:ILE:CG2   | 2.41                     | 0.43              |
| 1:10C:338:LYS:HE3 | 1:10C:338:LYS:HB2  | 1.76                     | 0.43              |
| 1:10E:139:HIS:HE1 | 1:10E:141:PHE:CE1  | 2.36                     | 0.43              |
| 2:11B:286:VAL:CG2 | 2:11B:321:MET:HE3  | 2.48                     | 0.43              |
| 2:11D:109:GLY:O   | 2:11D:113:VAL:HB   | 2.18                     | 0.43              |
| 1:11E:220:GLU:OE1 | 1:11E:220:GLU:N    | 2.47                     | 0.43              |
| 1:12A:90:GLU:OE2  | 1:12A:90:GLU:N     | 2.36                     | 0.43              |
| 1:13E:208:ALA:O   | 1:13E:212:ILE:HD12 | 2.17                     | 0.43              |
| 1:1A:88:HIS:HD2   | 1:2A:283:HIS:HB3   | 1.82                     | 0.43              |
| 1:1C:377:MET:SD   | 1:1C:379:SER:HB3   | 2.58                     | 0.43              |
| 1:2C:356:ASN:OD1  | 1:2C:357:TYR:N     | 2.52                     | 0.43              |
| 1:4A:390:ARG:HE   | 1:4A:391:LEU:HD12  | 1.83                     | 0.43              |
| 2:4B:219:THR:HG22 | 1:4C:326:LYS:HE2   | 2.00                     | 0.43              |
| 1:4C:430:LYS:O    | 1:4C:433:GLU:HG3   | 2.18                     | 0.43              |
| 2:4D:61:PRO:HD3   | 2:4D:84:ILE:HG22   | 2.00                     | 0.43              |
| 2:4D:167:TYR:CE1  | 2:4D:233:MET:HG2   | 2.54                     | 0.43              |
| 2:5B:209:ASP:CG   | 2:5B:213:ARG:HH12  | 2.24                     | 0.43              |
| 2:5D:328:GLU:O    | 2:5D:331:LEU:HG    | 2.19                     | 0.43              |
| 2:6B:358:PRO:HG2  | 2:6B:364:SER:OG    | 2.18                     | 0.43              |
| 1:6C:31:GLN:CG    | 1:6C:32:PRO:HD2    | 2.48                     | 0.43              |
| 2:6D:328:GLU:O    | 2:6D:331:LEU:HG    | 2.17                     | 0.43              |
| 2:7B:285:THR:O    | 2:7B:288:GLU:HG2   | 2.18                     | 0.43              |
| 2:7B:303:CYS:SG   | 2:7B:377:LEU:HG    | 2.58                     | 0.43              |
| 2:7D:130:LEU:CD1  | 2:7D:162:ARG:HD3   | 2.48                     | 0.43              |
| 2:7D:394:PHE:CD1  | 1:7E:261:PRO:HA    | 2.53                     | 0.43              |
| 2:8D:158:GLU:C    | 2:8D:160:PRO:HD3   | 2.44                     | 0.43              |
| 1:9C:214:ARG:HH21 | 2:9D:324:LYS:HE2   | 1.83                     | 0.43              |
| 2:9D:104:GLY:HA3  | 2:9D:146:GLY:HA3   | 2.00                     | 0.43              |
| 1:9E:20:CYS:HB3   | 1:9E:24:TYR:CE2    | 2.52                     | 0.43              |
| 1:10A:21:TRP:HZ3  | 1:10A:53:PHE:HE1   | 1.67                     | 0.43              |
| 2:10D:31:ASP:CG   | 2:10D:32:ALA:H     | 2.27                     | 0.43              |
| 1:10E:321:GLY:HA3 | 1:10E:372:GLN:O    | 2.18                     | 0.43              |
| 1:11C:220:GLU:HG2 | 1:11C:221:ARG:H    | 1.83                     | 0.43              |
| 2:11D:61:PRO:CD   | 2:11D:84:ILE:HG22  | 2.43                     | 0.43              |
| 2:11D:220:PRO:HD2 | 1:11E:326:LYS:CD   | 2.48                     | 0.43              |
| 1:11E:401:LYS:HZ2 | 1:11E:403:ALA:HB2  | 1.83                     | 0.43              |
| 1:12A:100:ALA:O   | 2:12B:255:VAL:HG11 | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:100:ASN:OD1  | 2:12B:398:TYR:HE1  | 2.01                     | 0.43              |
| 2:12B:146:GLY:O    | 2:12B:149:THR:HG22 | 2.18                     | 0.43              |
| 2:12B:190:HIS:NE2  | 2:12B:414:ASN:OD1  | 2.50                     | 0.43              |
| 1:12C:88:HIS:HA    | 1:12C:89:PRO:HD3   | 1.93                     | 0.43              |
| 2:12D:109:GLY:O    | 2:12D:113:VAL:HB   | 2.18                     | 0.43              |
| 2:13D:22:GLU:OE2   | 2:13D:80:PRO:HG2   | 2.19                     | 0.43              |
| 1:13E:205:ASP:OD1  | 1:13E:206:ASN:N    | 2.49                     | 0.43              |
| 2:1D:183:TYR:OH    | 2:1D:388:MET:HB3   | 2.18                     | 0.43              |
| 2:2D:178:THR:HG22  | 2:2D:180:VAL:H     | 1.83                     | 0.43              |
| 1:2E:377:MET:SD    | 1:2E:379:SER:HB3   | 2.59                     | 0.43              |
| 1:3C:5:ILE:HB      | 1:3C:135:PHE:CD1   | 2.53                     | 0.43              |
| 2:3D:5:VAL:HG22    | 2:3D:133:PHE:CD1   | 2.53                     | 0.43              |
| 1:3E:47:ASP:HB3    | 1:3E:48:SER:H      | 1.60                     | 0.43              |
| 1:3E:303:VAL:O     | 1:3E:305:CYS:N     | 2.51                     | 0.43              |
| 2:4B:390:ARG:NH1   | 2:4B:391:ARG:HE    | 2.16                     | 0.43              |
| 1:4E:53:PHE:O      | 1:4E:64:ARG:NH1    | 2.52                     | 0.43              |
| 1:5A:201:ALA:O     | 1:5A:268:PRO:HD2   | 2.18                     | 0.43              |
| 2:5D:183:TYR:CE1   | 2:5D:388:MET:HB3   | 2.53                     | 0.43              |
| 1:5E:265:ILE:HG23  | 1:5E:432:TYR:CZ    | 2.54                     | 0.43              |
| 2:6B:159:TYR:HD1   | 2:6B:162:ARG:HH21  | 1.65                     | 0.43              |
| 1:6E:210:TYR:CE1   | 1:6E:227:LEU:HD11  | 2.53                     | 0.43              |
| 1:6E:332:ILE:HD12  | 1:6E:351:PHE:CE2   | 2.54                     | 0.43              |
| 1:7A:205:ASP:O     | 1:7A:209:ILE:HG12  | 2.18                     | 0.43              |
| 1:7C:207:GLU:O     | 1:7C:210:TYR:HB2   | 2.18                     | 0.43              |
| 1:7C:414:GLU:OE2   | 1:7C:417:GLU:N     | 2.51                     | 0.43              |
| 1:7E:265:ILE:HG23  | 1:7E:432:TYR:CE1   | 2.53                     | 0.43              |
| 1:8A:71:GLU:HG2    | 1:8A:73:THR:H      | 1.83                     | 0.43              |
| 1:9A:193:THR:O     | 1:9A:197:HIS:HB2   | 2.18                     | 0.43              |
| 2:9B:286:VAL:HG22  | 2:9B:321:MET:HE3   | 2.00                     | 0.43              |
| 2:9D:310:TYR:O     | 2:9D:342:VAL:HG23  | 2.19                     | 0.43              |
| 1:9E:34:GLY:O      | 1:9E:61:HIS:N      | 2.51                     | 0.43              |
| 1:10A:265:ILE:HG23 | 1:10A:432:TYR:CZ   | 2.53                     | 0.43              |
| 2:10D:398:TYR:O    | 2:10D:403:MET:HE3  | 2.17                     | 0.43              |
| 1:11A:31:GLN:HB3   | 1:11A:35:GLN:HG3   | 2.00                     | 0.43              |
| 2:11B:101:TRP:HE1  | 2:11B:149:THR:HG21 | 1.84                     | 0.43              |
| 2:11B:303:CYS:SG   | 2:11B:377:LEU:HG   | 2.58                     | 0.43              |
| 1:11C:207:GLU:O    | 1:11C:210:TYR:HB2  | 2.19                     | 0.43              |
| 2:12D:285:THR:O    | 2:12D:288:GLU:HG3  | 2.19                     | 0.43              |
| 1:13C:269:LEU:HB2  | 1:13C:379:SER:O    | 2.17                     | 0.43              |
| 1:1C:8:HIS:HD2     | 1:1C:67:PHE:CE1    | 2.36                     | 0.43              |
| 1:2C:188:ILE:HG22  | 1:2C:421:ALA:HB1   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2C:338:LYS:HD3   | 1:2C:338:LYS:HA    | 1.75                     | 0.43              |
| 1:3A:269:LEU:HD11  | 1:3A:384:ILE:HB    | 2.01                     | 0.43              |
| 2:3B:31:ASP:CG     | 2:3B:32:ALA:H      | 2.27                     | 0.43              |
| 2:3B:219:THR:HA    | 1:3C:326:LYS:HD3   | 2.00                     | 0.43              |
| 1:3C:193:THR:O     | 1:3C:197:HIS:HB2   | 2.18                     | 0.43              |
| 1:3E:98:ASP:OD2    | 1:3E:99:ALA:N      | 2.50                     | 0.43              |
| 1:4C:184:PRO:O     | 1:4C:188:ILE:HG12  | 2.18                     | 0.43              |
| 1:4C:414:GLU:HG2   | 1:4C:415:GLU:N     | 2.34                     | 0.43              |
| 1:5A:407:TRP:O     | 1:5A:411:GLU:HG2   | 2.19                     | 0.43              |
| 1:7A:201:ALA:O     | 1:7A:268:PRO:HD2   | 2.18                     | 0.43              |
| 2:7D:173:PRO:HD2   | 2:7D:380:ARG:HH11  | 1.83                     | 0.43              |
| 2:8B:11:GLN:HB2    | 2:8B:72:THR:HG21   | 2.00                     | 0.43              |
| 1:9E:9:VAL:HG11    | 1:9E:150:THR:OG1   | 2.18                     | 0.43              |
| 2:10B:311:LEU:HD23 | 2:10B:342:VAL:HG21 | 2.01                     | 0.43              |
| 1:10C:298:PRO:HG3  | 1:10C:308:ARG:NE   | 2.33                     | 0.43              |
| 2:13B:295:ASP:OD1  | 2:13B:296:ALA:N    | 2.52                     | 0.43              |
| 2:13D:305:PRO:HA   | 2:13D:373:ALA:HB2  | 2.00                     | 0.43              |
| 2:1B:257:MET:HE1   | 2:1B:313:VAL:O     | 2.18                     | 0.43              |
| 2:1D:73:MET:HG3    | 2:1D:92:PHE:HB3    | 2.01                     | 0.43              |
| 1:2A:301:GLN:HE22  | 1:2A:377:MET:HE1   | 1.84                     | 0.43              |
| 1:2A:313:MET:HB3   | 1:2A:380:ASN:O     | 2.19                     | 0.43              |
| 1:2C:55:GLU:OE2    | 1:2C:61:HIS:NE2    | 2.52                     | 0.43              |
| 1:2C:425:LEU:HD23  | 1:2C:425:LEU:HA    | 1.90                     | 0.43              |
| 2:3B:211:CYS:HB2   | 2:3B:217:LEU:HD12  | 2.01                     | 0.43              |
| 1:3C:184:PRO:O     | 1:3C:188:ILE:HG12  | 2.17                     | 0.43              |
| 1:3C:265:ILE:HG23  | 1:3C:432:TYR:CZ    | 2.54                     | 0.43              |
| 1:4A:332:ILE:HD12  | 1:4A:351:PHE:CE2   | 2.54                     | 0.43              |
| 2:4D:111:GLU:OE1   | 2:4D:111:GLU:N     | 2.51                     | 0.43              |
| 1:5C:88:HIS:ND1    | 1:6C:283:HIS:HB3   | 2.34                     | 0.43              |
| 1:6A:320:ARG:HG3   | 1:6A:360:PRO:HD3   | 2.00                     | 0.43              |
| 2:6B:52:ASN:HB3    | 2:6B:62:ARG:HH12   | 1.82                     | 0.43              |
| 1:6C:252:LEU:O     | 1:6C:256:GLN:HG2   | 2.19                     | 0.43              |
| 2:6D:376:GLU:HA    | 2:6D:379:LYS:HZ1   | 1.83                     | 0.43              |
| 1:6E:425:LEU:HD23  | 1:6E:425:LEU:HA    | 1.91                     | 0.43              |
| 1:7A:344:VAL:HG11  | 1:7A:346:TRP:CE2   | 2.54                     | 0.43              |
| 2:7B:412:GLU:O     | 2:7B:416:ASN:N     | 2.47                     | 0.43              |
| 1:7C:100:ALA:HA    | 2:7D:252:LYS:CG    | 2.48                     | 0.43              |
| 1:7E:91:GLN:HA     | 1:7E:121:ARG:HH12  | 1.83                     | 0.43              |
| 1:8C:219:ILE:HG21  | 1:8C:367:ASP:OD1   | 2.18                     | 0.43              |
| 1:8C:291:ILE:HD12  | 1:8C:375:VAL:HG23  | 2.01                     | 0.43              |
| 2:8D:208:TYR:HE1   | 2:8D:225:LEU:HD11  | 1.84                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:9D:178:THR:HG22  | 2:9D:180:VAL:H     | 1.82                     | 0.43              |
| 1:10A:294:ALA:O    | 1:10A:297:GLU:HG2  | 2.19                     | 0.43              |
| 1:10E:265:ILE:HG23 | 1:10E:432:TYR:CZ   | 2.53                     | 0.43              |
| 1:12A:184:PRO:O    | 1:12A:188:ILE:HG12 | 2.19                     | 0.43              |
| 1:12A:220:GLU:HG2  | 1:12A:221:ARG:H    | 1.84                     | 0.43              |
| 1:12C:75:VAL:O     | 1:12C:78:VAL:HG22  | 2.19                     | 0.43              |
| 1:12E:185:TYR:OH   | 1:12E:403:ALA:O    | 2.27                     | 0.43              |
| 1:13A:112:LYS:HA   | 1:13A:115:VAL:CG1  | 2.45                     | 0.43              |
| 1:13A:184:PRO:HA   | 1:13A:187:SER:HB2  | 2.01                     | 0.43              |
| 1:13A:314:ALA:HA   | 1:13A:350:GLY:O    | 2.18                     | 0.43              |
| 1:13A:320:ARG:HG2  | 1:13A:374:ALA:O    | 2.19                     | 0.43              |
| 2:13B:330:MET:O    | 2:13B:334:GLN:HG3  | 2.18                     | 0.43              |
| 2:1D:130:LEU:HD23  | 2:1D:130:LEU:H     | 1.83                     | 0.43              |
| 2:4D:31:ASP:CG     | 2:4D:32:ALA:H      | 2.27                     | 0.43              |
| 2:5B:30:ILE:HD11   | 2:5B:47:ILE:HD11   | 2.00                     | 0.43              |
| 2:5B:128:ASP:N     | 2:5B:128:ASP:OD1   | 2.52                     | 0.43              |
| 2:5D:215:LEU:HG    | 2:5D:217:LEU:HG    | 2.00                     | 0.43              |
| 1:5E:8:HIS:HD2     | 1:5E:67:PHE:CE1    | 2.37                     | 0.43              |
| 2:6D:388:MET:HE1   | 1:6E:348:PRO:HD2   | 2.01                     | 0.43              |
| 2:7B:379:LYS:HA    | 2:7B:382:SER:HB3   | 2.01                     | 0.43              |
| 2:8B:175:VAL:HG23  | 2:8B:205:GLU:HG3   | 2.00                     | 0.43              |
| 2:10B:3:GLU:O      | 2:10B:130:LEU:HB2  | 2.19                     | 0.43              |
| 2:10B:5:VAL:HG12   | 2:10B:62:ARG:CD    | 2.49                     | 0.43              |
| 1:10C:298:PRO:HG3  | 1:10C:308:ARG:CZ   | 2.49                     | 0.43              |
| 2:10D:178:THR:HG22 | 2:10D:180:VAL:H    | 1.83                     | 0.43              |
| 1:10E:207:GLU:O    | 1:10E:210:TYR:HB2  | 2.19                     | 0.43              |
| 1:11E:122:ILE:HD13 | 1:11E:157:LEU:HD21 | 2.01                     | 0.43              |
| 2:12B:385:PHE:CZ   | 2:12B:408:PHE:HD2  | 2.37                     | 0.43              |
| 1:12E:5:ILE:HD13   | 1:12E:125:LEU:HB3  | 2.01                     | 0.43              |
| 1:12E:53:PHE:HD2   | 1:12E:61:HIS:HB3   | 1.84                     | 0.43              |
| 1:12E:56:THR:HG23  | 1:13E:285:GLN:HB2  | 1.99                     | 0.43              |
| 1:13A:283:HIS:HB2  | 1:13A:284:GLU:OE1  | 2.18                     | 0.43              |
| 1:13A:292:THR:HG21 | 1:13A:331:ALA:HB1  | 2.01                     | 0.43              |
| 2:13B:293:MET:HE1  | 2:13B:365:ALA:CB   | 2.48                     | 0.43              |
| 1:13C:64:ARG:HG3   | 1:13C:125:LEU:HD13 | 2.00                     | 0.43              |
| 2:13D:287:PRO:HB3  | 2:13D:329:GLN:HG3  | 2.01                     | 0.43              |
| 1:13E:318:LEU:O    | 1:13E:375:VAL:HA   | 2.19                     | 0.43              |
| 2:1B:267:MET:HE3   | 2:1B:301:ALA:HB3   | 2.00                     | 0.43              |
| 1:1E:326:LYS:HG3   | 1:1E:327:ASP:N     | 2.34                     | 0.43              |
| 1:2A:177:VAL:HG13  | 2:2B:327:ASP:HB2   | 2.01                     | 0.43              |
| 1:2E:63:PRO:HD3    | 1:2E:86:LEU:HD23   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:332:ILE:HD12  | 1:3A:351:PHE:CD2   | 2.54                     | 0.43              |
| 2:3D:373:ALA:O     | 2:3D:376:GLU:HG2   | 2.19                     | 0.43              |
| 2:4B:178:THR:HG22  | 2:4B:180:VAL:H     | 1.82                     | 0.43              |
| 2:6B:133:PHE:HB2   | 2:6B:164:MET:SD    | 2.59                     | 0.43              |
| 2:6D:20:PHE:CD1    | 2:6D:233:MET:HE3   | 2.54                     | 0.43              |
| 1:6E:75:VAL:O      | 1:6E:78:VAL:HG22   | 2.17                     | 0.43              |
| 1:6E:244:PHE:HB2   | 1:6E:356:ASN:HD21  | 1.83                     | 0.43              |
| 1:7A:118:VAL:HA    | 1:7A:121:ARG:HB2   | 1.99                     | 0.43              |
| 1:7A:269:LEU:HD11  | 1:7A:384:ILE:HB    | 2.00                     | 0.43              |
| 1:7E:172:TYR:HE2   | 1:7E:391:LEU:HD13  | 1.83                     | 0.43              |
| 1:7E:245:ASP:OD1   | 1:7E:245:ASP:N     | 2.49                     | 0.43              |
| 2:8B:20:PHE:CD1    | 2:8B:233:MET:HE3   | 2.53                     | 0.43              |
| 1:8C:265:ILE:HG23  | 1:8C:432:TYR:CZ    | 2.53                     | 0.43              |
| 2:9B:101:TRP:CE3   | 2:9B:187:LEU:HD13  | 2.53                     | 0.43              |
| 2:9B:267:MET:CE    | 2:9B:303:CYS:HB2   | 2.48                     | 0.43              |
| 1:9C:102:ASN:OD1   | 1:9C:408:TYR:HE1   | 2.02                     | 0.43              |
| 2:10B:141:GLY:HA3  | 5:10B:600:GDP:O2A  | 2.18                     | 0.43              |
| 1:12A:332:ILE:O    | 1:12A:336:LYS:HG2  | 2.19                     | 0.43              |
| 2:12D:12:CYS:CB    | 2:12D:138:SER:HG   | 2.32                     | 0.43              |
| 2:13B:300:MET:O    | 2:13B:300:MET:HG3  | 2.18                     | 0.43              |
| 1:13C:115:VAL:HG22 | 1:13C:119:LEU:HD12 | 2.01                     | 0.43              |
| 1:13C:270:VAL:HA   | 1:13C:377:MET:O    | 2.19                     | 0.43              |
| 2:13D:382:SER:O    | 2:13D:386:THR:OG1  | 2.31                     | 0.43              |
| 2:1D:203:ASP:O     | 2:1D:207:LEU:HD13  | 2.19                     | 0.43              |
| 1:2A:31:GLN:HE21   | 1:2A:37:PRO:HG2    | 1.84                     | 0.43              |
| 2:2D:279:GLN:H     | 2:2D:279:GLN:HG3   | 1.67                     | 0.43              |
| 1:2E:174:ALA:HB1   | 1:2E:207:GLU:OE2   | 2.18                     | 0.43              |
| 1:3A:21:TRP:HZ3    | 1:3A:53:PHE:HE1    | 1.67                     | 0.43              |
| 1:3C:5:ILE:HB      | 1:3C:135:PHE:HD1   | 1.82                     | 0.43              |
| 1:5A:265:ILE:HG23  | 1:5A:432:TYR:CZ    | 2.54                     | 0.43              |
| 1:5E:53:PHE:C      | 1:5E:64:ARG:HH12   | 2.22                     | 0.43              |
| 2:6B:303:CYS:SG    | 2:6B:377:LEU:HG    | 2.59                     | 0.43              |
| 1:6E:69:ASP:OD1    | 1:6E:70:LEU:N      | 2.49                     | 0.43              |
| 1:7A:53:PHE:HD2    | 1:7A:61:HIS:HB3    | 1.83                     | 0.43              |
| 2:7B:373:ALA:O     | 2:7B:376:GLU:HG2   | 2.19                     | 0.43              |
| 1:7C:245:ASP:OD1   | 1:7C:245:ASP:N     | 2.50                     | 0.43              |
| 2:7D:285:THR:HG23  | 2:7D:287:PRO:HD2   | 2.01                     | 0.43              |
| 1:8A:139:HIS:CG    | 1:8A:150:THR:HG21  | 2.54                     | 0.43              |
| 1:8A:222:PRO:HD2   | 2:8B:324:LYS:HD3   | 2.01                     | 0.43              |
| 1:9A:265:ILE:HD11  | 1:9A:435:VAL:HG21  | 2.00                     | 0.43              |
| 2:9B:293:MET:HE1   | 2:9B:315:ALA:HB1   | 2.00                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:9D:3:GLU:HB3     | 2:9D:62:ARG:NH1   | 2.33                     | 0.43              |
| 1:10A:168:GLU:HG2  | 1:10A:201:ALA:HA  | 2.00                     | 0.42              |
| 1:10C:225:THR:O    | 1:10C:229:ARG:HG3 | 2.19                     | 0.42              |
| 2:10D:219:THR:HA   | 1:10E:326:LYS:HD3 | 2.01                     | 0.42              |
| 1:11E:201:ALA:O    | 1:11E:268:PRO:HD2 | 2.18                     | 0.42              |
| 2:12B:267:MET:SD   | 2:12B:299:MET:HE3 | 2.59                     | 0.42              |
| 2:12B:406:MET:SD   | 2:12B:407:GLU:HG3 | 2.59                     | 0.42              |
| 2:13B:165:ASN:HB3  | 2:13B:167:TYR:CE2 | 2.52                     | 0.42              |
| 2:13B:416:ASN:O    | 2:13B:420:SER:N   | 2.31                     | 0.42              |
| 2:13D:256:ASN:HB2  | 2:13D:350:LYS:NZ  | 2.34                     | 0.42              |
| 1:1A:102:ASN:HB3   | 1:1A:105:ARG:HB2  | 2.01                     | 0.42              |
| 1:1C:328:VAL:O     | 1:1C:332:ILE:HG12 | 2.19                     | 0.42              |
| 2:2D:113:VAL:O     | 2:2D:117:LEU:HD23 | 2.19                     | 0.42              |
| 1:2E:93:ILE:HG22   | 1:2E:114:ILE:HD11 | 2.00                     | 0.42              |
| 1:2E:303:VAL:O     | 1:2E:305:CYS:N    | 2.52                     | 0.42              |
| 1:2E:322:ASP:HB3   | 1:2E:373:ARG:HH21 | 1.84                     | 0.42              |
| 1:3A:71:GLU:HG2    | 1:3A:73:THR:H     | 1.83                     | 0.42              |
| 2:3B:114:ASP:OD1   | 2:3B:114:ASP:N    | 2.51                     | 0.42              |
| 1:3C:71:GLU:HG2    | 1:3C:73:THR:H     | 1.83                     | 0.42              |
| 1:3C:129:CYS:SG    | 1:3C:132:LEU:HD13 | 2.59                     | 0.42              |
| 1:3C:402:ARG:HG3   | 1:3C:402:ARG:NH1  | 2.33                     | 0.42              |
| 2:3D:167:TYR:CD2   | 2:3D:233:MET:HG3  | 2.54                     | 0.42              |
| 2:4B:193:VAL:HG13  | 2:4B:194:GLU:OE1  | 2.19                     | 0.42              |
| 1:4E:68:VAL:HG11   | 1:4E:149:PHE:HE2  | 1.84                     | 0.42              |
| 1:4E:430:LYS:O     | 1:4E:433:GLU:HG3  | 2.19                     | 0.42              |
| 1:5A:164:LYS:HE2   | 1:5A:164:LYS:HB2  | 1.73                     | 0.42              |
| 2:5B:130:LEU:CD1   | 2:5B:162:ARG:HD2  | 2.49                     | 0.42              |
| 1:6E:184:PRO:O     | 1:6E:188:ILE:HG12 | 2.18                     | 0.42              |
| 1:6E:265:ILE:HG23  | 1:6E:432:TYR:CZ   | 2.54                     | 0.42              |
| 1:6E:286:LEU:O     | 1:6E:373:ARG:NH1  | 2.52                     | 0.42              |
| 1:7E:201:ALA:O     | 1:7E:268:PRO:HD2  | 2.19                     | 0.42              |
| 1:8A:407:TRP:CD1   | 2:8B:255:VAL:HG23 | 2.54                     | 0.42              |
| 2:8B:111:GLU:N     | 2:8B:111:GLU:OE1  | 2.52                     | 0.42              |
| 1:8E:31:GLN:HG3    | 1:8E:32:PRO:HD2   | 2.01                     | 0.42              |
| 1:9A:213:CYS:SG    | 1:9A:222:PRO:HB3  | 2.59                     | 0.42              |
| 1:9A:398:MET:CE    | 2:9B:346:PRO:HD2  | 2.47                     | 0.42              |
| 1:9C:234:ILE:HD11  | 1:9C:302:MET:HE3  | 2.00                     | 0.42              |
| 1:9C:305:CYS:HA    | 1:9C:386:GLU:OE2  | 2.19                     | 0.42              |
| 1:10E:294:ALA:O    | 1:10E:297:GLU:HG2 | 2.19                     | 0.42              |
| 1:10E:332:ILE:O    | 1:10E:336:LYS:HG2 | 2.19                     | 0.42              |
| 2:11D:156:ARG:HH12 | 2:11D:197:ASP:CG  | 2.26                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:11E:173:PRO:HG3  | 1:11E:187:SER:OG   | 2.19                     | 0.42              |
| 2:12B:313:VAL:HA   | 2:12B:369:GLY:HA2  | 2.00                     | 0.42              |
| 2:12D:99:ASN:ND2   | 1:12E:254:GLU:OE2  | 2.50                     | 0.42              |
| 2:12D:141:GLY:HA3  | 5:12D:600:GDP:O2A  | 2.19                     | 0.42              |
| 2:12D:289:LEU:O    | 2:12D:293:MET:N    | 2.52                     | 0.42              |
| 1:13A:20:CYS:HB3   | 1:13A:24:TYR:CE2   | 2.54                     | 0.42              |
| 1:13A:193:THR:O    | 1:13A:197:HIS:N    | 2.52                     | 0.42              |
| 2:13B:390:ARG:HG3  | 2:13B:391:ARG:NE   | 2.33                     | 0.42              |
| 1:13C:224:TYR:HD1  | 1:13C:227:LEU:HD13 | 1.84                     | 0.42              |
| 2:13D:330:MET:O    | 2:13D:334:GLN:HG3  | 2.18                     | 0.42              |
| 2:13D:375:GLN:C    | 2:13D:379:LYS:HE3  | 2.44                     | 0.42              |
| 1:13E:21:TRP:CH2   | 1:13E:52:PHE:HB3   | 2.54                     | 0.42              |
| 2:1D:67:ASP:OD2    | 2:1D:68:LEU:N      | 2.52                     | 0.42              |
| 2:2B:326:VAL:O     | 2:2B:330:MET:HG2   | 2.19                     | 0.42              |
| 2:2D:293:MET:HB3   | 2:2D:367:PHE:HB2   | 2.00                     | 0.42              |
| 1:3A:132:LEU:HD23  | 1:3A:164:LYS:HE3   | 2.01                     | 0.42              |
| 2:3D:195:ASN:HD22  | 2:3D:195:ASN:HA    | 1.64                     | 0.42              |
| 1:4A:430:LYS:O     | 1:4A:433:GLU:HG3   | 2.19                     | 0.42              |
| 1:4C:102:ASN:ND2   | 1:4C:105:ARG:HD3   | 2.27                     | 0.42              |
| 1:4C:311:LYS:H     | 1:4C:382:THR:HG22  | 1.84                     | 0.42              |
| 1:4E:172:TYR:HB3   | 1:4E:205:ASP:OD2   | 2.19                     | 0.42              |
| 1:5A:245:ASP:N     | 1:5A:245:ASP:OD1   | 2.51                     | 0.42              |
| 2:5B:127:CYS:SG    | 2:5B:130:LEU:HB3   | 2.59                     | 0.42              |
| 2:5D:216:LYS:HD3   | 2:5D:216:LYS:HA    | 1.89                     | 0.42              |
| 2:5D:257:MET:HE1   | 2:5D:313:VAL:C     | 2.45                     | 0.42              |
| 1:5E:172:TYR:CE2   | 1:5E:391:LEU:HD13  | 2.54                     | 0.42              |
| 1:6C:91:GLN:HA     | 1:6C:121:ARG:NH1   | 2.34                     | 0.42              |
| 2:7B:384:GLN:OE1   | 1:7C:348:PRO:HB2   | 2.19                     | 0.42              |
| 2:8B:190:HIS:NE2   | 2:8B:414:ASN:OD1   | 2.52                     | 0.42              |
| 2:9B:67:ASP:O      | 2:9B:92:PHE:HA     | 2.19                     | 0.42              |
| 2:9B:213:ARG:CZ    | 2:9B:297:LYS:HE3   | 2.48                     | 0.42              |
| 1:9E:205:ASP:O     | 1:9E:209:ILE:HG12  | 2.19                     | 0.42              |
| 1:9E:286:LEU:HA    | 1:9E:290:GLU:OE1   | 2.20                     | 0.42              |
| 1:10A:69:ASP:CG    | 1:10A:71:GLU:H     | 2.27                     | 0.42              |
| 1:10A:372:GLN:OE1  | 1:10A:372:GLN:N    | 2.51                     | 0.42              |
| 2:10B:2:ARG:N      | 2:10B:3:GLU:OE1    | 2.53                     | 0.42              |
| 2:10B:190:HIS:HD2  | 2:10B:414:ASN:HB2  | 1.83                     | 0.42              |
| 1:10C:315:CYS:HA   | 1:10C:379:SER:HA   | 2.01                     | 0.42              |
| 2:11B:289:LEU:HD23 | 2:11B:365:ALA:HB2  | 2.00                     | 0.42              |
| 1:11E:129:CYS:SG   | 1:11E:132:LEU:HB2  | 2.60                     | 0.42              |
| 2:12B:61:PRO:HD3   | 2:12B:84:ILE:CG2   | 2.47                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:12B:131:GLN:O    | 2:12B:162:ARG:HB2  | 2.18                     | 0.42              |
| 2:12B:423:GLN:HG3  | 2:12B:424:GLN:H    | 1.84                     | 0.42              |
| 1:12C:405:VAL:HG22 | 1:12C:409:VAL:HG23 | 2.01                     | 0.42              |
| 2:12D:371:SER:O    | 2:12D:374:ILE:HG12 | 2.19                     | 0.42              |
| 1:13A:31:GLN:HG3   | 1:13A:32:PRO:HD2   | 2.00                     | 0.42              |
| 1:1C:201:ALA:O     | 1:1C:268:PRO:HD2   | 2.18                     | 0.42              |
| 2:2B:73:MET:HA     | 2:2B:76:VAL:HG12   | 2.01                     | 0.42              |
| 2:2B:279:GLN:H     | 2:2B:279:GLN:HG3   | 1.68                     | 0.42              |
| 1:2C:56:THR:HG21   | 1:3C:283:HIS:O     | 2.19                     | 0.42              |
| 1:2E:265:ILE:HG23  | 1:2E:432:TYR:CE2   | 2.55                     | 0.42              |
| 1:3C:316:CYS:SG    | 1:3C:352:LYS:HB3   | 2.59                     | 0.42              |
| 1:3E:113:GLU:N     | 1:3E:113:GLU:OE2   | 2.53                     | 0.42              |
| 1:3E:147:SER:HB2   | 1:3E:190:THR:CG2   | 2.49                     | 0.42              |
| 2:4B:4:ILE:HG13    | 2:4B:132:GLY:C     | 2.44                     | 0.42              |
| 1:4C:47:ASP:HB3    | 1:4C:48:SER:H      | 1.60                     | 0.42              |
| 1:5E:269:LEU:HD11  | 1:5E:384:ILE:HB    | 2.02                     | 0.42              |
| 1:5E:370:LYS:HB3   | 1:5E:370:LYS:HE3   | 1.74                     | 0.42              |
| 2:6B:213:ARG:HE    | 2:6B:213:ARG:HB3   | 1.54                     | 0.42              |
| 1:6E:125:LEU:HD23  | 1:6E:125:LEU:HA    | 1.90                     | 0.42              |
| 1:7A:245:ASP:OD1   | 1:7A:245:ASP:N     | 2.50                     | 0.42              |
| 2:7D:294:PHE:HE1   | 2:7D:341:PHE:HZ    | 1.68                     | 0.42              |
| 1:8A:323:VAL:HG23  | 1:8A:355:ILE:HG23  | 2.00                     | 0.42              |
| 1:8C:67:PHE:HB2    | 1:8C:92:LEU:HD23   | 2.01                     | 0.42              |
| 1:9C:9:VAL:HG11    | 1:9C:150:THR:OG1   | 2.20                     | 0.42              |
| 1:9C:315:CYS:HA    | 1:9C:379:SER:HA    | 2.02                     | 0.42              |
| 2:9D:317:PHE:HB3   | 2:9D:321:MET:SD    | 2.60                     | 0.42              |
| 1:9E:316:CYS:SG    | 1:9E:352:LYS:HB3   | 2.60                     | 0.42              |
| 1:9E:319:TYR:CD2   | 1:9E:375:VAL:HG22  | 2.53                     | 0.42              |
| 1:10A:165:SER:HA   | 1:10A:199:ASP:OD2  | 2.20                     | 0.42              |
| 1:10A:339:ARG:O    | 1:10A:342:GLN:NE2  | 2.53                     | 0.42              |
| 1:10C:210:TYR:CE1  | 1:10C:227:LEU:HD21 | 2.54                     | 0.42              |
| 2:11B:13:GLY:O     | 2:11B:17:GLY:N     | 2.48                     | 0.42              |
| 2:11D:317:PHE:HB3  | 2:11D:321:MET:SD   | 2.60                     | 0.42              |
| 1:11E:3:GLU:OE1    | 1:11E:3:GLU:N      | 2.53                     | 0.42              |
| 1:12A:206:ASN:O    | 1:12A:209:ILE:HB   | 2.20                     | 0.42              |
| 2:12B:414:ASN:O    | 2:12B:418:LEU:N    | 2.34                     | 0.42              |
| 1:12E:302:MET:HG3  | 1:12E:302:MET:O    | 2.20                     | 0.42              |
| 2:13B:6:HIS:HD1    | 2:13B:21:TRP:NE1   | 2.17                     | 0.42              |
| 1:1A:121:ARG:HH21  | 1:1A:125:LEU:HG    | 1.84                     | 0.42              |
| 1:1A:322:ASP:H     | 1:1A:373:ARG:HG2   | 1.84                     | 0.42              |
| 1:1C:367:ASP:OD1   | 1:1C:367:ASP:N     | 2.43                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:2B:213:ARG:NE    | 2:2B:297:LYS:HD2   | 2.34                     | 0.42              |
| 1:2C:4:CYS:SG      | 1:2C:133:GLN:HB2   | 2.59                     | 0.42              |
| 1:2E:118:VAL:O     | 1:2E:122:ILE:N     | 2.47                     | 0.42              |
| 1:2E:184:PRO:O     | 1:2E:188:ILE:HG12  | 2.19                     | 0.42              |
| 1:3C:21:TRP:HZ3    | 1:3C:53:PHE:CE1    | 2.38                     | 0.42              |
| 1:3C:119:LEU:O     | 1:3C:123:ARG:HG2   | 2.19                     | 0.42              |
| 1:3C:338:LYS:HD3   | 1:3C:338:LYS:HA    | 1.75                     | 0.42              |
| 1:4E:172:TYR:CG    | 1:4E:173:PRO:HD2   | 2.54                     | 0.42              |
| 1:4E:173:PRO:HG3   | 1:4E:187:SER:OG    | 2.19                     | 0.42              |
| 2:5B:219:THR:HG22  | 1:5C:326:LYS:HE2   | 2.01                     | 0.42              |
| 2:5D:326:VAL:O     | 2:5D:330:MET:HG2   | 2.19                     | 0.42              |
| 1:5E:201:ALA:O     | 1:5E:268:PRO:HD2   | 2.19                     | 0.42              |
| 1:6C:63:PRO:HD3    | 1:6C:86:LEU:HG     | 2.01                     | 0.42              |
| 2:6D:212:PHE:CE1   | 2:6D:220:PRO:HG3   | 2.54                     | 0.42              |
| 1:7A:188:ILE:HG23  | 1:7A:425:LEU:HD12  | 2.01                     | 0.42              |
| 1:7A:413:MET:HE2   | 1:7A:413:MET:HB3   | 1.90                     | 0.42              |
| 1:7C:255:PHE:CZ    | 1:7C:378:LEU:HD11  | 2.54                     | 0.42              |
| 2:7D:73:MET:HG3    | 2:7D:92:PHE:HD1    | 1.83                     | 0.42              |
| 1:8C:208:ALA:O     | 1:8C:212:ILE:HG13  | 2.20                     | 0.42              |
| 2:10B:61:PRO:CD    | 2:10B:84:ILE:HG22  | 2.44                     | 0.42              |
| 1:10C:69:ASP:CG    | 1:10C:71:GLU:H     | 2.28                     | 0.42              |
| 1:11A:271:THR:HG22 | 1:11A:377:MET:SD   | 2.60                     | 0.42              |
| 1:11C:420:GLU:O    | 1:11C:424:ASP:N    | 2.37                     | 0.42              |
| 1:11E:47:ASP:HB3   | 1:11E:48:SER:H     | 1.68                     | 0.42              |
| 1:12A:195:LEU:HD21 | 1:12A:264:ARG:HG2  | 2.02                     | 0.42              |
| 1:12A:220:GLU:OE1  | 1:12A:220:GLU:N    | 2.51                     | 0.42              |
| 2:12B:411:ALA:O    | 2:12B:415:MET:HG3  | 2.19                     | 0.42              |
| 1:12C:201:ALA:O    | 1:12C:268:PRO:HD2  | 2.19                     | 0.42              |
| 2:12D:406:MET:N    | 2:12D:406:MET:SD   | 2.92                     | 0.42              |
| 1:12E:265:ILE:HG23 | 1:12E:432:TYR:OH   | 2.18                     | 0.42              |
| 1:13A:7:ILE:HG22   | 1:13A:9:VAL:HG23   | 2.02                     | 0.42              |
| 1:13C:327:ASP:O    | 1:13C:331:ALA:N    | 2.42                     | 0.42              |
| 1:13C:338:LYS:HD3  | 1:13C:338:LYS:HA   | 1.70                     | 0.42              |
| 2:13D:313:VAL:HA   | 2:13D:369:GLY:HA2  | 2.00                     | 0.42              |
| 1:13E:224:TYR:HA   | 1:13E:227:LEU:HD13 | 2.01                     | 0.42              |
| 1:1E:88:HIS:HD2    | 1:2E:283:HIS:HB3   | 1.82                     | 0.42              |
| 1:1E:367:ASP:OD1   | 1:1E:367:ASP:N     | 2.41                     | 0.42              |
| 2:3B:152:ILE:HG22  | 2:3B:195:ASN:HB3   | 2.01                     | 0.42              |
| 2:4B:173:PRO:HB3   | 2:4B:384:GLN:HE21  | 1.83                     | 0.42              |
| 1:4C:98:ASP:OD1    | 1:4C:145:THR:OG1   | 2.32                     | 0.42              |
| 2:4D:420:SER:O     | 2:4D:423:GLN:HG3   | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:5C:338:LYS:HD3   | 1:5C:338:LYS:HA    | 1.73                     | 0.42              |
| 1:6E:201:ALA:O     | 1:6E:268:PRO:HD2   | 2.20                     | 0.42              |
| 1:7A:407:TRP:O     | 1:7A:411:GLU:HG2   | 2.19                     | 0.42              |
| 2:7B:69:GLU:HG3    | 2:7B:96:GLY:HA2    | 2.01                     | 0.42              |
| 1:7C:10:GLY:O      | 1:7C:14:VAL:HG23   | 2.20                     | 0.42              |
| 2:7D:208:TYR:HE1   | 2:7D:225:LEU:HD11  | 1.84                     | 0.42              |
| 1:7E:298:PRO:HB3   | 1:7E:307:PRO:HD2   | 2.00                     | 0.42              |
| 2:8B:388:MET:HE1   | 1:8C:348:PRO:CD    | 2.49                     | 0.42              |
| 1:8C:134:GLY:HA3   | 1:8C:165:SER:O     | 2.19                     | 0.42              |
| 2:8D:130:LEU:HD23  | 2:8D:130:LEU:H     | 1.85                     | 0.42              |
| 2:8D:213:ARG:NE    | 2:8D:297:LYS:HE3   | 2.34                     | 0.42              |
| 1:8E:205:ASP:HB2   | 1:8E:303:VAL:HG22  | 2.01                     | 0.42              |
| 1:9A:121:ARG:HB3   | 1:9A:121:ARG:CZ    | 2.49                     | 0.42              |
| 1:9A:203:MET:HE2   | 1:9A:203:MET:HB2   | 1.96                     | 0.42              |
| 1:9C:195:LEU:HD21  | 1:9C:264:ARG:HE    | 1.84                     | 0.42              |
| 1:9C:344:VAL:HG11  | 1:9C:346:TRP:CZ2   | 2.55                     | 0.42              |
| 2:9D:317:PHE:CD2   | 2:9D:321:MET:HE1   | 2.55                     | 0.42              |
| 1:9E:177:VAL:HB    | 1:9E:207:GLU:HB3   | 2.01                     | 0.42              |
| 2:10B:317:PHE:CD2  | 2:10B:321:MET:HE1  | 2.54                     | 0.42              |
| 1:10C:9:VAL:HG11   | 1:10C:150:THR:OG1  | 2.19                     | 0.42              |
| 1:10C:398:MET:HE2  | 2:10D:346:PRO:HD2  | 2.02                     | 0.42              |
| 2:10D:5:VAL:HG12   | 2:10D:62:ARG:HG2   | 2.02                     | 0.42              |
| 2:10D:311:LEU:HD23 | 2:10D:342:VAL:HG21 | 2.02                     | 0.42              |
| 1:10E:8:HIS:CD2    | 1:10E:67:PHE:HE1   | 2.37                     | 0.42              |
| 1:10E:303:VAL:O    | 1:10E:305:CYS:N    | 2.52                     | 0.42              |
| 1:13A:3:GLU:HB2    | 1:13A:64:ARG:HH12  | 1.85                     | 0.42              |
| 1:13A:105:ARG:NE   | 1:13A:411:GLU:HG3  | 2.35                     | 0.42              |
| 2:13B:218:THR:HG23 | 2:13B:219:THR:HG23 | 2.01                     | 0.42              |
| 1:13C:31:GLN:HG3   | 1:13C:32:PRO:HD2   | 2.00                     | 0.42              |
| 1:1E:173:PRO:HG3   | 1:1E:187:SER:OG    | 2.19                     | 0.42              |
| 2:2D:143:THR:HB    | 5:2D:600:GDP:O3B   | 2.19                     | 0.42              |
| 1:2E:102:ASN:ND2   | 1:2E:105:ARG:HD3   | 2.21                     | 0.42              |
| 1:3C:21:TRP:HZ3    | 1:3C:53:PHE:HE1    | 1.68                     | 0.42              |
| 2:4B:265:PHE:C     | 2:4B:266:PHE:HD1   | 2.28                     | 0.42              |
| 1:4C:56:THR:HA     | 1:5C:285:GLN:HB2   | 2.00                     | 0.42              |
| 2:4D:304:ASP:HB2   | 2:4D:307:HIS:CD2   | 2.55                     | 0.42              |
| 1:5A:49:PHE:HD2    | 1:5A:53:PHE:HB2    | 1.85                     | 0.42              |
| 2:5B:299:MET:HE2   | 2:5B:299:MET:HB2   | 1.91                     | 0.42              |
| 1:5C:91:GLN:HA     | 1:5C:121:ARG:HH12  | 1.84                     | 0.42              |
| 1:5E:338:LYS:HD3   | 1:5E:338:LYS:HA    | 1.73                     | 0.42              |
| 2:6D:358:PRO:HG2   | 2:6D:364:SER:OG    | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:6E:171:ILE:HD11  | 1:6E:206:ASN:OD1   | 2.20                     | 0.42              |
| 1:7A:251:ASP:O     | 1:7A:255:PHE:HB2   | 2.19                     | 0.42              |
| 2:7B:302:ALA:HB3   | 2:7B:377:LEU:HD21  | 2.01                     | 0.42              |
| 1:7C:378:LEU:HD12  | 1:7C:378:LEU:O     | 2.19                     | 0.42              |
| 2:7D:116:VAL:HG23  | 2:7D:117:LEU:HD12  | 2.02                     | 0.42              |
| 1:7E:102:ASN:HB3   | 1:7E:105:ARG:H     | 1.85                     | 0.42              |
| 1:8A:70:LEU:HD12   | 1:8A:114:ILE:HD12  | 2.00                     | 0.42              |
| 2:8B:324:LYS:HG3   | 2:8B:325:GLU:N     | 2.34                     | 0.42              |
| 2:9B:267:MET:HG3   | 2:9B:374:ILE:HD11  | 2.02                     | 0.42              |
| 2:9D:95:SER:OG     | 2:9D:96:GLY:N      | 2.52                     | 0.42              |
| 1:9E:326:LYS:HG3   | 1:9E:327:ASP:N     | 2.35                     | 0.42              |
| 1:10A:168:GLU:O    | 1:10A:202:PHE:HB2  | 2.20                     | 0.42              |
| 1:10C:168:GLU:HG2  | 1:10C:201:ALA:HA   | 2.02                     | 0.42              |
| 1:10C:220:GLU:HG2  | 1:10C:221:ARG:H    | 1.84                     | 0.42              |
| 2:11B:379:LYS:HA   | 2:11B:382:SER:HB3  | 2.01                     | 0.42              |
| 1:11C:202:PHE:CE1  | 1:11C:378:LEU:HD23 | 2.54                     | 0.42              |
| 2:11D:334:GLN:HE22 | 2:11D:347:ASN:HA   | 1.84                     | 0.42              |
| 2:12B:175:VAL:HG13 | 1:12C:329:ASN:ND2  | 2.34                     | 0.42              |
| 2:12D:303:CYS:SG   | 2:12D:376:GLU:HG3  | 2.60                     | 0.42              |
| 2:12D:371:SER:OG   | 2:12D:372:THR:N    | 2.52                     | 0.42              |
| 1:12E:98:ASP:OD1   | 1:12E:98:ASP:N     | 2.53                     | 0.42              |
| 1:13A:5:ILE:O      | 1:13A:135:PHE:HA   | 2.19                     | 0.42              |
| 1:13C:212:ILE:O    | 1:13C:216:ASN:HB2  | 2.20                     | 0.42              |
| 1:13C:328:VAL:HA   | 1:13C:331:ALA:HB3  | 2.01                     | 0.42              |
| 2:13D:6:HIS:HD1    | 2:13D:21:TRP:HE1   | 1.68                     | 0.42              |
| 2:13D:138:SER:HA   | 2:13D:169:VAL:HG12 | 2.02                     | 0.42              |
| 2:13D:176:SER:OG   | 1:13E:349:THR:HG21 | 2.20                     | 0.42              |
| 1:1A:31:GLN:HE21   | 1:1A:31:GLN:HB3    | 1.72                     | 0.42              |
| 2:1D:299:MET:HE3   | 2:1D:299:MET:HB2   | 1.82                     | 0.42              |
| 1:1E:121:ARG:HH21  | 1:1E:125:LEU:HG    | 1.84                     | 0.42              |
| 1:2E:103:TYR:CE1   | 1:2E:148:GLY:HA2   | 2.55                     | 0.42              |
| 1:3A:21:TRP:HZ3    | 1:3A:53:PHE:CE1    | 2.38                     | 0.42              |
| 2:3D:263:LEU:HG    | 2:3D:422:TYR:CE2   | 2.54                     | 0.42              |
| 1:4A:217:LEU:HD23  | 1:4A:367:ASP:OD2   | 2.20                     | 0.42              |
| 2:4B:141:GLY:HA3   | 5:4B:600:GDP:O3A   | 2.18                     | 0.42              |
| 1:5A:414:GLU:OE1   | 1:5A:416:GLY:N     | 2.40                     | 0.42              |
| 1:6A:3:GLU:N       | 1:6A:3:GLU:OE2     | 2.52                     | 0.42              |
| 2:6B:100:ASN:HD22  | 2:6B:103:LYS:HG3   | 1.85                     | 0.42              |
| 1:6C:315:CYS:HA    | 1:6C:379:SER:HA    | 2.02                     | 0.42              |
| 1:6E:123:ARG:NE    | 1:6E:123:ARG:HA    | 2.35                     | 0.42              |
| 1:6E:189:LEU:HD21  | 1:6E:413:MET:HE1   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:7D:232:THR:HG21  | 2:7D:268:PRO:HB3  | 2.02                     | 0.42              |
| 1:7E:203:MET:SD    | 1:7E:203:MET:N    | 2.93                     | 0.42              |
| 2:8B:67:ASP:OD1    | 2:8B:68:LEU:N     | 2.52                     | 0.42              |
| 2:8B:114:ASP:OD1   | 2:8B:115:SER:N    | 2.53                     | 0.42              |
| 1:8C:269:LEU:HD13  | 1:8C:381:THR:HG22 | 2.01                     | 0.42              |
| 1:10A:185:TYR:HD2  | 1:10A:408:TYR:HE1 | 1.68                     | 0.42              |
| 2:10D:3:GLU:O      | 2:10D:130:LEU:HB2 | 2.20                     | 0.42              |
| 2:10D:45:GLU:C     | 2:10D:46:ARG:HD2  | 2.44                     | 0.42              |
| 1:10E:339:ARG:O    | 1:10E:342:GLN:NE2 | 2.53                     | 0.42              |
| 1:11A:3:GLU:OE2    | 1:11A:130:THR:N   | 2.52                     | 0.42              |
| 1:11A:175:PRO:HB3  | 1:11A:390:ARG:CZ  | 2.49                     | 0.42              |
| 1:11C:102:ASN:HD22 | 1:11C:105:ARG:CD  | 2.33                     | 0.42              |
| 2:11D:8:GLN:O      | 2:11D:66:VAL:HB   | 2.20                     | 0.42              |
| 1:11E:156:ARG:HD3  | 1:11E:156:ARG:N   | 2.34                     | 0.42              |
| 1:12C:210:TYR:CE2  | 2:12D:324:LYS:HB3 | 2.55                     | 0.42              |
| 2:13B:6:HIS:HD1    | 2:13B:21:TRP:HZ2  | 1.67                     | 0.42              |
| 1:13E:63:PRO:O     | 1:13E:91:GLN:NE2  | 2.48                     | 0.42              |
| 1:1A:205:ASP:O     | 1:1A:209:ILE:HG12 | 2.19                     | 0.42              |
| 2:1B:153:SER:HB2   | 2:1B:191:GLN:NE2  | 2.35                     | 0.42              |
| 2:1D:13:GLY:HA2    | 2:1D:136:THR:HG22 | 2.02                     | 0.42              |
| 2:1D:326:VAL:O     | 2:1D:330:MET:HG2  | 2.20                     | 0.42              |
| 1:1E:201:ALA:O     | 1:1E:268:PRO:HD2  | 2.19                     | 0.42              |
| 1:2A:221:ARG:HA    | 2:2B:324:LYS:CE   | 2.39                     | 0.42              |
| 1:2E:286:LEU:HA    | 1:2E:290:GLU:OE1  | 2.20                     | 0.42              |
| 1:3A:210:TYR:HE1   | 1:3A:227:LEU:HD11 | 1.85                     | 0.42              |
| 1:4C:73:THR:HG23   | 2:4D:2:ARG:HH22   | 1.85                     | 0.42              |
| 1:5E:3:GLU:OE1     | 1:5E:64:ARG:NE    | 2.53                     | 0.42              |
| 2:6B:310:TYR:O     | 2:6B:342:VAL:HG23 | 2.19                     | 0.42              |
| 1:6C:56:THR:HG23   | 1:7C:285:GLN:HB2  | 2.01                     | 0.42              |
| 2:6D:130:LEU:HD23  | 2:6D:130:LEU:H    | 1.85                     | 0.42              |
| 1:7A:173:PRO:HG3   | 1:7A:187:SER:OG   | 2.19                     | 0.42              |
| 1:8A:394:LYS:HG2   | 2:8B:346:PRO:HG3  | 2.00                     | 0.42              |
| 2:8B:20:PHE:HD1    | 2:8B:233:MET:HE3  | 1.85                     | 0.42              |
| 1:8C:71:GLU:HG2    | 1:8C:73:THR:H     | 1.85                     | 0.42              |
| 2:8D:391:ARG:HA    | 2:8D:391:ARG:HD3  | 1.73                     | 0.42              |
| 2:9B:317:PHE:CD2   | 2:9B:321:MET:HE1  | 2.54                     | 0.42              |
| 1:9C:245:ASP:OD1   | 1:9C:245:ASP:N    | 2.53                     | 0.42              |
| 1:9C:405:VAL:HG12  | 1:9C:409:VAL:HG23 | 2.02                     | 0.42              |
| 2:9D:303:CYS:SG    | 2:9D:377:LEU:HG   | 2.60                     | 0.42              |
| 1:9E:11:GLN:HG2    | 1:9E:15:GLN:HE22  | 1.85                     | 0.42              |
| 2:10B:404:ASP:O    | 2:10B:407:GLU:HB2 | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10D:4:ILE:HG23   | 2:10D:50:TYR:CE1   | 2.54                     | 0.42              |
| 2:10D:117:LEU:HD23 | 2:10D:117:LEU:HA   | 1.83                     | 0.42              |
| 2:10D:174:LYS:HB2  | 2:10D:174:LYS:HE2  | 1.86                     | 0.42              |
| 1:11A:291:ILE:HD12 | 1:11A:375:VAL:HG23 | 2.02                     | 0.42              |
| 1:11C:213:CYS:HB2  | 1:11C:219:ILE:CD1  | 2.47                     | 0.42              |
| 2:11D:326:VAL:O    | 2:11D:330:MET:N    | 2.48                     | 0.42              |
| 2:12D:27:GLU:CD    | 2:12D:241:ARG:HH21 | 2.28                     | 0.42              |
| 2:12D:226:ASN:OD1  | 5:12D:600:GDP:N1   | 2.53                     | 0.42              |
| 2:13B:8:GLN:OE1    | 2:13B:17:GLY:HA3   | 2.20                     | 0.42              |
| 2:13B:409:THR:HA   | 2:13B:412:GLU:HB3  | 2.02                     | 0.42              |
| 1:13C:102:ASN:N    | 1:13C:144:GLY:HA3  | 2.34                     | 0.42              |
| 1:13C:359:PRO:HA   | 1:13C:360:PRO:HD3  | 1.96                     | 0.42              |
| 2:13D:4:ILE:HG23   | 2:13D:132:GLY:O    | 2.20                     | 0.42              |
| 2:13D:73:MET:HE3   | 2:13D:92:PHE:CG    | 2.55                     | 0.42              |
| 1:13E:70:LEU:CB    | 1:13E:98:ASP:HA    | 2.49                     | 0.42              |
| 1:1A:338:LYS:HA    | 1:1A:338:LYS:HD3   | 1.75                     | 0.42              |
| 1:1C:73:THR:O      | 1:1C:77:GLU:HG3    | 2.19                     | 0.42              |
| 1:2A:215:ARG:HH22  | 1:2A:299:ALA:HB1   | 1.84                     | 0.42              |
| 2:2B:12:CYS:SG     | 2:2B:13:GLY:N      | 2.93                     | 0.42              |
| 2:2B:127:CYS:SG    | 2:2B:130:LEU:HB3   | 2.60                     | 0.42              |
| 2:2B:209:ASP:CG    | 2:2B:213:ARG:HH21  | 2.28                     | 0.42              |
| 2:2B:371:SER:OG    | 2:2B:372:THR:N     | 2.53                     | 0.42              |
| 1:2C:139:HIS:HE1   | 1:2C:141:PHE:HE1   | 1.68                     | 0.42              |
| 1:3A:338:LYS:HD3   | 1:3A:338:LYS:HA    | 1.75                     | 0.42              |
| 2:3B:209:ASP:CG    | 2:3B:213:ARG:HH12  | 2.26                     | 0.42              |
| 1:3C:69:ASP:OD2    | 1:3C:74:VAL:HG22   | 2.19                     | 0.42              |
| 1:3C:102:ASN:HB2   | 1:3C:105:ARG:HB2   | 2.01                     | 0.42              |
| 1:3C:328:VAL:O     | 1:3C:332:ILE:HG12  | 2.20                     | 0.42              |
| 2:3D:152:ILE:HG22  | 2:3D:195:ASN:HB3   | 2.02                     | 0.42              |
| 2:3D:386:THR:O     | 2:3D:390:ARG:HG3   | 2.20                     | 0.42              |
| 2:4B:45:GLU:O      | 2:4B:46:ARG:NH1    | 2.51                     | 0.42              |
| 1:4C:144:GLY:O     | 1:4C:148:GLY:N     | 2.47                     | 0.42              |
| 1:4C:147:SER:HB2   | 1:4C:190:THR:CG2   | 2.50                     | 0.42              |
| 2:4D:68:LEU:HD12   | 2:4D:143:THR:HG23  | 2.01                     | 0.42              |
| 1:4E:425:LEU:HD23  | 1:4E:425:LEU:HA    | 1.87                     | 0.42              |
| 1:5E:186:ASN:O     | 1:5E:190:THR:HG23  | 2.19                     | 0.42              |
| 1:5E:213:CYS:O     | 1:5E:219:ILE:HG22  | 2.20                     | 0.42              |
| 1:6A:271:THR:HG22  | 1:6A:377:MET:HB3   | 2.02                     | 0.42              |
| 1:6A:338:LYS:HA    | 1:6A:338:LYS:HD3   | 1.74                     | 0.42              |
| 2:6B:45:GLU:O      | 2:6B:46:ARG:HD2    | 2.19                     | 0.42              |
| 1:6C:201:ALA:O     | 1:6C:268:PRO:HD2   | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:7B:285:THR:HB    | 2:7B:287:PRO:HD2   | 2.02                     | 0.42              |
| 1:7C:193:THR:O     | 1:7C:197:HIS:HB2   | 2.20                     | 0.42              |
| 2:8B:33:THR:O      | 2:8B:58:LYS:HE3    | 2.20                     | 0.42              |
| 2:8B:139:LEU:HD23  | 2:8B:170:VAL:HG23  | 2.01                     | 0.42              |
| 2:8D:3:GLU:OE1     | 2:8D:3:GLU:N       | 2.53                     | 0.42              |
| 2:8D:324:LYS:HG3   | 2:8D:325:GLU:N     | 2.34                     | 0.42              |
| 2:9D:5:VAL:HG12    | 2:9D:62:ARG:CD     | 2.50                     | 0.42              |
| 2:9D:114:ASP:OD1   | 2:9D:115:SER:N     | 2.52                     | 0.42              |
| 1:10A:203:MET:HE2  | 1:10A:203:MET:HB2  | 1.86                     | 0.42              |
| 2:10B:152:ILE:HG22 | 2:10B:195:ASN:HB3  | 2.02                     | 0.42              |
| 1:10E:8:HIS:CE1    | 1:10E:17:GLY:HA2   | 2.55                     | 0.42              |
| 1:11C:210:TYR:HA   | 1:11C:213:CYS:SG   | 2.60                     | 0.42              |
| 2:11D:98:GLY:HA2   | 1:11E:254:GLU:HB2  | 2.02                     | 0.42              |
| 2:11D:135:LEU:HD23 | 2:11D:152:ILE:HD11 | 2.02                     | 0.42              |
| 2:11D:280:GLN:OE1  | 2:11D:280:GLN:N    | 2.51                     | 0.42              |
| 1:11E:252:LEU:O    | 1:11E:256:GLN:HG2  | 2.20                     | 0.42              |
| 1:11E:276:ILE:HD11 | 1:11E:280:LYS:HB3  | 2.02                     | 0.42              |
| 1:11E:305:CYS:SG   | 1:11E:384:ILE:HA   | 2.60                     | 0.42              |
| 1:12A:315:CYS:HA   | 1:12A:379:SER:HA   | 2.01                     | 0.42              |
| 2:12B:99:ASN:ND2   | 1:12C:254:GLU:OE2  | 2.52                     | 0.42              |
| 1:12C:54:SER:HB2   | 1:12C:64:ARG:HH12  | 1.85                     | 0.42              |
| 2:12D:309:ARG:H    | 2:12D:372:THR:HG1  | 1.64                     | 0.42              |
| 1:13A:102:ASN:N    | 1:13A:144:GLY:HA3  | 2.34                     | 0.42              |
| 1:13A:115:VAL:HG22 | 1:13A:119:LEU:HD12 | 2.02                     | 0.42              |
| 1:13E:69:ASP:CG    | 1:13E:71:GLU:H     | 2.28                     | 0.42              |
| 1:13E:169:PHE:HE1  | 1:13E:235:VAL:HG22 | 1.83                     | 0.42              |
| 1:1A:377:MET:SD    | 1:1A:379:SER:HB3   | 2.59                     | 0.42              |
| 2:1D:164:MET:O     | 2:1D:197:ASP:HB2   | 2.19                     | 0.42              |
| 2:1D:190:HIS:HD2   | 2:1D:411:ALA:HA    | 1.84                     | 0.42              |
| 2:3B:130:LEU:H     | 2:3B:130:LEU:HD23  | 1.85                     | 0.42              |
| 2:3B:191:GLN:HE21  | 2:3B:195:ASN:HD22  | 1.66                     | 0.42              |
| 2:3B:285:THR:HG23  | 2:3B:287:PRO:HD2   | 2.01                     | 0.42              |
| 1:3C:144:GLY:O     | 1:3C:148:GLY:N     | 2.50                     | 0.42              |
| 2:4B:31:ASP:CG     | 2:4B:32:ALA:H      | 2.28                     | 0.42              |
| 2:4B:279:GLN:H     | 2:4B:279:GLN:HG3   | 1.70                     | 0.42              |
| 2:4D:100:ASN:HD22  | 2:4D:103:LYS:CD    | 2.33                     | 0.42              |
| 1:5A:210:TYR:CE2   | 1:5A:227:LEU:HD11  | 2.55                     | 0.42              |
| 1:5C:377:MET:SD    | 1:5C:379:SER:HB3   | 2.60                     | 0.42              |
| 1:5E:251:ASP:H     | 1:5E:254:GLU:HB3   | 1.83                     | 0.42              |
| 2:6B:11:GLN:N      | 5:6B:600:GDP:O2B   | 2.47                     | 0.42              |
| 1:7A:221:ARG:C     | 2:7B:324:LYS:HZ1   | 2.28                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7E:115:VAL:HG22  | 1:7E:119:LEU:HD12  | 2.00                     | 0.42              |
| 1:8A:56:THR:HG23   | 1:9A:285:GLN:HA    | 2.02                     | 0.42              |
| 2:8D:371:SER:OG    | 2:8D:372:THR:N     | 2.52                     | 0.42              |
| 1:9A:407:TRP:NE1   | 2:9B:255:VAL:HA    | 2.35                     | 0.42              |
| 1:9E:287:SER:O     | 1:9E:291:ILE:HG12  | 2.19                     | 0.42              |
| 1:11C:165:SER:HA   | 1:11C:199:ASP:OD2  | 2.20                     | 0.41              |
| 2:11D:31:ASP:CG    | 2:11D:32:ALA:H     | 2.28                     | 0.41              |
| 2:12B:5:VAL:HG22   | 2:12B:133:PHE:CD1  | 2.55                     | 0.41              |
| 2:12B:28:HIS:NE2   | 2:12B:241:ARG:HD2  | 2.35                     | 0.41              |
| 2:12B:97:ALA:O     | 2:12B:100:ASN:ND2  | 2.52                     | 0.41              |
| 1:12C:54:SER:CB    | 1:12C:64:ARG:HH22  | 2.33                     | 0.41              |
| 1:12C:90:GLU:OE2   | 1:12C:90:GLU:N     | 2.44                     | 0.41              |
| 2:13B:387:ALA:HB1  | 2:13B:391:ARG:HH21 | 1.85                     | 0.41              |
| 1:13C:405:VAL:HG12 | 1:13C:409:VAL:HG23 | 2.01                     | 0.41              |
| 2:13D:8:GLN:CD     | 2:13D:17:GLY:HA3   | 2.44                     | 0.41              |
| 1:1A:201:ALA:O     | 1:1A:268:PRO:HD2   | 2.20                     | 0.41              |
| 1:1A:202:PHE:HE1   | 1:1A:378:LEU:HD23  | 1.84                     | 0.41              |
| 2:1B:203:ASP:O     | 2:1B:207:LEU:HD13  | 2.19                     | 0.41              |
| 1:1C:271:THR:HG22  | 1:1C:377:MET:HE3   | 2.02                     | 0.41              |
| 1:1C:338:LYS:HA    | 1:1C:338:LYS:HD3   | 1.74                     | 0.41              |
| 1:1E:27:GLU:OE1    | 1:1E:243:ARG:NH2   | 2.52                     | 0.41              |
| 1:2C:5:ILE:HB      | 1:2C:135:PHE:HD1   | 1.84                     | 0.41              |
| 1:2E:186:ASN:O     | 1:2E:190:THR:HG23  | 2.20                     | 0.41              |
| 1:2E:201:ALA:O     | 1:2E:268:PRO:HD2   | 2.19                     | 0.41              |
| 1:2E:338:LYS:HD3   | 1:2E:338:LYS:HA    | 1.76                     | 0.41              |
| 1:3A:174:ALA:HB1   | 1:3A:207:GLU:OE1   | 2.19                     | 0.41              |
| 1:3A:259:LEU:HD21  | 1:3A:380:ASN:HB2   | 2.01                     | 0.41              |
| 2:3D:131:GLN:OE1   | 2:3D:131:GLN:N     | 2.53                     | 0.41              |
| 1:3E:269:LEU:HD11  | 1:3E:384:ILE:HB    | 2.02                     | 0.41              |
| 1:3E:338:LYS:HA    | 1:3E:338:LYS:HD3   | 1.75                     | 0.41              |
| 1:4C:169:PHE:CE2   | 1:4C:235:VAL:HG22  | 2.55                     | 0.41              |
| 2:4D:183:TYR:CE1   | 2:4D:388:MET:HB3   | 2.55                     | 0.41              |
| 2:4D:398:TYR:HB3   | 2:4D:403:MET:HE3   | 2.02                     | 0.41              |
| 1:4E:313:MET:HB3   | 1:4E:380:ASN:O     | 2.20                     | 0.41              |
| 1:5C:239:THR:OG1   | 1:5C:243:ARG:NH1   | 2.52                     | 0.41              |
| 2:5D:111:GLU:OE1   | 2:5D:111:GLU:N     | 2.53                     | 0.41              |
| 2:5D:392:LYS:HB3   | 2:5D:395:LEU:HD23  | 2.02                     | 0.41              |
| 1:5E:315:CYS:HA    | 1:5E:379:SER:HA    | 2.02                     | 0.41              |
| 1:6E:91:GLN:HA     | 1:6E:121:ARG:NH1   | 2.34                     | 0.41              |
| 2:7B:64:VAL:HG21   | 2:7B:120:VAL:HG12  | 2.02                     | 0.41              |
| 1:7C:47:ASP:HB3    | 1:7C:48:SER:H      | 1.60                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:28:HIS:CE1    | 2:8B:241:ARG:HD2   | 2.55                     | 0.41              |
| 2:8B:313:VAL:HA    | 2:8B:369:GLY:HA2   | 2.01                     | 0.41              |
| 2:8D:3:GLU:OE2     | 2:8D:127:CYS:HB2   | 2.20                     | 0.41              |
| 2:8D:175:VAL:HG23  | 2:8D:205:GLU:HG3   | 2.01                     | 0.41              |
| 1:9A:205:ASP:O     | 1:9A:209:ILE:HG12  | 2.20                     | 0.41              |
| 1:9C:287:SER:O     | 1:9C:290:GLU:HG3   | 2.19                     | 0.41              |
| 1:10A:209:ILE:HG23 | 1:10A:230:LEU:HD22 | 2.03                     | 0.41              |
| 1:10A:269:LEU:HD11 | 1:10A:384:ILE:HB   | 2.01                     | 0.41              |
| 1:11A:104:ALA:HB2  | 1:11A:408:TYR:HB3  | 2.02                     | 0.41              |
| 1:11A:184:PRO:O    | 1:11A:188:ILE:HG12 | 2.20                     | 0.41              |
| 2:11B:167:TYR:HA   | 2:11B:200:TYR:HB2  | 2.00                     | 0.41              |
| 2:11B:372:THR:HG21 | 2:11B:426:GLN:HA   | 2.02                     | 0.41              |
| 1:11C:270:VAL:HA   | 1:11C:377:MET:O    | 2.19                     | 0.41              |
| 2:11D:292:GLN:NE2  | 2:11D:298:ASN:HD22 | 2.09                     | 0.41              |
| 1:12A:265:ILE:HD11 | 1:12A:435:VAL:HG21 | 2.02                     | 0.41              |
| 1:12E:8:HIS:CD2    | 1:12E:67:PHE:HE1   | 2.38                     | 0.41              |
| 2:13D:374:ILE:O    | 2:13D:377:LEU:HB2  | 2.20                     | 0.41              |
| 1:13E:231:ILE:O    | 1:13E:235:VAL:HG23 | 2.21                     | 0.41              |
| 1:13E:421:ALA:O    | 1:13E:425:LEU:N    | 2.41                     | 0.41              |
| 1:1A:265:ILE:HG23  | 1:1A:432:TYR:CZ    | 2.55                     | 0.41              |
| 1:1A:398:MET:HE3   | 2:1B:345:ILE:HG12  | 2.01                     | 0.41              |
| 2:1B:117:LEU:HD23  | 2:1B:117:LEU:HA    | 1.83                     | 0.41              |
| 1:1C:191:THR:O     | 1:1C:195:LEU:HB2   | 2.20                     | 0.41              |
| 1:1C:329:ASN:C     | 1:1C:329:ASN:HD22  | 2.28                     | 0.41              |
| 2:1D:220:PRO:HD2   | 1:1E:326:LYS:CD    | 2.44                     | 0.41              |
| 2:1D:406:MET:O     | 2:1D:410:GLU:HG3   | 2.20                     | 0.41              |
| 1:2C:35:GLN:O      | 1:2C:37:PRO:HD3    | 2.20                     | 0.41              |
| 1:2C:215:ARG:HH22  | 1:2C:299:ALA:HB1   | 1.84                     | 0.41              |
| 1:3C:425:LEU:HD23  | 1:3C:425:LEU:HA    | 1.89                     | 0.41              |
| 2:4B:183:TYR:CE1   | 2:4B:388:MET:HB3   | 2.55                     | 0.41              |
| 1:4E:9:VAL:HG12    | 1:4E:146:GLY:HA2   | 2.02                     | 0.41              |
| 1:6C:222:PRO:CD    | 2:6D:324:LYS:HD2   | 2.50                     | 0.41              |
| 1:6C:332:ILE:HD12  | 1:6C:351:PHE:CE2   | 2.56                     | 0.41              |
| 2:6D:390:ARG:O     | 2:6D:392:LYS:NZ    | 2.53                     | 0.41              |
| 1:7A:31:GLN:HG3    | 1:7A:32:PRO:HD2    | 2.02                     | 0.41              |
| 1:7A:414:GLU:OE1   | 1:7A:416:GLY:N     | 2.36                     | 0.41              |
| 1:7C:119:LEU:O     | 1:7C:123:ARG:HG2   | 2.20                     | 0.41              |
| 1:8A:205:ASP:HB2   | 1:8A:303:VAL:HG22  | 2.02                     | 0.41              |
| 1:8A:245:ASP:OD1   | 1:8A:245:ASP:N     | 2.53                     | 0.41              |
| 2:8B:117:LEU:HA    | 2:8B:117:LEU:HD23  | 1.84                     | 0.41              |
| 2:8B:167:TYR:CE2   | 2:8B:233:MET:HG2   | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:8B:285:THR:CG2   | 2:8B:287:PRO:HD2   | 2.49                     | 0.41              |
| 2:8D:164:MET:HE2   | 2:8D:164:MET:HB2   | 1.79                     | 0.41              |
| 2:8D:190:HIS:CD2   | 2:8D:414:ASN:HD22  | 2.38                     | 0.41              |
| 1:8E:103:TYR:HD2   | 1:8E:147:SER:HB2   | 1.84                     | 0.41              |
| 1:8E:172:TYR:HE1   | 1:8E:391:LEU:HD13  | 1.85                     | 0.41              |
| 1:8E:255:PHE:CE2   | 1:8E:259:LEU:HD22  | 2.55                     | 0.41              |
| 1:9A:151:SER:OG    | 1:9A:193:THR:HG21  | 2.20                     | 0.41              |
| 1:10A:142:GLY:O    | 1:10A:186:ASN:ND2  | 2.53                     | 0.41              |
| 1:12A:50:ASN:HA    | 1:12A:53:PHE:O     | 2.20                     | 0.41              |
| 1:12A:106:GLY:CA   | 1:12A:148:GLY:HA3  | 2.48                     | 0.41              |
| 1:12A:306:ASP:OD1  | 1:12A:306:ASP:N    | 2.53                     | 0.41              |
| 2:12B:256:ASN:C    | 2:12B:350:LYS:HZ1  | 2.27                     | 0.41              |
| 1:12C:129:CYS:SG   | 1:12C:132:LEU:HB2  | 2.60                     | 0.41              |
| 1:12C:225:THR:O    | 1:12C:229:ARG:HG3  | 2.20                     | 0.41              |
| 1:13A:3:GLU:OE2    | 1:13A:131:GLY:N    | 2.46                     | 0.41              |
| 1:13A:21:TRP:CH2   | 1:13A:52:PHE:HB3   | 2.55                     | 0.41              |
| 1:13A:50:ASN:O     | 1:13A:64:ARG:NH2   | 2.53                     | 0.41              |
| 1:13A:145:THR:OG1  | 1:13A:146:GLY:N    | 2.53                     | 0.41              |
| 2:13B:381:ILE:O    | 2:13B:384:GLN:HB2  | 2.20                     | 0.41              |
| 1:13E:291:ILE:HD12 | 1:13E:375:VAL:HG23 | 2.01                     | 0.41              |
| 1:1C:102:ASN:HB3   | 1:1C:105:ARG:HB2   | 2.02                     | 0.41              |
| 1:2A:193:THR:O     | 1:2A:197:HIS:HB2   | 2.20                     | 0.41              |
| 1:3A:91:GLN:HG2    | 1:3A:121:ARG:HH22  | 1.85                     | 0.41              |
| 1:3A:303:VAL:O     | 1:3A:305:CYS:N     | 2.53                     | 0.41              |
| 1:3C:356:ASN:OD1   | 1:3C:357:TYR:N     | 2.53                     | 0.41              |
| 2:4B:111:GLU:OE1   | 2:4B:111:GLU:N     | 2.53                     | 0.41              |
| 1:5E:225:THR:O     | 1:5E:229:ARG:HG3   | 2.19                     | 0.41              |
| 2:6B:163:ILE:HA    | 2:6B:197:ASP:OD2   | 2.21                     | 0.41              |
| 1:6C:121:ARG:HH21  | 1:6C:125:LEU:HG    | 1.86                     | 0.41              |
| 2:6D:356:ILE:HD12  | 2:6D:357:PRO:HD2   | 2.02                     | 0.41              |
| 1:6E:401:LYS:HA    | 1:6E:401:LYS:HD3   | 1.78                     | 0.41              |
| 2:8B:172:SER:HB2   | 2:8B:205:GLU:OE1   | 2.19                     | 0.41              |
| 1:8C:174:ALA:HB1   | 1:8C:207:GLU:OE2   | 2.20                     | 0.41              |
| 1:8C:175:PRO:HD2   | 1:8C:207:GLU:OE2   | 2.20                     | 0.41              |
| 2:8D:114:ASP:OD1   | 2:8D:115:SER:N     | 2.53                     | 0.41              |
| 2:8D:167:TYR:CG    | 2:8D:233:MET:HE1   | 2.55                     | 0.41              |
| 1:9A:169:PHE:HE2   | 1:9A:235:VAL:HG13  | 1.86                     | 0.41              |
| 1:9C:140:SER:OG    | 3:9C:500:GTP:O2A   | 2.33                     | 0.41              |
| 2:9D:268:PRO:HG2   | 2:9D:300:MET:HB3   | 2.03                     | 0.41              |
| 2:10B:215:LEU:HD23 | 2:10B:215:LEU:O    | 2.20                     | 0.41              |
| 2:10D:220:PRO:HD2  | 1:10E:326:LYS:CD   | 2.48                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:10D:415:MET:HE2  | 2:10D:415:MET:HB3  | 1.87                     | 0.41              |
| 1:11C:156:ARG:HD3  | 1:11C:156:ARG:N    | 2.34                     | 0.41              |
| 1:12A:205:ASP:OD1  | 1:12A:206:ASN:N    | 2.51                     | 0.41              |
| 2:12B:109:GLY:O    | 2:12B:113:VAL:HB   | 2.20                     | 0.41              |
| 2:13B:405:GLU:HA   | 2:13B:408:PHE:CE1  | 2.55                     | 0.41              |
| 1:13C:3:GLU:OE2    | 1:13C:131:GLY:N    | 2.48                     | 0.41              |
| 1:13C:31:GLN:HG2   | 1:13C:32:PRO:HD2   | 2.00                     | 0.41              |
| 2:13D:228:LEU:HD23 | 2:13D:300:MET:HE1  | 2.02                     | 0.41              |
| 2:1B:164:MET:N     | 2:1B:197:ASP:OD2   | 2.52                     | 0.41              |
| 1:1C:177:VAL:HG13  | 2:1D:327:ASP:HB2   | 2.02                     | 0.41              |
| 1:2A:201:ALA:O     | 1:2A:268:PRO:HD2   | 2.19                     | 0.41              |
| 1:2C:201:ALA:O     | 1:2C:268:PRO:HD2   | 2.19                     | 0.41              |
| 2:3B:20:PHE:CD1    | 2:3B:233:MET:HE3   | 2.55                     | 0.41              |
| 1:4A:425:LEU:HD23  | 1:4A:425:LEU:HA    | 1.93                     | 0.41              |
| 2:4B:36:TYR:CZ     | 2:4B:44:LEU:HD21   | 2.55                     | 0.41              |
| 2:4B:409:THR:O     | 2:4B:412:GLU:HG3   | 2.20                     | 0.41              |
| 1:5A:9:VAL:HG11    | 1:5A:150:THR:OG1   | 2.21                     | 0.41              |
| 1:5A:169:PHE:CE1   | 1:5A:235:VAL:HG22  | 2.55                     | 0.41              |
| 1:5E:422:ARG:O     | 1:5E:426:ALA:N     | 2.47                     | 0.41              |
| 2:6B:178:THR:HG22  | 2:6B:180:VAL:H     | 1.84                     | 0.41              |
| 1:6E:88:HIS:ND1    | 1:6E:90:GLU:OE2    | 2.53                     | 0.41              |
| 1:6E:145:THR:HG1   | 3:6E:500:GTP:PG    | 2.41                     | 0.41              |
| 1:7A:9:VAL:HG11    | 1:7A:150:THR:OG1   | 2.20                     | 0.41              |
| 1:7A:121:ARG:HH21  | 1:7A:125:LEU:HG    | 1.86                     | 0.41              |
| 2:7D:132:GLY:HA2   | 2:7D:163:ILE:O     | 2.20                     | 0.41              |
| 2:8D:326:VAL:HG11  | 2:8D:351:THR:HG21  | 2.01                     | 0.41              |
| 2:9B:4:ILE:HG13    | 2:9B:132:GLY:C     | 2.46                     | 0.41              |
| 2:9D:286:VAL:HB    | 2:9D:287:PRO:HD3   | 2.02                     | 0.41              |
| 1:9E:388:TRP:CD1   | 1:9E:388:TRP:N     | 2.88                     | 0.41              |
| 2:11D:6:HIS:HD2    | 2:11D:7:ILE:N      | 2.18                     | 0.41              |
| 1:12A:102:ASN:HB2  | 1:12A:105:ARG:HB2  | 2.03                     | 0.41              |
| 1:12C:195:LEU:HD12 | 1:12C:428:LEU:HD22 | 2.01                     | 0.41              |
| 1:12C:344:VAL:HG12 | 1:12C:346:TRP:H    | 1.84                     | 0.41              |
| 1:12C:433:GLU:HA   | 1:12C:433:GLU:OE2  | 2.21                     | 0.41              |
| 2:12D:329:GLN:O    | 2:12D:332:ASN:HB2  | 2.20                     | 0.41              |
| 1:12E:157:LEU:HB3  | 1:12E:166:LYS:HD3  | 2.01                     | 0.41              |
| 2:13D:309:ARG:H    | 2:13D:372:THR:HG1  | 1.63                     | 0.41              |
| 1:13E:272:TYR:CE2  | 1:13E:368:LEU:HD21 | 2.55                     | 0.41              |
| 1:1A:173:PRO:HG3   | 1:1A:187:SER:OG    | 2.20                     | 0.41              |
| 2:1D:232:THR:O     | 2:1D:236:VAL:HG23  | 2.21                     | 0.41              |
| 1:2A:174:ALA:HB3   | 1:2A:177:VAL:O     | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2E:225:THR:O     | 1:2E:229:ARG:HG3   | 2.20                     | 0.41              |
| 1:4A:222:PRO:O     | 2:4B:324:LYS:HB3   | 2.20                     | 0.41              |
| 1:4A:338:LYS:HA    | 1:4A:338:LYS:HD3   | 1.73                     | 0.41              |
| 2:4D:192:LEU:O     | 2:4D:196:THR:HG22  | 2.20                     | 0.41              |
| 1:5A:216:ASN:N     | 1:5A:216:ASN:ND2   | 2.67                     | 0.41              |
| 2:5B:376:GLU:HA    | 2:5B:379:LYS:HE2   | 2.02                     | 0.41              |
| 2:5D:23:ILE:HG13   | 2:5D:24:ILE:N      | 2.35                     | 0.41              |
| 2:5D:320:ARG:HE    | 2:5D:320:ARG:HB3   | 1.51                     | 0.41              |
| 1:6A:298:PRO:HG2   | 1:6A:308:ARG:NE    | 2.36                     | 0.41              |
| 1:6C:74:VAL:HA     | 1:6C:77:GLU:OE1    | 2.19                     | 0.41              |
| 1:6C:112:LYS:HE3   | 1:6C:112:LYS:HB3   | 1.69                     | 0.41              |
| 1:6C:137:ILE:HG21  | 1:6C:154:MET:HE3   | 2.02                     | 0.41              |
| 2:8B:143:THR:HB    | 5:8B:600:GDP:O3B   | 2.20                     | 0.41              |
| 2:8B:391:ARG:HA    | 2:8B:391:ARG:HD3   | 1.71                     | 0.41              |
| 1:9C:169:PHE:CE2   | 1:9C:235:VAL:HG22  | 2.56                     | 0.41              |
| 2:9D:374:ILE:HB    | 2:9D:422:TYR:CE2   | 2.56                     | 0.41              |
| 1:10A:271:THR:CG2  | 1:10A:377:MET:HB3  | 2.51                     | 0.41              |
| 2:10B:405:GLU:HA   | 2:10B:408:PHE:CD1  | 2.51                     | 0.41              |
| 1:10C:47:ASP:HB3   | 1:10C:48:SER:H     | 1.63                     | 0.41              |
| 2:10D:8:GLN:NE2    | 2:10D:65:LEU:HD22  | 2.36                     | 0.41              |
| 2:10D:405:GLU:HA   | 2:10D:408:PHE:CD1  | 2.52                     | 0.41              |
| 1:11A:51:THR:HG21  | 1:11A:243:ARG:HG2  | 2.03                     | 0.41              |
| 1:11A:286:LEU:HA   | 1:11A:290:GLU:OE2  | 2.19                     | 0.41              |
| 1:11A:398:MET:HE1  | 2:11B:345:ILE:HD13 | 2.02                     | 0.41              |
| 1:12A:171:ILE:HA   | 1:12A:204:VAL:O    | 2.20                     | 0.41              |
| 1:12E:91:GLN:OE1   | 1:12E:121:ARG:NH2  | 2.53                     | 0.41              |
| 1:12E:200:CYS:HA   | 1:12E:266:HIS:HB2  | 2.03                     | 0.41              |
| 1:12E:209:ILE:HG21 | 1:12E:227:LEU:HG   | 2.02                     | 0.41              |
| 1:12E:287:SER:HB3  | 1:12E:290:GLU:HB2  | 2.01                     | 0.41              |
| 1:12E:317:MET:HG3  | 1:12E:319:TYR:CE1  | 2.56                     | 0.41              |
| 2:13D:293:MET:HE1  | 2:13D:365:ALA:CB   | 2.50                     | 0.41              |
| 1:13E:116:ASP:HA   | 1:13E:119:LEU:HB2  | 2.03                     | 0.41              |
| 1:13E:135:PHE:HD2  | 1:13E:166:LYS:HG2  | 1.85                     | 0.41              |
| 1:1C:221:ARG:HA    | 2:1D:324:LYS:HE2   | 2.03                     | 0.41              |
| 2:1D:65:LEU:HB2    | 2:1D:73:MET:HE1    | 2.02                     | 0.41              |
| 2:1D:117:LEU:HA    | 2:1D:120:VAL:HG22  | 2.01                     | 0.41              |
| 1:1E:291:ILE:HD12  | 1:1E:375:VAL:HG23  | 2.03                     | 0.41              |
| 2:2B:267:MET:CE    | 2:2B:299:MET:HE2   | 2.42                     | 0.41              |
| 2:3B:5:VAL:HG12    | 2:3B:62:ARG:HD3    | 2.02                     | 0.41              |
| 2:3B:128:ASP:OD1   | 2:3B:129:CYS:N     | 2.48                     | 0.41              |
| 1:3C:90:GLU:CD     | 1:4C:280:LYS:HD2   | 2.46                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:3E:265:ILE:HG23 | 1:3E:432:TYR:CZ    | 2.55                     | 0.41              |
| 1:4C:175:PRO:HB3  | 1:4C:390:ARG:CD    | 2.50                     | 0.41              |
| 2:5B:232:THR:HG21 | 2:5B:268:PRO:HB3   | 2.02                     | 0.41              |
| 2:5D:149:THR:HG23 | 2:5D:191:GLN:HG2   | 2.02                     | 0.41              |
| 2:5D:237:THR:OG1  | 2:5D:241:ARG:NH1   | 2.53                     | 0.41              |
| 1:6A:220:GLU:O    | 2:6B:324:LYS:HE2   | 2.20                     | 0.41              |
| 1:6C:204:VAL:HG23 | 1:6C:302:MET:HG3   | 2.02                     | 0.41              |
| 1:6E:245:ASP:OD1  | 1:6E:245:ASP:N     | 2.52                     | 0.41              |
| 1:7E:203:MET:HE3  | 1:7E:203:MET:HB3   | 1.88                     | 0.41              |
| 1:7E:317:MET:SD   | 1:7E:377:MET:HB2   | 2.60                     | 0.41              |
| 1:8A:150:THR:O    | 1:8A:154:MET:HG3   | 2.20                     | 0.41              |
| 1:8A:407:TRP:NE1  | 2:8B:255:VAL:HA    | 2.36                     | 0.41              |
| 2:8B:359:ARG:HD3  | 2:8B:359:ARG:H     | 1.86                     | 0.41              |
| 1:9C:319:TYR:CD2  | 1:9C:375:VAL:HG22  | 2.55                     | 0.41              |
| 2:9D:130:LEU:HG   | 2:9D:162:ARG:NH1   | 2.36                     | 0.41              |
| 2:9D:131:GLN:O    | 2:9D:163:ILE:HG22  | 2.20                     | 0.41              |
| 1:9E:214:ARG:HD3  | 1:9E:214:ARG:HA    | 1.86                     | 0.41              |
| 2:10D:30:ILE:HD11 | 2:10D:51:TYR:CZ    | 2.55                     | 0.41              |
| 2:10D:146:GLY:O   | 2:10D:149:THR:HG22 | 2.21                     | 0.41              |
| 2:10D:404:ASP:O   | 2:10D:407:GLU:HB2  | 2.19                     | 0.41              |
| 1:11A:15:GLN:HG3  | 3:11A:500:GTP:C5   | 2.55                     | 0.41              |
| 2:11B:40:SER:O    | 2:11B:43:GLN:HB2   | 2.21                     | 0.41              |
| 1:11C:180:ALA:HB3 | 1:11C:183:GLU:HG3  | 2.03                     | 0.41              |
| 1:11C:398:MET:HE3 | 2:11D:346:PRO:HD2  | 2.01                     | 0.41              |
| 2:11D:105:HIS:HD2 | 2:11D:150:LEU:HD23 | 1.85                     | 0.41              |
| 1:11E:49:PHE:HE2  | 1:11E:61:HIS:CD2   | 2.38                     | 0.41              |
| 1:12A:330:ALA:O   | 1:12A:334:THR:N    | 2.54                     | 0.41              |
| 2:12B:61:PRO:CD   | 2:12B:84:ILE:HG22  | 2.46                     | 0.41              |
| 2:13B:91:VAL:HG11 | 2:13B:116:VAL:HG13 | 2.02                     | 0.41              |
| 2:13B:121:ARG:NH1 | 2:13B:158:GLU:OE1  | 2.54                     | 0.41              |
| 1:13C:369:ALA:O   | 1:13C:371:VAL:HG13 | 2.20                     | 0.41              |
| 2:13D:385:PHE:HA  | 2:13D:388:MET:HG2  | 2.02                     | 0.41              |
| 2:1B:20:PHE:O     | 2:1B:23:ILE:HG22   | 2.20                     | 0.41              |
| 1:1C:53:PHE:O     | 1:1C:64:ARG:NH1    | 2.53                     | 0.41              |
| 1:2A:88:HIS:ND1   | 1:3A:283:HIS:HB3   | 2.35                     | 0.41              |
| 1:2A:338:LYS:HD3  | 1:2A:338:LYS:HA    | 1.76                     | 0.41              |
| 2:2D:304:ASP:HB2  | 2:2D:307:HIS:CD2   | 2.55                     | 0.41              |
| 2:2D:388:MET:HE2  | 1:2E:348:PRO:HD2   | 2.03                     | 0.41              |
| 1:2E:121:ARG:HD2  | 1:2E:121:ARG:HA    | 1.97                     | 0.41              |
| 1:3A:147:SER:HB2  | 1:3A:190:THR:HG21  | 2.01                     | 0.41              |
| 2:3B:139:LEU:HD13 | 2:3B:168:SER:HB3   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3D:147:MET:HE2   | 2:3D:147:MET:HB3   | 1.96                     | 0.41              |
| 2:4D:279:GLN:H     | 2:4D:279:GLN:HG3   | 1.72                     | 0.41              |
| 1:4E:102:ASN:ND2   | 1:4E:105:ARG:HD3   | 2.26                     | 0.41              |
| 1:4E:225:THR:O     | 1:4E:229:ARG:HG3   | 2.20                     | 0.41              |
| 1:4E:338:LYS:HA    | 1:4E:338:LYS:HD3   | 1.73                     | 0.41              |
| 2:5B:215:LEU:HD12  | 2:5B:215:LEU:O     | 2.21                     | 0.41              |
| 1:6A:101:ASN:ND2   | 3:6A:500:GTP:O3G   | 2.54                     | 0.41              |
| 1:7A:5:ILE:O       | 1:7A:135:PHE:HA    | 2.20                     | 0.41              |
| 1:7C:11:GLN:HG2    | 1:7C:15:GLN:HE22   | 1.85                     | 0.41              |
| 1:7C:204:VAL:HG22  | 1:7C:209:ILE:HD11  | 2.03                     | 0.41              |
| 2:8B:89:ASN:O      | 2:8B:91:VAL:HG23   | 2.20                     | 0.41              |
| 1:8C:298:PRO:HG3   | 1:8C:308:ARG:NE    | 2.35                     | 0.41              |
| 1:10C:8:HIS:CE1    | 1:10C:17:GLY:HA2   | 2.56                     | 0.41              |
| 1:10C:141:PHE:HB3  | 1:10C:187:SER:OG   | 2.21                     | 0.41              |
| 1:10C:195:LEU:HD12 | 1:10C:428:LEU:HD22 | 2.03                     | 0.41              |
| 1:10C:425:LEU:HD23 | 1:10C:425:LEU:HA   | 1.95                     | 0.41              |
| 1:11A:5:ILE:O      | 1:11A:135:PHE:HA   | 2.21                     | 0.41              |
| 2:11B:61:PRO:CD    | 2:11B:84:ILE:HG22  | 2.43                     | 0.41              |
| 1:11C:3:GLU:HB2    | 1:11C:64:ARG:HH12  | 1.85                     | 0.41              |
| 1:11C:5:ILE:HG12   | 1:11C:64:ARG:CG    | 2.51                     | 0.41              |
| 2:11D:28:HIS:CE1   | 2:11D:241:ARG:HD2  | 2.56                     | 0.41              |
| 2:11D:33:THR:O     | 2:11D:58:LYS:HE3   | 2.20                     | 0.41              |
| 1:12A:327:ASP:OD1  | 1:12A:328:VAL:N    | 2.53                     | 0.41              |
| 1:12C:324:VAL:HA   | 1:12C:325:PRO:HD3  | 1.97                     | 0.41              |
| 2:12D:28:HIS:CE1   | 2:12D:241:ARG:HD2  | 2.55                     | 0.41              |
| 1:12E:319:TYR:CD2  | 1:12E:375:VAL:HG22 | 2.56                     | 0.41              |
| 1:13A:3:GLU:HA     | 1:13A:51:THR:HG23  | 2.02                     | 0.41              |
| 1:13A:172:TYR:HB2  | 1:13A:203:MET:SD   | 2.60                     | 0.41              |
| 1:13A:224:TYR:HD1  | 1:13A:224:TYR:HA   | 1.72                     | 0.41              |
| 1:13C:69:ASP:CG    | 1:13C:71:GLU:H     | 2.29                     | 0.41              |
| 1:13C:184:PRO:O    | 1:13C:188:ILE:N    | 2.52                     | 0.41              |
| 2:13D:293:MET:HE1  | 2:13D:365:ALA:HB1  | 2.02                     | 0.41              |
| 1:13E:245:ASP:O    | 1:13E:357:TYR:HB2  | 2.21                     | 0.41              |
| 1:13E:306:ASP:OD1  | 1:13E:306:ASP:N    | 2.54                     | 0.41              |
| 2:1B:293:MET:HE2   | 2:1B:367:PHE:HB2   | 2.03                     | 0.41              |
| 1:1C:222:PRO:HD2   | 2:1D:324:LYS:CE    | 2.50                     | 0.41              |
| 1:2A:225:THR:O     | 1:2A:229:ARG:HG3   | 2.21                     | 0.41              |
| 2:2B:154:LYS:O     | 2:2B:158:GLU:HG3   | 2.21                     | 0.41              |
| 1:2C:184:PRO:O     | 1:2C:188:ILE:HG12  | 2.20                     | 0.41              |
| 2:3B:120:VAL:HG21  | 2:3B:155:ILE:HD11  | 2.02                     | 0.41              |
| 1:4A:169:PHE:CE2   | 1:4A:235:VAL:HG22  | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:4B:310:TYR:O     | 2:4B:342:VAL:HG23  | 2.21                     | 0.41              |
| 1:4C:119:LEU:O     | 1:4C:123:ARG:HG2   | 2.21                     | 0.41              |
| 1:4E:47:ASP:HB3    | 1:4E:48:SER:H      | 1.60                     | 0.41              |
| 1:5C:186:ASN:O     | 1:5C:190:THR:HG23  | 2.20                     | 0.41              |
| 2:6B:219:THR:HA    | 1:6C:326:LYS:HE2   | 2.02                     | 0.41              |
| 1:6E:195:LEU:HD12  | 1:6E:428:LEU:HD22  | 2.03                     | 0.41              |
| 1:7C:31:GLN:OE1    | 1:7C:35:GLN:NE2    | 2.54                     | 0.41              |
| 1:7C:204:VAL:CG2   | 1:7C:209:ILE:HD11  | 2.50                     | 0.41              |
| 2:7D:285:THR:OG1   | 2:7D:287:PRO:HD2   | 2.19                     | 0.41              |
| 1:7E:9:VAL:HG11    | 1:7E:150:THR:OG1   | 2.21                     | 0.41              |
| 1:7E:53:PHE:HD2    | 1:7E:61:HIS:HB3    | 1.84                     | 0.41              |
| 2:8D:36:TYR:CZ     | 2:8D:44:LEU:HD21   | 2.56                     | 0.41              |
| 1:8E:15:GLN:HG3    | 3:8E:500:GTP:N1    | 2.35                     | 0.41              |
| 2:9D:69:GLU:HG3    | 2:9D:96:GLY:HA2    | 2.02                     | 0.41              |
| 2:9D:112:LEU:O     | 2:9D:112:LEU:HD23  | 2.21                     | 0.41              |
| 1:10A:332:ILE:O    | 1:10A:336:LYS:HG2  | 2.20                     | 0.41              |
| 2:10B:33:THR:O     | 2:10B:58:LYS:HE3   | 2.21                     | 0.41              |
| 2:10B:267:MET:HG3  | 2:10B:374:ILE:HD11 | 2.03                     | 0.41              |
| 2:10D:409:THR:O    | 2:10D:413:SER:N    | 2.53                     | 0.41              |
| 1:10E:104:ALA:HB1  | 1:10E:411:GLU:HB2  | 2.02                     | 0.41              |
| 1:11A:145:THR:N    | 3:11A:500:GTP:O2G  | 2.52                     | 0.41              |
| 2:11B:141:GLY:HA3  | 5:11B:600:GDP:O2A  | 2.21                     | 0.41              |
| 1:11C:31:GLN:O     | 1:11C:33:ASP:N     | 2.54                     | 0.41              |
| 1:11C:121:ARG:HB3  | 1:11C:121:ARG:CZ   | 2.50                     | 0.41              |
| 2:11D:61:PRO:HD3   | 2:11D:84:ILE:CG2   | 2.43                     | 0.41              |
| 2:11D:391:ARG:HA   | 2:11D:391:ARG:HD3  | 1.88                     | 0.41              |
| 1:11E:31:GLN:O     | 1:11E:33:ASP:N     | 2.54                     | 0.41              |
| 1:11E:269:LEU:HD11 | 1:11E:384:ILE:HB   | 2.03                     | 0.41              |
| 1:12A:52:PHE:C     | 1:12A:53:PHE:HD1   | 2.29                     | 0.41              |
| 1:12A:98:ASP:OD1   | 1:12A:98:ASP:N     | 2.54                     | 0.41              |
| 1:12A:191:THR:OG1  | 1:12A:421:ALA:HB1  | 2.21                     | 0.41              |
| 1:12A:394:LYS:HG3  | 2:12B:346:PRO:HG3  | 2.03                     | 0.41              |
| 1:12C:101:ASN:HD21 | 2:12D:252:LYS:HE3  | 1.85                     | 0.41              |
| 2:12D:6:HIS:HB3    | 2:12D:63:ALA:HA    | 2.02                     | 0.41              |
| 1:12E:150:THR:HG22 | 1:12E:154:MET:HE3  | 2.02                     | 0.41              |
| 1:12E:250:VAL:HG23 | 1:12E:352:LYS:HE3  | 2.03                     | 0.41              |
| 1:13A:221:ARG:HG2  | 2:13B:324:LYS:NZ   | 2.36                     | 0.41              |
| 1:13A:231:ILE:O    | 1:13A:235:VAL:HG23 | 2.21                     | 0.41              |
| 2:13B:327:ASP:OD1  | 2:13B:328:GLU:N    | 2.54                     | 0.41              |
| 2:13D:210:ILE:HD11 | 2:13D:300:MET:HA   | 2.03                     | 0.41              |
| 1:13E:125:LEU:HD23 | 1:13E:125:LEU:HA   | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:13E:246:GLY:HA2 | 1:13E:357:TYR:CG  | 2.56                     | 0.41              |
| 1:13E:307:PRO:HB3 | 1:13E:312:TYR:OH  | 2.21                     | 0.41              |
| 1:13E:331:ALA:O   | 1:13E:334:THR:HB  | 2.20                     | 0.41              |
| 1:1A:255:PHE:HD2  | 1:1A:256:GLN:OE1  | 2.04                     | 0.41              |
| 1:1E:287:SER:O    | 1:1E:290:GLU:HG2  | 2.20                     | 0.41              |
| 1:1E:317:MET:SD   | 1:1E:377:MET:HG2  | 2.61                     | 0.41              |
| 1:2C:224:TYR:O    | 1:2C:228:ASN:ND2  | 2.53                     | 0.41              |
| 1:2C:315:CYS:HA   | 1:2C:379:SER:HA   | 2.01                     | 0.41              |
| 2:2D:374:ILE:HD13 | 2:2D:374:ILE:HA   | 1.88                     | 0.41              |
| 1:3A:53:PHE:O     | 1:3A:64:ARG:NH1   | 2.53                     | 0.41              |
| 1:3A:123:ARG:NE   | 1:3A:123:ARG:HA   | 2.36                     | 0.41              |
| 1:3A:407:TRP:CD1  | 2:3B:255:VAL:HG23 | 2.55                     | 0.41              |
| 2:3B:164:MET:HE3  | 2:3B:164:MET:HB2  | 1.95                     | 0.41              |
| 2:3B:220:PRO:HD2  | 1:3C:326:LYS:HD2  | 2.02                     | 0.41              |
| 2:3D:211:CYS:HB2  | 2:3D:217:LEU:HD12 | 2.03                     | 0.41              |
| 2:4D:112:LEU:HD23 | 2:4D:112:LEU:O    | 2.21                     | 0.41              |
| 2:4D:141:GLY:HA3  | 5:4D:600:GDP:O3A  | 2.20                     | 0.41              |
| 2:4D:279:GLN:NE2  | 2:4D:280:GLN:HG2  | 2.35                     | 0.41              |
| 1:5A:8:HIS:HD2    | 1:5A:67:PHE:CE1   | 2.39                     | 0.41              |
| 1:5C:177:VAL:HG13 | 2:5D:327:ASP:HB3  | 2.02                     | 0.41              |
| 1:5C:251:ASP:H    | 1:5C:254:GLU:HB3  | 1.85                     | 0.41              |
| 2:5D:299:MET:HE2  | 2:5D:299:MET:HB2  | 1.91                     | 0.41              |
| 1:5E:91:GLN:HA    | 1:5E:121:ARG:NH1  | 2.36                     | 0.41              |
| 1:6A:245:ASP:OD1  | 1:6A:245:ASP:N    | 2.53                     | 0.41              |
| 1:6A:278:ALA:HA   | 1:6A:369:ALA:HB2  | 2.02                     | 0.41              |
| 2:6B:267:MET:SD   | 2:6B:299:MET:SD   | 3.18                     | 0.41              |
| 2:6B:328:GLU:O    | 2:6B:331:LEU:HG   | 2.20                     | 0.41              |
| 2:6B:375:GLN:H    | 2:6B:375:GLN:HG3  | 1.73                     | 0.41              |
| 2:6D:132:GLY:HA2  | 2:6D:163:ILE:O    | 2.20                     | 0.41              |
| 1:6E:3:GLU:OE1    | 1:6E:64:ARG:NE    | 2.54                     | 0.41              |
| 1:6E:55:GLU:OE2   | 1:6E:61:HIS:NE2   | 2.54                     | 0.41              |
| 1:6E:377:MET:SD   | 1:6E:379:SER:HB3  | 2.61                     | 0.41              |
| 1:7A:414:GLU:OE2  | 1:7A:417:GLU:N    | 2.54                     | 0.41              |
| 2:7B:175:VAL:HG12 | 2:7B:175:VAL:O    | 2.21                     | 0.41              |
| 2:7B:390:ARG:O    | 2:7B:392:LYS:NZ   | 2.54                     | 0.41              |
| 1:7C:221:ARG:HG2  | 2:7D:324:LYS:HE3  | 2.03                     | 0.41              |
| 1:7C:332:ILE:HD12 | 1:7C:351:PHE:CD2  | 2.56                     | 0.41              |
| 2:7D:89:ASN:O     | 2:7D:91:VAL:HG23  | 2.21                     | 0.41              |
| 2:7D:324:LYS:HG3  | 2:7D:325:GLU:N    | 2.35                     | 0.41              |
| 1:7E:121:ARG:HH21 | 1:7E:125:LEU:HG   | 1.86                     | 0.41              |
| 1:7E:296:PHE:CE1  | 1:7E:312:TYR:HE2  | 2.39                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7E:425:LEU:HD23  | 1:7E:425:LEU:HA    | 1.96                     | 0.41              |
| 1:8A:21:TRP:HZ3    | 1:8A:53:PHE:HE1    | 1.68                     | 0.41              |
| 1:8A:134:GLY:HA3   | 1:8A:165:SER:O     | 2.21                     | 0.41              |
| 2:8B:242:PHE:CD1   | 2:8B:356:ILE:HG13  | 2.56                     | 0.41              |
| 2:8D:218:THR:HG23  | 2:8D:219:THR:HG23  | 2.03                     | 0.41              |
| 2:8D:362:LYS:HD3   | 2:8D:362:LYS:HA    | 1.76                     | 0.41              |
| 1:9A:245:ASP:OD1   | 1:9A:245:ASP:N     | 2.54                     | 0.41              |
| 2:9B:257:MET:HE1   | 2:9B:266:PHE:CZ    | 2.56                     | 0.41              |
| 2:9B:359:ARG:HD3   | 2:9B:359:ARG:N     | 2.36                     | 0.41              |
| 1:9C:121:ARG:HB3   | 1:9C:121:ARG:CZ    | 2.50                     | 0.41              |
| 2:9D:290:THR:HG21  | 2:9D:329:GLN:OE1   | 2.20                     | 0.41              |
| 1:10A:184:PRO:O    | 1:10A:188:ILE:HG12 | 2.21                     | 0.41              |
| 1:10A:245:ASP:OD1  | 1:10A:245:ASP:N    | 2.54                     | 0.41              |
| 2:10D:141:GLY:HA3  | 5:10D:600:GDP:O2A  | 2.21                     | 0.41              |
| 2:11D:140:GLY:O    | 2:11D:184:ASN:ND2  | 2.54                     | 0.41              |
| 2:12B:236:VAL:HG22 | 2:12B:368:ILE:HD11 | 2.03                     | 0.41              |
| 1:13A:102:ASN:HB3  | 1:13A:105:ARG:HH11 | 1.85                     | 0.41              |
| 1:13A:359:PRO:HA   | 1:13A:360:PRO:HD3  | 1.96                     | 0.41              |
| 2:13B:371:SER:O    | 2:13B:374:ILE:HG12 | 2.21                     | 0.41              |
| 2:13B:372:THR:HG21 | 2:13B:426:GLN:HA   | 2.02                     | 0.41              |
| 1:13C:332:ILE:O    | 1:13C:336:LYS:HG2  | 2.21                     | 0.41              |
| 2:13D:223:GLY:O    | 2:13D:227:HIS:HB2  | 2.20                     | 0.41              |
| 2:1B:167:TYR:CE2   | 2:1B:233:MET:HG3   | 2.56                     | 0.41              |
| 1:1C:340:THR:OG1   | 1:1C:341:ILE:HD12  | 2.21                     | 0.41              |
| 1:1E:53:PHE:O      | 1:1E:64:ARG:NH1    | 2.54                     | 0.41              |
| 1:1E:91:GLN:HA     | 1:1E:121:ARG:NH1   | 2.34                     | 0.41              |
| 1:2E:220:GLU:OE1   | 1:2E:220:GLU:N     | 2.46                     | 0.41              |
| 2:3B:65:LEU:CB     | 2:3B:73:MET:HE1    | 2.50                     | 0.41              |
| 1:3E:261:PRO:HG3   | 1:3E:313:MET:HE3   | 2.02                     | 0.41              |
| 1:4A:201:ALA:O     | 1:4A:268:PRO:HD2   | 2.20                     | 0.41              |
| 2:4B:192:LEU:O     | 2:4B:196:THR:HG22  | 2.21                     | 0.41              |
| 2:4B:285:THR:HG23  | 2:4B:287:PRO:HD2   | 2.02                     | 0.41              |
| 2:4D:175:VAL:HG13  | 1:4E:329:ASN:ND2   | 2.36                     | 0.41              |
| 1:4E:113:GLU:N     | 1:4E:113:GLU:OE2   | 2.54                     | 0.41              |
| 1:6C:2:ARG:HA      | 1:6C:133:GLN:NE2   | 2.35                     | 0.41              |
| 1:6C:69:ASP:OD1    | 1:6C:70:LEU:N      | 2.54                     | 0.41              |
| 2:6D:174:LYS:HD3   | 2:6D:174:LYS:HA    | 1.82                     | 0.41              |
| 1:7A:255:PHE:CE2   | 1:7A:378:LEU:HD22  | 2.56                     | 0.41              |
| 1:7E:71:GLU:HG2    | 1:7E:73:THR:H      | 1.86                     | 0.41              |
| 1:8A:136:LEU:HA    | 1:8A:167:LEU:O     | 2.21                     | 0.41              |
| 2:8B:213:ARG:NE    | 2:8B:297:LYS:HE3   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:8E:56:THR:HG23  | 1:9E:285:GLN:HB2   | 2.03                     | 0.41              |
| 1:9A:340:THR:HG23 | 1:9A:341:ILE:HD12  | 2.03                     | 0.41              |
| 2:9B:67:ASP:HB3   | 2:9B:92:PHE:HB3    | 2.02                     | 0.41              |
| 2:9B:174:LYS:HD3  | 2:9B:174:LYS:HA    | 1.85                     | 0.41              |
| 1:9C:323:VAL:HG23 | 1:9C:355:ILE:HG23  | 2.02                     | 0.41              |
| 1:9E:121:ARG:HB3  | 1:9E:121:ARG:CZ    | 2.51                     | 0.41              |
| 1:10E:30:ILE:HG23 | 1:10E:61:HIS:HD2   | 1.86                     | 0.40              |
| 1:10E:69:ASP:CG   | 1:10E:71:GLU:H     | 2.29                     | 0.40              |
| 1:10E:151:SER:OG  | 1:10E:193:THR:HG21 | 2.22                     | 0.40              |
| 1:10E:165:SER:HA  | 1:10E:199:ASP:OD2  | 2.21                     | 0.40              |
| 1:10E:255:PHE:HZ  | 1:10E:378:LEU:HD22 | 1.85                     | 0.40              |
| 1:11A:165:SER:HA  | 1:11A:199:ASP:OD2  | 2.21                     | 0.40              |
| 1:11A:339:ARG:O   | 1:11A:342:GLN:NE2  | 2.55                     | 0.40              |
| 2:11B:345:ILE:O   | 2:11B:348:ASN:ND2  | 2.54                     | 0.40              |
| 1:11C:224:TYR:CE2 | 2:11D:323:MET:HG3  | 2.56                     | 0.40              |
| 2:12B:69:GLU:O    | 2:12B:73:MET:HE1   | 2.21                     | 0.40              |
| 1:12C:15:GLN:HG3  | 3:12C:500:GTP:C5   | 2.57                     | 0.40              |
| 1:13A:207:GLU:HA  | 1:13A:210:TYR:HD2  | 1.85                     | 0.40              |
| 1:13C:64:ARG:HE   | 1:13C:64:ARG:HB2   | 1.76                     | 0.40              |
| 1:13E:316:CYS:N   | 1:13E:378:LEU:O    | 2.29                     | 0.40              |
| 1:1E:169:PHE:CE2  | 1:1E:235:VAL:HG22  | 2.56                     | 0.40              |
| 2:2B:211:CYS:HB2  | 2:2B:217:LEU:HD12  | 2.03                     | 0.40              |
| 1:2C:53:PHE:O     | 1:2C:64:ARG:NH1    | 2.54                     | 0.40              |
| 2:3B:310:TYR:O    | 2:3B:342:VAL:HG23  | 2.21                     | 0.40              |
| 1:3C:121:ARG:HH21 | 1:3C:125:LEU:HG    | 1.85                     | 0.40              |
| 2:3D:219:THR:HA   | 1:3E:326:LYS:HD3   | 2.03                     | 0.40              |
| 1:4A:119:LEU:O    | 1:4A:123:ARG:HG2   | 2.21                     | 0.40              |
| 2:4B:378:PHE:HD2  | 2:4B:418:LEU:HD22  | 1.87                     | 0.40              |
| 1:4C:215:ARG:NH2  | 1:4C:299:ALA:HB1   | 2.36                     | 0.40              |
| 2:5B:20:PHE:CD2   | 2:5B:233:MET:HE3   | 2.54                     | 0.40              |
| 2:5B:293:MET:HE1  | 2:5B:315:ALA:HB1   | 2.02                     | 0.40              |
| 1:7C:100:ALA:HA   | 2:7D:252:LYS:HG3   | 2.02                     | 0.40              |
| 1:7C:405:VAL:HG12 | 1:7C:409:VAL:HG23  | 2.03                     | 0.40              |
| 2:8B:2:ARG:HE     | 2:8B:240:LEU:HD22  | 1.86                     | 0.40              |
| 2:8B:246:LEU:HA   | 2:8B:246:LEU:HD12  | 1.80                     | 0.40              |
| 2:8D:20:PHE:HE1   | 2:8D:24:ILE:HD12   | 1.85                     | 0.40              |
| 1:8E:47:ASP:HB3   | 1:8E:48:SER:H      | 1.61                     | 0.40              |
| 1:9A:20:CYS:HB3   | 1:9A:24:TYR:CE2    | 2.55                     | 0.40              |
| 1:9A:49:PHE:HD2   | 1:9A:53:PHE:HB2    | 1.86                     | 0.40              |
| 1:9E:115:VAL:HG22 | 1:9E:119:LEU:HD12  | 2.03                     | 0.40              |
| 1:9E:193:THR:O    | 1:9E:197:HIS:HB2   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9E:311:LYS:HB3   | 1:9E:344:VAL:HG22  | 2.03                     | 0.40              |
| 1:10A:271:THR:HG22 | 1:10A:377:MET:HB3  | 2.02                     | 0.40              |
| 1:10C:326:LYS:HG3  | 1:10C:327:ASP:N    | 2.36                     | 0.40              |
| 1:11A:125:LEU:HD23 | 1:11A:125:LEU:HA   | 1.92                     | 0.40              |
| 1:11A:250:VAL:HG11 | 1:11A:318:LEU:CD2  | 2.51                     | 0.40              |
| 2:11B:390:ARG:HG3  | 2:11B:391:ARG:HD3  | 2.04                     | 0.40              |
| 1:11C:377:MET:HE1  | 1:11C:379:SER:HB3  | 2.03                     | 0.40              |
| 2:11D:377:LEU:HD23 | 2:11D:380:ARG:HH22 | 1.86                     | 0.40              |
| 1:12C:193:THR:O    | 1:12C:197:HIS:N    | 2.53                     | 0.40              |
| 1:12C:291:ILE:HD13 | 1:12C:291:ILE:HG21 | 1.73                     | 0.40              |
| 1:12C:320:ARG:O    | 1:12C:373:ARG:HA   | 2.21                     | 0.40              |
| 1:12E:102:ASN:HD22 | 1:12E:105:ARG:CG   | 2.30                     | 0.40              |
| 2:13B:334:GLN:HG2  | 2:13B:341:PHE:CZ   | 2.56                     | 0.40              |
| 1:13E:102:ASN:H    | 1:13E:144:GLY:HA3  | 1.86                     | 0.40              |
| 1:1E:338:LYS:HA    | 1:1E:338:LYS:HD3   | 1.76                     | 0.40              |
| 2:2B:110:ALA:O     | 2:2B:113:VAL:HG12  | 2.21                     | 0.40              |
| 1:2E:195:LEU:HD23  | 1:2E:196:GLU:HG2   | 2.03                     | 0.40              |
| 1:3A:201:ALA:O     | 1:3A:268:PRO:HD2   | 2.21                     | 0.40              |
| 1:3A:367:ASP:OD2   | 1:3A:367:ASP:N     | 2.52                     | 0.40              |
| 1:3E:21:TRP:HZ3    | 1:3E:53:PHE:HE1    | 1.69                     | 0.40              |
| 1:4A:20:CYS:HB3    | 1:4A:24:TYR:CE2    | 2.56                     | 0.40              |
| 2:4D:388:MET:HE2   | 2:4D:388:MET:N     | 2.35                     | 0.40              |
| 1:4E:210:TYR:CE1   | 1:4E:227:LEU:HD21  | 2.57                     | 0.40              |
| 1:4E:402:ARG:HB2   | 1:4E:402:ARG:CZ    | 2.51                     | 0.40              |
| 1:5A:425:LEU:HD23  | 1:5A:425:LEU:HA    | 1.93                     | 0.40              |
| 1:5E:2:ARG:HG3     | 1:5E:133:GLN:NE2   | 2.35                     | 0.40              |
| 2:6B:257:MET:HE2   | 2:6B:257:MET:HB2   | 1.96                     | 0.40              |
| 1:7A:31:GLN:OE1    | 1:7A:35:GLN:NE2    | 2.54                     | 0.40              |
| 1:7A:67:PHE:HB2    | 1:7A:92:LEU:HD23   | 2.02                     | 0.40              |
| 1:7A:205:ASP:OD1   | 1:7A:206:ASN:N     | 2.54                     | 0.40              |
| 1:7A:407:TRP:CG    | 2:7B:255:VAL:HG23  | 2.56                     | 0.40              |
| 2:7D:11:GLN:HB2    | 2:7D:72:THR:HG21   | 2.03                     | 0.40              |
| 1:7E:8:HIS:HD2     | 1:7E:67:PHE:CE1    | 2.39                     | 0.40              |
| 1:8A:329:ASN:OD1   | 1:8A:330:ALA:N     | 2.54                     | 0.40              |
| 1:8C:404:PHE:CE2   | 2:8D:256:ASN:HA    | 2.47                     | 0.40              |
| 2:8D:279:GLN:H     | 2:8D:279:GLN:HG3   | 1.68                     | 0.40              |
| 1:8E:332:ILE:HD12  | 1:8E:351:PHE:CE2   | 2.56                     | 0.40              |
| 1:9A:11:GLN:NE2    | 2:9B:245:GLN:O     | 2.54                     | 0.40              |
| 1:9A:53:PHE:O      | 1:9A:64:ARG:NH2    | 2.46                     | 0.40              |
| 1:9A:228:ASN:OD1   | 3:9A:500:GTP:N2    | 2.29                     | 0.40              |
| 1:9C:21:TRP:HZ3    | 1:9C:53:PHE:HE1    | 1.70                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:9C:115:VAL:HG22  | 1:9C:119:LEU:HD12  | 2.04                     | 0.40              |
| 1:9C:182:VAL:O     | 1:9C:182:VAL:HG22  | 2.21                     | 0.40              |
| 2:9D:170:VAL:HG13  | 2:9D:203:ASP:OD1   | 2.21                     | 0.40              |
| 1:9E:362:VAL:HG11  | 1:9E:370:LYS:HA    | 2.03                     | 0.40              |
| 2:10B:310:TYR:O    | 2:10B:342:VAL:HG23 | 2.20                     | 0.40              |
| 2:10D:117:LEU:HA   | 2:10D:120:VAL:HG22 | 2.03                     | 0.40              |
| 2:10D:156:ARG:HH12 | 2:10D:197:ASP:CG   | 2.29                     | 0.40              |
| 2:11B:286:VAL:HB   | 2:11B:325:GLU:HG2  | 2.03                     | 0.40              |
| 2:11D:5:VAL:HG12   | 2:11D:62:ARG:CD    | 2.51                     | 0.40              |
| 2:11D:252:LYS:HE3  | 2:11D:350:LYS:HZ3  | 1.87                     | 0.40              |
| 1:11E:195:LEU:HD21 | 1:11E:264:ARG:HG2  | 2.03                     | 0.40              |
| 1:11E:406:HIS:CE1  | 1:11E:407:TRP:CE2  | 3.10                     | 0.40              |
| 1:12A:200:CYS:HA   | 1:12A:266:HIS:HB2  | 2.04                     | 0.40              |
| 1:12E:320:ARG:O    | 1:12E:373:ARG:HA   | 2.22                     | 0.40              |
| 1:13A:79:ARG:O     | 1:13A:84:ARG:HD3   | 2.20                     | 0.40              |
| 1:13A:291:ILE:HD12 | 1:13A:375:VAL:CG2  | 2.52                     | 0.40              |
| 2:13D:109:GLY:HA2  | 2:13D:147:MET:HE1  | 2.03                     | 0.40              |
| 2:1B:232:THR:OG1   | 2:1B:300:MET:HE1   | 2.22                     | 0.40              |
| 2:1D:215:LEU:HB3   | 2:1D:217:LEU:HG    | 2.02                     | 0.40              |
| 1:1E:316:CYS:SG    | 1:1E:352:LYS:HB3   | 2.62                     | 0.40              |
| 2:2B:151:LEU:HD23  | 2:2B:151:LEU:HA    | 1.92                     | 0.40              |
| 1:3C:70:LEU:HD22   | 1:3C:114:ILE:HD12  | 2.03                     | 0.40              |
| 2:3D:21:TRP:HZ3    | 2:3D:51:TYR:HE1    | 1.69                     | 0.40              |
| 2:3D:317:PHE:HB3   | 2:3D:321:MET:SD    | 2.62                     | 0.40              |
| 1:3E:121:ARG:HD2   | 1:3E:121:ARG:HA    | 2.00                     | 0.40              |
| 1:4A:47:ASP:HB3    | 1:4A:48:SER:H      | 1.59                     | 0.40              |
| 2:4B:67:ASP:OD1    | 2:4B:68:LEU:N      | 2.54                     | 0.40              |
| 1:4E:271:THR:OG1   | 1:4E:377:MET:HB3   | 2.22                     | 0.40              |
| 2:5B:216:LYS:HA    | 2:5B:216:LYS:HD3   | 1.90                     | 0.40              |
| 1:5C:407:TRP:CG    | 2:5D:255:VAL:HG23  | 2.56                     | 0.40              |
| 1:5E:47:ASP:HB3    | 1:5E:48:SER:H      | 1.62                     | 0.40              |
| 2:6B:131:GLN:O     | 2:6B:163:ILE:HG22  | 2.21                     | 0.40              |
| 2:6B:155:ILE:HG22  | 2:6B:164:MET:HE1   | 2.02                     | 0.40              |
| 2:6B:279:GLN:NE2   | 2:6B:280:GLN:HG2   | 2.36                     | 0.40              |
| 1:7A:47:ASP:HB3    | 1:7A:48:SER:H      | 1.55                     | 0.40              |
| 1:7A:153:LEU:HD23  | 1:7A:153:LEU:HA    | 1.90                     | 0.40              |
| 1:7A:251:ASP:O     | 1:7A:255:PHE:N     | 2.55                     | 0.40              |
| 2:7B:121:ARG:O     | 2:7B:125:GLU:HG2   | 2.21                     | 0.40              |
| 2:7B:211:CYS:SG    | 2:7B:212:PHE:N     | 2.93                     | 0.40              |
| 1:7C:11:GLN:NE2    | 2:7D:245:GLN:O     | 2.53                     | 0.40              |
| 1:8A:102:ASN:HB3   | 1:8A:105:ARG:HB2   | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:8A:265:ILE:HD11  | 1:8A:435:VAL:HG21  | 2.03                     | 0.40              |
| 1:8C:25:CYS:HB3    | 1:8C:30:ILE:O      | 2.22                     | 0.40              |
| 2:8D:12:CYS:SG     | 2:8D:13:GLY:N      | 2.94                     | 0.40              |
| 1:8E:213:CYS:HB2   | 1:8E:219:ILE:CD1   | 2.49                     | 0.40              |
| 1:8E:265:ILE:HG23  | 1:8E:432:TYR:OH    | 2.21                     | 0.40              |
| 2:9B:99:ASN:ND2    | 1:9C:254:GLU:OE2   | 2.55                     | 0.40              |
| 2:9B:112:LEU:HD23  | 2:9B:112:LEU:O     | 2.21                     | 0.40              |
| 2:9B:175:VAL:HG12  | 2:9B:175:VAL:O     | 2.21                     | 0.40              |
| 1:9C:304:LYS:HE2   | 1:9C:304:LYS:HB3   | 1.75                     | 0.40              |
| 1:9C:317:MET:SD    | 1:9C:377:MET:HG2   | 2.61                     | 0.40              |
| 2:9D:284:LEU:HD23  | 2:9D:284:LEU:HA    | 1.95                     | 0.40              |
| 2:9D:326:VAL:O     | 2:9D:330:MET:HG2   | 2.21                     | 0.40              |
| 1:9E:245:ASP:N     | 1:9E:245:ASP:OD1   | 2.52                     | 0.40              |
| 1:10E:245:ASP:OD1  | 1:10E:245:ASP:N    | 2.55                     | 0.40              |
| 1:11C:47:ASP:HB3   | 1:11C:48:SER:H     | 1.70                     | 0.40              |
| 1:11C:174:ALA:HB1  | 1:11C:207:GLU:OE1  | 2.22                     | 0.40              |
| 2:12B:200:TYR:HD1  | 2:12B:266:PHE:HB2  | 1.85                     | 0.40              |
| 1:12C:270:VAL:O    | 1:12C:302:MET:HB2  | 2.22                     | 0.40              |
| 1:12C:414:GLU:CD   | 1:12C:416:GLY:H    | 2.28                     | 0.40              |
| 1:12E:306:ASP:OD1  | 1:12E:306:ASP:N    | 2.53                     | 0.40              |
| 1:13A:6:SER:OG     | 1:13A:21:TRP:HZ2   | 2.04                     | 0.40              |
| 1:13A:125:LEU:HA   | 1:13A:125:LEU:HD23 | 1.82                     | 0.40              |
| 1:13A:318:LEU:HD23 | 1:13A:354:GLY:HA3  | 2.03                     | 0.40              |
| 2:13D:214:THR:HG21 | 2:13D:298:ASN:HD21 | 1.84                     | 0.40              |
| 2:13D:385:PHE:HA   | 2:13D:388:MET:HE3  | 2.03                     | 0.40              |
| 1:2C:174:ALA:HB1   | 1:2C:207:GLU:OE2   | 2.20                     | 0.40              |
| 1:3A:108:TYR:O     | 1:3A:112:LYS:NZ    | 2.43                     | 0.40              |
| 2:3D:111:GLU:OE2   | 2:3D:111:GLU:N     | 2.54                     | 0.40              |
| 2:3D:131:GLN:O     | 2:3D:163:ILE:HG22  | 2.21                     | 0.40              |
| 2:3D:190:HIS:NE2   | 2:3D:414:ASN:OD1   | 2.54                     | 0.40              |
| 1:3E:201:ALA:O     | 1:3E:268:PRO:HD2   | 2.21                     | 0.40              |
| 1:3E:316:CYS:SG    | 1:3E:352:LYS:HB3   | 2.62                     | 0.40              |
| 1:4C:234:ILE:HD11  | 1:4C:302:MET:HE3   | 2.02                     | 0.40              |
| 2:4D:110:ALA:O     | 2:4D:113:VAL:HG12  | 2.21                     | 0.40              |
| 1:4E:204:VAL:HG11  | 1:4E:231:ILE:HD11  | 2.03                     | 0.40              |
| 2:5D:231:LEU:HD23  | 2:5D:231:LEU:HA    | 1.96                     | 0.40              |
| 2:6D:164:MET:N     | 2:6D:197:ASP:OD2   | 2.55                     | 0.40              |
| 2:6D:178:THR:HG22  | 2:6D:180:VAL:H     | 1.85                     | 0.40              |
| 2:6D:213:ARG:NE    | 2:6D:297:LYS:HE3   | 2.36                     | 0.40              |
| 2:6D:317:PHE:HB3   | 2:6D:321:MET:SD    | 2.61                     | 0.40              |
| 1:7A:193:THR:O     | 1:7A:197:HIS:HB2   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:7A:316:CYS:SG    | 1:7A:352:LYS:HB3   | 2.62                     | 0.40              |
| 2:7B:215:LEU:O     | 2:7B:215:LEU:HD23  | 2.21                     | 0.40              |
| 2:7B:263:LEU:HG    | 2:7B:422:TYR:CE2   | 2.57                     | 0.40              |
| 2:7B:324:LYS:CG    | 2:7B:325:GLU:N     | 2.84                     | 0.40              |
| 1:7C:102:ASN:OD1   | 1:7C:408:TYR:HE1   | 2.03                     | 0.40              |
| 2:7D:209:ASP:OD2   | 2:7D:213:ARG:NH2   | 2.51                     | 0.40              |
| 2:8B:130:LEU:H     | 2:8B:130:LEU:HD23  | 1.87                     | 0.40              |
| 1:8C:367:ASP:C     | 1:8C:368:LEU:HD12  | 2.47                     | 0.40              |
| 1:8E:328:VAL:O     | 1:8E:332:ILE:HG12  | 2.21                     | 0.40              |
| 2:9D:173:PRO:HG2   | 2:9D:380:ARG:HH21  | 1.86                     | 0.40              |
| 1:9E:3:GLU:HG3     | 1:9E:130:THR:H     | 1.86                     | 0.40              |
| 1:10A:213:CYS:HA   | 1:10A:217:LEU:HD13 | 2.03                     | 0.40              |
| 1:10A:219:ILE:HG21 | 1:10A:367:ASP:OD1  | 2.21                     | 0.40              |
| 2:10B:173:PRO:HG3  | 2:10B:380:ARG:NH1  | 2.36                     | 0.40              |
| 2:10D:175:VAL:HG13 | 1:10E:329:ASN:ND2  | 2.35                     | 0.40              |
| 1:10E:175:PRO:HB3  | 1:10E:390:ARG:CZ   | 2.52                     | 0.40              |
| 2:11B:61:PRO:HD3   | 2:11B:84:ILE:CG2   | 2.43                     | 0.40              |
| 1:11C:175:PRO:HB3  | 1:11C:390:ARG:NE   | 2.35                     | 0.40              |
| 2:11D:290:THR:HA   | 2:11D:293:MET:HB2  | 2.04                     | 0.40              |
| 1:12A:88:HIS:HA    | 1:12A:89:PRO:HD3   | 1.96                     | 0.40              |
| 1:12A:101:ASN:HA   | 1:12A:144:GLY:H    | 1.87                     | 0.40              |
| 1:12A:321:GLY:HA3  | 1:12A:372:GLN:O    | 2.21                     | 0.40              |
| 1:12C:265:ILE:HG23 | 1:12C:432:TYR:CZ   | 2.56                     | 0.40              |
| 1:12C:312:TYR:O    | 1:12C:344:VAL:N    | 2.48                     | 0.40              |
| 2:13B:33:THR:O     | 2:13B:58:LYS:HE3   | 2.21                     | 0.40              |
| 2:13B:110:ALA:O    | 2:13B:113:VAL:HG12 | 2.21                     | 0.40              |
| 2:13D:175:VAL:HG21 | 2:13D:205:GLU:HA   | 2.03                     | 0.40              |
| 1:1C:245:ASP:N     | 1:1C:245:ASP:OD1   | 2.54                     | 0.40              |
| 1:1C:425:LEU:HA    | 1:1C:425:LEU:HD23  | 1.90                     | 0.40              |
| 1:2A:35:GLN:O      | 1:2A:37:PRO:HD3    | 2.22                     | 0.40              |
| 1:2A:271:THR:HG22  | 1:2A:377:MET:HB3   | 2.04                     | 0.40              |
| 2:2D:128:ASP:OD1   | 2:2D:129:CYS:N     | 2.53                     | 0.40              |
| 1:2E:91:GLN:HA     | 1:2E:121:ARG:NH1   | 2.35                     | 0.40              |
| 1:3A:175:PRO:HD2   | 1:3A:207:GLU:OE1   | 2.21                     | 0.40              |
| 1:3A:265:ILE:HG23  | 1:3A:432:TYR:CZ    | 2.56                     | 0.40              |
| 1:3E:207:GLU:O     | 1:3E:210:TYR:HB2   | 2.21                     | 0.40              |
| 1:4A:11:GLN:HB3    | 3:4A:500:GTP:O2B   | 2.22                     | 0.40              |
| 1:4C:213:CYS:O     | 1:4C:219:ILE:HG22  | 2.21                     | 0.40              |
| 1:4C:360:PRO:HG3   | 1:4C:374:ALA:HB2   | 2.02                     | 0.40              |
| 2:5B:317:PHE:CD2   | 2:5B:321:MET:HE1   | 2.57                     | 0.40              |
| 2:6D:220:PRO:HD2   | 1:6E:326:LYS:CD    | 2.51                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:6E:220:GLU:OE1 | 1:6E:220:GLU:N   | 2.40                     | 0.40              |
| 1:7C:407:TRP:O   | 1:7C:411:GLU:HG2 | 2.21                     | 0.40              |
| 1:7E:69:ASP:OD1  | 1:7E:70:LEU:N    | 2.54                     | 0.40              |
| 1:8C:168:GLU:C   | 1:8C:169:PHE:HD1 | 2.29                     | 0.40              |
| 2:9D:2:ARG:HB2   | 2:9D:2:ARG:NH1   | 2.36                     | 0.40              |
| 2:9D:327:ASP:OD1 | 2:9D:328:GLU:N   | 2.55                     | 0.40              |
| 1:9E:129:CYS:SG  | 1:9E:132:LEU:HB2 | 2.62                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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   | 10A   | 422/475 (89%) | 409 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | 10C   | 422/475 (89%) | 409 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | 10E   | 422/475 (89%) | 407 (96%) | 15 (4%) | 0        | 100         | 100 |
| 1   | 11A   | 422/475 (89%) | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 11C   | 422/475 (89%) | 404 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 11E   | 422/475 (89%) | 401 (95%) | 21 (5%) | 0        | 100         | 100 |
| 1   | 12A   | 422/475 (89%) | 409 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | 12C   | 422/475 (89%) | 410 (97%) | 12 (3%) | 0        | 100         | 100 |
| 1   | 12E   | 422/475 (89%) | 406 (96%) | 16 (4%) | 0        | 100         | 100 |
| 1   | 13A   | 422/475 (89%) | 402 (95%) | 20 (5%) | 0        | 100         | 100 |
| 1   | 13C   | 422/475 (89%) | 403 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | 13E   | 422/475 (89%) | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 1A    | 422/475 (89%) | 406 (96%) | 16 (4%) | 0        | 100         | 100 |
| 1   | 1C    | 422/475 (89%) | 405 (96%) | 17 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | 1E    | 422/475 (89%)  | 404 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2A    | 422/475 (89%)  | 407 (96%) | 15 (4%) | 0        | 100         | 100 |
| 1   | 2C    | 422/475 (89%)  | 407 (96%) | 15 (4%) | 0        | 100         | 100 |
| 1   | 2E    | 422/475 (89%)  | 408 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | 3A    | 422/475 (89%)  | 404 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3C    | 422/475 (89%)  | 406 (96%) | 16 (4%) | 0        | 100         | 100 |
| 1   | 3E    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 4A    | 422/475 (89%)  | 408 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | 4C    | 422/475 (89%)  | 406 (96%) | 16 (4%) | 0        | 100         | 100 |
| 1   | 4E    | 422/475 (89%)  | 406 (96%) | 16 (4%) | 0        | 100         | 100 |
| 1   | 5A    | 422/475 (89%)  | 407 (96%) | 15 (4%) | 0        | 100         | 100 |
| 1   | 5C    | 422/475 (89%)  | 411 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | 5E    | 422/475 (89%)  | 409 (97%) | 13 (3%) | 0        | 100         | 100 |
| 1   | 6A    | 422/475 (89%)  | 403 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | 6C    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 6E    | 422/475 (89%)  | 404 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 7A    | 422/475 (89%)  | 403 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | 7C    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 7E    | 422/475 (89%)  | 404 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 8A    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 8C    | 422/475 (89%)  | 403 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | 8E    | 422/475 (89%)  | 403 (96%) | 19 (4%) | 0        | 100         | 100 |
| 1   | 9A    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | 9C    | 422/475 (89%)  | 408 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | 9E    | 422/475 (89%)  | 405 (96%) | 17 (4%) | 0        | 100         | 100 |
| 2   | 10B   | 423/425 (100%) | 405 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 10D   | 423/425 (100%) | 404 (96%) | 19 (4%) | 0        | 100         | 100 |
| 2   | 11B   | 423/425 (100%) | 403 (95%) | 20 (5%) | 0        | 100         | 100 |
| 2   | 11D   | 423/425 (100%) | 405 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 12B   | 423/425 (100%) | 398 (94%) | 25 (6%) | 0        | 100         | 100 |
| 2   | 12D   | 423/425 (100%) | 398 (94%) | 25 (6%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 2   | 13B   | 423/425 (100%)    | 396 (94%)   | 27 (6%)   | 0        | 100         | 100 |
| 2   | 13D   | 423/425 (100%)    | 400 (95%)   | 23 (5%)   | 0        | 100         | 100 |
| 2   | 1B    | 423/425 (100%)    | 411 (97%)   | 12 (3%)   | 0        | 100         | 100 |
| 2   | 1D    | 423/425 (100%)    | 404 (96%)   | 19 (4%)   | 0        | 100         | 100 |
| 2   | 2B    | 423/425 (100%)    | 411 (97%)   | 12 (3%)   | 0        | 100         | 100 |
| 2   | 2D    | 423/425 (100%)    | 407 (96%)   | 16 (4%)   | 0        | 100         | 100 |
| 2   | 3B    | 423/425 (100%)    | 412 (97%)   | 11 (3%)   | 0        | 100         | 100 |
| 2   | 3D    | 423/425 (100%)    | 412 (97%)   | 11 (3%)   | 0        | 100         | 100 |
| 2   | 4B    | 423/425 (100%)    | 408 (96%)   | 15 (4%)   | 0        | 100         | 100 |
| 2   | 4D    | 423/425 (100%)    | 411 (97%)   | 12 (3%)   | 0        | 100         | 100 |
| 2   | 5B    | 423/425 (100%)    | 404 (96%)   | 19 (4%)   | 0        | 100         | 100 |
| 2   | 5D    | 423/425 (100%)    | 405 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 6B    | 423/425 (100%)    | 399 (94%)   | 24 (6%)   | 0        | 100         | 100 |
| 2   | 6D    | 423/425 (100%)    | 397 (94%)   | 26 (6%)   | 0        | 100         | 100 |
| 2   | 7B    | 423/425 (100%)    | 401 (95%)   | 22 (5%)   | 0        | 100         | 100 |
| 2   | 7D    | 423/425 (100%)    | 402 (95%)   | 21 (5%)   | 0        | 100         | 100 |
| 2   | 8B    | 423/425 (100%)    | 404 (96%)   | 19 (4%)   | 0        | 100         | 100 |
| 2   | 8D    | 423/425 (100%)    | 406 (96%)   | 17 (4%)   | 0        | 100         | 100 |
| 2   | 9B    | 423/425 (100%)    | 412 (97%)   | 11 (3%)   | 0        | 100         | 100 |
| 2   | 9D    | 423/425 (100%)    | 405 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| All | All   | 27456/29575 (93%) | 26342 (96%) | 1114 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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   | 10A   | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 10C   | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 10E   | 359/395 (91%) | 357 (99%)  | 2 (1%)   | 78          | 79  |
| 1   | 11A   | 359/395 (91%) | 357 (99%)  | 2 (1%)   | 78          | 79  |
| 1   | 11C   | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 11E   | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 12A   | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 12C   | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 12E   | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 13A   | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 13C   | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 13E   | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 1A    | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 1C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 1E    | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 2A    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 2C    | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 2E    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 3A    | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 3C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 3E    | 359/395 (91%) | 358 (100%) | 1 (0%)   | 86          | 84  |
| 1   | 4A    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 4C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 4E    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 5A    | 359/395 (91%) | 357 (99%)  | 2 (1%)   | 78          | 79  |
| 1   | 5C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 5E    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 6A    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 6C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 6E    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 7A    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |
| 1   | 7C    | 359/395 (91%) | 359 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 7E    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 8A    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 8C    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 8E    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 9A    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 9C    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | 9E    | 359/395 (91%)  | 359 (100%) | 0        | 100         | 100 |
| 2   | 10B   | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 10D   | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 11B   | 364/364 (100%) | 362 (100%) | 2 (0%)   | 81          | 81  |
| 2   | 11D   | 364/364 (100%) | 363 (100%) | 1 (0%)   | 86          | 84  |
| 2   | 12B   | 364/364 (100%) | 362 (100%) | 2 (0%)   | 81          | 81  |
| 2   | 12D   | 364/364 (100%) | 362 (100%) | 2 (0%)   | 81          | 81  |
| 2   | 13B   | 364/364 (100%) | 360 (99%)  | 4 (1%)   | 65          | 73  |
| 2   | 13D   | 364/364 (100%) | 361 (99%)  | 3 (1%)   | 73          | 76  |
| 2   | 1B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 1D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 2B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 2D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 3B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 3D    | 364/364 (100%) | 363 (100%) | 1 (0%)   | 86          | 84  |
| 2   | 4B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 4D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 5B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 5D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 6B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 6D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 7B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 7D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 8B    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |
| 2   | 8D    | 364/364 (100%) | 364 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 2   | 9B    | 364/364 (100%)    | 364 (100%)   | 0        | 100         | 100 |
| 2   | 9D    | 364/364 (100%)    | 364 (100%)   | 0        | 100         | 100 |
| All | All   | 23465/24869 (94%) | 23434 (100%) | 31 (0%)  | 87          | 89  |

All (31) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 10C   | 300 | ASN  |
| 1   | 10E   | 313 | MET  |
| 1   | 10E   | 373 | ARG  |
| 1   | 11A   | 280 | LYS  |
| 1   | 11A   | 313 | MET  |
| 2   | 11B   | 204 | ASN  |
| 2   | 11B   | 391 | ARG  |
| 2   | 11D   | 204 | ASN  |
| 1   | 12A   | 128 | GLN  |
| 2   | 12B   | 329 | GLN  |
| 2   | 12B   | 391 | ARG  |
| 1   | 12C   | 402 | ARG  |
| 2   | 12D   | 204 | ASN  |
| 2   | 12D   | 391 | ARG  |
| 1   | 12E   | 128 | GLN  |
| 2   | 13B   | 204 | ASN  |
| 2   | 13B   | 320 | ARG  |
| 2   | 13B   | 363 | MET  |
| 2   | 13B   | 391 | ARG  |
| 2   | 13D   | 204 | ASN  |
| 2   | 13D   | 320 | ARG  |
| 2   | 13D   | 391 | ARG  |
| 1   | 13E   | 329 | ASN  |
| 1   | 1A    | 31  | GLN  |
| 1   | 1E    | 309 | HIS  |
| 1   | 2C    | 31  | GLN  |
| 1   | 3A    | 133 | GLN  |
| 2   | 3D    | 195 | ASN  |
| 1   | 3E    | 133 | GLN  |
| 1   | 5A    | 216 | ASN  |
| 1   | 5A    | 300 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 197 | HIS  |
| 2   | 1B    | 43  | GLN  |
| 2   | 1B    | 264 | HIS  |
| 2   | 1B    | 280 | GLN  |
| 1   | 1C    | 128 | GLN  |
| 1   | 1C    | 256 | GLN  |
| 1   | 1C    | 309 | HIS  |
| 1   | 1C    | 380 | ASN  |
| 2   | 1D    | 43  | GLN  |
| 2   | 1D    | 134 | GLN  |
| 2   | 1D    | 191 | GLN  |
| 2   | 1D    | 195 | ASN  |
| 1   | 1E    | 102 | ASN  |
| 1   | 1E    | 197 | HIS  |
| 1   | 1E    | 216 | ASN  |
| 1   | 1E    | 300 | ASN  |
| 1   | 1E    | 329 | ASN  |
| 1   | 2A    | 31  | GLN  |
| 1   | 2A    | 88  | HIS  |
| 1   | 2A    | 102 | ASN  |
| 1   | 2A    | 249 | ASN  |
| 1   | 2A    | 301 | GLN  |
| 2   | 2B    | 43  | GLN  |
| 2   | 2B    | 291 | GLN  |
| 2   | 2B    | 335 | ASN  |
| 1   | 2C    | 8   | HIS  |
| 1   | 2C    | 101 | ASN  |
| 1   | 2C    | 256 | GLN  |
| 2   | 2D    | 191 | GLN  |
| 2   | 2D    | 335 | ASN  |
| 2   | 2D    | 396 | HIS  |
| 2   | 2D    | 423 | GLN  |
| 1   | 2E    | 31  | GLN  |
| 1   | 2E    | 61  | HIS  |
| 1   | 2E    | 102 | ASN  |
| 1   | 2E    | 197 | HIS  |
| 1   | 2E    | 293 | ASN  |
| 1   | 3A    | 133 | GLN  |
| 1   | 3A    | 186 | ASN  |
| 1   | 3A    | 249 | ASN  |
| 1   | 3A    | 283 | HIS  |
| 2   | 3B    | 14  | ASN  |
| 2   | 3B    | 99  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3B    | 191 | GLN  |
| 2   | 3B    | 335 | ASN  |
| 2   | 3B    | 426 | GLN  |
| 1   | 3C    | 31  | GLN  |
| 1   | 3C    | 88  | HIS  |
| 1   | 3C    | 101 | ASN  |
| 1   | 3C    | 133 | GLN  |
| 1   | 3C    | 249 | ASN  |
| 1   | 3C    | 283 | HIS  |
| 2   | 3D    | 43  | GLN  |
| 2   | 3D    | 191 | GLN  |
| 2   | 3D    | 195 | ASN  |
| 2   | 3D    | 256 | ASN  |
| 2   | 3D    | 335 | ASN  |
| 2   | 3D    | 384 | GLN  |
| 2   | 3D    | 423 | GLN  |
| 1   | 3E    | 88  | HIS  |
| 1   | 3E    | 102 | ASN  |
| 1   | 3E    | 133 | GLN  |
| 1   | 3E    | 186 | ASN  |
| 1   | 3E    | 249 | ASN  |
| 1   | 3E    | 283 | HIS  |
| 1   | 4A    | 216 | ASN  |
| 1   | 4A    | 258 | ASN  |
| 1   | 4A    | 285 | GLN  |
| 1   | 4A    | 300 | ASN  |
| 2   | 4B    | 8   | GLN  |
| 2   | 4B    | 191 | GLN  |
| 2   | 4B    | 291 | GLN  |
| 2   | 4B    | 384 | GLN  |
| 1   | 4C    | 88  | HIS  |
| 1   | 4C    | 192 | HIS  |
| 1   | 4C    | 197 | HIS  |
| 1   | 4C    | 216 | ASN  |
| 1   | 4C    | 285 | GLN  |
| 1   | 4C    | 300 | ASN  |
| 2   | 4D    | 43  | GLN  |
| 2   | 4D    | 191 | GLN  |
| 2   | 4D    | 195 | ASN  |
| 1   | 4E    | 102 | ASN  |
| 1   | 4E    | 139 | HIS  |
| 1   | 4E    | 329 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5A    | 11  | GLN  |
| 1   | 5A    | 133 | GLN  |
| 1   | 5A    | 226 | ASN  |
| 1   | 5A    | 249 | ASN  |
| 1   | 5A    | 283 | HIS  |
| 1   | 5A    | 285 | GLN  |
| 2   | 5B    | 43  | GLN  |
| 2   | 5B    | 134 | GLN  |
| 2   | 5B    | 396 | HIS  |
| 1   | 5C    | 11  | GLN  |
| 1   | 5C    | 50  | ASN  |
| 1   | 5C    | 88  | HIS  |
| 1   | 5C    | 206 | ASN  |
| 1   | 5C    | 283 | HIS  |
| 1   | 5C    | 301 | GLN  |
| 2   | 5D    | 43  | GLN  |
| 2   | 5D    | 131 | GLN  |
| 2   | 5D    | 195 | ASN  |
| 1   | 5E    | 88  | HIS  |
| 1   | 5E    | 186 | ASN  |
| 1   | 5E    | 206 | ASN  |
| 1   | 5E    | 226 | ASN  |
| 1   | 5E    | 249 | ASN  |
| 1   | 5E    | 283 | HIS  |
| 1   | 5E    | 285 | GLN  |
| 1   | 6A    | 11  | GLN  |
| 1   | 6A    | 102 | ASN  |
| 1   | 6A    | 256 | GLN  |
| 1   | 6A    | 285 | GLN  |
| 1   | 6A    | 301 | GLN  |
| 2   | 6B    | 99  | ASN  |
| 2   | 6B    | 191 | GLN  |
| 2   | 6B    | 195 | ASN  |
| 2   | 6B    | 298 | ASN  |
| 1   | 6C    | 11  | GLN  |
| 1   | 6C    | 101 | ASN  |
| 1   | 6C    | 102 | ASN  |
| 1   | 6C    | 133 | GLN  |
| 1   | 6C    | 256 | GLN  |
| 1   | 6C    | 285 | GLN  |
| 1   | 6C    | 300 | ASN  |
| 1   | 6C    | 329 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 6D    | 99  | ASN  |
| 2   | 6D    | 191 | GLN  |
| 2   | 6D    | 291 | GLN  |
| 2   | 6D    | 307 | HIS  |
| 2   | 6D    | 384 | GLN  |
| 1   | 6E    | 101 | ASN  |
| 1   | 6E    | 102 | ASN  |
| 1   | 6E    | 197 | HIS  |
| 1   | 6E    | 206 | ASN  |
| 1   | 6E    | 216 | ASN  |
| 1   | 6E    | 226 | ASN  |
| 1   | 6E    | 283 | HIS  |
| 1   | 6E    | 285 | GLN  |
| 1   | 6E    | 300 | ASN  |
| 1   | 6E    | 329 | ASN  |
| 1   | 7A    | 133 | GLN  |
| 1   | 7A    | 186 | ASN  |
| 1   | 7A    | 206 | ASN  |
| 1   | 7A    | 258 | ASN  |
| 1   | 7A    | 283 | HIS  |
| 1   | 7A    | 285 | GLN  |
| 2   | 7B    | 43  | GLN  |
| 2   | 7B    | 99  | ASN  |
| 1   | 7C    | 11  | GLN  |
| 1   | 7C    | 88  | HIS  |
| 1   | 7C    | 102 | ASN  |
| 1   | 7C    | 133 | GLN  |
| 1   | 7C    | 186 | ASN  |
| 1   | 7C    | 285 | GLN  |
| 1   | 7C    | 301 | GLN  |
| 1   | 7C    | 329 | ASN  |
| 2   | 7D    | 43  | GLN  |
| 2   | 7D    | 195 | ASN  |
| 2   | 7D    | 426 | GLN  |
| 1   | 7E    | 35  | GLN  |
| 1   | 7E    | 101 | ASN  |
| 1   | 7E    | 133 | GLN  |
| 1   | 7E    | 226 | ASN  |
| 1   | 7E    | 283 | HIS  |
| 1   | 7E    | 285 | GLN  |
| 1   | 7E    | 301 | GLN  |
| 1   | 8A    | 186 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8A    | 226 | ASN  |
| 1   | 8A    | 266 | HIS  |
| 1   | 8A    | 283 | HIS  |
| 1   | 8A    | 285 | GLN  |
| 1   | 8A    | 309 | HIS  |
| 1   | 8A    | 406 | HIS  |
| 2   | 8B    | 137 | HIS  |
| 1   | 8C    | 133 | GLN  |
| 1   | 8C    | 206 | ASN  |
| 1   | 8C    | 266 | HIS  |
| 1   | 8C    | 283 | HIS  |
| 1   | 8C    | 309 | HIS  |
| 1   | 8C    | 380 | ASN  |
| 2   | 8D    | 396 | HIS  |
| 2   | 8D    | 414 | ASN  |
| 2   | 8D    | 426 | GLN  |
| 1   | 8E    | 101 | ASN  |
| 1   | 8E    | 128 | GLN  |
| 1   | 8E    | 226 | ASN  |
| 1   | 8E    | 266 | HIS  |
| 1   | 8E    | 283 | HIS  |
| 1   | 8E    | 285 | GLN  |
| 1   | 9A    | 11  | GLN  |
| 1   | 9A    | 88  | HIS  |
| 1   | 9A    | 226 | ASN  |
| 1   | 9A    | 266 | HIS  |
| 2   | 9B    | 14  | ASN  |
| 2   | 9B    | 43  | GLN  |
| 2   | 9B    | 105 | HIS  |
| 2   | 9B    | 329 | GLN  |
| 1   | 9C    | 266 | HIS  |
| 1   | 9C    | 301 | GLN  |
| 2   | 9D    | 43  | GLN  |
| 2   | 9D    | 348 | ASN  |
| 2   | 9D    | 426 | GLN  |
| 1   | 9E    | 102 | ASN  |
| 1   | 9E    | 226 | ASN  |
| 1   | 9E    | 266 | HIS  |
| 1   | 9E    | 301 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 104 ligands modelled in this entry, 39 are monoatomic - leaving 65 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 3   | GTP  | 11A   | 500 | 4    | 33,34,34     | 0.99 | 2 (6%)      | 50,54,54    | 1.64 | 9 (18%)     |
| 3   | GTP  | 7E    | 500 | -    | 33,34,34     | 0.95 | 2 (6%)      | 50,54,54    | 1.57 | 8 (16%)     |
| 3   | GTP  | 1A    | 500 | 4    | 33,34,34     | 0.94 | 2 (6%)      | 50,54,54    | 1.64 | 9 (18%)     |
| 3   | GTP  | 8E    | 500 | 4    | 33,34,34     | 1.30 | 5 (15%)     | 50,54,54    | 1.86 | 11 (22%)    |
| 5   | GDP  | 3D    | 600 | -    | 29,30,30     | 1.14 | 3 (10%)     | 45,47,47    | 1.76 | 7 (15%)     |
| 3   | GTP  | 3E    | 500 | 4    | 33,34,34     | 0.87 | 2 (6%)      | 50,54,54    | 1.62 | 9 (18%)     |
| 5   | GDP  | 13B   | 600 | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 3   | GTP  | 13C   | 500 | 4    | 33,34,34     | 0.97 | 1 (3%)      | 50,54,54    | 1.71 | 10 (20%)    |
| 3   | GTP  | 2A    | 500 | 4    | 33,34,34     | 0.89 | 2 (6%)      | 50,54,54    | 1.64 | 9 (18%)     |
| 5   | GDP  | 12D   | 600 | -    | 29,30,30     | 1.13 | 4 (13%)     | 45,47,47    | 1.75 | 8 (17%)     |
| 5   | GDP  | 13D   | 600 | -    | 29,30,30     | 1.15 | 3 (10%)     | 45,47,47    | 1.72 | 6 (13%)     |
| 5   | GDP  | 2D    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)     | 45,47,47    | 1.79 | 8 (17%)     |
| 3   | GTP  | 13A   | 500 | 4    | 33,34,34     | 0.97 | 2 (6%)      | 50,54,54    | 1.63 | 11 (22%)    |
| 5   | GDP  | 5D    | 600 | -    | 29,30,30     | 1.14 | 3 (10%)     | 45,47,47    | 1.78 | 8 (17%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | GTP  | 9E    | 500 | 4    | 33,34,34     | 0.94 | 2 (6%)   | 50,54,54    | 1.65 | 10 (20%) |
| 3   | GTP  | 8C    | 500 | 4    | 33,34,34     | 0.97 | 2 (6%)   | 50,54,54    | 1.56 | 8 (16%)  |
| 5   | GDP  | 1B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.79 | 8 (17%)  |
| 3   | GTP  | 9C    | 500 | 4    | 33,34,34     | 0.90 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 3   | GTP  | 11E   | 500 | 4    | 33,34,34     | 0.98 | 2 (6%)   | 50,54,54    | 1.63 | 9 (18%)  |
| 5   | GDP  | 6B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.75 | 8 (17%)  |
| 5   | GDP  | 7B    | 600 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.81 | 8 (17%)  |
| 5   | GDP  | 11D   | 600 | -    | 29,30,30     | 1.16 | 4 (13%)  | 45,47,47    | 1.72 | 8 (17%)  |
| 5   | GDP  | 4B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.78 | 8 (17%)  |
| 3   | GTP  | 5A    | 500 | 4    | 33,34,34     | 0.91 | 1 (3%)   | 50,54,54    | 1.53 | 8 (16%)  |
| 5   | GDP  | 9D    | 600 | -    | 29,30,30     | 1.13 | 3 (10%)  | 45,47,47    | 1.80 | 7 (15%)  |
| 3   | GTP  | 4A    | 500 | 4    | 33,34,34     | 0.89 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 5   | GDP  | 10D   | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.77 | 7 (15%)  |
| 3   | GTP  | 7C    | 500 | 4    | 33,34,34     | 0.93 | 2 (6%)   | 50,54,54    | 1.65 | 10 (20%) |
| 5   | GDP  | 2B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.79 | 8 (17%)  |
| 5   | GDP  | 10B   | 600 | -    | 29,30,30     | 1.13 | 3 (10%)  | 45,47,47    | 1.77 | 8 (17%)  |
| 3   | GTP  | 8A    | 500 | 4    | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.54 | 9 (18%)  |
| 3   | GTP  | 13E   | 500 | 4    | 33,34,34     | 0.95 | 2 (6%)   | 50,54,54    | 1.61 | 11 (22%) |
| 5   | GDP  | 6D    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.76 | 8 (17%)  |
| 5   | GDP  | 11B   | 600 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.72 | 8 (17%)  |
| 3   | GTP  | 10E   | 500 | 4    | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.58 | 9 (18%)  |
| 3   | GTP  | 1E    | 500 | 4    | 33,34,34     | 0.96 | 2 (6%)   | 50,54,54    | 1.64 | 10 (20%) |
| 3   | GTP  | 10A   | 500 | 4    | 33,34,34     | 0.98 | 2 (6%)   | 50,54,54    | 1.61 | 9 (18%)  |
| 5   | GDP  | 8B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.76 | 8 (17%)  |
| 5   | GDP  | 7D    | 600 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.80 | 8 (17%)  |
| 3   | GTP  | 1C    | 500 | 4    | 33,34,34     | 0.93 | 2 (6%)   | 50,54,54    | 1.63 | 9 (18%)  |
| 3   | GTP  | 5E    | 500 | 4    | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.53 | 8 (16%)  |
| 3   | GTP  | 7A    | 500 | 4    | 33,34,34     | 0.93 | 2 (6%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 3A    | 500 | 4    | 33,34,34     | 0.86 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 3   | GTP  | 5C    | 500 | 4    | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.58 | 9 (18%)  |
| 3   | GTP  | 2C    | 500 | 4    | 33,34,34     | 0.90 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 5   | GDP  | 4D    | 600 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.78 | 8 (17%)  |
| 5   | GDP  | 9B    | 600 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.79 | 7 (15%)  |
| 3   | GTP  | 11C   | 500 | 4    | 33,34,34     | 0.96 | 1 (3%)   | 50,54,54    | 1.65 | 9 (18%)  |
| 3   | GTP  | 10C   | 500 | 4    | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.62 | 10 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | GTP  | 12E   | 500 | 4    | 33,34,34     | 1.01 | 2 (6%)   | 50,54,54    | 1.56 | 8 (16%)  |
| 5   | GDP  | 1D    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.79 | 8 (17%)  |
| 5   | GDP  | 8D    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.75 | 8 (17%)  |
| 3   | GTP  | 3C    | 500 | 4    | 33,34,34     | 0.89 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 3   | GTP  | 6A    | 500 | 4    | 33,34,34     | 0.93 | 2 (6%)   | 50,54,54    | 1.58 | 8 (16%)  |
| 3   | GTP  | 2E    | 500 | 4    | 33,34,34     | 0.90 | 2 (6%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 3   | GTP  | 6C    | 500 | 4    | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.56 | 8 (16%)  |
| 3   | GTP  | 12A   | 500 | 4    | 33,34,34     | 0.98 | 3 (9%)   | 50,54,54    | 1.66 | 10 (20%) |
| 3   | GTP  | 12C   | 500 | 4    | 33,34,34     | 0.96 | 3 (9%)   | 50,54,54    | 1.70 | 10 (20%) |
| 3   | GTP  | 4C    | 500 | 4    | 33,34,34     | 0.86 | 2 (6%)   | 50,54,54    | 1.61 | 9 (18%)  |
| 3   | GTP  | 6E    | 500 | 4    | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.60 | 9 (18%)  |
| 5   | GDP  | 12B   | 600 | -    | 29,30,30     | 1.13 | 3 (10%)  | 45,47,47    | 1.76 | 7 (15%)  |
| 5   | GDP  | 5B    | 600 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.79 | 8 (17%)  |
| 3   | GTP  | 9A    | 500 | 4    | 33,34,34     | 0.94 | 2 (6%)   | 50,54,54    | 1.64 | 10 (20%) |
| 5   | GDP  | 3B    | 600 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.77 | 6 (13%)  |
| 3   | GTP  | 4E    | 500 | 4    | 33,34,34     | 0.85 | 2 (6%)   | 50,54,54    | 1.60 | 9 (18%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | GTP  | 11A   | 500 | 4    | -       | 9/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 7E    | 500 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1A    | 500 | 4    | -       | 7/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 8E    | 500 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3D    | 600 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3E    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 13B   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 13C   | 500 | 4    | -       | 3/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2A    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 12D   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 13D   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2D    | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 13A   | 500 | 4    | -       | 7/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | GDP  | 5D    | 600 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 9E    | 500 | 4    | -       | 3/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 8C    | 500 | 4    | -       | 5/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1B    | 600 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 9C    | 500 | 4    | -       | 3/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 11E   | 500 | 4    | -       | 8/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 6B    | 600 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 7B    | 600 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 11D   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4B    | 600 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 5A    | 500 | 4    | -       | 5/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 9D    | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4A    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 10D   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 7C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2B    | 600 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 10B   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 8A    | 500 | 4    | -       | 5/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 13E   | 500 | 4    | -       | 5/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 6D    | 600 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 11B   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 10E   | 500 | 4    | -       | 7/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1E    | 500 | 4    | -       | 8/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 10A   | 500 | 4    | -       | 8/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 8B    | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 7D    | 600 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1C    | 500 | 4    | -       | 7/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 5E    | 500 | 4    | -       | 5/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 7A    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3A    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 5C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 4D    | 600 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 9B    | 600 | -    | -       | 3/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | GTP  | 11C   | 500 | 4    | -       | 8/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 10C   | 500 | 4    | -       | 7/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 12E   | 500 | 4    | -       | 2/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1D    | 600 | -    | -       | 0/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 8D    | 600 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 6A    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2E    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 6C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 12A   | 500 | 4    | -       | 1/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 12C   | 500 | 4    | -       | 2/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4C    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 6E    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 12B   | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 5B    | 600 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 9A    | 500 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3B    | 600 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4E    | 500 | 4    | -       | 4/22/38/38 | 0/3/3/3 |

All (156) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | 8E    | 500 | GTP  | C5-N7 | -3.33 | 1.32        | 1.39     |
| 5   | 1B    | 600 | GDP  | C5-C4 | 2.97  | 1.46        | 1.38     |
| 5   | 3D    | 600 | GDP  | C5-C4 | 2.97  | 1.46        | 1.38     |
| 5   | 3B    | 600 | GDP  | C5-C4 | 2.97  | 1.46        | 1.38     |
| 5   | 1D    | 600 | GDP  | C5-C4 | 2.96  | 1.46        | 1.38     |
| 5   | 2D    | 600 | GDP  | C5-C4 | 2.95  | 1.46        | 1.38     |
| 5   | 6D    | 600 | GDP  | C5-C4 | 2.94  | 1.46        | 1.38     |
| 5   | 4D    | 600 | GDP  | C5-C4 | 2.93  | 1.46        | 1.38     |
| 5   | 2B    | 600 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 5   | 6B    | 600 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 5   | 13D   | 600 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 5   | 13B   | 600 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 5   | 4B    | 600 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 5   | 8B    | 600 | GDP  | C5-C4 | 2.90  | 1.46        | 1.38     |
| 5   | 5B    | 600 | GDP  | C5-C4 | 2.89  | 1.46        | 1.38     |
| 5   | 5D    | 600 | GDP  | C5-C4 | 2.87  | 1.46        | 1.38     |
| 5   | 9D    | 600 | GDP  | C5-C4 | 2.86  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | 8D    | 600 | GDP  | C5-C4   | 2.85  | 1.46        | 1.38     |
| 5   | 7D    | 600 | GDP  | C5-C4   | 2.84  | 1.46        | 1.38     |
| 5   | 7B    | 600 | GDP  | C5-C4   | 2.84  | 1.46        | 1.38     |
| 5   | 7B    | 600 | GDP  | C6-N1   | -2.83 | 1.33        | 1.38     |
| 5   | 9B    | 600 | GDP  | C5-C4   | 2.83  | 1.46        | 1.38     |
| 5   | 10B   | 600 | GDP  | C5-C4   | 2.82  | 1.46        | 1.38     |
| 5   | 7D    | 600 | GDP  | C6-N1   | -2.81 | 1.33        | 1.38     |
| 5   | 10D   | 600 | GDP  | C5-C4   | 2.81  | 1.46        | 1.38     |
| 5   | 11D   | 600 | GDP  | C5-C4   | 2.78  | 1.46        | 1.38     |
| 5   | 11B   | 600 | GDP  | C5-C4   | 2.77  | 1.46        | 1.38     |
| 5   | 2D    | 600 | GDP  | C6-N1   | -2.76 | 1.33        | 1.38     |
| 5   | 12D   | 600 | GDP  | C5-C4   | 2.76  | 1.46        | 1.38     |
| 5   | 10D   | 600 | GDP  | C6-N1   | -2.76 | 1.33        | 1.38     |
| 5   | 12B   | 600 | GDP  | C5-C4   | 2.76  | 1.46        | 1.38     |
| 5   | 2B    | 600 | GDP  | C6-N1   | -2.75 | 1.33        | 1.38     |
| 5   | 11B   | 600 | GDP  | C6-N1   | -2.73 | 1.33        | 1.38     |
| 5   | 5B    | 600 | GDP  | C6-N1   | -2.73 | 1.33        | 1.38     |
| 5   | 8B    | 600 | GDP  | C6-N1   | -2.71 | 1.33        | 1.38     |
| 5   | 6B    | 600 | GDP  | C6-N1   | -2.71 | 1.33        | 1.38     |
| 5   | 11D   | 600 | GDP  | C6-N1   | -2.70 | 1.33        | 1.38     |
| 5   | 8D    | 600 | GDP  | C6-N1   | -2.69 | 1.33        | 1.38     |
| 5   | 1B    | 600 | GDP  | C6-N1   | -2.69 | 1.33        | 1.38     |
| 5   | 6D    | 600 | GDP  | C6-N1   | -2.69 | 1.33        | 1.38     |
| 5   | 5D    | 600 | GDP  | C6-N1   | -2.68 | 1.33        | 1.38     |
| 3   | 8E    | 500 | GTP  | C2-N2   | -2.68 | 1.27        | 1.34     |
| 5   | 1D    | 600 | GDP  | C6-N1   | -2.67 | 1.33        | 1.38     |
| 5   | 10B   | 600 | GDP  | C6-N1   | -2.66 | 1.33        | 1.38     |
| 5   | 4B    | 600 | GDP  | C6-N1   | -2.66 | 1.33        | 1.38     |
| 5   | 13B   | 600 | GDP  | C6-N1   | -2.65 | 1.33        | 1.38     |
| 5   | 9D    | 600 | GDP  | C6-N1   | -2.64 | 1.33        | 1.38     |
| 5   | 4D    | 600 | GDP  | C6-N1   | -2.63 | 1.33        | 1.38     |
| 5   | 3B    | 600 | GDP  | C6-N1   | -2.63 | 1.33        | 1.38     |
| 5   | 12B   | 600 | GDP  | C6-N1   | -2.63 | 1.33        | 1.38     |
| 5   | 12D   | 600 | GDP  | C6-N1   | -2.62 | 1.33        | 1.38     |
| 5   | 9B    | 600 | GDP  | C6-N1   | -2.62 | 1.33        | 1.38     |
| 5   | 3D    | 600 | GDP  | C6-N1   | -2.61 | 1.34        | 1.38     |
| 5   | 13D   | 600 | GDP  | C6-N1   | -2.60 | 1.34        | 1.38     |
| 3   | 8E    | 500 | GTP  | O4'-C4' | -2.51 | 1.39        | 1.45     |
| 3   | 8E    | 500 | GTP  | PB-O3A  | 2.37  | 1.62        | 1.59     |
| 5   | 5B    | 600 | GDP  | C5-N7   | -2.30 | 1.34        | 1.39     |
| 3   | 13A   | 500 | GTP  | PB-O3B  | 2.29  | 1.62        | 1.59     |
| 5   | 11B   | 600 | GDP  | C5-N7   | -2.29 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 11D   | 600 | GDP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 3   | 7A    | 500 | GTP  | C5-N7  | -2.27 | 1.34        | 1.39     |
| 5   | 7B    | 600 | GDP  | C5-N7  | -2.24 | 1.34        | 1.39     |
| 5   | 7D    | 600 | GDP  | C5-N7  | -2.23 | 1.34        | 1.39     |
| 3   | 7E    | 500 | GTP  | C5-N7  | -2.22 | 1.34        | 1.39     |
| 3   | 1A    | 500 | GTP  | C2-N3  | 2.22  | 1.38        | 1.33     |
| 3   | 1C    | 500 | GTP  | C2-N3  | 2.22  | 1.38        | 1.33     |
| 3   | 1E    | 500 | GTP  | C2-N3  | 2.21  | 1.38        | 1.33     |
| 5   | 1D    | 600 | GDP  | C5-N7  | -2.21 | 1.34        | 1.39     |
| 5   | 5D    | 600 | GDP  | C5-N7  | -2.21 | 1.34        | 1.39     |
| 5   | 10D   | 600 | GDP  | C5-N7  | -2.21 | 1.34        | 1.39     |
| 5   | 12B   | 600 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 5   | 6B    | 600 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 5   | 6D    | 600 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 3   | 13E   | 500 | GTP  | PB-O3B | 2.20  | 1.61        | 1.59     |
| 3   | 8C    | 500 | GTP  | C5-N7  | -2.19 | 1.34        | 1.39     |
| 3   | 5C    | 500 | GTP  | C5-N7  | -2.19 | 1.34        | 1.39     |
| 3   | 2E    | 500 | GTP  | C2-N3  | 2.19  | 1.38        | 1.33     |
| 3   | 13C   | 500 | GTP  | C5-N7  | -2.19 | 1.34        | 1.39     |
| 5   | 2D    | 600 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 3   | 2C    | 500 | GTP  | C2-N3  | 2.18  | 1.38        | 1.33     |
| 5   | 3D    | 600 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 5   | 1B    | 600 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 5   | 2B    | 600 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 5   | 3B    | 600 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 5   | 12D   | 600 | GDP  | C5-N7  | -2.17 | 1.34        | 1.39     |
| 5   | 4B    | 600 | GDP  | C5-N7  | -2.17 | 1.34        | 1.39     |
| 3   | 9C    | 500 | GTP  | C2-N3  | 2.16  | 1.38        | 1.33     |
| 5   | 9B    | 600 | GDP  | C5-N7  | -2.16 | 1.34        | 1.39     |
| 5   | 10B   | 600 | GDP  | C5-N7  | -2.16 | 1.34        | 1.39     |
| 3   | 2A    | 500 | GTP  | C2-N3  | 2.16  | 1.38        | 1.33     |
| 5   | 4D    | 600 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 3   | 12C   | 500 | GTP  | C2-N3  | 2.15  | 1.38        | 1.33     |
| 3   | 12A   | 500 | GTP  | PB-O3B | 2.15  | 1.61        | 1.59     |
| 3   | 10C   | 500 | GTP  | C2-N3  | 2.14  | 1.38        | 1.33     |
| 5   | 13D   | 600 | GDP  | C5-N7  | -2.14 | 1.34        | 1.39     |
| 3   | 6E    | 500 | GTP  | C2-N3  | 2.14  | 1.38        | 1.33     |
| 3   | 4A    | 500 | GTP  | C2-N3  | 2.13  | 1.38        | 1.33     |
| 3   | 12A   | 500 | GTP  | C5-N7  | -2.13 | 1.34        | 1.39     |
| 5   | 13B   | 600 | GDP  | C5-N7  | -2.13 | 1.34        | 1.39     |
| 3   | 4E    | 500 | GTP  | C2-N3  | 2.13  | 1.38        | 1.33     |
| 3   | 10C   | 500 | GTP  | C5-N7  | -2.13 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 9E    | 500 | GTP  | C2-N3   | 2.13  | 1.38        | 1.33     |
| 3   | 13E   | 500 | GTP  | C5-N7   | -2.13 | 1.34        | 1.39     |
| 3   | 10A   | 500 | GTP  | C5-N7   | -2.13 | 1.34        | 1.39     |
| 5   | 8D    | 600 | GDP  | C5-N7   | -2.13 | 1.34        | 1.39     |
| 3   | 5E    | 500 | GTP  | C5-N7   | -2.12 | 1.34        | 1.39     |
| 3   | 9A    | 500 | GTP  | C2-N3   | 2.12  | 1.38        | 1.33     |
| 3   | 12E   | 500 | GTP  | C5-N7   | -2.12 | 1.34        | 1.39     |
| 3   | 10E   | 500 | GTP  | C5-N7   | -2.12 | 1.34        | 1.39     |
| 3   | 12A   | 500 | GTP  | C2-N3   | 2.12  | 1.38        | 1.33     |
| 3   | 10E   | 500 | GTP  | C2-N3   | 2.12  | 1.38        | 1.33     |
| 3   | 12C   | 500 | GTP  | C5-N7   | -2.11 | 1.34        | 1.39     |
| 5   | 8B    | 600 | GDP  | C5-N7   | -2.11 | 1.34        | 1.39     |
| 3   | 11E   | 500 | GTP  | C2-N3   | 2.11  | 1.38        | 1.33     |
| 3   | 12E   | 500 | GTP  | PB-O3B  | 2.11  | 1.61        | 1.59     |
| 3   | 13A   | 500 | GTP  | C5-N7   | -2.10 | 1.34        | 1.39     |
| 3   | 6A    | 500 | GTP  | C2-N3   | 2.09  | 1.38        | 1.33     |
| 3   | 11C   | 500 | GTP  | C2-N3   | 2.09  | 1.38        | 1.33     |
| 3   | 3C    | 500 | GTP  | C2-N3   | 2.09  | 1.38        | 1.33     |
| 3   | 4C    | 500 | GTP  | C2-N3   | 2.09  | 1.38        | 1.33     |
| 3   | 3E    | 500 | GTP  | C2-N3   | 2.09  | 1.38        | 1.33     |
| 3   | 9E    | 500 | GTP  | C5-N7   | -2.09 | 1.34        | 1.39     |
| 3   | 9A    | 500 | GTP  | C5-N7   | -2.08 | 1.34        | 1.39     |
| 3   | 3A    | 500 | GTP  | C2-N3   | 2.08  | 1.38        | 1.33     |
| 3   | 7C    | 500 | GTP  | C5-N7   | -2.08 | 1.34        | 1.39     |
| 3   | 7C    | 500 | GTP  | C2-N3   | 2.07  | 1.38        | 1.33     |
| 3   | 6A    | 500 | GTP  | C5-N7   | -2.06 | 1.34        | 1.39     |
| 3   | 5A    | 500 | GTP  | C5-N7   | -2.06 | 1.34        | 1.39     |
| 3   | 10A   | 500 | GTP  | C2-N3   | 2.06  | 1.38        | 1.33     |
| 3   | 6C    | 500 | GTP  | C2-N3   | 2.06  | 1.38        | 1.33     |
| 3   | 3A    | 500 | GTP  | C5-N7   | -2.06 | 1.34        | 1.39     |
| 3   | 8E    | 500 | GTP  | PB-O3B  | 2.06  | 1.61        | 1.59     |
| 5   | 9D    | 600 | GDP  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 3   | 9C    | 500 | GTP  | C5-N7   | -2.05 | 1.35        | 1.39     |
| 3   | 11A   | 500 | GTP  | C2-N3   | 2.05  | 1.38        | 1.33     |
| 5   | 11D   | 600 | GDP  | C4-N9   | -2.05 | 1.32        | 1.38     |
| 3   | 8C    | 500 | GTP  | O4'-C4' | -2.04 | 1.40        | 1.45     |
| 3   | 1A    | 500 | GTP  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 3   | 2A    | 500 | GTP  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 3   | 7A    | 500 | GTP  | C2-N3   | 2.04  | 1.38        | 1.33     |
| 3   | 1E    | 500 | GTP  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 3   | 3C    | 500 | GTP  | C5-N7   | -2.04 | 1.35        | 1.39     |
| 3   | 1C    | 500 | GTP  | C5-N7   | -2.03 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | 12C   | 500 | GTP  | PB-O3B | 2.03  | 1.61        | 1.59     |
| 3   | 11E   | 500 | GTP  | C5-N7  | -2.03 | 1.35        | 1.39     |
| 3   | 2C    | 500 | GTP  | C5-N7  | -2.02 | 1.35        | 1.39     |
| 3   | 3E    | 500 | GTP  | C5-N7  | -2.02 | 1.35        | 1.39     |
| 3   | 11A   | 500 | GTP  | C5-N7  | -2.02 | 1.35        | 1.39     |
| 3   | 4A    | 500 | GTP  | C5-N7  | -2.01 | 1.35        | 1.39     |
| 3   | 8A    | 500 | GTP  | C5-N7  | -2.01 | 1.35        | 1.39     |
| 3   | 4E    | 500 | GTP  | C5-N7  | -2.01 | 1.35        | 1.39     |
| 3   | 2E    | 500 | GTP  | C5-N7  | -2.01 | 1.35        | 1.39     |
| 3   | 7E    | 500 | GTP  | C2-N3  | 2.01  | 1.38        | 1.33     |
| 3   | 8A    | 500 | GTP  | C2-N3  | 2.01  | 1.38        | 1.33     |
| 3   | 4C    | 500 | GTP  | C5-N7  | -2.00 | 1.35        | 1.39     |
| 5   | 12D   | 600 | GDP  | C4-N9  | -2.00 | 1.33        | 1.38     |

All (554) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 2D    | 600 | GDP  | C5-C4-N3 | -6.34 | 118.31      | 128.39   |
| 5   | 2B    | 600 | GDP  | C5-C4-N3 | -6.31 | 118.35      | 128.39   |
| 5   | 1B    | 600 | GDP  | C5-C4-N3 | -6.27 | 118.41      | 128.39   |
| 5   | 1D    | 600 | GDP  | C5-C4-N3 | -6.25 | 118.45      | 128.39   |
| 5   | 7B    | 600 | GDP  | C5-C4-N3 | -6.22 | 118.49      | 128.39   |
| 5   | 5D    | 600 | GDP  | C5-C4-N3 | -6.22 | 118.50      | 128.39   |
| 5   | 5B    | 600 | GDP  | C5-C4-N3 | -6.22 | 118.50      | 128.39   |
| 5   | 3B    | 600 | GDP  | C5-C4-N3 | -6.20 | 118.52      | 128.39   |
| 5   | 4B    | 600 | GDP  | C5-C4-N3 | -6.20 | 118.52      | 128.39   |
| 5   | 4D    | 600 | GDP  | C5-C4-N3 | -6.17 | 118.58      | 128.39   |
| 5   | 6B    | 600 | GDP  | C5-C4-N3 | -6.12 | 118.65      | 128.39   |
| 5   | 6D    | 600 | GDP  | C5-C4-N3 | -6.11 | 118.67      | 128.39   |
| 5   | 7D    | 600 | GDP  | C5-C4-N3 | -6.10 | 118.68      | 128.39   |
| 5   | 3D    | 600 | GDP  | C5-C4-N3 | -6.09 | 118.70      | 128.39   |
| 5   | 8B    | 600 | GDP  | C5-C4-N3 | -6.03 | 118.80      | 128.39   |
| 5   | 10D   | 600 | GDP  | C5-C4-N3 | -6.00 | 118.84      | 128.39   |
| 5   | 9B    | 600 | GDP  | C5-C4-N3 | -5.98 | 118.87      | 128.39   |
| 5   | 9D    | 600 | GDP  | C5-C4-N3 | -5.96 | 118.90      | 128.39   |
| 5   | 10B   | 600 | GDP  | C5-C4-N3 | -5.94 | 118.93      | 128.39   |
| 5   | 13B   | 600 | GDP  | C5-C4-N3 | -5.89 | 119.02      | 128.39   |
| 5   | 13D   | 600 | GDP  | C5-C4-N3 | -5.87 | 119.04      | 128.39   |
| 5   | 12B   | 600 | GDP  | C5-C4-N3 | -5.86 | 119.07      | 128.39   |
| 5   | 8D    | 600 | GDP  | C5-C4-N3 | -5.84 | 119.09      | 128.39   |
| 5   | 11B   | 600 | GDP  | C5-C4-N3 | -5.82 | 119.13      | 128.39   |
| 5   | 12D   | 600 | GDP  | C5-C4-N3 | -5.81 | 119.14      | 128.39   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 11D   | 600 | GDP  | C5-C4-N3 | -5.68 | 119.35      | 128.39   |
| 3   | 8E    | 500 | GTP  | C5-C4-N3 | -5.66 | 119.39      | 128.39   |
| 3   | 12C   | 500 | GTP  | C5-C4-N3 | -5.47 | 119.69      | 128.39   |
| 3   | 2A    | 500 | GTP  | C5-C4-N3 | -5.40 | 119.80      | 128.39   |
| 3   | 1A    | 500 | GTP  | C5-C4-N3 | -5.39 | 119.81      | 128.39   |
| 3   | 1E    | 500 | GTP  | C5-C4-N3 | -5.35 | 119.88      | 128.39   |
| 3   | 1C    | 500 | GTP  | C5-C4-N3 | -5.33 | 119.91      | 128.39   |
| 3   | 2C    | 500 | GTP  | C5-C4-N3 | -5.29 | 119.97      | 128.39   |
| 3   | 2E    | 500 | GTP  | C5-C4-N3 | -5.28 | 119.98      | 128.39   |
| 3   | 4A    | 500 | GTP  | C5-C4-N3 | -5.28 | 119.99      | 128.39   |
| 3   | 9C    | 500 | GTP  | C5-C4-N3 | -5.26 | 120.01      | 128.39   |
| 3   | 3C    | 500 | GTP  | C5-C4-N3 | -5.24 | 120.05      | 128.39   |
| 3   | 10A   | 500 | GTP  | C5-C4-N3 | -5.24 | 120.05      | 128.39   |
| 3   | 3A    | 500 | GTP  | C5-C4-N3 | -5.21 | 120.10      | 128.39   |
| 3   | 11C   | 500 | GTP  | C5-C4-N3 | -5.19 | 120.12      | 128.39   |
| 3   | 4C    | 500 | GTP  | C5-C4-N3 | -5.18 | 120.14      | 128.39   |
| 3   | 3E    | 500 | GTP  | C5-C4-N3 | -5.17 | 120.16      | 128.39   |
| 3   | 10C   | 500 | GTP  | C5-C4-N3 | -5.17 | 120.16      | 128.39   |
| 3   | 9A    | 500 | GTP  | C5-C4-N3 | -5.17 | 120.17      | 128.39   |
| 3   | 7C    | 500 | GTP  | C5-C4-N3 | -5.17 | 120.17      | 128.39   |
| 3   | 4E    | 500 | GTP  | C5-C4-N3 | -5.16 | 120.18      | 128.39   |
| 3   | 6E    | 500 | GTP  | C5-C4-N3 | -5.16 | 120.18      | 128.39   |
| 3   | 10E   | 500 | GTP  | C5-C4-N3 | -5.15 | 120.19      | 128.39   |
| 3   | 6A    | 500 | GTP  | C5-C4-N3 | -5.15 | 120.20      | 128.39   |
| 3   | 11A   | 500 | GTP  | C5-C4-N3 | -5.15 | 120.20      | 128.39   |
| 5   | 7D    | 600 | GDP  | C2-N3-C4 | 5.14  | 121.16      | 112.30   |
| 5   | 2D    | 600 | GDP  | C2-N3-C4 | 5.14  | 121.16      | 112.30   |
| 3   | 11E   | 500 | GTP  | C5-C4-N3 | -5.14 | 120.21      | 128.39   |
| 3   | 8C    | 500 | GTP  | C5-C4-N3 | -5.14 | 120.21      | 128.39   |
| 3   | 9E    | 500 | GTP  | C5-C4-N3 | -5.13 | 120.23      | 128.39   |
| 3   | 12A   | 500 | GTP  | C5-C4-N3 | -5.13 | 120.23      | 128.39   |
| 5   | 1B    | 600 | GDP  | C2-N3-C4 | 5.12  | 121.12      | 112.30   |
| 5   | 7B    | 600 | GDP  | C2-N3-C4 | 5.12  | 121.11      | 112.30   |
| 3   | 13C   | 500 | GTP  | C5-C4-N3 | -5.11 | 120.26      | 128.39   |
| 5   | 5D    | 600 | GDP  | C2-N3-C4 | 5.11  | 121.10      | 112.30   |
| 5   | 9D    | 600 | GDP  | C2-N3-C4 | 5.10  | 121.09      | 112.30   |
| 5   | 1D    | 600 | GDP  | C2-N3-C4 | 5.10  | 121.09      | 112.30   |
| 5   | 5B    | 600 | GDP  | C2-N3-C4 | 5.09  | 121.06      | 112.30   |
| 5   | 4D    | 600 | GDP  | C2-N3-C4 | 5.09  | 121.06      | 112.30   |
| 5   | 8B    | 600 | GDP  | C2-N3-C4 | 5.08  | 121.06      | 112.30   |
| 5   | 9B    | 600 | GDP  | C2-N3-C4 | 5.08  | 121.06      | 112.30   |
| 5   | 3B    | 600 | GDP  | C2-N3-C4 | 5.08  | 121.05      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 3D    | 600 | GDP  | C2-N3-C4 | 5.07  | 121.03      | 112.30   |
| 5   | 4B    | 600 | GDP  | C2-N3-C4 | 5.06  | 121.01      | 112.30   |
| 5   | 2B    | 600 | GDP  | C2-N3-C4 | 5.05  | 121.00      | 112.30   |
| 5   | 10B   | 600 | GDP  | C2-N3-C4 | 5.05  | 120.99      | 112.30   |
| 5   | 8D    | 600 | GDP  | C2-N3-C4 | 5.03  | 120.97      | 112.30   |
| 3   | 7A    | 500 | GTP  | C5-C4-N3 | -5.02 | 120.40      | 128.39   |
| 5   | 6D    | 600 | GDP  | C2-N3-C4 | 5.02  | 120.94      | 112.30   |
| 5   | 10D   | 600 | GDP  | C2-N3-C4 | 5.01  | 120.94      | 112.30   |
| 3   | 8A    | 500 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 6C    | 500 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 5   | 12D   | 600 | GDP  | C2-N3-C4 | 4.97  | 120.86      | 112.30   |
| 5   | 6B    | 600 | GDP  | C2-N3-C4 | 4.96  | 120.84      | 112.30   |
| 5   | 11B   | 600 | GDP  | C2-N3-C4 | 4.95  | 120.83      | 112.30   |
| 5   | 11D   | 600 | GDP  | C2-N3-C4 | 4.94  | 120.81      | 112.30   |
| 5   | 12B   | 600 | GDP  | C2-N3-C4 | 4.93  | 120.79      | 112.30   |
| 3   | 5C    | 500 | GTP  | C5-C4-N3 | -4.91 | 120.57      | 128.39   |
| 3   | 7E    | 500 | GTP  | C5-C4-N3 | -4.90 | 120.59      | 128.39   |
| 5   | 13B   | 600 | GDP  | C2-N3-C4 | 4.89  | 120.72      | 112.30   |
| 3   | 5A    | 500 | GTP  | C5-C4-N3 | -4.84 | 120.68      | 128.39   |
| 5   | 13D   | 600 | GDP  | C2-N3-C4 | 4.82  | 120.61      | 112.30   |
| 3   | 5E    | 500 | GTP  | C5-C4-N3 | -4.82 | 120.72      | 128.39   |
| 3   | 13A   | 500 | GTP  | C5-C4-N3 | -4.81 | 120.73      | 128.39   |
| 3   | 8E    | 500 | GTP  | C2-N3-C4 | 4.81  | 120.58      | 112.30   |
| 5   | 1B    | 600 | GDP  | N9-C4-N3 | 4.80  | 135.54      | 125.95   |
| 5   | 1D    | 600 | GDP  | N9-C4-N3 | 4.78  | 135.51      | 125.95   |
| 5   | 2B    | 600 | GDP  | N9-C4-N3 | 4.73  | 135.40      | 125.95   |
| 3   | 12E   | 500 | GTP  | C5-C4-N3 | -4.71 | 120.89      | 128.39   |
| 5   | 5B    | 600 | GDP  | N9-C4-N3 | 4.69  | 135.34      | 125.95   |
| 5   | 2D    | 600 | GDP  | N9-C4-N3 | 4.67  | 135.30      | 125.95   |
| 5   | 6B    | 600 | GDP  | N9-C4-N3 | 4.63  | 135.21      | 125.95   |
| 5   | 5D    | 600 | GDP  | N9-C4-N3 | 4.62  | 135.20      | 125.95   |
| 3   | 13E   | 500 | GTP  | C5-C4-N3 | -4.62 | 121.03      | 128.39   |
| 5   | 4B    | 600 | GDP  | N9-C4-N3 | 4.61  | 135.18      | 125.95   |
| 3   | 1A    | 500 | GTP  | C2-N3-C4 | 4.60  | 120.22      | 112.30   |
| 3   | 1E    | 500 | GTP  | C2-N3-C4 | 4.59  | 120.21      | 112.30   |
| 5   | 6D    | 600 | GDP  | N9-C4-N3 | 4.59  | 135.14      | 125.95   |
| 5   | 3B    | 600 | GDP  | N9-C4-N3 | 4.59  | 135.13      | 125.95   |
| 3   | 2A    | 500 | GTP  | C2-N3-C4 | 4.56  | 120.16      | 112.30   |
| 3   | 1C    | 500 | GTP  | C2-N3-C4 | 4.55  | 120.14      | 112.30   |
| 3   | 4A    | 500 | GTP  | C2-N3-C4 | 4.55  | 120.13      | 112.30   |
| 3   | 3C    | 500 | GTP  | C2-N3-C4 | 4.54  | 120.12      | 112.30   |
| 3   | 4C    | 500 | GTP  | C2-N3-C4 | 4.54  | 120.11      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | 3A    | 500 | GTP  | C2-N3-C4 | 4.53 | 120.11      | 112.30   |
| 3   | 2E    | 500 | GTP  | C2-N3-C4 | 4.53 | 120.11      | 112.30   |
| 3   | 3E    | 500 | GTP  | C2-N3-C4 | 4.52 | 120.08      | 112.30   |
| 3   | 2C    | 500 | GTP  | C2-N3-C4 | 4.52 | 120.08      | 112.30   |
| 5   | 4D    | 600 | GDP  | N9-C4-N3 | 4.51 | 134.97      | 125.95   |
| 3   | 8C    | 500 | GTP  | C2-N3-C4 | 4.51 | 120.06      | 112.30   |
| 3   | 4E    | 500 | GTP  | C2-N3-C4 | 4.51 | 120.06      | 112.30   |
| 3   | 12C   | 500 | GTP  | C2-N3-C4 | 4.50 | 120.05      | 112.30   |
| 3   | 9C    | 500 | GTP  | C2-N3-C4 | 4.45 | 119.96      | 112.30   |
| 5   | 3D    | 600 | GDP  | N9-C4-N3 | 4.44 | 134.84      | 125.95   |
| 5   | 12B   | 600 | GDP  | N9-C4-N3 | 4.44 | 134.83      | 125.95   |
| 3   | 13C   | 500 | GTP  | C2-N3-C4 | 4.44 | 119.94      | 112.30   |
| 5   | 7B    | 600 | GDP  | N9-C4-N3 | 4.43 | 134.82      | 125.95   |
| 3   | 11A   | 500 | GTP  | C2-N3-C4 | 4.38 | 119.84      | 112.30   |
| 3   | 11C   | 500 | GTP  | C2-N3-C4 | 4.37 | 119.83      | 112.30   |
| 5   | 12D   | 600 | GDP  | N9-C4-N3 | 4.36 | 134.68      | 125.95   |
| 3   | 8E    | 500 | GTP  | N9-C4-N3 | 4.36 | 134.68      | 125.95   |
| 3   | 8A    | 500 | GTP  | C2-N3-C4 | 4.35 | 119.79      | 112.30   |
| 5   | 7D    | 600 | GDP  | N9-C4-N3 | 4.34 | 134.64      | 125.95   |
| 3   | 11E   | 500 | GTP  | C2-N3-C4 | 4.31 | 119.72      | 112.30   |
| 5   | 13D   | 600 | GDP  | N9-C4-N3 | 4.30 | 134.55      | 125.95   |
| 5   | 10B   | 600 | GDP  | N9-C4-N3 | 4.30 | 134.55      | 125.95   |
| 3   | 9A    | 500 | GTP  | C2-N3-C4 | 4.30 | 119.70      | 112.30   |
| 5   | 13B   | 600 | GDP  | N9-C4-N3 | 4.30 | 134.54      | 125.95   |
| 3   | 6C    | 500 | GTP  | C2-N3-C4 | 4.29 | 119.68      | 112.30   |
| 3   | 6E    | 500 | GTP  | C2-N3-C4 | 4.29 | 119.68      | 112.30   |
| 5   | 10D   | 600 | GDP  | N9-C4-N3 | 4.28 | 134.51      | 125.95   |
| 5   | 8B    | 600 | GDP  | N9-C4-N3 | 4.28 | 134.50      | 125.95   |
| 3   | 10A   | 500 | GTP  | C2-N3-C4 | 4.27 | 119.65      | 112.30   |
| 5   | 11B   | 600 | GDP  | N9-C4-N3 | 4.26 | 134.47      | 125.95   |
| 5   | 9B    | 600 | GDP  | N9-C4-N3 | 4.24 | 134.42      | 125.95   |
| 3   | 9E    | 500 | GTP  | C2-N3-C4 | 4.24 | 119.59      | 112.30   |
| 5   | 11D   | 600 | GDP  | N9-C4-N3 | 4.23 | 134.42      | 125.95   |
| 5   | 9D    | 600 | GDP  | N9-C4-N3 | 4.23 | 134.41      | 125.95   |
| 3   | 5A    | 500 | GTP  | C2-N3-C4 | 4.23 | 119.59      | 112.30   |
| 3   | 12A   | 500 | GTP  | C2-N3-C4 | 4.23 | 119.58      | 112.30   |
| 3   | 7C    | 500 | GTP  | C2-N3-C4 | 4.22 | 119.57      | 112.30   |
| 3   | 10C   | 500 | GTP  | C2-N3-C4 | 4.22 | 119.57      | 112.30   |
| 3   | 13A   | 500 | GTP  | C2-N3-C4 | 4.21 | 119.55      | 112.30   |
| 3   | 10E   | 500 | GTP  | C2-N3-C4 | 4.21 | 119.55      | 112.30   |
| 3   | 6A    | 500 | GTP  | C2-N3-C4 | 4.20 | 119.54      | 112.30   |
| 3   | 5E    | 500 | GTP  | C2-N3-C4 | 4.17 | 119.47      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 5C    | 500 | GTP  | C2-N3-C4 | 4.15  | 119.44      | 112.30   |
| 3   | 7A    | 500 | GTP  | C2-N3-C4 | 4.12  | 119.40      | 112.30   |
| 5   | 8D    | 600 | GDP  | N9-C4-N3 | 4.10  | 134.16      | 125.95   |
| 3   | 13E   | 500 | GTP  | C2-N3-C4 | 4.10  | 119.35      | 112.30   |
| 3   | 7E    | 500 | GTP  | C2-N3-C4 | 4.07  | 119.31      | 112.30   |
| 3   | 12E   | 500 | GTP  | C2-N3-C4 | 3.97  | 119.14      | 112.30   |
| 3   | 12C   | 500 | GTP  | N9-C4-N3 | 3.94  | 133.83      | 125.95   |
| 3   | 12A   | 500 | GTP  | N9-C4-N3 | 3.84  | 133.62      | 125.95   |
| 3   | 10A   | 500 | GTP  | N9-C4-N3 | 3.82  | 133.58      | 125.95   |
| 3   | 9E    | 500 | GTP  | N9-C4-N3 | 3.77  | 133.50      | 125.95   |
| 3   | 2A    | 500 | GTP  | N9-C4-N3 | 3.77  | 133.49      | 125.95   |
| 3   | 8E    | 500 | GTP  | C2-N1-C6 | -3.75 | 118.31      | 125.11   |
| 3   | 10C   | 500 | GTP  | N9-C4-N3 | 3.74  | 133.43      | 125.95   |
| 3   | 11E   | 500 | GTP  | N9-C4-N3 | 3.73  | 133.40      | 125.95   |
| 3   | 1A    | 500 | GTP  | N9-C4-N3 | 3.72  | 133.40      | 125.95   |
| 3   | 7C    | 500 | GTP  | N9-C4-N3 | 3.72  | 133.40      | 125.95   |
| 3   | 9C    | 500 | GTP  | N9-C4-N3 | 3.72  | 133.39      | 125.95   |
| 3   | 9A    | 500 | GTP  | N9-C4-N3 | 3.72  | 133.39      | 125.95   |
| 3   | 1C    | 500 | GTP  | N9-C4-N3 | 3.69  | 133.33      | 125.95   |
| 3   | 2C    | 500 | GTP  | N9-C4-N3 | 3.69  | 133.33      | 125.95   |
| 3   | 1E    | 500 | GTP  | N9-C4-N3 | 3.68  | 133.30      | 125.95   |
| 3   | 2E    | 500 | GTP  | N9-C4-N3 | 3.67  | 133.29      | 125.95   |
| 3   | 11C   | 500 | GTP  | N9-C4-N3 | 3.66  | 133.28      | 125.95   |
| 3   | 7A    | 500 | GTP  | N9-C4-N3 | 3.66  | 133.27      | 125.95   |
| 3   | 10E   | 500 | GTP  | N9-C4-N3 | 3.65  | 133.26      | 125.95   |
| 5   | 9D    | 600 | GDP  | C6-C5-N7 | 3.65  | 136.93      | 130.29   |
| 3   | 7E    | 500 | GTP  | N9-C4-N3 | 3.62  | 133.20      | 125.95   |
| 5   | 8D    | 600 | GDP  | C6-C5-N7 | 3.62  | 136.88      | 130.29   |
| 5   | 9B    | 600 | GDP  | C6-C5-N7 | 3.57  | 136.78      | 130.29   |
| 3   | 11A   | 500 | GTP  | N9-C4-N3 | 3.56  | 133.08      | 125.95   |
| 3   | 6E    | 500 | GTP  | N9-C4-N3 | 3.55  | 133.06      | 125.95   |
| 3   | 13C   | 500 | GTP  | N9-C4-N3 | 3.53  | 133.01      | 125.95   |
| 5   | 7D    | 600 | GDP  | C6-C5-N7 | 3.53  | 136.71      | 130.29   |
| 5   | 8B    | 600 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 10B   | 600 | GDP  | C6-C5-N7 | 3.49  | 136.65      | 130.29   |
| 5   | 10D   | 600 | GDP  | C6-C5-N7 | 3.49  | 136.65      | 130.29   |
| 3   | 3A    | 500 | GTP  | N9-C4-N3 | 3.45  | 132.86      | 125.95   |
| 3   | 13C   | 500 | GTP  | O6-C6-C5 | -3.45 | 117.42      | 126.53   |
| 5   | 13B   | 600 | GDP  | C6-C5-N7 | 3.45  | 136.57      | 130.29   |
| 3   | 6A    | 500 | GTP  | N9-C4-N3 | 3.45  | 132.84      | 125.95   |
| 5   | 11D   | 600 | GDP  | C6-C5-N7 | 3.44  | 136.55      | 130.29   |
| 3   | 4A    | 500 | GTP  | N9-C4-N3 | 3.43  | 132.81      | 125.95   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 3E    | 500 | GTP  | N9-C4-N3   | 3.43  | 132.81      | 125.95   |
| 3   | 13A   | 500 | GTP  | N9-C4-N3   | 3.43  | 132.81      | 125.95   |
| 5   | 3D    | 600 | GDP  | C6-C5-N7   | 3.42  | 136.51      | 130.29   |
| 3   | 3C    | 500 | GTP  | N9-C4-N3   | 3.41  | 132.78      | 125.95   |
| 3   | 8A    | 500 | GTP  | N9-C4-N3   | 3.41  | 132.77      | 125.95   |
| 5   | 13D   | 600 | GDP  | C6-C5-N7   | 3.40  | 136.49      | 130.29   |
| 5   | 7B    | 600 | GDP  | C6-C5-N7   | 3.39  | 136.46      | 130.29   |
| 3   | 12C   | 500 | GTP  | C2-N1-C6   | -3.39 | 118.96      | 125.11   |
| 5   | 11B   | 600 | GDP  | C6-C5-N7   | 3.37  | 136.42      | 130.29   |
| 5   | 4D    | 600 | GDP  | C6-C5-N7   | 3.34  | 136.37      | 130.29   |
| 3   | 6C    | 500 | GTP  | N9-C4-N3   | 3.34  | 132.63      | 125.95   |
| 3   | 4E    | 500 | GTP  | N9-C4-N3   | 3.34  | 132.62      | 125.95   |
| 5   | 12D   | 600 | GDP  | C6-C5-N7   | 3.31  | 136.32      | 130.29   |
| 3   | 4C    | 500 | GTP  | N9-C4-N3   | 3.31  | 132.58      | 125.95   |
| 3   | 5E    | 500 | GTP  | N9-C4-N3   | 3.28  | 132.52      | 125.95   |
| 3   | 5A    | 500 | GTP  | N9-C4-N3   | 3.27  | 132.49      | 125.95   |
| 5   | 3B    | 600 | GDP  | C6-C5-N7   | 3.25  | 136.20      | 130.29   |
| 5   | 12B   | 600 | GDP  | C6-C5-N7   | 3.25  | 136.20      | 130.29   |
| 3   | 12E   | 500 | GTP  | N9-C4-N3   | 3.24  | 132.43      | 125.95   |
| 5   | 6D    | 600 | GDP  | C6-C5-N7   | 3.23  | 136.17      | 130.29   |
| 3   | 2A    | 500 | GTP  | C2-N1-C6   | -3.22 | 119.26      | 125.11   |
| 3   | 4C    | 500 | GTP  | C2-N1-C6   | -3.22 | 119.27      | 125.11   |
| 5   | 2D    | 600 | GDP  | C6-C5-N7   | 3.21  | 136.13      | 130.29   |
| 3   | 2E    | 500 | GTP  | C2-N1-C6   | -3.21 | 119.29      | 125.11   |
| 3   | 4A    | 500 | GTP  | C2-N1-C6   | -3.21 | 119.29      | 125.11   |
| 3   | 1C    | 500 | GTP  | C2-N1-C6   | -3.21 | 119.29      | 125.11   |
| 5   | 4B    | 600 | GDP  | C6-C5-N7   | 3.21  | 136.12      | 130.29   |
| 3   | 1A    | 500 | GTP  | C2-N1-C6   | -3.20 | 119.31      | 125.11   |
| 3   | 1E    | 500 | GTP  | C2-N1-C6   | -3.20 | 119.31      | 125.11   |
| 3   | 13E   | 500 | GTP  | N9-C4-N3   | 3.18  | 132.32      | 125.95   |
| 3   | 2C    | 500 | GTP  | C2-N1-C6   | -3.18 | 119.34      | 125.11   |
| 5   | 5D    | 600 | GDP  | C6-C5-N7   | 3.18  | 136.07      | 130.29   |
| 3   | 3C    | 500 | GTP  | C2-N1-C6   | -3.15 | 119.39      | 125.11   |
| 3   | 3A    | 500 | GTP  | C2-N1-C6   | -3.14 | 119.41      | 125.11   |
| 5   | 2B    | 600 | GDP  | C6-C5-N7   | 3.14  | 136.00      | 130.29   |
| 3   | 4E    | 500 | GTP  | C2-N1-C6   | -3.14 | 119.42      | 125.11   |
| 3   | 12C   | 500 | GTP  | O6-C6-C5   | -3.13 | 118.26      | 126.53   |
| 5   | 1D    | 600 | GDP  | C6-C5-N7   | 3.12  | 135.98      | 130.29   |
| 5   | 1B    | 600 | GDP  | C6-C5-N7   | 3.12  | 135.97      | 130.29   |
| 5   | 6B    | 600 | GDP  | C6-C5-N7   | 3.12  | 135.96      | 130.29   |
| 3   | 3E    | 500 | GTP  | C2-N1-C6   | -3.10 | 119.48      | 125.11   |
| 3   | 8E    | 500 | GTP  | O4'-C1'-N9 | -3.09 | 101.36      | 108.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 5B    | 600 | GDP  | C6-C5-N7    | 3.09  | 135.91      | 130.29   |
| 3   | 5C    | 500 | GTP  | N9-C4-N3    | 3.08  | 132.12      | 125.95   |
| 3   | 11C   | 500 | GTP  | C2-N1-C6    | -3.07 | 119.54      | 125.11   |
| 3   | 9C    | 500 | GTP  | C2-N1-C6    | -3.05 | 119.57      | 125.11   |
| 3   | 8C    | 500 | GTP  | N9-C4-N3    | 3.04  | 132.04      | 125.95   |
| 3   | 10A   | 500 | GTP  | C2-N1-C6    | -3.02 | 119.63      | 125.11   |
| 3   | 8E    | 500 | GTP  | C3'-C2'-C1' | 3.02  | 107.17      | 101.46   |
| 3   | 8A    | 500 | GTP  | C2-N1-C6    | -3.00 | 119.66      | 125.11   |
| 3   | 12A   | 500 | GTP  | O6-C6-C5    | -2.98 | 118.66      | 126.53   |
| 3   | 12A   | 500 | GTP  | C2-N1-C6    | -2.95 | 119.76      | 125.11   |
| 3   | 11A   | 500 | GTP  | C2-N1-C6    | -2.94 | 119.79      | 125.11   |
| 3   | 11C   | 500 | GTP  | O6-C6-C5    | -2.92 | 118.81      | 126.53   |
| 3   | 11E   | 500 | GTP  | C2-N1-C6    | -2.92 | 119.81      | 125.11   |
| 3   | 13A   | 500 | GTP  | O6-C6-C5    | -2.92 | 118.83      | 126.53   |
| 3   | 13C   | 500 | GTP  | C2-N1-C6    | -2.91 | 119.84      | 125.11   |
| 3   | 10A   | 500 | GTP  | O6-C6-C5    | -2.90 | 118.87      | 126.53   |
| 3   | 9A    | 500 | GTP  | C2-N1-C6    | -2.90 | 119.85      | 125.11   |
| 3   | 5C    | 500 | GTP  | O6-C6-C5    | -2.90 | 118.89      | 126.53   |
| 3   | 9E    | 500 | GTP  | C2-N1-C6    | -2.88 | 119.88      | 125.11   |
| 3   | 13E   | 500 | GTP  | N9-C8-N7    | -2.82 | 108.17      | 113.40   |
| 3   | 7C    | 500 | GTP  | C2-N1-C6    | -2.82 | 120.00      | 125.11   |
| 3   | 13A   | 500 | GTP  | C2-N1-C6    | -2.82 | 120.00      | 125.11   |
| 3   | 11E   | 500 | GTP  | O6-C6-C5    | -2.82 | 119.10      | 126.53   |
| 3   | 13A   | 500 | GTP  | N9-C8-N7    | -2.82 | 108.18      | 113.40   |
| 3   | 5C    | 500 | GTP  | C2-N1-C6    | -2.81 | 120.02      | 125.11   |
| 3   | 10C   | 500 | GTP  | C2-N1-C6    | -2.79 | 120.05      | 125.11   |
| 3   | 10E   | 500 | GTP  | C2-N1-C6    | -2.79 | 120.06      | 125.11   |
| 3   | 6E    | 500 | GTP  | C2-N1-C6    | -2.79 | 120.06      | 125.11   |
| 3   | 9E    | 500 | GTP  | O6-C6-C5    | -2.78 | 119.18      | 126.53   |
| 3   | 10C   | 500 | GTP  | O6-C6-C5    | -2.77 | 119.22      | 126.53   |
| 3   | 13C   | 500 | GTP  | N9-C8-N7    | -2.76 | 108.29      | 113.40   |
| 5   | 9D    | 600 | GDP  | C4-C5-N7    | -2.75 | 106.31      | 110.67   |
| 3   | 8C    | 500 | GTP  | C3'-C2'-C1' | 2.74  | 106.65      | 101.46   |
| 3   | 9A    | 500 | GTP  | O6-C6-C5    | -2.73 | 119.32      | 126.53   |
| 3   | 11A   | 500 | GTP  | N9-C8-N7    | -2.73 | 108.33      | 113.40   |
| 3   | 11A   | 500 | GTP  | O6-C6-C5    | -2.73 | 119.32      | 126.53   |
| 3   | 13E   | 500 | GTP  | C2-N1-C6    | -2.73 | 120.17      | 125.11   |
| 3   | 2A    | 500 | GTP  | O6-C6-C5    | -2.72 | 119.35      | 126.53   |
| 3   | 9C    | 500 | GTP  | O6-C6-C5    | -2.72 | 119.35      | 126.53   |
| 3   | 2C    | 500 | GTP  | O6-C6-C5    | -2.72 | 119.36      | 126.53   |
| 5   | 9B    | 600 | GDP  | C4-C5-N7    | -2.71 | 106.37      | 110.67   |
| 3   | 12A   | 500 | GTP  | N9-C8-N7    | -2.71 | 108.38      | 113.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 2C    | 500 | GTP  | N9-C8-N7    | -2.70 | 108.39      | 113.40   |
| 3   | 7C    | 500 | GTP  | N9-C8-N7    | -2.70 | 108.39      | 113.40   |
| 3   | 1C    | 500 | GTP  | O6-C6-C5    | -2.70 | 119.39      | 126.53   |
| 3   | 2E    | 500 | GTP  | O6-C6-C5    | -2.69 | 119.42      | 126.53   |
| 3   | 11E   | 500 | GTP  | N9-C8-N7    | -2.69 | 108.41      | 113.40   |
| 3   | 12C   | 500 | GTP  | N9-C8-N7    | -2.69 | 108.42      | 113.40   |
| 3   | 2E    | 500 | GTP  | N9-C8-N7    | -2.69 | 108.42      | 113.40   |
| 3   | 11C   | 500 | GTP  | N9-C8-N7    | -2.68 | 108.42      | 113.40   |
| 5   | 13B   | 600 | GDP  | C4-C5-N7    | -2.68 | 106.42      | 110.67   |
| 3   | 1E    | 500 | GTP  | O6-C6-C5    | -2.68 | 119.45      | 126.53   |
| 3   | 1A    | 500 | GTP  | O6-C6-C5    | -2.68 | 119.46      | 126.53   |
| 3   | 8E    | 500 | GTP  | N9-C8-N7    | -2.67 | 108.45      | 113.40   |
| 3   | 2A    | 500 | GTP  | N9-C8-N7    | -2.67 | 108.46      | 113.40   |
| 3   | 3E    | 500 | GTP  | N9-C8-N7    | -2.67 | 108.46      | 113.40   |
| 3   | 8E    | 500 | GTP  | C5'-C4'-C3' | -2.66 | 105.62      | 115.21   |
| 3   | 8A    | 500 | GTP  | N9-C8-N7    | -2.66 | 108.46      | 113.40   |
| 5   | 13D   | 600 | GDP  | C4-C5-N7    | -2.66 | 106.45      | 110.67   |
| 3   | 1C    | 500 | GTP  | C5-C6-N1    | 2.66  | 120.02      | 113.25   |
| 3   | 10A   | 500 | GTP  | N9-C8-N7    | -2.65 | 108.48      | 113.40   |
| 3   | 12E   | 500 | GTP  | N9-C8-N7    | -2.65 | 108.48      | 113.40   |
| 3   | 3C    | 500 | GTP  | N9-C8-N7    | -2.65 | 108.48      | 113.40   |
| 3   | 3A    | 500 | GTP  | N9-C8-N7    | -2.65 | 108.49      | 113.40   |
| 3   | 1E    | 500 | GTP  | C5-C6-N1    | 2.65  | 120.00      | 113.25   |
| 3   | 9E    | 500 | GTP  | N9-C8-N7    | -2.65 | 108.49      | 113.40   |
| 3   | 6A    | 500 | GTP  | C8-N7-C5    | 2.65  | 108.98      | 104.26   |
| 3   | 3A    | 500 | GTP  | O6-C6-C5    | -2.65 | 119.54      | 126.53   |
| 5   | 10D   | 600 | GDP  | C4-C5-N7    | -2.65 | 106.48      | 110.67   |
| 3   | 1A    | 500 | GTP  | C5-C6-N1    | 2.65  | 119.99      | 113.25   |
| 3   | 10C   | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 10E   | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 10E   | 500 | GTP  | O6-C6-C5    | -2.64 | 119.56      | 126.53   |
| 3   | 1E    | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 4A    | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 9A    | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 9C    | 500 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 3   | 7C    | 500 | GTP  | O6-C6-C5    | -2.64 | 119.57      | 126.53   |
| 5   | 3D    | 600 | GDP  | C4-C5-N7    | -2.63 | 106.50      | 110.67   |
| 3   | 3C    | 500 | GTP  | O6-C6-C5    | -2.63 | 119.59      | 126.53   |
| 5   | 8D    | 600 | GDP  | C4-C5-N7    | -2.63 | 106.50      | 110.67   |
| 3   | 1C    | 500 | GTP  | N9-C8-N7    | -2.63 | 108.52      | 113.40   |
| 3   | 4C    | 500 | GTP  | N9-C8-N7    | -2.63 | 108.52      | 113.40   |
| 3   | 3E    | 500 | GTP  | O6-C6-C5    | -2.63 | 119.60      | 126.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 1A    | 500 | GTP  | N9-C8-N7    | -2.63 | 108.53      | 113.40   |
| 3   | 7A    | 500 | GTP  | C3'-C2'-C1' | 2.62  | 106.42      | 101.46   |
| 3   | 13E   | 500 | GTP  | O6-C6-C5    | -2.62 | 119.62      | 126.53   |
| 3   | 4E    | 500 | GTP  | N9-C8-N7    | -2.61 | 108.55      | 113.40   |
| 5   | 7B    | 600 | GDP  | C4-C5-N7    | -2.61 | 106.53      | 110.67   |
| 3   | 6C    | 500 | GTP  | N9-C8-N7    | -2.61 | 108.56      | 113.40   |
| 5   | 8B    | 600 | GDP  | C4-C5-N7    | -2.60 | 106.54      | 110.67   |
| 3   | 6E    | 500 | GTP  | N9-C8-N7    | -2.60 | 108.57      | 113.40   |
| 3   | 8A    | 500 | GTP  | O6-C6-C5    | -2.60 | 119.68      | 126.53   |
| 3   | 2E    | 500 | GTP  | C5-C6-N1    | 2.59  | 119.86      | 113.25   |
| 3   | 2A    | 500 | GTP  | C5-C6-N1    | 2.59  | 119.85      | 113.25   |
| 5   | 7D    | 600 | GDP  | C4-C5-N7    | -2.59 | 106.57      | 110.67   |
| 3   | 5A    | 500 | GTP  | N9-C8-N7    | -2.59 | 108.61      | 113.40   |
| 5   | 10B   | 600 | GDP  | C4-C5-N7    | -2.58 | 106.57      | 110.67   |
| 3   | 5E    | 500 | GTP  | N9-C8-N7    | -2.58 | 108.61      | 113.40   |
| 3   | 4A    | 500 | GTP  | O6-C6-C5    | -2.58 | 119.72      | 126.53   |
| 3   | 6C    | 500 | GTP  | C8-N7-C5    | 2.58  | 108.85      | 104.26   |
| 3   | 4E    | 500 | GTP  | O6-C6-C5    | -2.58 | 119.73      | 126.53   |
| 5   | 4D    | 600 | GDP  | C4-C5-N7    | -2.57 | 106.59      | 110.67   |
| 5   | 3B    | 600 | GDP  | C4-C5-N7    | -2.57 | 106.59      | 110.67   |
| 3   | 2C    | 500 | GTP  | C5-C6-N1    | 2.57  | 119.80      | 113.25   |
| 3   | 4C    | 500 | GTP  | O6-C6-C5    | -2.56 | 119.77      | 126.53   |
| 3   | 4C    | 500 | GTP  | C5-C6-N1    | 2.56  | 119.77      | 113.25   |
| 3   | 6A    | 500 | GTP  | C2-N1-C6    | -2.56 | 120.47      | 125.11   |
| 5   | 12B   | 600 | GDP  | O6-C6-C5    | -2.55 | 119.80      | 126.53   |
| 3   | 12E   | 500 | GTP  | C8-N7-C5    | 2.55  | 108.80      | 104.26   |
| 3   | 4A    | 500 | GTP  | C5-C6-N1    | 2.54  | 119.72      | 113.25   |
| 3   | 13E   | 500 | GTP  | O2B-PB-O3B  | 2.54  | 114.14      | 107.27   |
| 3   | 7C    | 500 | GTP  | C8-N7-C5    | 2.54  | 108.78      | 104.26   |
| 3   | 7E    | 500 | GTP  | N9-C8-N7    | -2.53 | 108.70      | 113.40   |
| 3   | 3C    | 500 | GTP  | C8-N7-C5    | 2.53  | 108.76      | 104.26   |
| 3   | 3A    | 500 | GTP  | C8-N7-C5    | 2.53  | 108.76      | 104.26   |
| 3   | 4E    | 500 | GTP  | C5-C6-N1    | 2.52  | 119.68      | 113.25   |
| 5   | 2D    | 600 | GDP  | C4-C5-N7    | -2.52 | 106.68      | 110.67   |
| 3   | 5E    | 500 | GTP  | C2-N1-C6    | -2.52 | 120.54      | 125.11   |
| 3   | 6A    | 500 | GTP  | N9-C8-N7    | -2.52 | 108.73      | 113.40   |
| 3   | 6E    | 500 | GTP  | C8-N7-C5    | 2.52  | 108.75      | 104.26   |
| 3   | 4A    | 500 | GTP  | C8-N7-C5    | 2.52  | 108.74      | 104.26   |
| 3   | 3E    | 500 | GTP  | C8-N7-C5    | 2.51  | 108.74      | 104.26   |
| 3   | 8C    | 500 | GTP  | C2-N1-C6    | -2.51 | 120.56      | 125.11   |
| 5   | 4B    | 600 | GDP  | C4-C5-N7    | -2.51 | 106.70      | 110.67   |
| 3   | 10E   | 500 | GTP  | C8-N7-C5    | 2.50  | 108.71      | 104.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 11A   | 500 | GTP  | C8-N7-C5    | 2.50  | 108.71      | 104.26   |
| 5   | 2B    | 600 | GDP  | C4-C5-N7    | -2.50 | 106.71      | 110.67   |
| 5   | 12D   | 600 | GDP  | O6-C6-C5    | -2.49 | 119.95      | 126.53   |
| 3   | 7E    | 500 | GTP  | C3'-C2'-C1' | 2.49  | 106.18      | 101.46   |
| 3   | 6C    | 500 | GTP  | C2-N1-C6    | -2.49 | 120.60      | 125.11   |
| 3   | 4C    | 500 | GTP  | C8-N7-C5    | 2.48  | 108.69      | 104.26   |
| 3   | 10C   | 500 | GTP  | C8-N7-C5    | 2.48  | 108.69      | 104.26   |
| 3   | 6E    | 500 | GTP  | O6-C6-C5    | -2.48 | 119.99      | 126.53   |
| 3   | 12C   | 500 | GTP  | C5-C6-N1    | 2.48  | 119.56      | 113.25   |
| 3   | 12C   | 500 | GTP  | C8-N7-C5    | 2.47  | 108.67      | 104.26   |
| 3   | 10A   | 500 | GTP  | C8-N7-C5    | 2.47  | 108.67      | 104.26   |
| 3   | 11E   | 500 | GTP  | C8-N7-C5    | 2.47  | 108.67      | 104.26   |
| 3   | 5E    | 500 | GTP  | C8-N7-C5    | 2.47  | 108.66      | 104.26   |
| 3   | 11C   | 500 | GTP  | C8-N7-C5    | 2.47  | 108.66      | 104.26   |
| 3   | 5C    | 500 | GTP  | N9-C8-N7    | -2.47 | 108.82      | 113.40   |
| 3   | 8E    | 500 | GTP  | C4'-O4'-C1' | 2.46  | 114.90      | 109.47   |
| 3   | 5A    | 500 | GTP  | C8-N7-C5    | 2.46  | 108.64      | 104.26   |
| 3   | 13C   | 500 | GTP  | C8-N7-C5    | 2.46  | 108.64      | 104.26   |
| 3   | 2C    | 500 | GTP  | C8-N7-C5    | 2.46  | 108.64      | 104.26   |
| 3   | 9A    | 500 | GTP  | C8-N7-C5    | 2.45  | 108.63      | 104.26   |
| 3   | 1A    | 500 | GTP  | C8-N7-C5    | 2.45  | 108.62      | 104.26   |
| 3   | 1E    | 500 | GTP  | C8-N7-C5    | 2.45  | 108.62      | 104.26   |
| 3   | 9E    | 500 | GTP  | C8-N7-C5    | 2.45  | 108.62      | 104.26   |
| 3   | 7A    | 500 | GTP  | N9-C8-N7    | -2.45 | 108.86      | 113.40   |
| 3   | 2A    | 500 | GTP  | C8-N7-C5    | 2.45  | 108.62      | 104.26   |
| 3   | 13A   | 500 | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 3   | 1C    | 500 | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 3   | 4E    | 500 | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 3   | 2E    | 500 | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 3   | 13C   | 500 | GTP  | O6-C6-N1    | 2.44  | 124.70      | 120.11   |
| 3   | 5A    | 500 | GTP  | C2-N1-C6    | -2.44 | 120.69      | 125.11   |
| 3   | 3A    | 500 | GTP  | C5-C6-N1    | 2.43  | 119.44      | 113.25   |
| 5   | 5B    | 600 | GDP  | O6-C6-C5    | -2.43 | 120.12      | 126.53   |
| 5   | 5D    | 600 | GDP  | C4-C5-N7    | -2.43 | 106.83      | 110.67   |
| 3   | 9C    | 500 | GTP  | C5-C6-N1    | 2.42  | 119.42      | 113.25   |
| 3   | 12A   | 500 | GTP  | C8-N7-C5    | 2.42  | 108.56      | 104.26   |
| 3   | 13E   | 500 | GTP  | C8-N7-C5    | 2.41  | 108.56      | 104.26   |
| 3   | 3E    | 500 | GTP  | C5-C6-N1    | 2.41  | 119.39      | 113.25   |
| 3   | 9C    | 500 | GTP  | C8-N7-C5    | 2.41  | 108.56      | 104.26   |
| 3   | 3C    | 500 | GTP  | C5-C6-N1    | 2.41  | 119.39      | 113.25   |
| 3   | 7A    | 500 | GTP  | C8-N7-C5    | 2.41  | 108.55      | 104.26   |
| 3   | 8C    | 500 | GTP  | N9-C8-N7    | -2.41 | 108.94      | 113.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 8A    | 500 | GTP  | C8-N7-C5    | 2.40  | 108.54      | 104.26   |
| 3   | 7E    | 500 | GTP  | C8-N7-C5    | 2.40  | 108.54      | 104.26   |
| 3   | 5C    | 500 | GTP  | C8-N7-C5    | 2.39  | 108.52      | 104.26   |
| 5   | 6D    | 600 | GDP  | C4-C5-N7    | -2.39 | 106.88      | 110.67   |
| 3   | 12E   | 500 | GTP  | C2-N1-C6    | -2.38 | 120.79      | 125.11   |
| 5   | 1D    | 600 | GDP  | O6-C6-C5    | -2.38 | 120.25      | 126.53   |
| 3   | 12C   | 500 | GTP  | C3'-C2'-C1' | 2.38  | 105.96      | 101.46   |
| 3   | 7A    | 500 | GTP  | C2-N1-C6    | -2.37 | 120.81      | 125.11   |
| 3   | 8C    | 500 | GTP  | C8-N7-C5    | 2.37  | 108.48      | 104.26   |
| 5   | 11B   | 600 | GDP  | C4-C5-N7    | -2.37 | 106.91      | 110.67   |
| 5   | 1B    | 600 | GDP  | C4-C5-N7    | -2.36 | 106.93      | 110.67   |
| 5   | 1D    | 600 | GDP  | C4-C5-N7    | -2.36 | 106.94      | 110.67   |
| 5   | 12D   | 600 | GDP  | C4-C5-N7    | -2.35 | 106.94      | 110.67   |
| 3   | 8A    | 500 | GTP  | C5-C6-N1    | 2.35  | 119.24      | 113.25   |
| 5   | 6B    | 600 | GDP  | O6-C6-C5    | -2.35 | 120.33      | 126.53   |
| 5   | 6B    | 600 | GDP  | C3'-C2'-C1' | 2.35  | 105.90      | 101.46   |
| 5   | 6B    | 600 | GDP  | C4-C5-N7    | -2.35 | 106.95      | 110.67   |
| 3   | 6A    | 500 | GTP  | C3'-C2'-C1' | 2.34  | 105.89      | 101.46   |
| 5   | 6D    | 600 | GDP  | O6-C6-C5    | -2.34 | 120.35      | 126.53   |
| 3   | 7C    | 500 | GTP  | C3'-C2'-C1' | 2.34  | 105.88      | 101.46   |
| 3   | 9E    | 500 | GTP  | C3'-C2'-C1' | 2.33  | 105.88      | 101.46   |
| 3   | 5A    | 500 | GTP  | C3'-C2'-C1' | 2.33  | 105.87      | 101.46   |
| 5   | 5D    | 600 | GDP  | O6-C6-C5    | -2.33 | 120.39      | 126.53   |
| 5   | 5B    | 600 | GDP  | C3'-C2'-C1' | 2.33  | 105.87      | 101.46   |
| 5   | 5B    | 600 | GDP  | C4-C5-N7    | -2.33 | 106.98      | 110.67   |
| 5   | 12B   | 600 | GDP  | C4-C5-N7    | -2.33 | 106.98      | 110.67   |
| 5   | 11D   | 600 | GDP  | C4-C5-N7    | -2.32 | 106.99      | 110.67   |
| 5   | 1B    | 600 | GDP  | O6-C6-C5    | -2.32 | 120.40      | 126.53   |
| 3   | 6E    | 500 | GTP  | C3'-C2'-C1' | 2.32  | 105.85      | 101.46   |
| 5   | 7B    | 600 | GDP  | C3'-C2'-C1' | 2.31  | 105.84      | 101.46   |
| 3   | 11C   | 500 | GTP  | C5-C6-N1    | 2.31  | 119.13      | 113.25   |
| 3   | 5E    | 500 | GTP  | C3'-C2'-C1' | 2.31  | 105.83      | 101.46   |
| 5   | 6D    | 600 | GDP  | C3'-C2'-C1' | 2.30  | 105.82      | 101.46   |
| 3   | 11A   | 500 | GTP  | C3'-C2'-C1' | 2.29  | 105.79      | 101.46   |
| 3   | 12E   | 500 | GTP  | C3'-C2'-C1' | 2.28  | 105.78      | 101.46   |
| 3   | 6C    | 500 | GTP  | C3'-C2'-C1' | 2.28  | 105.78      | 101.46   |
| 3   | 11E   | 500 | GTP  | C5-C6-N1    | 2.28  | 119.06      | 113.25   |
| 5   | 13D   | 600 | GDP  | C3'-C2'-C1' | 2.28  | 105.78      | 101.46   |
| 3   | 10C   | 500 | GTP  | C3'-C2'-C1' | 2.27  | 105.77      | 101.46   |
| 5   | 13B   | 600 | GDP  | C3'-C2'-C1' | 2.27  | 105.75      | 101.46   |
| 3   | 10A   | 500 | GTP  | C3'-C2'-C1' | 2.26  | 105.74      | 101.46   |
| 3   | 11C   | 500 | GTP  | C3'-C2'-C1' | 2.25  | 105.72      | 101.46   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 5C    | 500 | GTP  | C3'-C2'-C1' | 2.25  | 105.72      | 101.46   |
| 5   | 4D    | 600 | GDP  | O6-C6-C5    | -2.25 | 120.60      | 126.53   |
| 3   | 8E    | 500 | GTP  | N2-C2-N3    | 2.25  | 124.06      | 119.67   |
| 3   | 1C    | 500 | GTP  | C3'-C2'-C1' | 2.25  | 105.71      | 101.46   |
| 3   | 6C    | 500 | GTP  | O6-C6-C5    | -2.25 | 120.61      | 126.53   |
| 3   | 7E    | 500 | GTP  | C2-N1-C6    | -2.24 | 121.04      | 125.11   |
| 5   | 8B    | 600 | GDP  | C3'-C2'-C1' | 2.24  | 105.70      | 101.46   |
| 3   | 12E   | 500 | GTP  | O6-C6-C5    | -2.24 | 120.62      | 126.53   |
| 3   | 1A    | 500 | GTP  | C3'-C2'-C1' | 2.24  | 105.70      | 101.46   |
| 5   | 2D    | 600 | GDP  | O6-C6-C5    | -2.24 | 120.63      | 126.53   |
| 3   | 5E    | 500 | GTP  | O6-C6-C5    | -2.24 | 120.63      | 126.53   |
| 5   | 7D    | 600 | GDP  | C3'-C2'-C1' | 2.24  | 105.69      | 101.46   |
| 3   | 12A   | 500 | GTP  | C3'-C2'-C1' | 2.24  | 105.69      | 101.46   |
| 5   | 11B   | 600 | GDP  | C3'-C2'-C1' | 2.23  | 105.69      | 101.46   |
| 3   | 9C    | 500 | GTP  | C3'-C2'-C1' | 2.23  | 105.68      | 101.46   |
| 5   | 4B    | 600 | GDP  | O6-C6-C5    | -2.23 | 120.64      | 126.53   |
| 3   | 1E    | 500 | GTP  | C3'-C2'-C1' | 2.23  | 105.68      | 101.46   |
| 3   | 11A   | 500 | GTP  | C5-C6-N1    | 2.23  | 118.92      | 113.25   |
| 5   | 2B    | 600 | GDP  | C3'-C2'-C1' | 2.23  | 105.68      | 101.46   |
| 5   | 7B    | 600 | GDP  | O6-C6-C5    | -2.23 | 120.66      | 126.53   |
| 3   | 9A    | 500 | GTP  | C3'-C2'-C1' | 2.23  | 105.67      | 101.46   |
| 3   | 10E   | 500 | GTP  | C3'-C2'-C1' | 2.22  | 105.67      | 101.46   |
| 3   | 8C    | 500 | GTP  | O6-C6-C5    | -2.22 | 120.67      | 126.53   |
| 3   | 2C    | 500 | GTP  | C3'-C2'-C1' | 2.22  | 105.66      | 101.46   |
| 3   | 4A    | 500 | GTP  | C3'-C2'-C1' | 2.22  | 105.66      | 101.46   |
| 5   | 2D    | 600 | GDP  | C3'-C2'-C1' | 2.22  | 105.66      | 101.46   |
| 5   | 2B    | 600 | GDP  | O6-C6-C5    | -2.22 | 120.68      | 126.53   |
| 3   | 2A    | 500 | GTP  | C3'-C2'-C1' | 2.21  | 105.65      | 101.46   |
| 3   | 13A   | 500 | GTP  | O2B-PB-O3B  | 2.21  | 113.25      | 107.27   |
| 5   | 11D   | 600 | GDP  | C3'-C2'-C1' | 2.21  | 105.64      | 101.46   |
| 3   | 2E    | 500 | GTP  | C3'-C2'-C1' | 2.20  | 105.63      | 101.46   |
| 3   | 4C    | 500 | GTP  | C3'-C2'-C1' | 2.20  | 105.63      | 101.46   |
| 5   | 10D   | 600 | GDP  | O6-C6-C5    | -2.20 | 120.72      | 126.53   |
| 5   | 11B   | 600 | GDP  | O6-C6-C5    | -2.20 | 120.72      | 126.53   |
| 3   | 10A   | 500 | GTP  | C5-C6-N1    | 2.20  | 118.85      | 113.25   |
| 5   | 7D    | 600 | GDP  | O6-C6-C5    | -2.20 | 120.73      | 126.53   |
| 3   | 12A   | 500 | GTP  | C5-C6-N1    | 2.20  | 118.85      | 113.25   |
| 3   | 5A    | 500 | GTP  | O6-C6-C5    | -2.20 | 120.73      | 126.53   |
| 3   | 9A    | 500 | GTP  | C5-C6-N1    | 2.19  | 118.83      | 113.25   |
| 5   | 5D    | 600 | GDP  | C3'-C2'-C1' | 2.19  | 105.61      | 101.46   |
| 3   | 6A    | 500 | GTP  | O6-C6-C5    | -2.18 | 120.77      | 126.53   |
| 5   | 9B    | 600 | GDP  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 3B    | 600 | GDP  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |
| 3   | 13A   | 500 | GTP  | O2G-PG-O3B  | 2.18  | 111.94      | 104.64   |
| 3   | 7E    | 500 | GTP  | O6-C6-C5    | -2.17 | 120.80      | 126.53   |
| 5   | 11D   | 600 | GDP  | O6-C6-C5    | -2.17 | 120.80      | 126.53   |
| 5   | 10B   | 600 | GDP  | O6-C6-C5    | -2.17 | 120.81      | 126.53   |
| 3   | 11E   | 500 | GTP  | C3'-C2'-C1' | 2.17  | 105.56      | 101.46   |
| 3   | 9E    | 500 | GTP  | C5-C6-N1    | 2.17  | 118.77      | 113.25   |
| 3   | 4E    | 500 | GTP  | C3'-C2'-C1' | 2.16  | 105.56      | 101.46   |
| 5   | 7D    | 600 | GDP  | C5-C6-N1    | 2.16  | 118.76      | 113.25   |
| 3   | 7A    | 500 | GTP  | O6-C6-C5    | -2.16 | 120.83      | 126.53   |
| 3   | 8E    | 500 | GTP  | O3A-PA-O1A  | -2.16 | 104.21      | 110.70   |
| 5   | 4B    | 600 | GDP  | C3'-C2'-C1' | 2.16  | 105.54      | 101.46   |
| 3   | 12C   | 500 | GTP  | O2B-PB-O3B  | 2.16  | 113.10      | 107.27   |
| 5   | 8D    | 600 | GDP  | C3'-C2'-C1' | 2.15  | 105.53      | 101.46   |
| 3   | 13C   | 500 | GTP  | N2-C2-N1    | 2.15  | 121.29      | 116.76   |
| 5   | 3D    | 600 | GDP  | O6-C6-C5    | -2.14 | 120.89      | 126.53   |
| 5   | 1D    | 600 | GDP  | C3'-C2'-C1' | 2.14  | 105.51      | 101.46   |
| 5   | 9D    | 600 | GDP  | O6-C6-C5    | -2.14 | 120.89      | 126.53   |
| 3   | 6E    | 500 | GTP  | C5-C6-N1    | 2.14  | 118.69      | 113.25   |
| 5   | 8B    | 600 | GDP  | O6-C6-C5    | -2.13 | 120.92      | 126.53   |
| 5   | 12B   | 600 | GDP  | C5-C6-N1    | 2.12  | 118.65      | 113.25   |
| 5   | 8D    | 600 | GDP  | O6-C6-C5    | -2.12 | 120.94      | 126.53   |
| 5   | 7B    | 600 | GDP  | C5-C6-N1    | 2.12  | 118.64      | 113.25   |
| 5   | 12D   | 600 | GDP  | C5-C6-N1    | 2.12  | 118.64      | 113.25   |
| 3   | 3A    | 500 | GTP  | C3'-C2'-C1' | 2.11  | 105.45      | 101.46   |
| 3   | 7C    | 500 | GTP  | C5-C6-N1    | 2.10  | 118.61      | 113.25   |
| 5   | 10B   | 600 | GDP  | C3'-C2'-C1' | 2.09  | 105.42      | 101.46   |
| 3   | 13A   | 500 | GTP  | C5-C6-N1    | 2.09  | 118.57      | 113.25   |
| 3   | 3C    | 500 | GTP  | C3'-C2'-C1' | 2.09  | 105.41      | 101.46   |
| 5   | 1D    | 600 | GDP  | C5-C6-N1    | 2.09  | 118.57      | 113.25   |
| 5   | 11D   | 600 | GDP  | C5-C6-N1    | 2.08  | 118.56      | 113.25   |
| 5   | 1B    | 600 | GDP  | C5-C6-N1    | 2.08  | 118.56      | 113.25   |
| 3   | 3E    | 500 | GTP  | C3'-C2'-C1' | 2.08  | 105.40      | 101.46   |
| 3   | 13E   | 500 | GTP  | O2G-PG-O3B  | 2.08  | 111.61      | 104.64   |
| 5   | 1B    | 600 | GDP  | C3'-C2'-C1' | 2.08  | 105.39      | 101.46   |
| 5   | 9D    | 600 | GDP  | C5-C6-N1    | 2.08  | 118.54      | 113.25   |
| 5   | 5B    | 600 | GDP  | C5-C6-N1    | 2.08  | 118.54      | 113.25   |
| 5   | 10B   | 600 | GDP  | C5-C6-N1    | 2.08  | 118.54      | 113.25   |
| 3   | 7C    | 500 | GTP  | C2'-C3'-C4' | 2.07  | 106.61      | 102.61   |
| 5   | 6D    | 600 | GDP  | C5-C6-N1    | 2.07  | 118.51      | 113.25   |
| 3   | 8A    | 500 | GTP  | C3'-C2'-C1' | 2.06  | 105.37      | 101.46   |
| 3   | 12A   | 500 | GTP  | O2B-PB-O3B  | 2.06  | 112.85      | 107.27   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 5   | 4D    | 600 | GDP  | C5-C6-N1    | 2.06 | 118.50      | 113.25   |
| 3   | 10C   | 500 | GTP  | C2'-C3'-C4' | 2.06 | 106.59      | 102.61   |
| 5   | 11B   | 600 | GDP  | C5-C6-N1    | 2.06 | 118.49      | 113.25   |
| 5   | 2D    | 600 | GDP  | C5-C6-N1    | 2.06 | 118.49      | 113.25   |
| 5   | 12D   | 600 | GDP  | C3'-C2'-C1' | 2.06 | 105.35      | 101.46   |
| 5   | 10D   | 600 | GDP  | C5-C6-N1    | 2.06 | 118.49      | 113.25   |
| 5   | 5D    | 600 | GDP  | C5-C6-N1    | 2.06 | 118.49      | 113.25   |
| 5   | 8B    | 600 | GDP  | C5-C6-N1    | 2.05 | 118.48      | 113.25   |
| 5   | 8D    | 600 | GDP  | C5-C6-N1    | 2.05 | 118.48      | 113.25   |
| 5   | 6B    | 600 | GDP  | C5-C6-N1    | 2.05 | 118.47      | 113.25   |
| 3   | 13C   | 500 | GTP  | C3'-C2'-C1' | 2.04 | 105.33      | 101.46   |
| 3   | 10C   | 500 | GTP  | C5-C6-N1    | 2.04 | 118.45      | 113.25   |
| 5   | 9B    | 600 | GDP  | C5-C6-N1    | 2.03 | 118.43      | 113.25   |
| 3   | 9A    | 500 | GTP  | C2'-C3'-C4' | 2.03 | 106.53      | 102.61   |
| 5   | 2B    | 600 | GDP  | C5-C6-N1    | 2.03 | 118.42      | 113.25   |
| 5   | 4B    | 600 | GDP  | C5-C6-N1    | 2.03 | 118.42      | 113.25   |
| 3   | 1E    | 500 | GTP  | C2'-C3'-C4' | 2.02 | 106.52      | 102.61   |
| 3   | 10E   | 500 | GTP  | C5-C6-N1    | 2.02 | 118.40      | 113.25   |
| 3   | 13E   | 500 | GTP  | C2'-C3'-C4' | 2.02 | 106.51      | 102.61   |
| 3   | 5C    | 500 | GTP  | C2'-C3'-C4' | 2.01 | 106.49      | 102.61   |
| 5   | 4D    | 600 | GDP  | C3'-C2'-C1' | 2.01 | 105.26      | 101.46   |
| 3   | 13A   | 500 | GTP  | C3'-C2'-C1' | 2.01 | 105.26      | 101.46   |
| 3   | 9E    | 500 | GTP  | C2'-C3'-C4' | 2.01 | 106.48      | 102.61   |
| 3   | 13E   | 500 | GTP  | C5-C6-N1    | 2.01 | 118.36      | 113.25   |
| 5   | 3D    | 600 | GDP  | C5-C6-N1    | 2.00 | 118.35      | 113.25   |

There are no chirality outliers.

All (268) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | 10A   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 10A   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 10C   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 10C   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 10E   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 10E   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 11A   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 11A   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 11A   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 11A   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 11A   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 11C   | 500 | GTP  | C5'-O5'-PA-O3A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | 11C   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 11C   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 11E   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 11E   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 11E   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 12C   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 12C   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 13A   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 13A   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 13C   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 1A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 1A    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 1A    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 1C    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 1C    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 1C    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 1E    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 1E    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 1E    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 2A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 2A    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 2A    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 2C    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 2C    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 2C    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 2E    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 2E    | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 2E    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 3A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 3A    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 3C    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 3C    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 3E    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 3E    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 4A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 4A    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 4C    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 4C    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 4E    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 4E    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 5A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 5A    | 500 | GTP  | C5'-O5'-PA-O1A  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 5A    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 5C    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 5C    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 5E    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 5E    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 5E    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 6A    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 6A    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 6A    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 6C    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 6C    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 6C    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 6E    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 6E    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 6E    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 7A    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 7A    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 7A    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 7C    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 7C    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 7C    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 7E    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 7E    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 7E    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 8A    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 8A    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 8A    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 8C    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 8C    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 8C    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 8E    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 8E    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 8E    | 500 | GTP  | C5'-O5'-PA-O2A |
| 3   | 9A    | 500 | GTP  | C5'-O5'-PA-O1A |
| 3   | 9C    | 500 | GTP  | C5'-O5'-PA-O3A |
| 3   | 9C    | 500 | GTP  | C5'-O5'-PA-O2A |
| 5   | 2B    | 600 | GDP  | PA-O3A-PB-O2B  |
| 5   | 2B    | 600 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2B    | 600 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2D    | 600 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2D    | 600 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3B    | 600 | GDP  | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | 4B    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 4B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 4B    | 600 | GDP  | C5'-O5'-PA-O1A  |
| 5   | 4B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 4D    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 4D    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 4D    | 600 | GDP  | C5'-O5'-PA-O1A  |
| 5   | 4D    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 5B    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 5B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 5B    | 600 | GDP  | C5'-O5'-PA-O1A  |
| 5   | 5B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 5D    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 5D    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 5D    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 6B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 6D    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 6D    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 7B    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 7B    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 7B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 7B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 7D    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 7D    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 7D    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 8B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 8B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 8D    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 8D    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 9B    | 600 | GDP  | C5'-O5'-PA-O1A  |
| 5   | 9B    | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 9D    | 600 | GDP  | O4'-C4'-C5'-O5' |
| 3   | 10A   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 11C   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 11E   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 13A   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 13C   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 10B   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 10B   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 10D   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 10D   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 11B   | 600 | GDP  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | 11B   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 12B   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 12B   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 12D   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 12D   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 9B    | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 9D    | 600 | GDP  | C3'-C4'-C5'-O5' |
| 3   | 3E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 4C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 4E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10C   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 11C   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 1E    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 11D   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 11D   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 3   | 3C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 4A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 11E   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 3A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 5   | 13B   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 3   | 8A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10A   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 12E   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 13B   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 3   | 1A    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 1E    | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 11C   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 11E   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 8C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 9C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10C   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 10A   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 11A   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 2A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 2E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 6C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 6E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 1C    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 8D    | 600 | GDP  | PA-O3A-PB-O2B   |
| 5   | 8D    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 13D   | 600 | GDP  | C3'-C4'-C5'-O5' |
| 5   | 6B    | 600 | GDP  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | 6D    | 600 | GDP  | C3'-C4'-C5'-O5' |
| 3   | 7C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10C   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 11C   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 11E   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 13A   | 500 | GTP  | PB-O3A-PA-O1A   |
| 3   | 1A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 5E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 7E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10A   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 10C   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 10E   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 12A   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 13A   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 13A   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 13E   | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 13E   | 500 | GTP  | C5'-O5'-PA-O1A  |
| 3   | 13E   | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 5C    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 3   | 9A    | 500 | GTP  | C5'-O5'-PA-O3A  |
| 3   | 9A    | 500 | GTP  | C5'-O5'-PA-O2A  |
| 5   | 1B    | 600 | GDP  | C5'-O5'-PA-O3A  |
| 5   | 3B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 5   | 6B    | 600 | GDP  | C5'-O5'-PA-O2A  |
| 3   | 10C   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10E   | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 1C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 1E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 2C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 5A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 5C    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 6A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 7A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 8E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 9A    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 10A   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 10E   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 11A   | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 1A    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 1E    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 9A    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 9E    | 500 | GTP  | PA-O3A-PB-O1B   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | 3D    | 600 | GDP  | C3'-C4'-C5'-O5' |
| 3   | 9E    | 500 | GTP  | C4'-C5'-O5'-PA  |
| 3   | 13E   | 500 | GTP  | PB-O3A-PA-O1A   |
| 3   | 1C    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 5E    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 8E    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 9E    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 10E   | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 13D   | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 4D    | 600 | GDP  | PA-O3A-PB-O1B   |
| 5   | 5B    | 600 | GDP  | PA-O3A-PB-O1B   |
| 5   | 7D    | 600 | GDP  | PA-O3A-PB-O1B   |
| 5   | 2B    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 4B    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 4D    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 5D    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 7D    | 600 | GDP  | PA-O3A-PB-O3B   |
| 5   | 6B    | 600 | GDP  | O4'-C4'-C5'-O5' |
| 3   | 8E    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 10E   | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 11A   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 11E   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 13C   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 13E   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 3A    | 500 | GTP  | PG-O3B-PB-O2B   |
| 3   | 3C    | 500 | GTP  | PG-O3B-PB-O1B   |
| 3   | 4E    | 500 | GTP  | PG-O3B-PB-O2B   |
| 3   | 7E    | 500 | GTP  | PA-O3A-PB-O2B   |
| 3   | 9A    | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 8A    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 5   | 6D    | 600 | GDP  | O4'-C4'-C5'-O5' |
| 5   | 2B    | 600 | GDP  | PA-O3A-PB-O1B   |
| 5   | 5D    | 600 | GDP  | PA-O3A-PB-O1B   |
| 3   | 12E   | 500 | GTP  | O4'-C4'-C5'-O5' |
| 3   | 8C    | 500 | GTP  | C3'-C4'-C5'-O5' |
| 3   | 10A   | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 11A   | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 11C   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 13A   | 500 | GTP  | PB-O3A-PA-O2A   |
| 3   | 1A    | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 1C    | 500 | GTP  | PA-O3A-PB-O1B   |
| 3   | 1E    | 500 | GTP  | PA-O3A-PB-O1B   |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | 3E    | 500 | GTP  | PG-O3B-PB-O2B |
| 3   | 4A    | 500 | GTP  | PG-O3B-PB-O2B |
| 3   | 4C    | 500 | GTP  | PG-O3B-PB-O2B |
| 3   | 5A    | 500 | GTP  | PA-O3A-PB-O2B |

There are no ring outliers.

49 monomers are involved in 101 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | 11A   | 500 | GTP  | 5       | 0            |
| 3   | 7E    | 500 | GTP  | 6       | 0            |
| 3   | 1A    | 500 | GTP  | 1       | 0            |
| 3   | 8E    | 500 | GTP  | 5       | 0            |
| 3   | 3E    | 500 | GTP  | 1       | 0            |
| 3   | 13C   | 500 | GTP  | 2       | 0            |
| 3   | 2A    | 500 | GTP  | 2       | 0            |
| 5   | 12D   | 600 | GDP  | 3       | 0            |
| 5   | 2D    | 600 | GDP  | 1       | 0            |
| 3   | 13A   | 500 | GTP  | 1       | 0            |
| 3   | 8C    | 500 | GTP  | 3       | 0            |
| 3   | 9C    | 500 | GTP  | 3       | 0            |
| 3   | 11E   | 500 | GTP  | 1       | 0            |
| 5   | 6B    | 600 | GDP  | 1       | 0            |
| 5   | 11D   | 600 | GDP  | 1       | 0            |
| 5   | 4B    | 600 | GDP  | 1       | 0            |
| 3   | 5A    | 500 | GTP  | 3       | 0            |
| 3   | 4A    | 500 | GTP  | 2       | 0            |
| 5   | 10D   | 600 | GDP  | 1       | 0            |
| 3   | 7C    | 500 | GTP  | 4       | 0            |
| 5   | 10B   | 600 | GDP  | 1       | 0            |
| 3   | 8A    | 500 | GTP  | 2       | 0            |
| 3   | 13E   | 500 | GTP  | 1       | 0            |
| 5   | 11B   | 600 | GDP  | 2       | 0            |
| 3   | 10E   | 500 | GTP  | 2       | 0            |
| 3   | 1E    | 500 | GTP  | 1       | 0            |
| 3   | 10A   | 500 | GTP  | 2       | 0            |
| 5   | 8B    | 600 | GDP  | 1       | 0            |
| 3   | 1C    | 500 | GTP  | 1       | 0            |
| 3   | 5E    | 500 | GTP  | 4       | 0            |
| 3   | 7A    | 500 | GTP  | 5       | 0            |
| 3   | 3A    | 500 | GTP  | 2       | 0            |
| 3   | 5C    | 500 | GTP  | 2       | 0            |

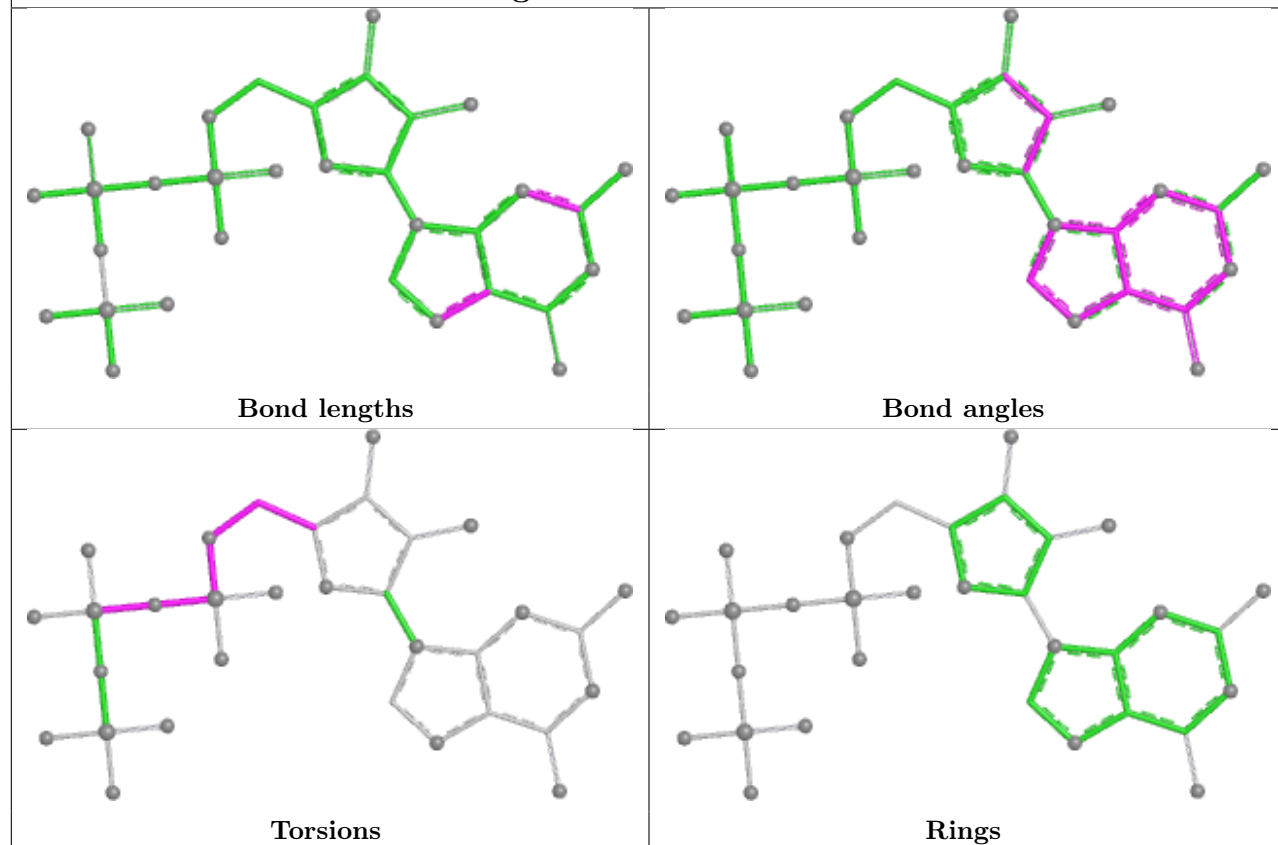
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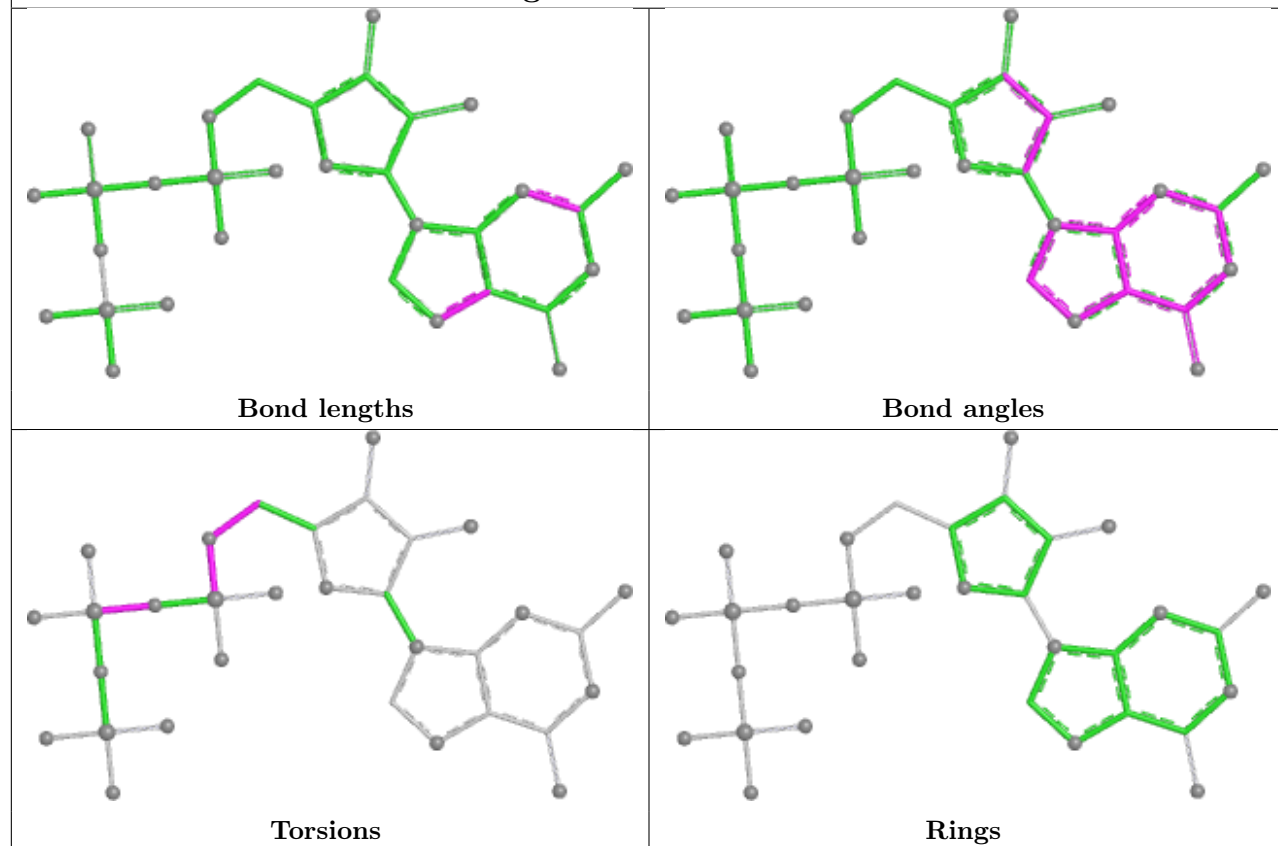
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | 2C    | 500 | GTP  | 2       | 0            |
| 5   | 4D    | 600 | GDP  | 1       | 0            |
| 3   | 11C   | 500 | GTP  | 1       | 0            |
| 3   | 10C   | 500 | GTP  | 1       | 0            |
| 3   | 12E   | 500 | GTP  | 1       | 0            |
| 3   | 3C    | 500 | GTP  | 2       | 0            |
| 3   | 6A    | 500 | GTP  | 4       | 0            |
| 3   | 2E    | 500 | GTP  | 1       | 0            |
| 3   | 6C    | 500 | GTP  | 3       | 0            |
| 3   | 12A   | 500 | GTP  | 1       | 0            |
| 3   | 12C   | 500 | GTP  | 2       | 0            |
| 3   | 4C    | 500 | GTP  | 2       | 0            |
| 3   | 6E    | 500 | GTP  | 3       | 0            |
| 5   | 12B   | 600 | GDP  | 2       | 0            |
| 3   | 9A    | 500 | GTP  | 1       | 0            |
| 3   | 4E    | 500 | GTP  | 1       | 0            |

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

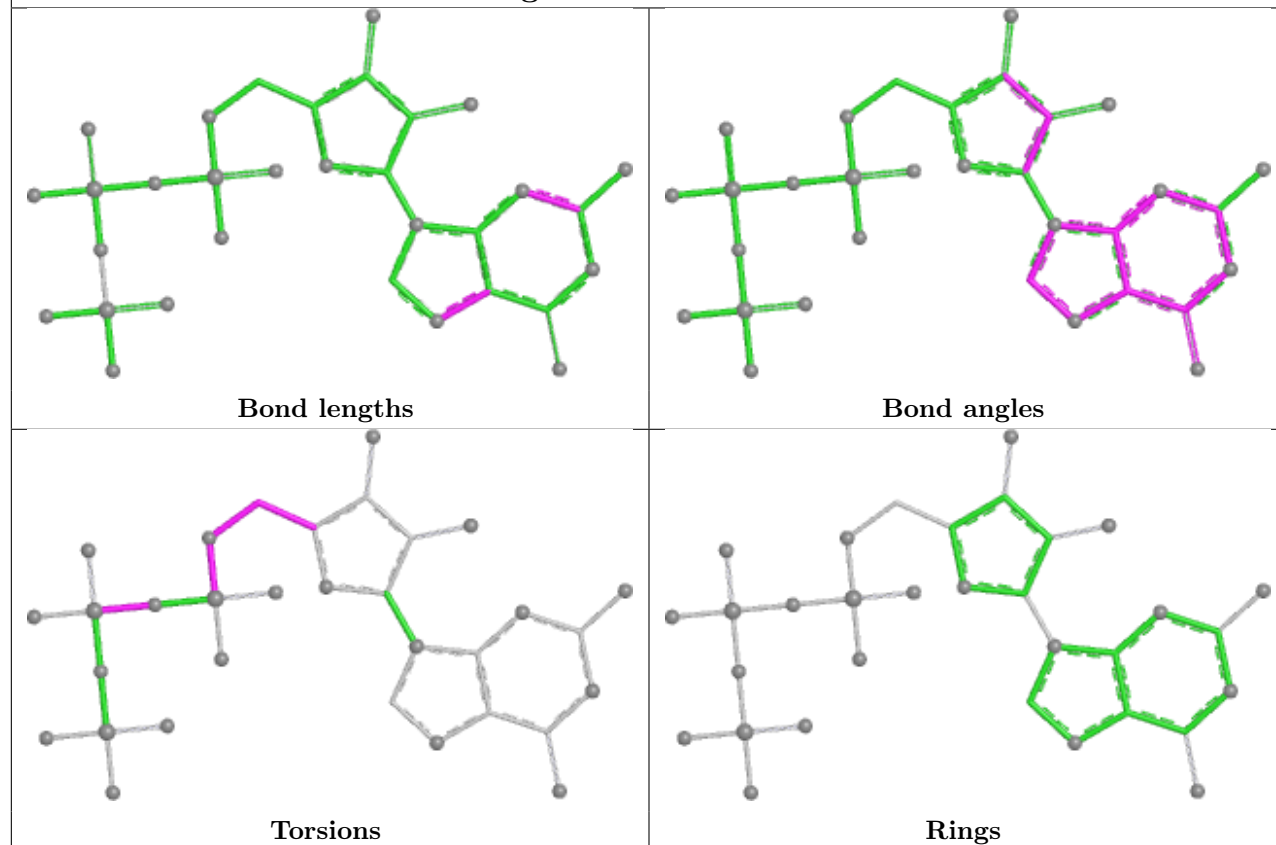
## Ligand GTP 11A 500



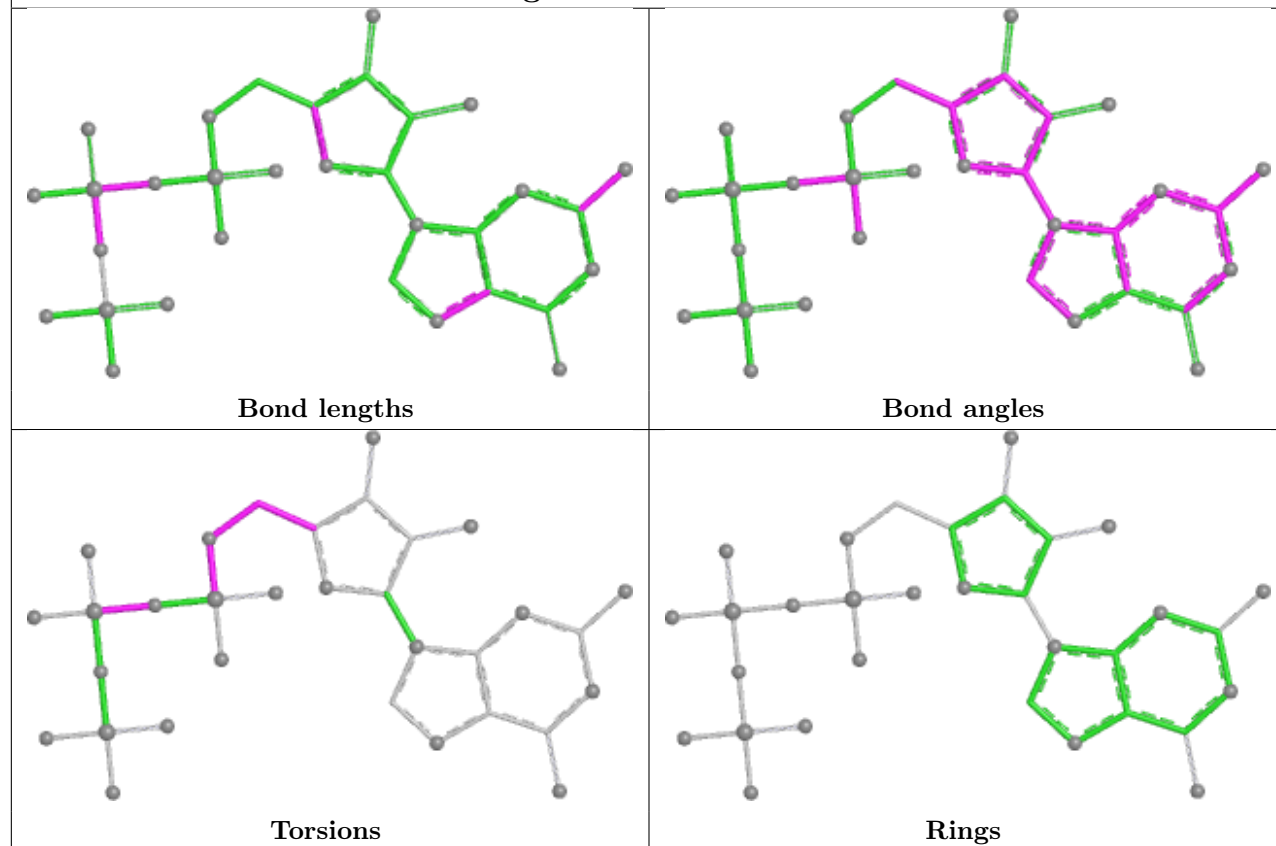
## Ligand GTP 7E 500

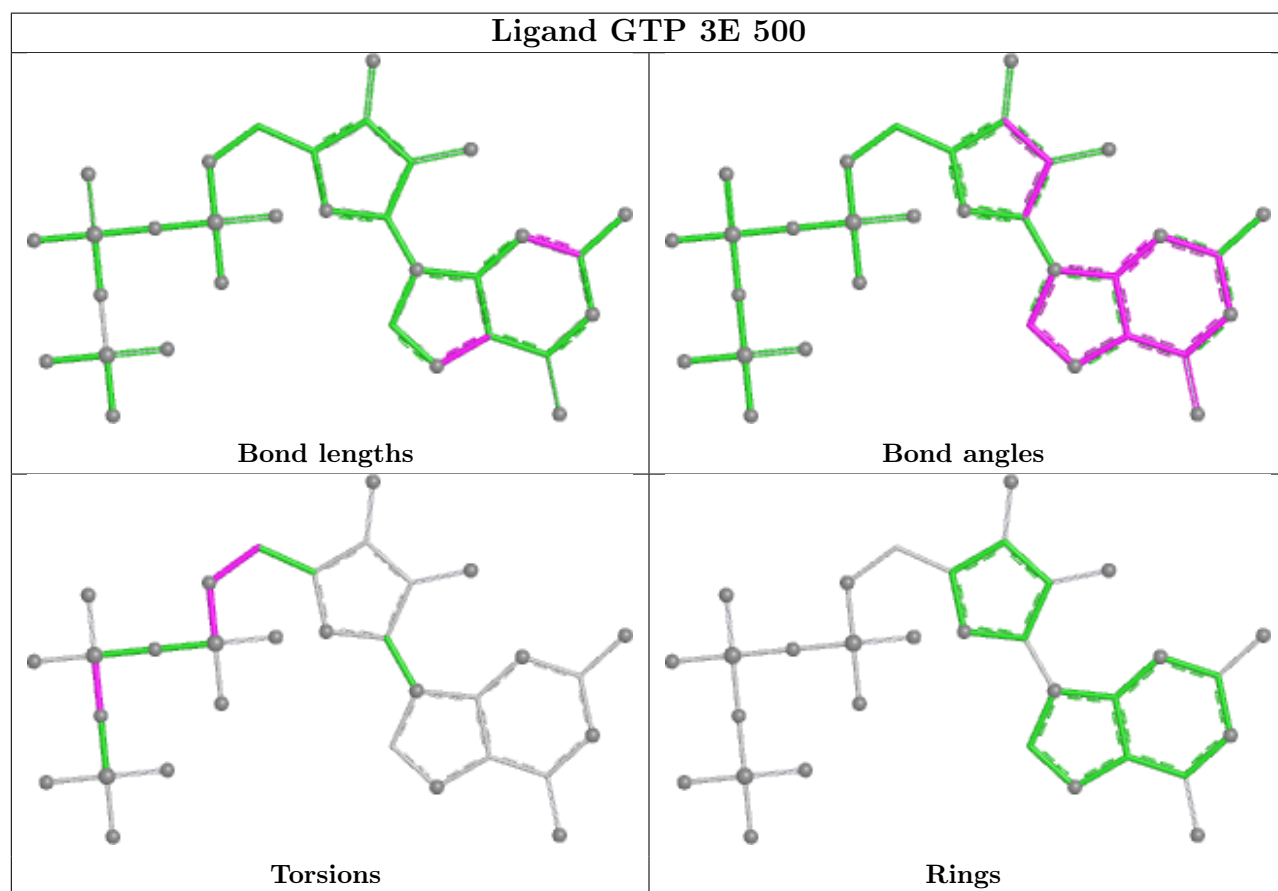
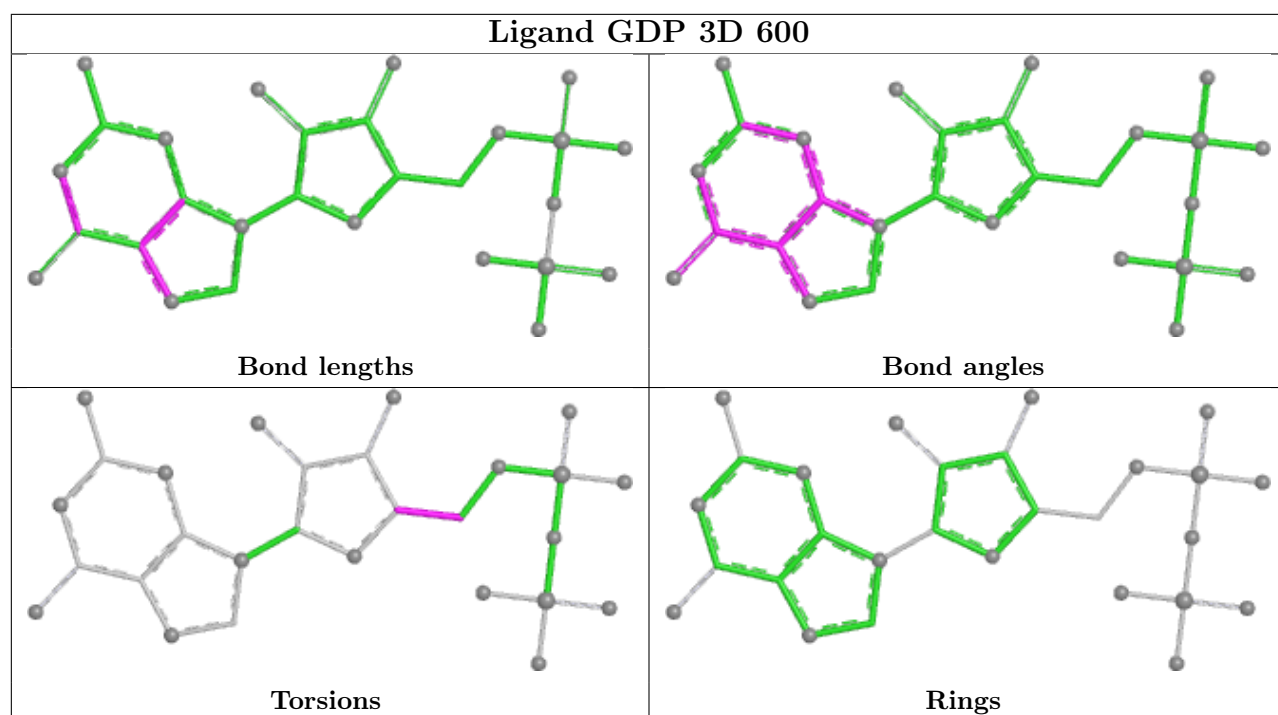


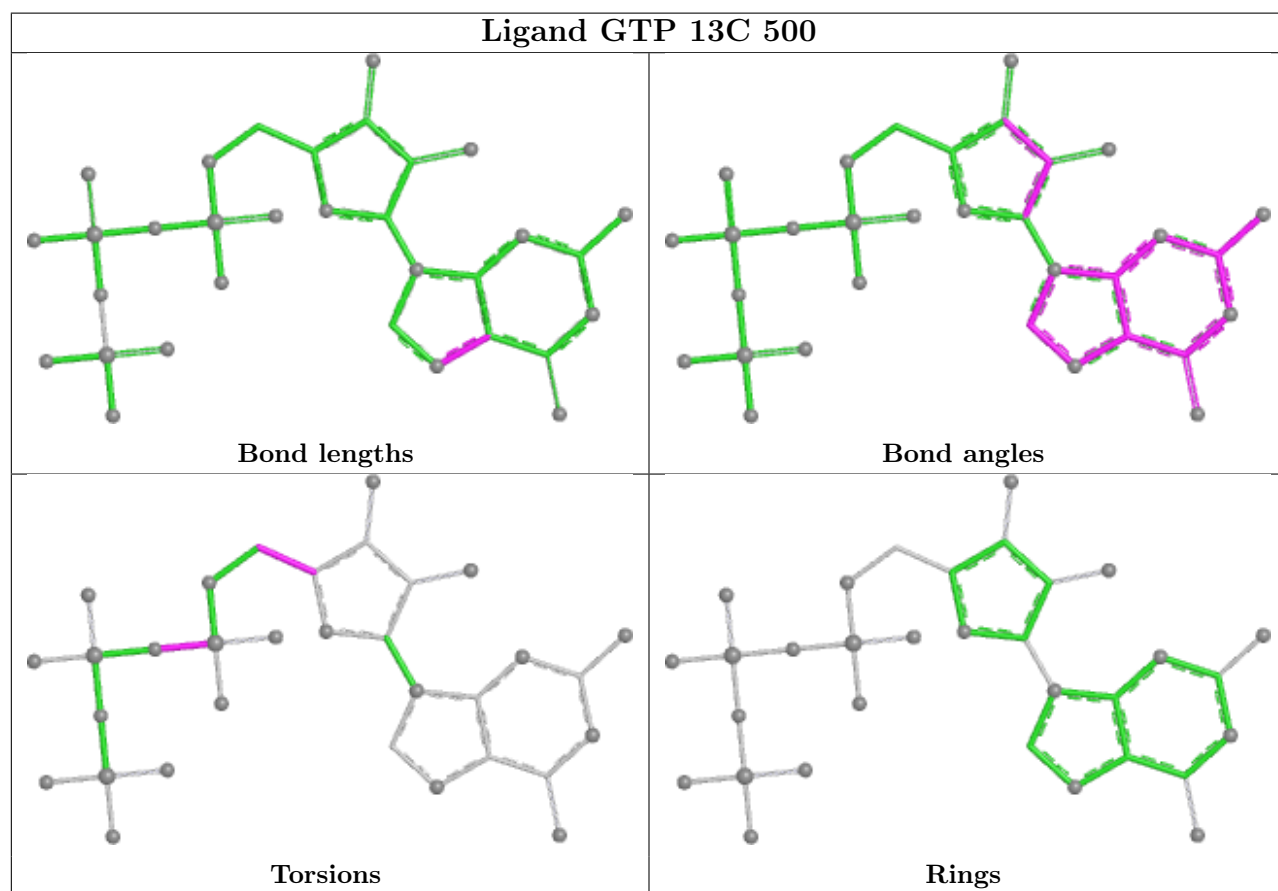
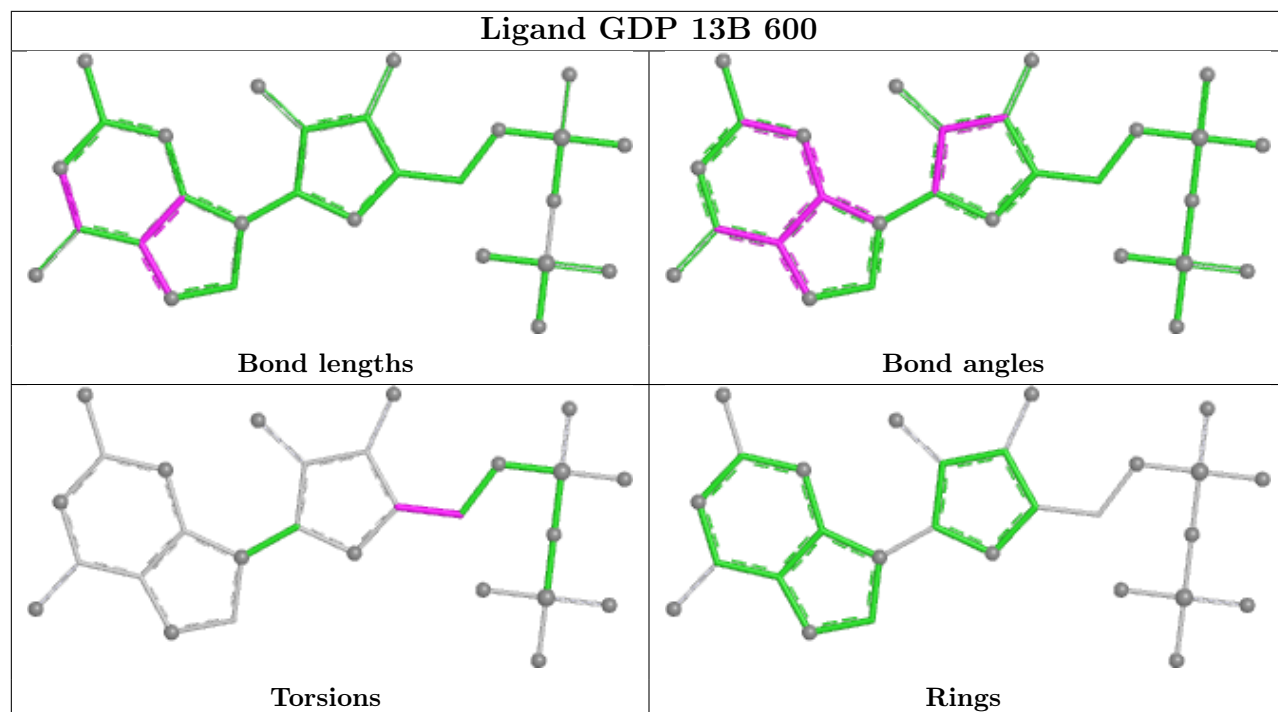
## Ligand GTP 1A 500

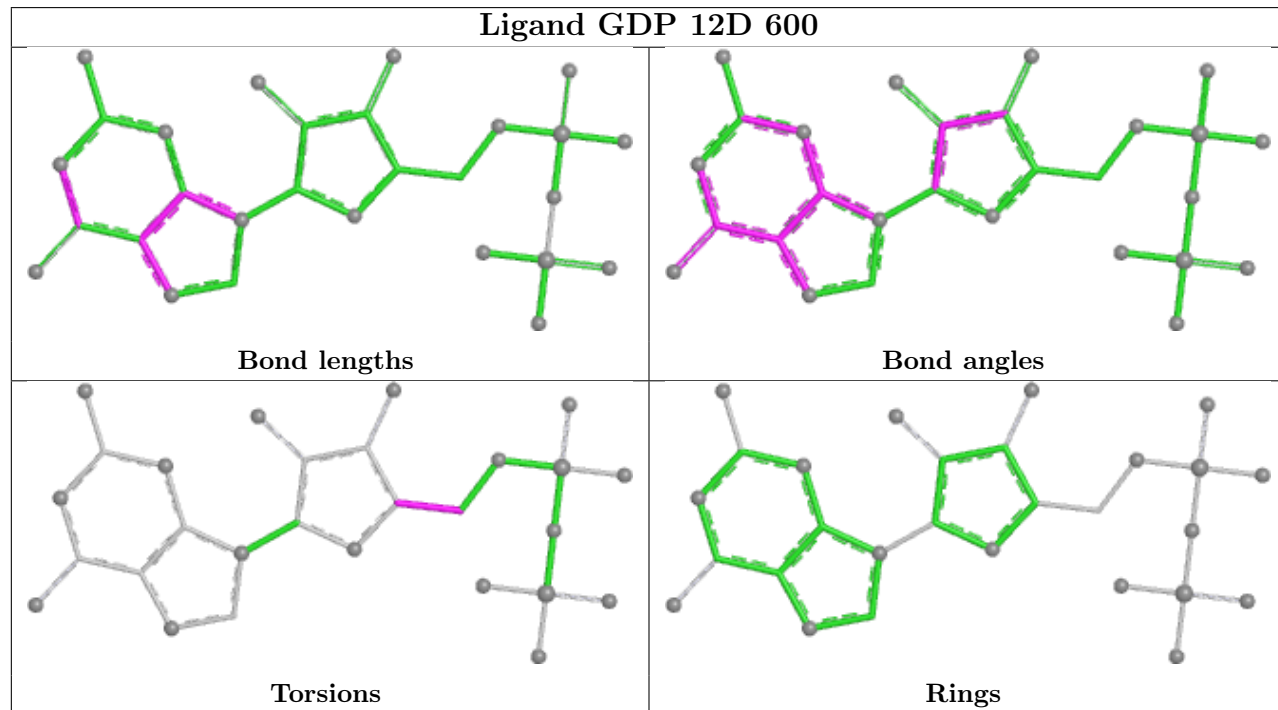
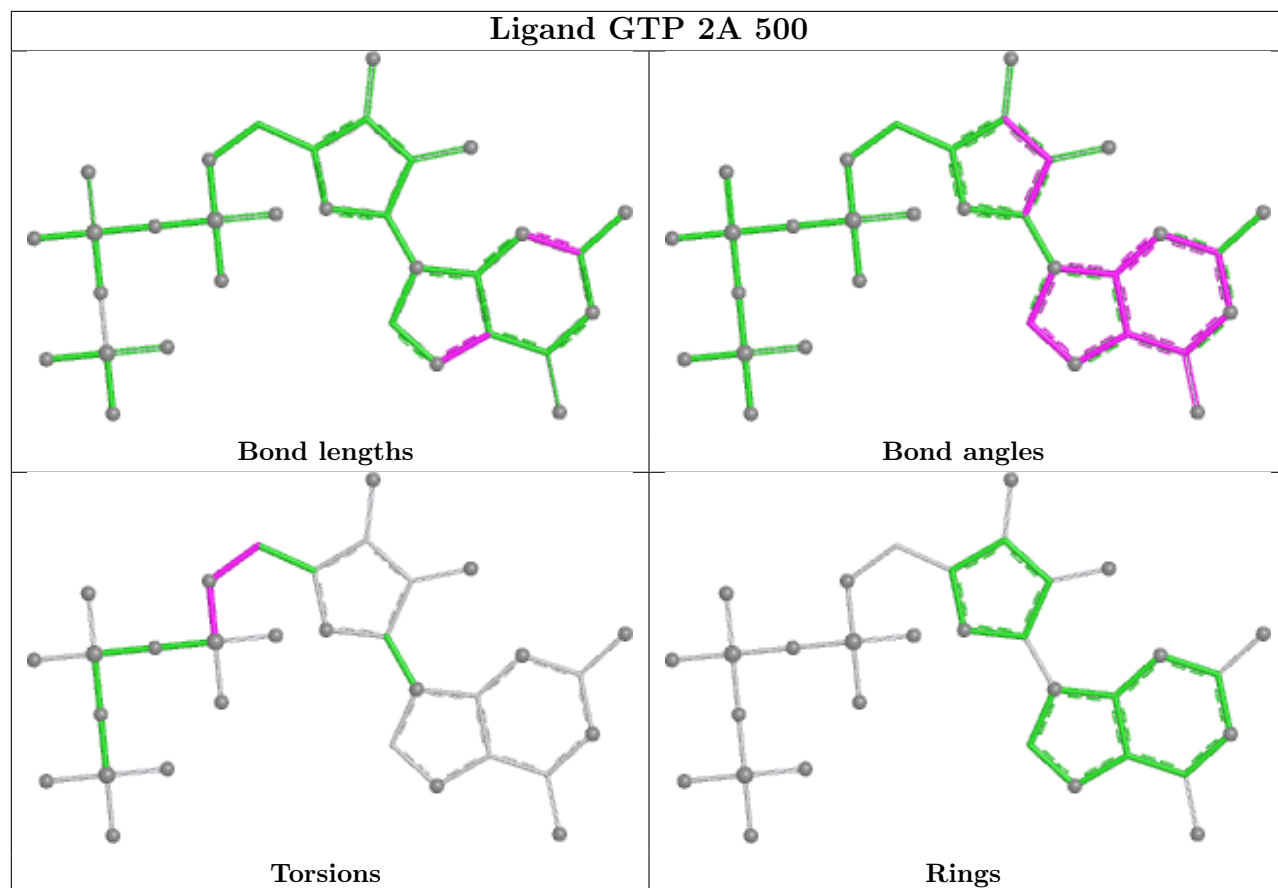


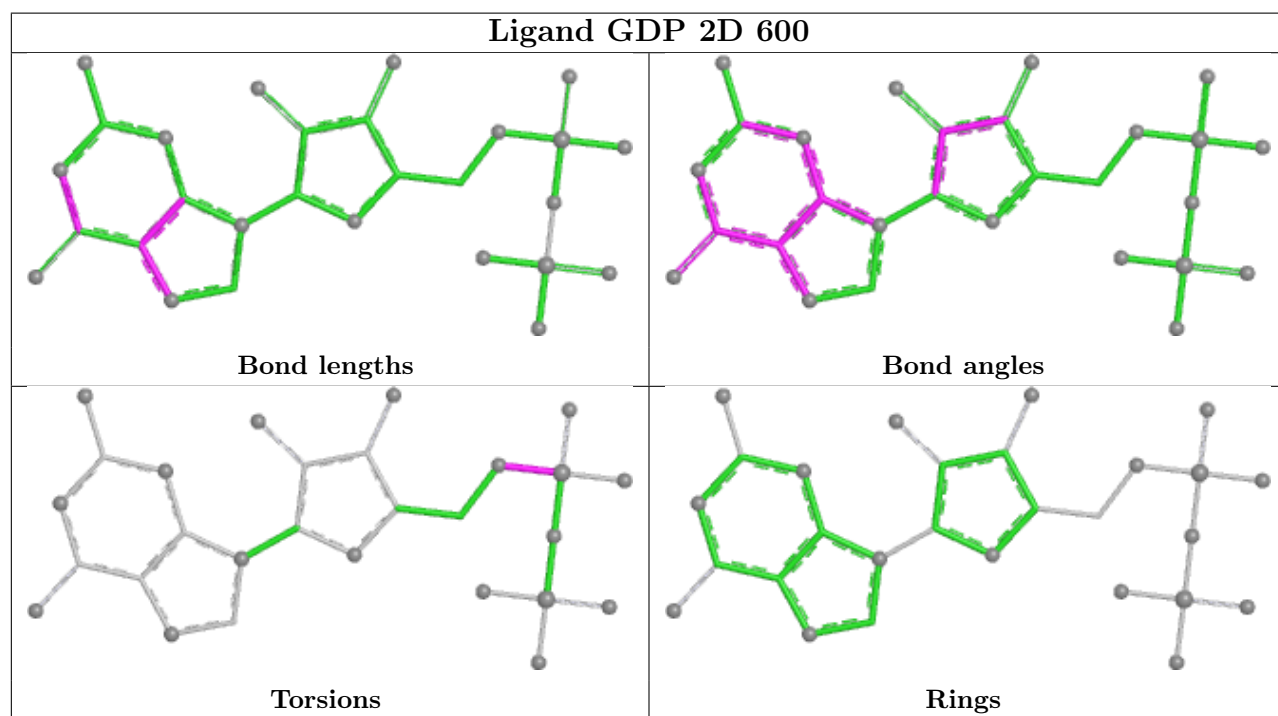
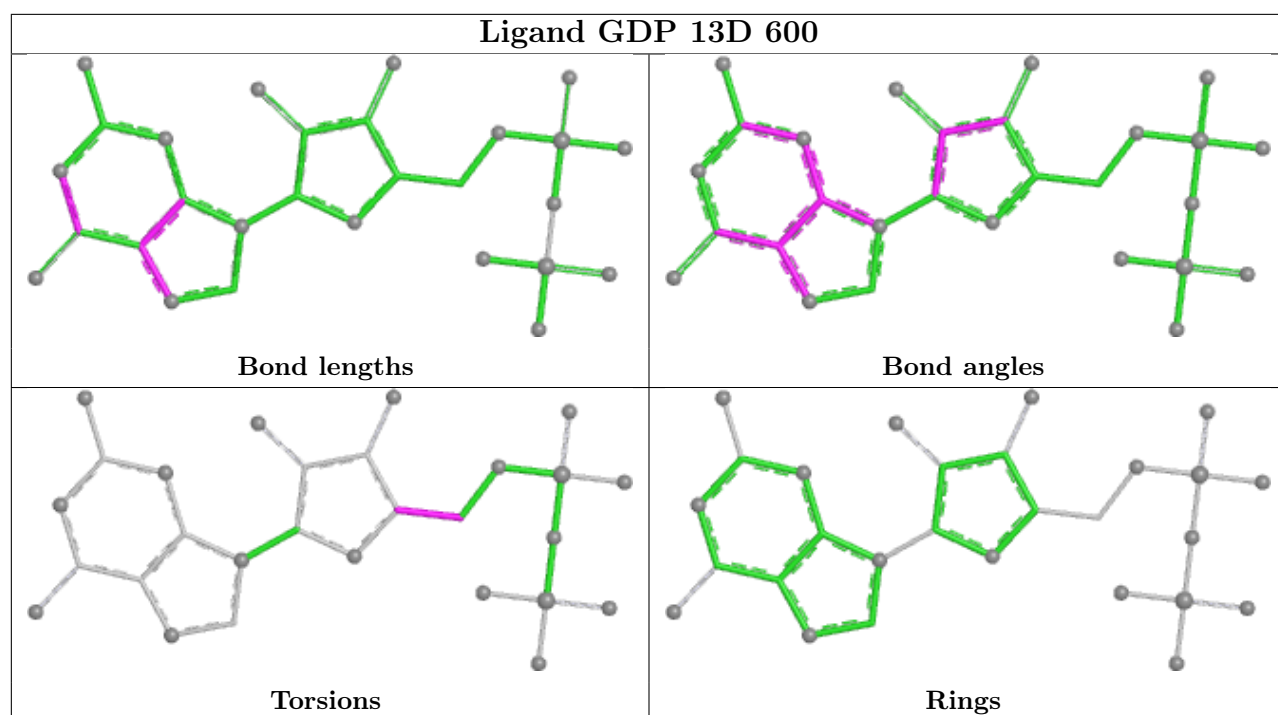
## Ligand GTP 8E 500



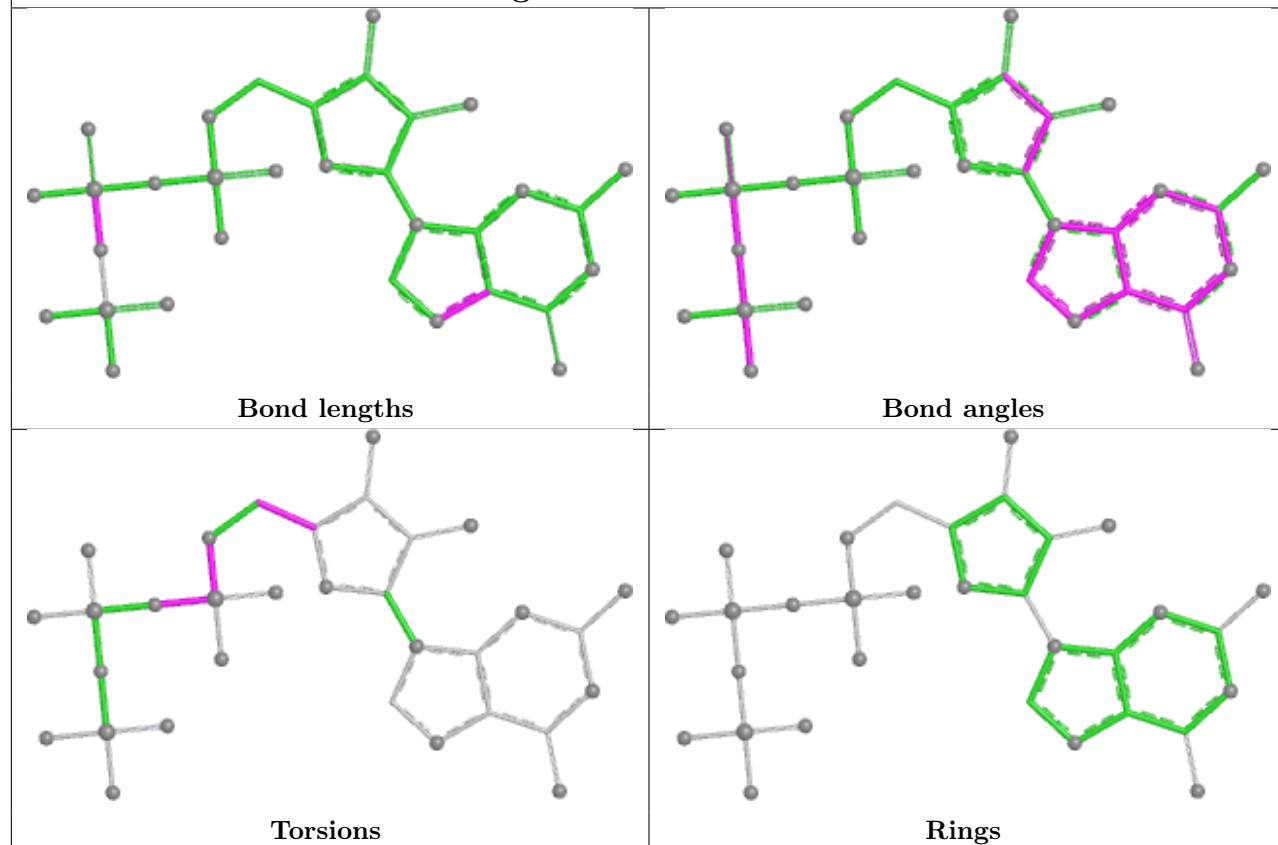




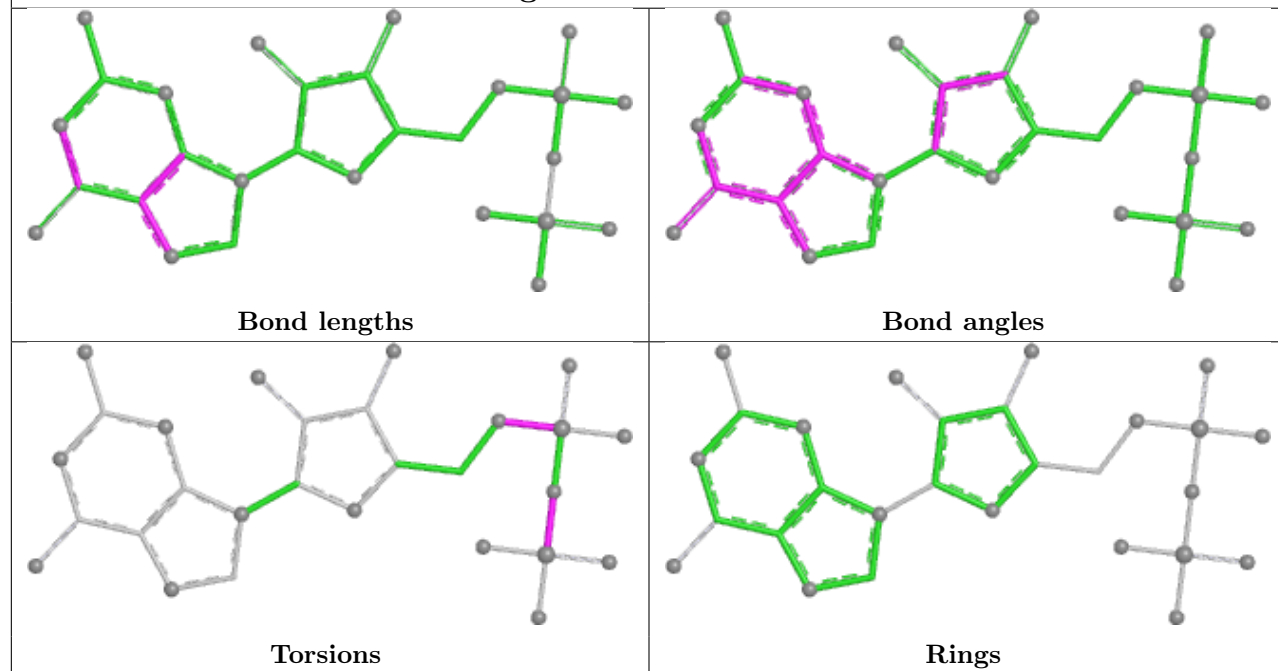




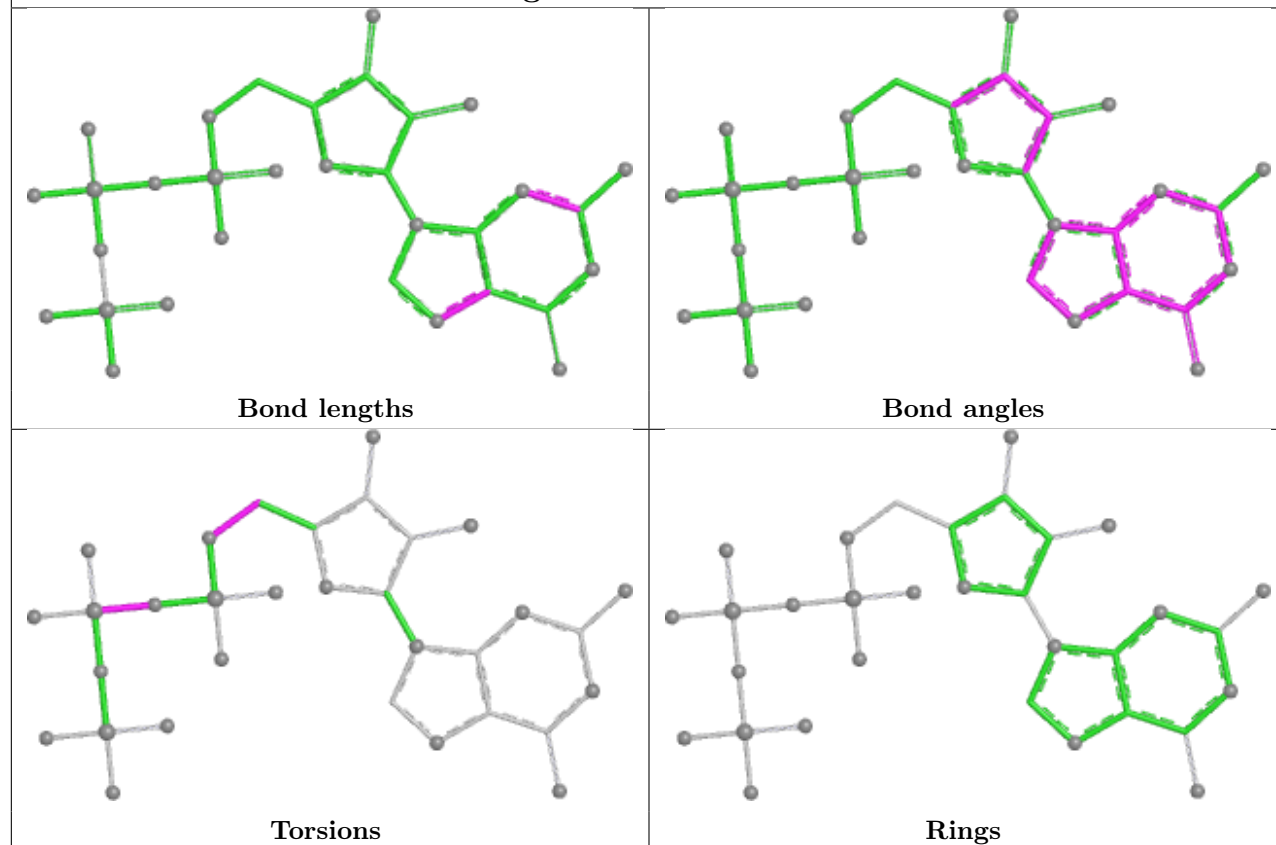
## Ligand GTP 13A 500



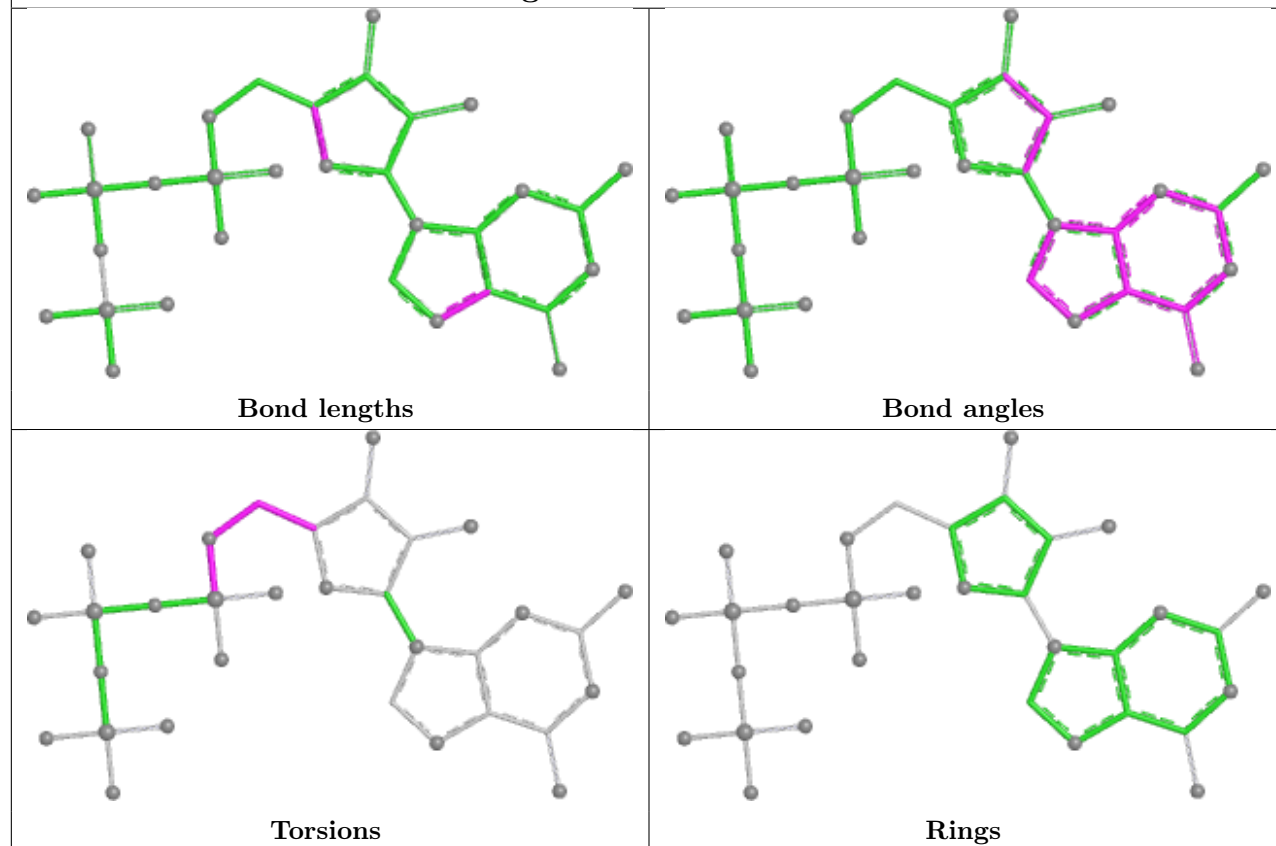
## Ligand GDP 5D 600

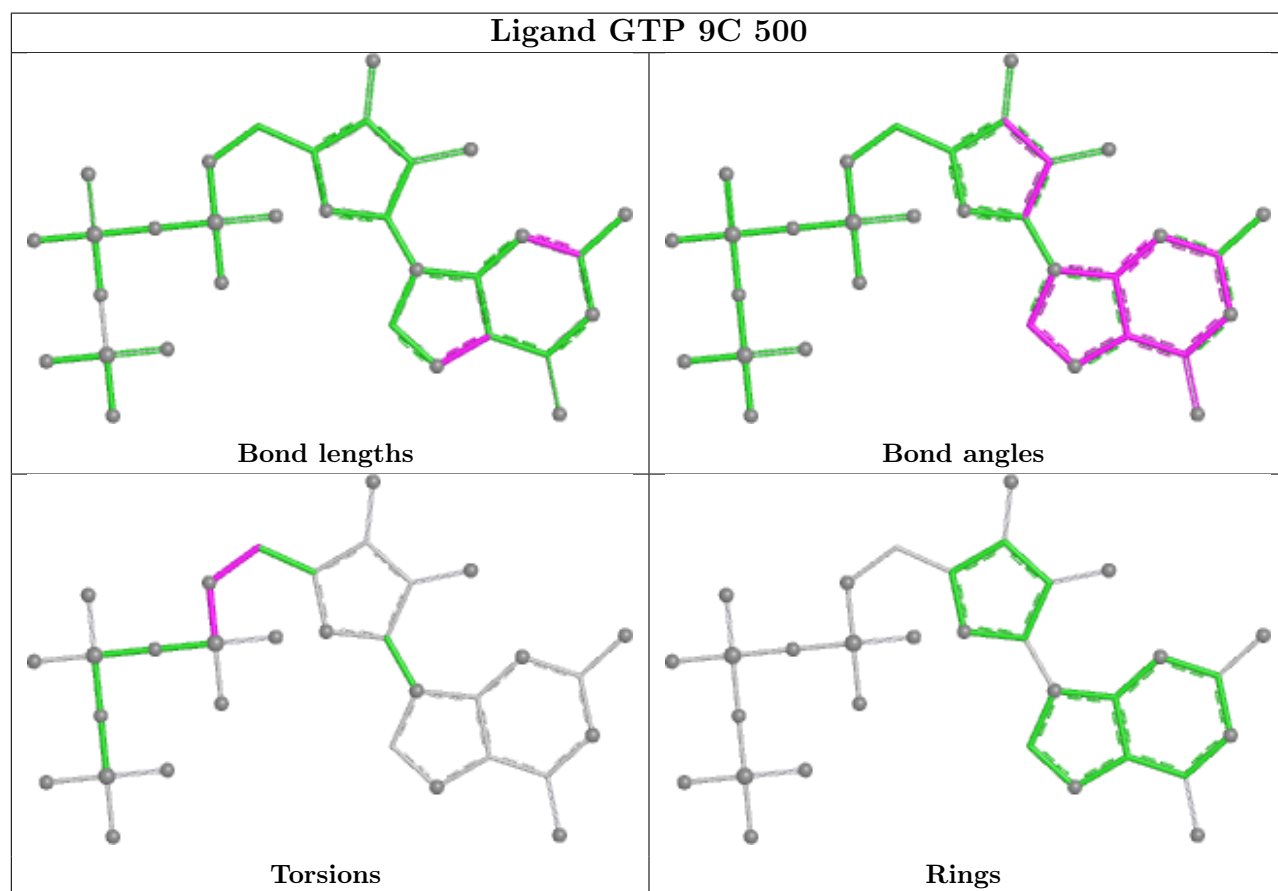
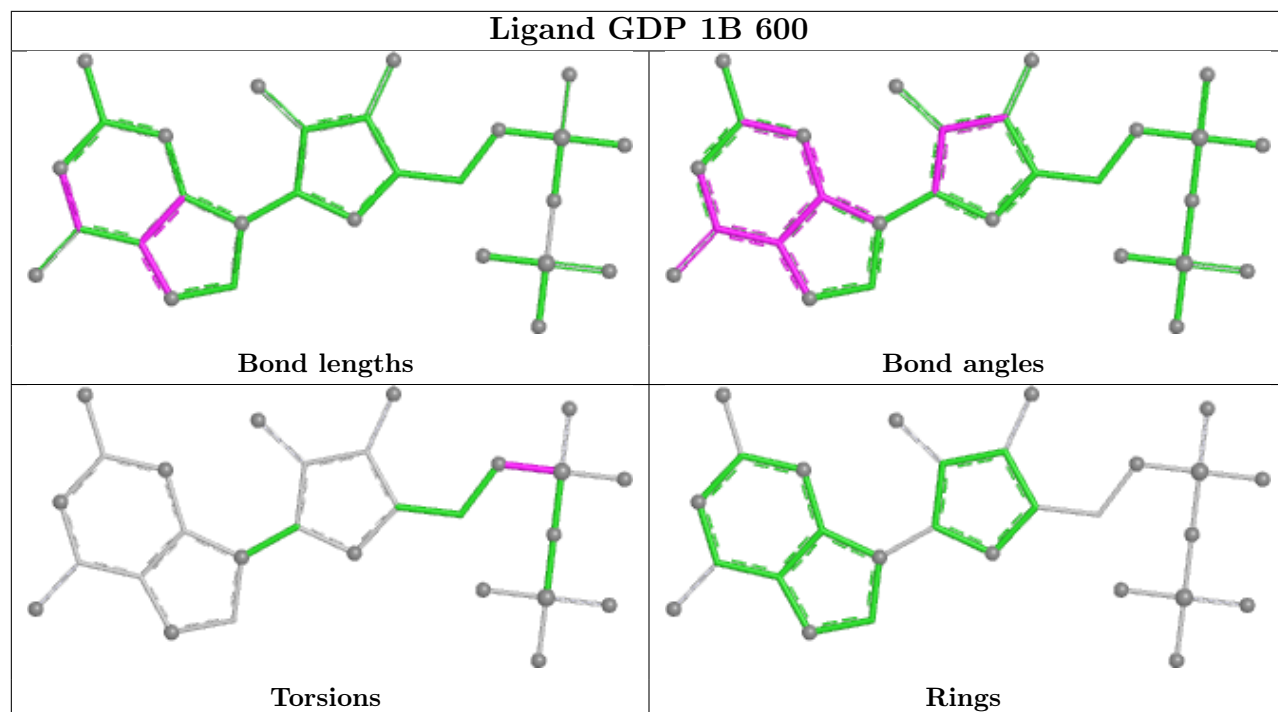


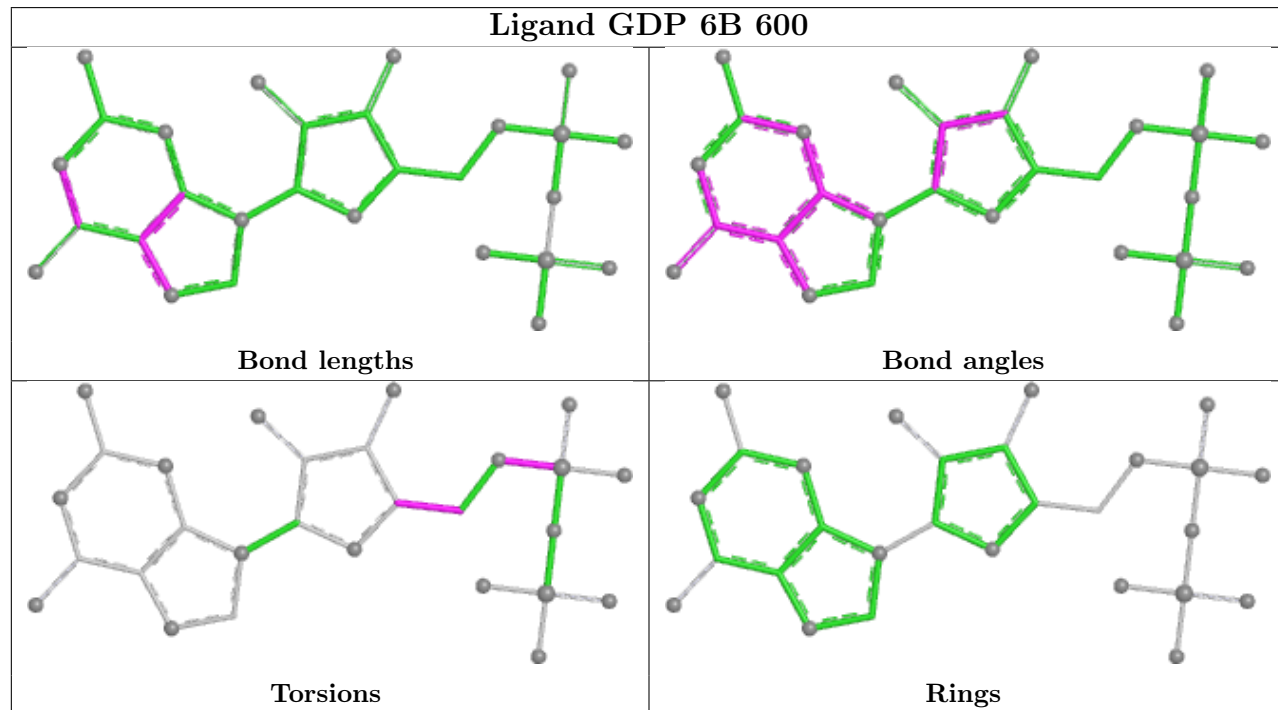
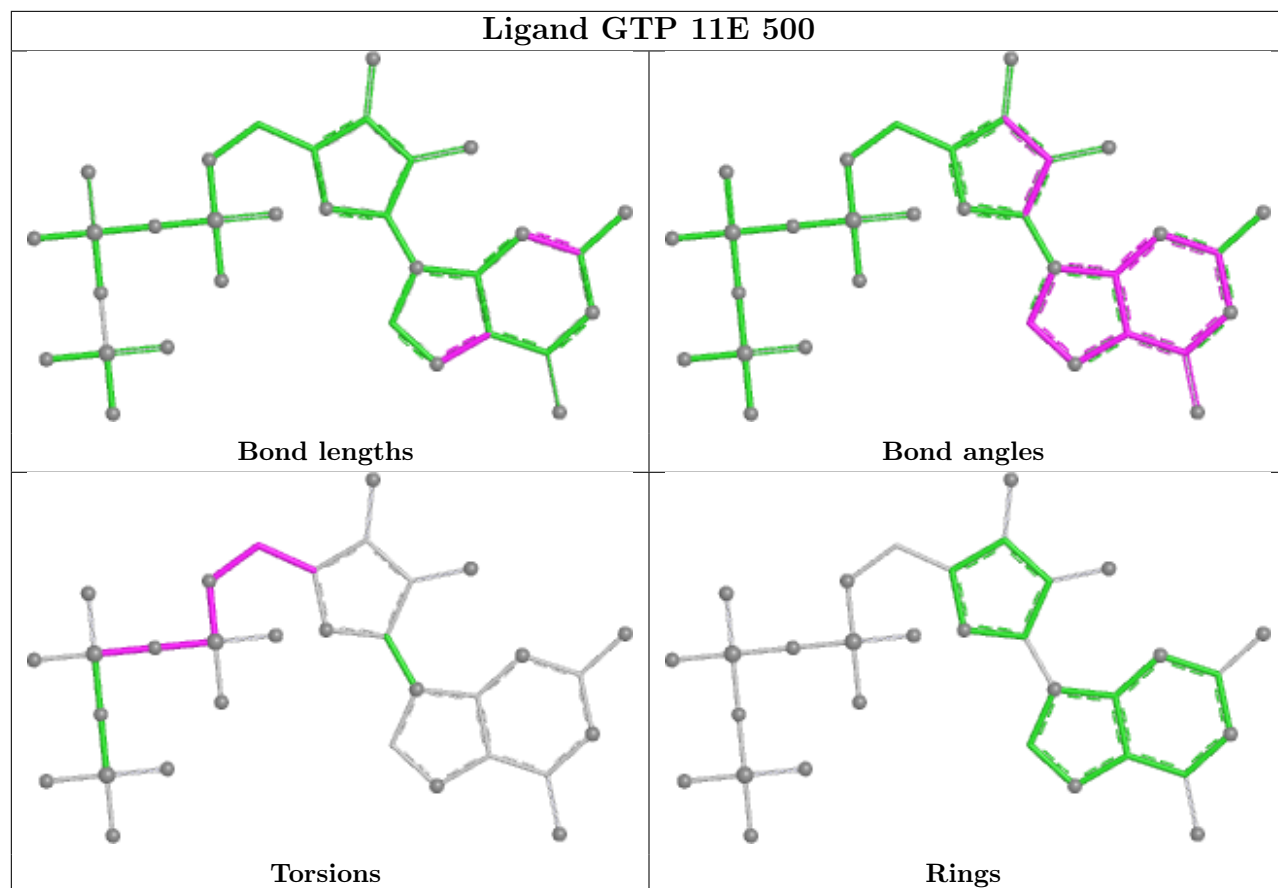
## Ligand GTP 9E 500

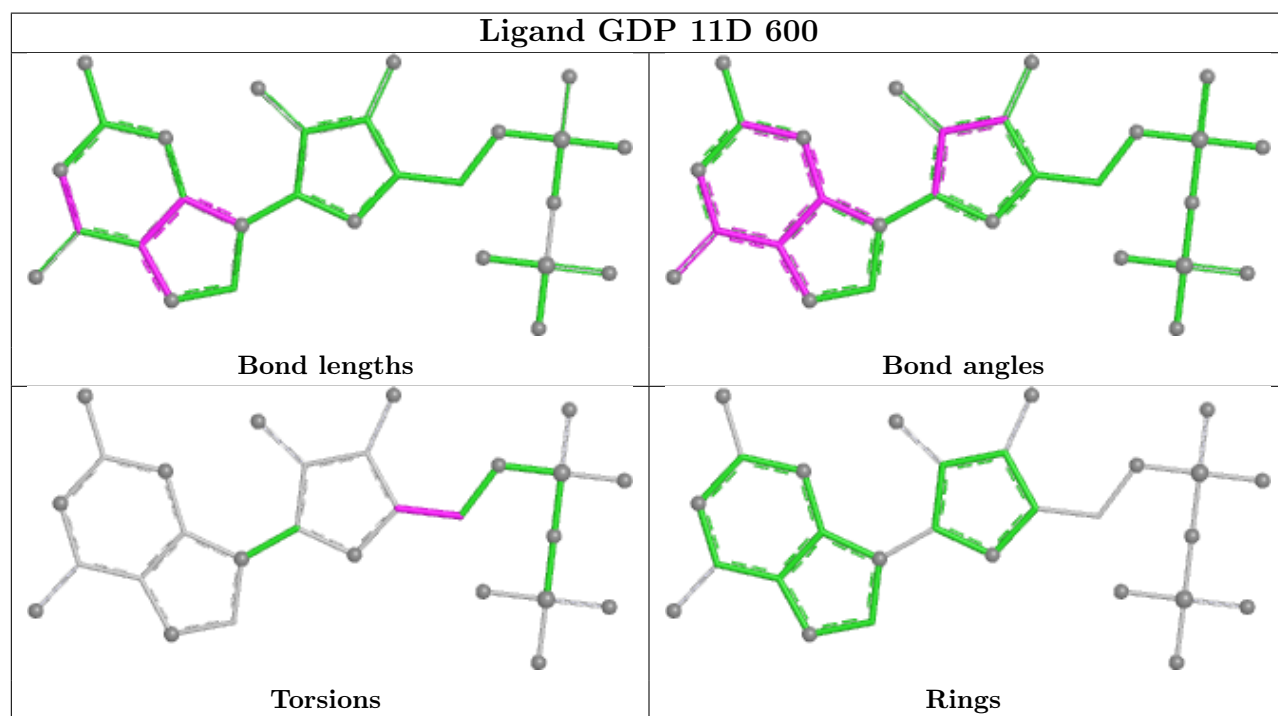
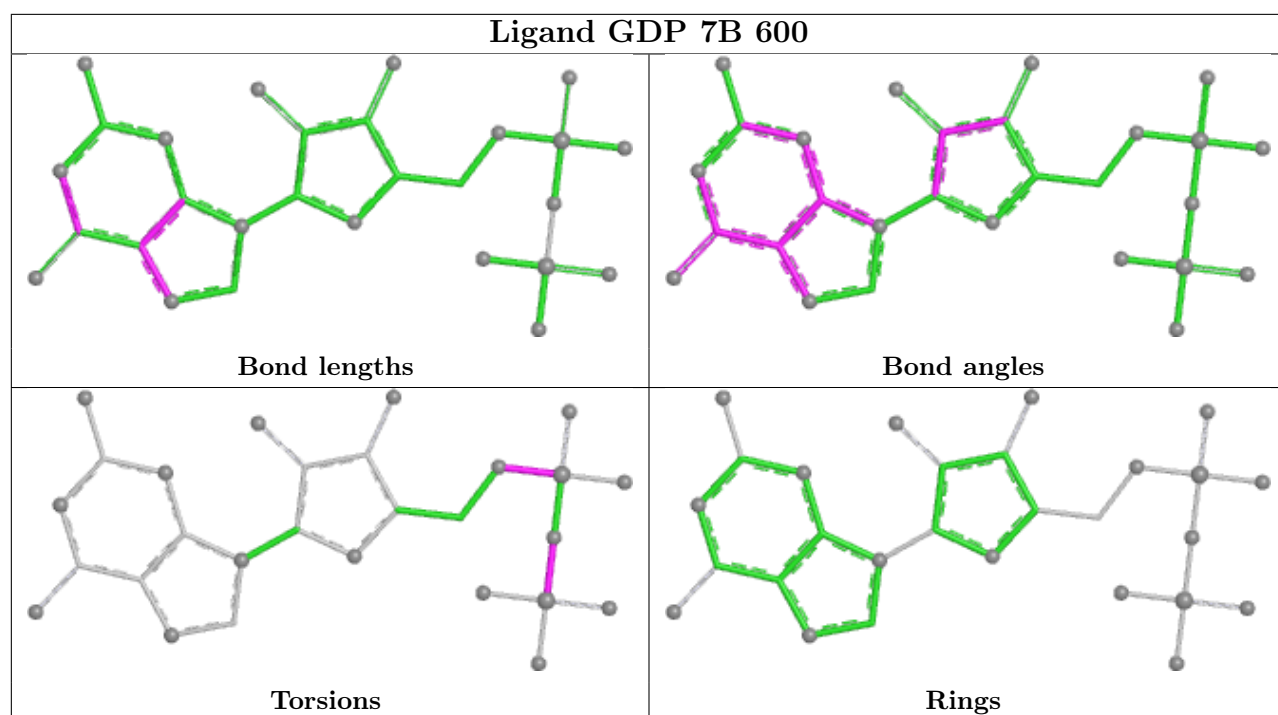


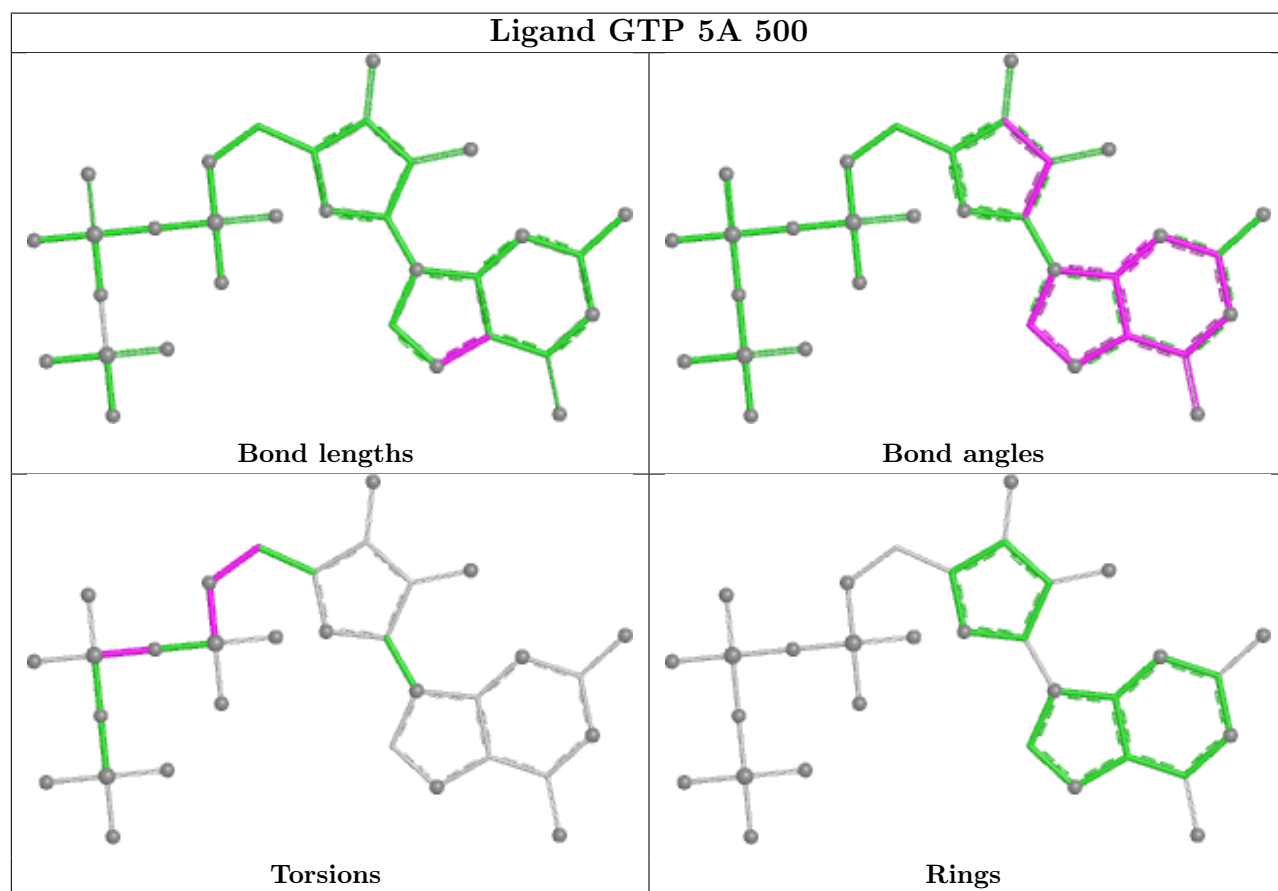
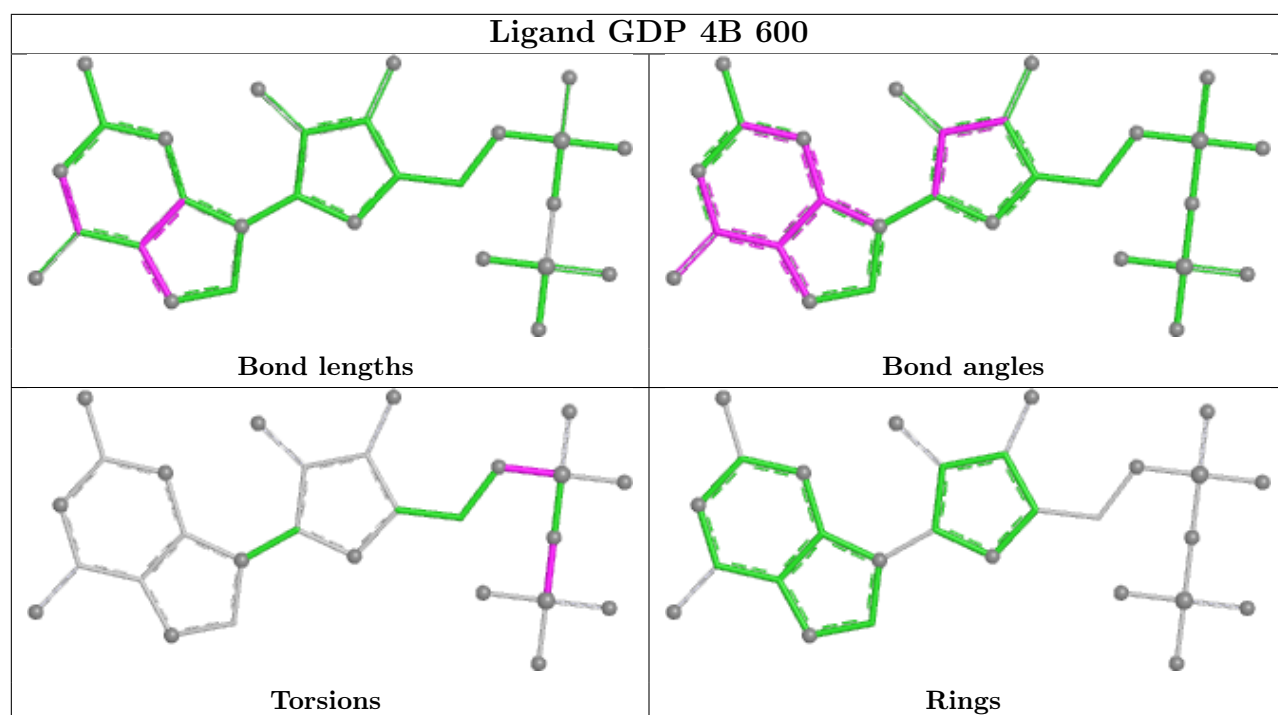
## Ligand GTP 8C 500

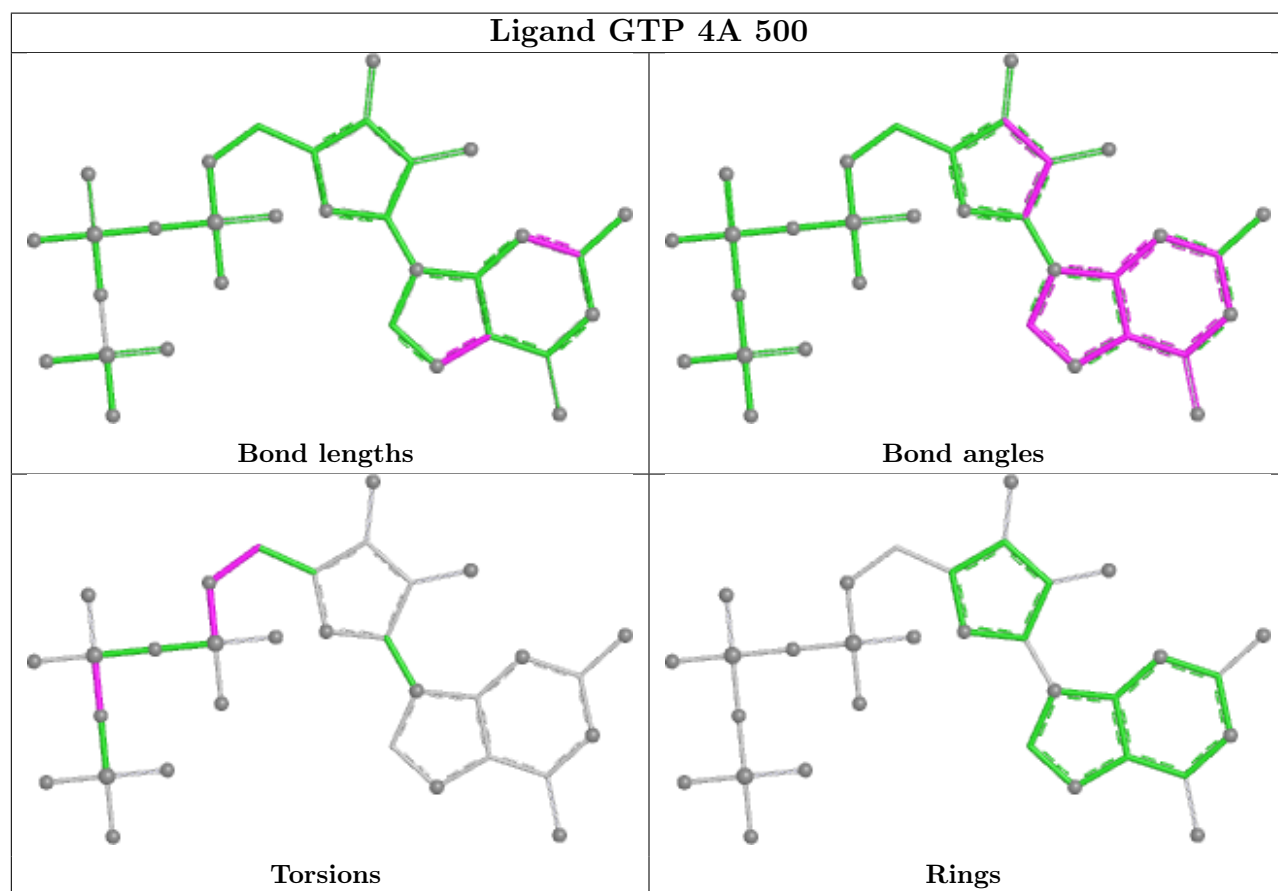
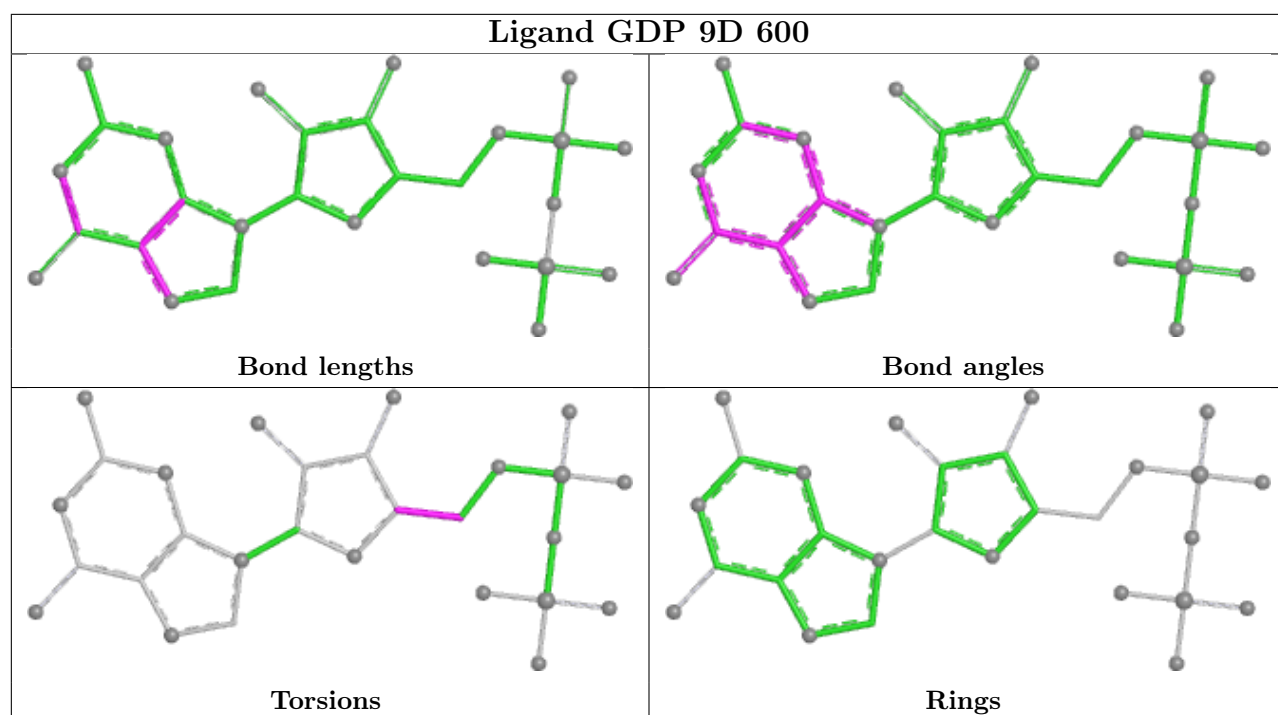


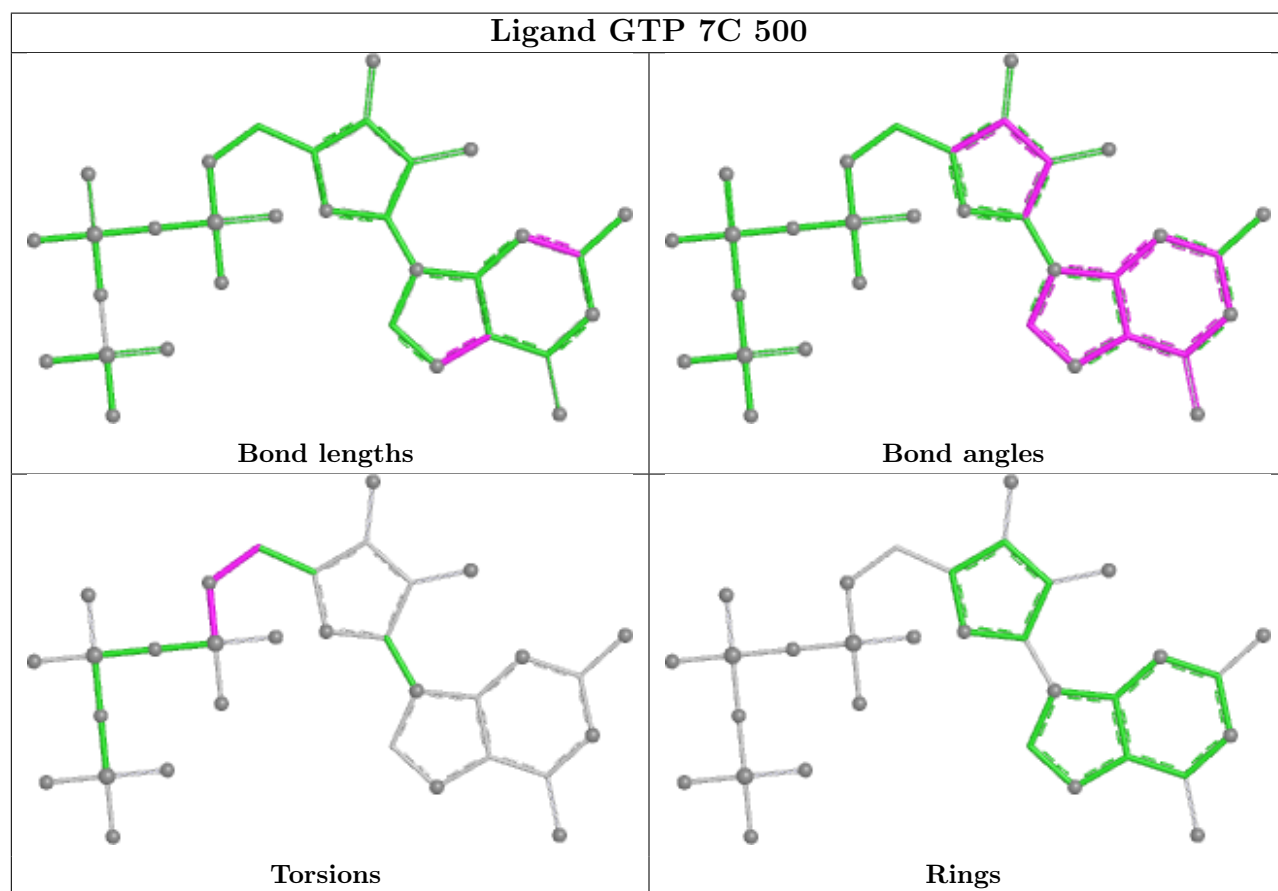
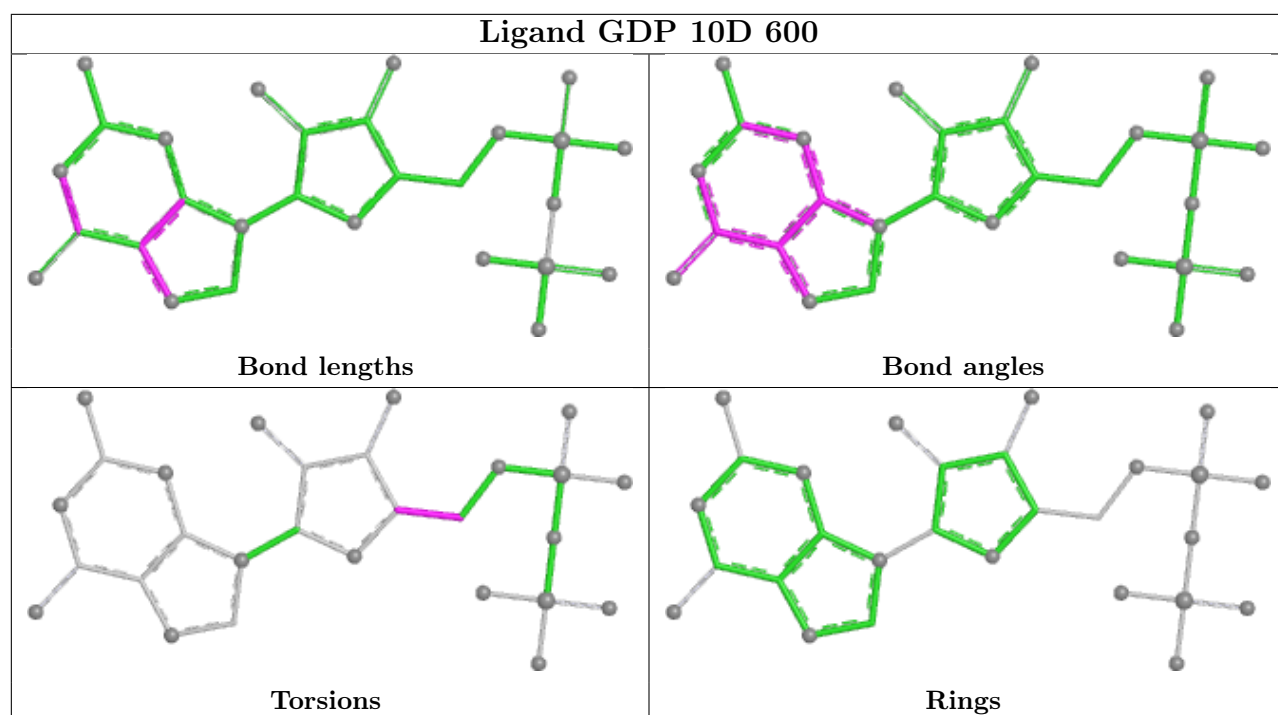


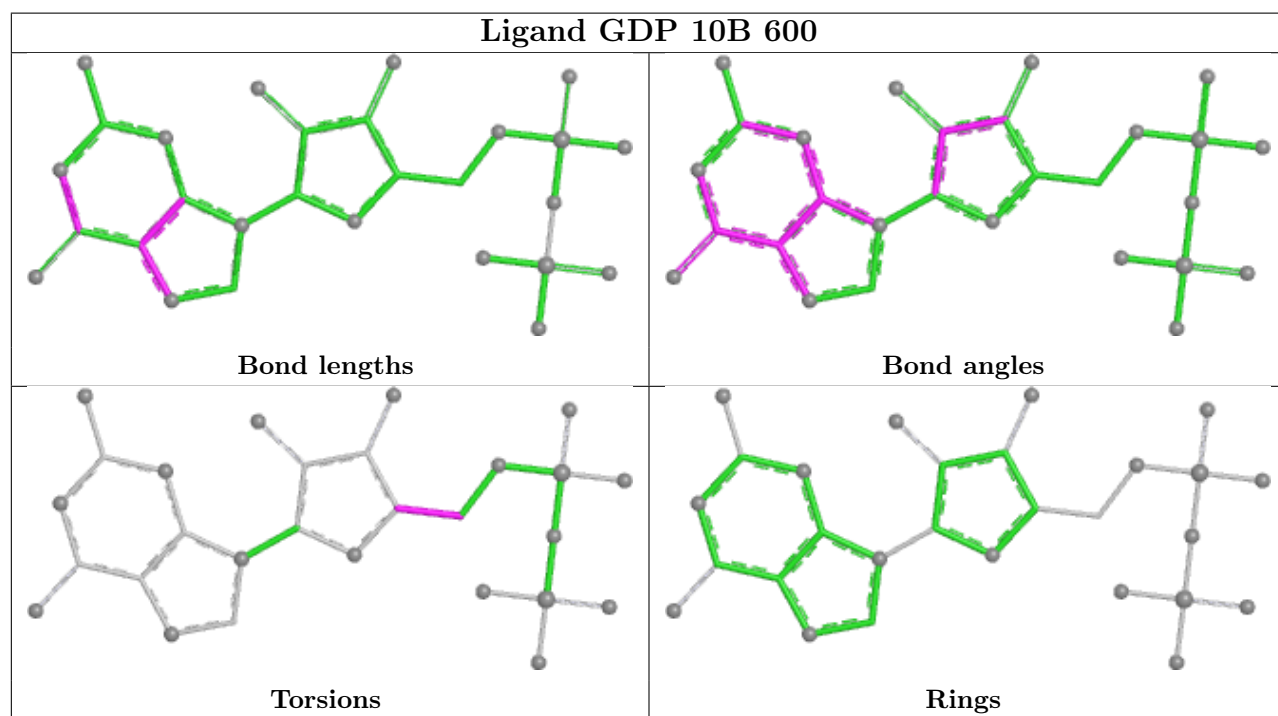
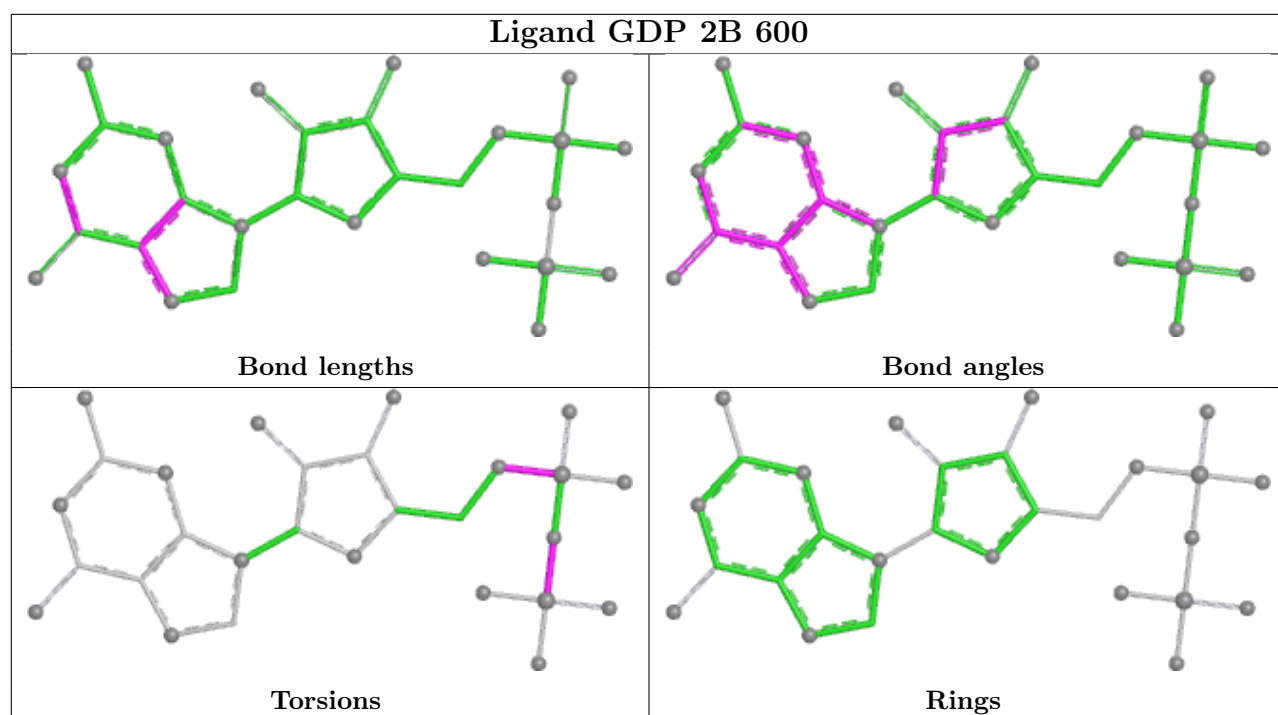




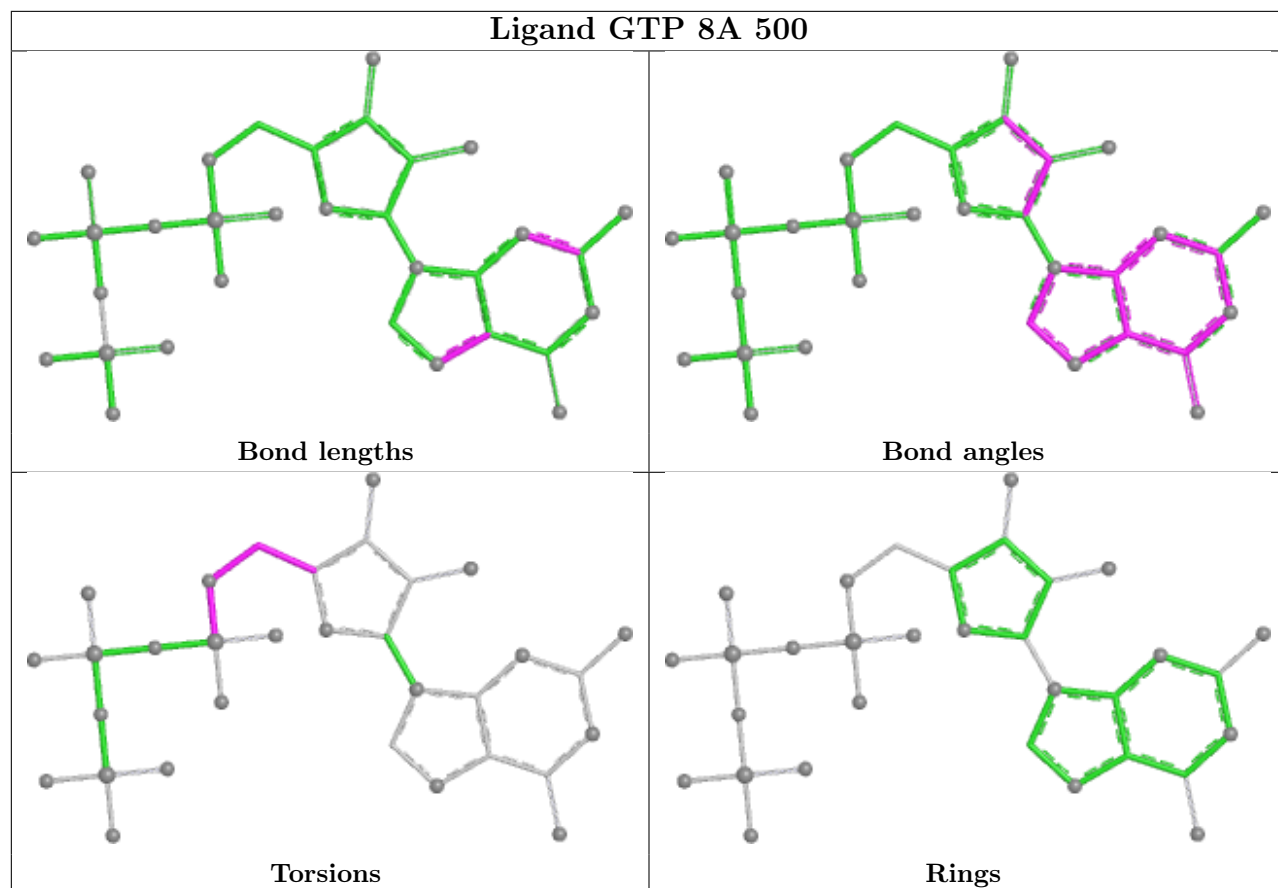




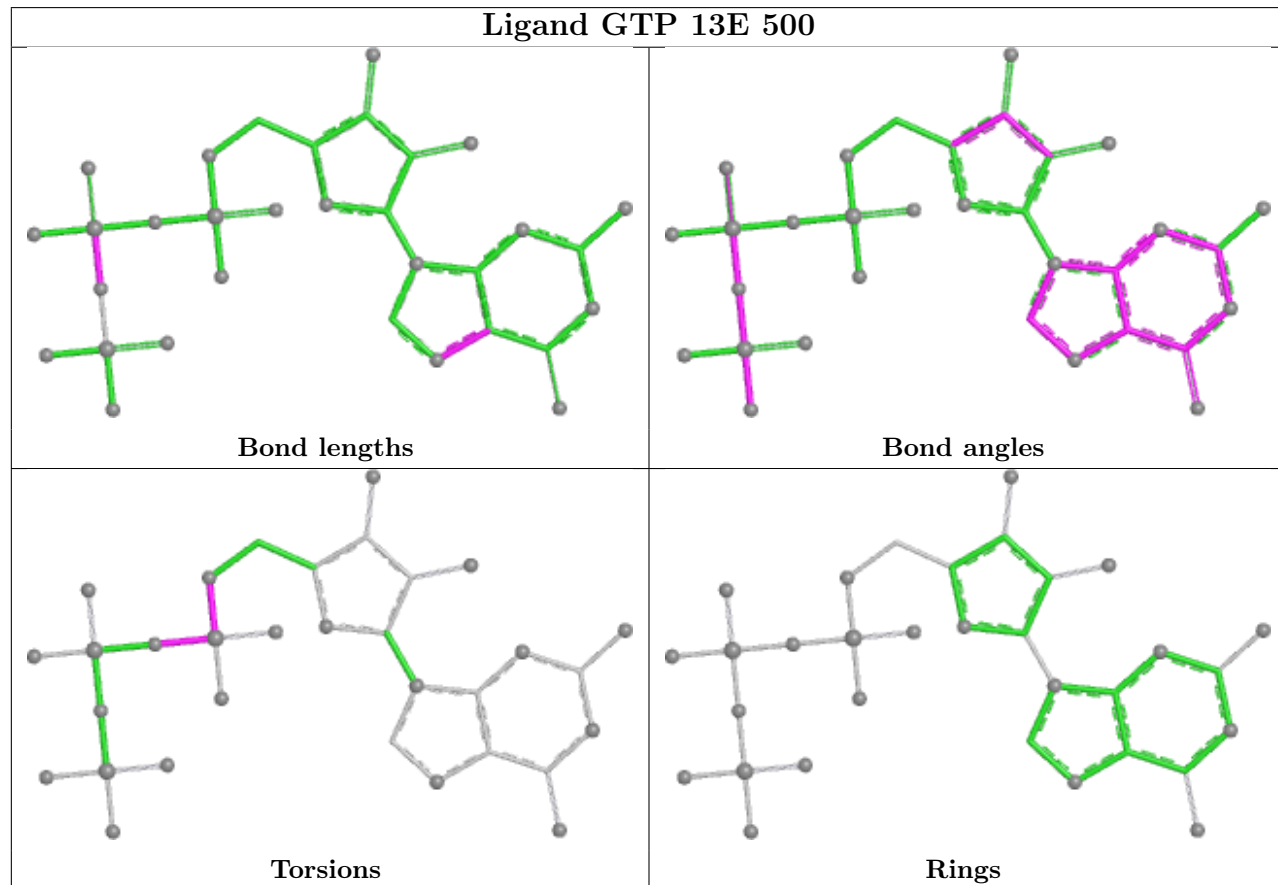


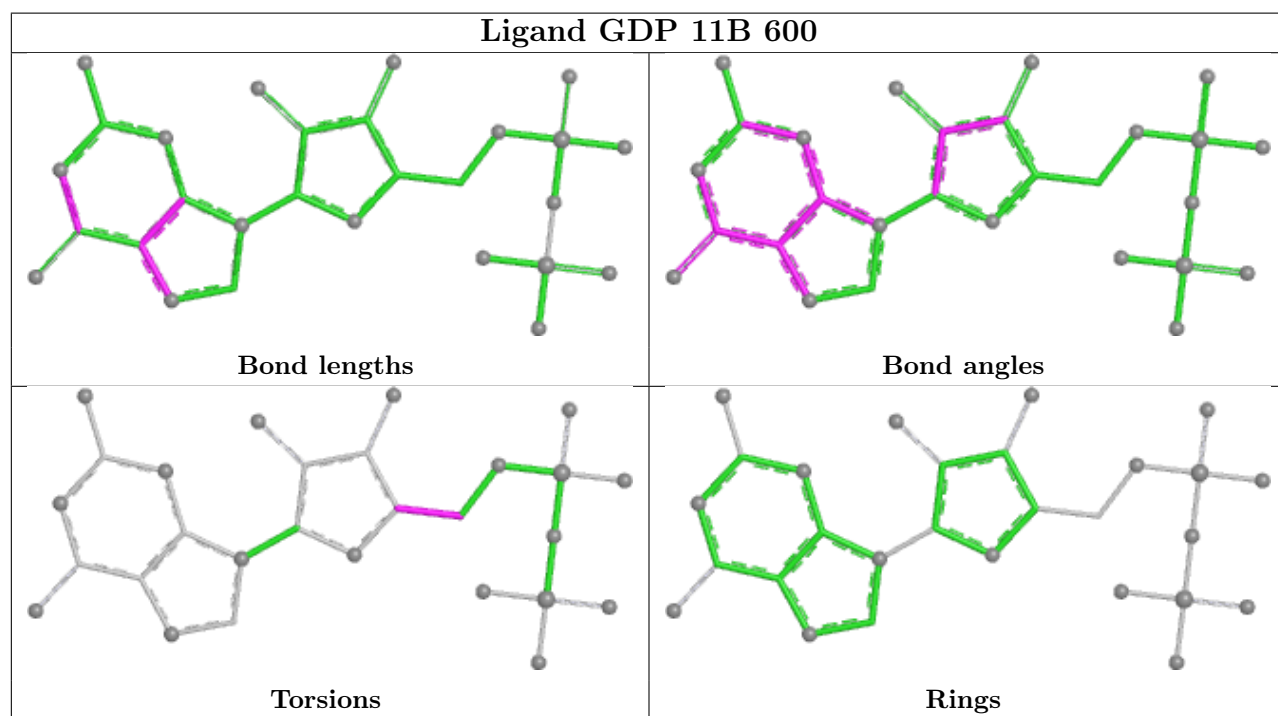
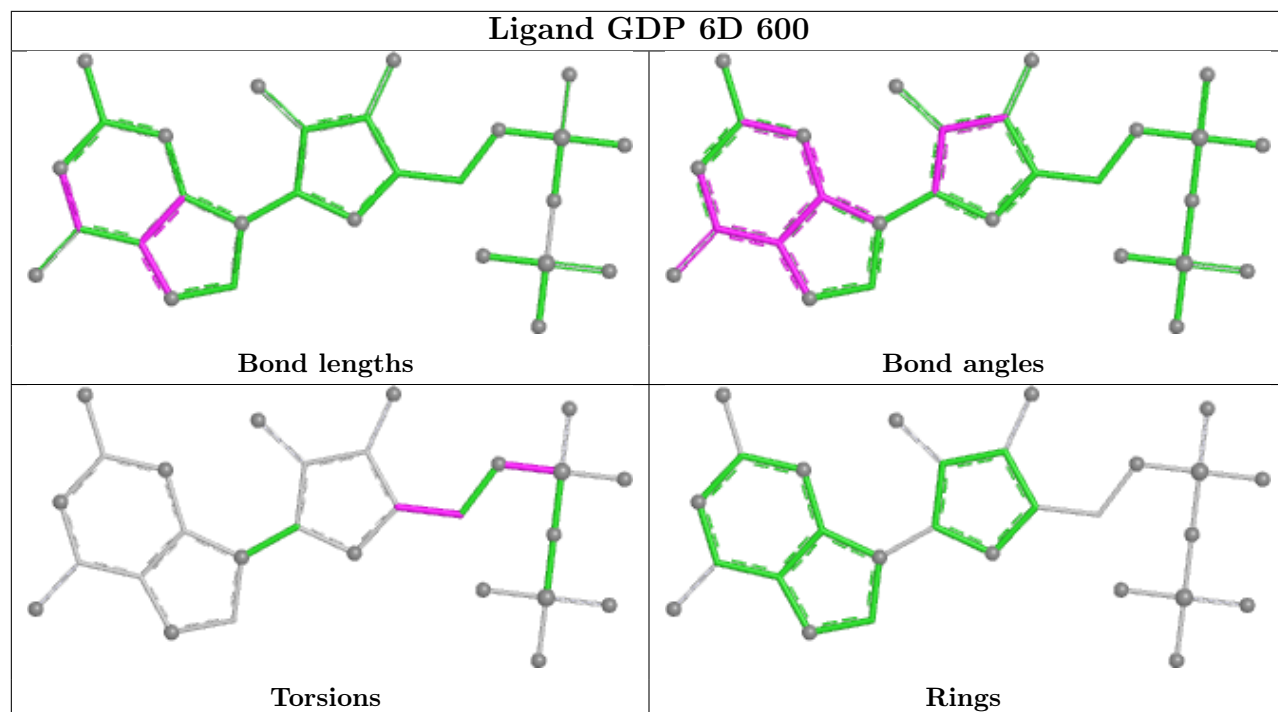


## Ligand GTP 8A 500

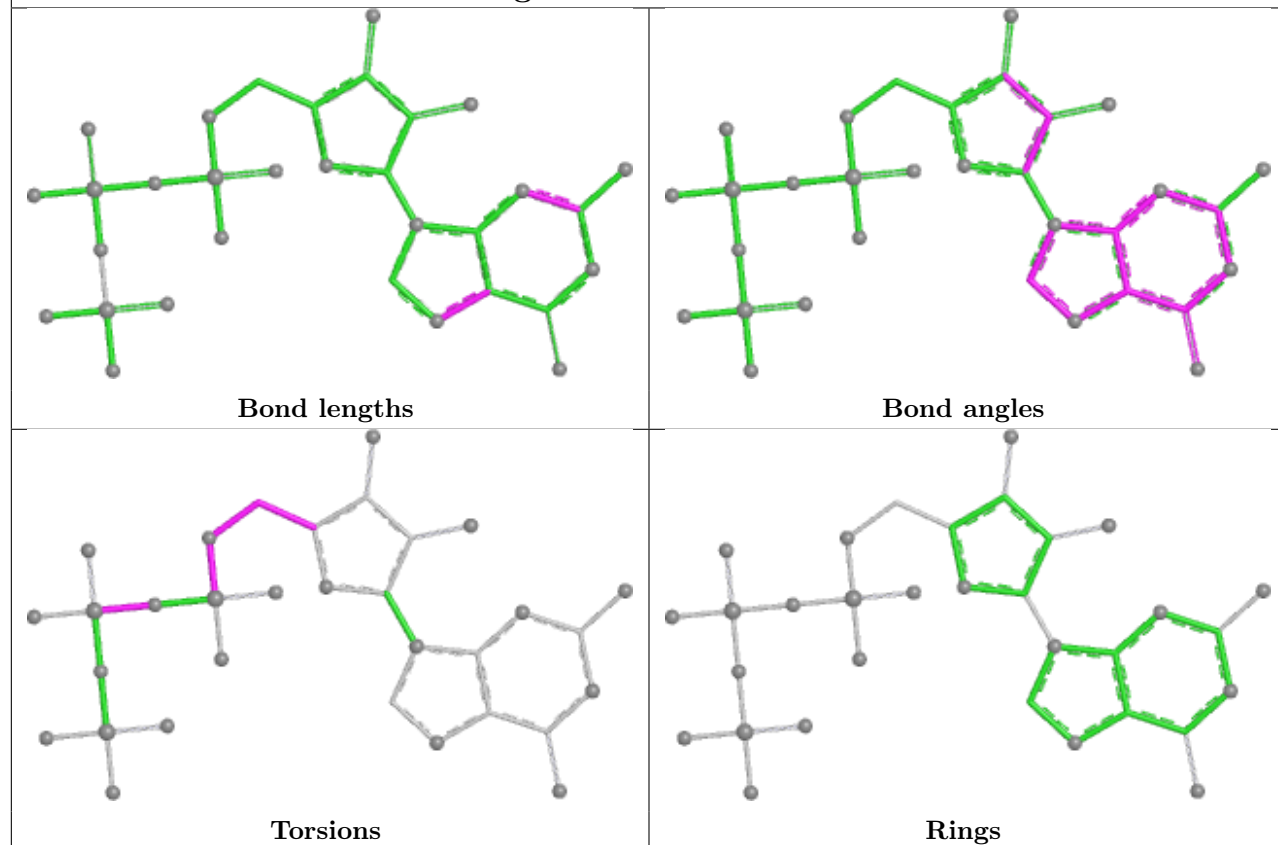


## Ligand GTP 13E 500

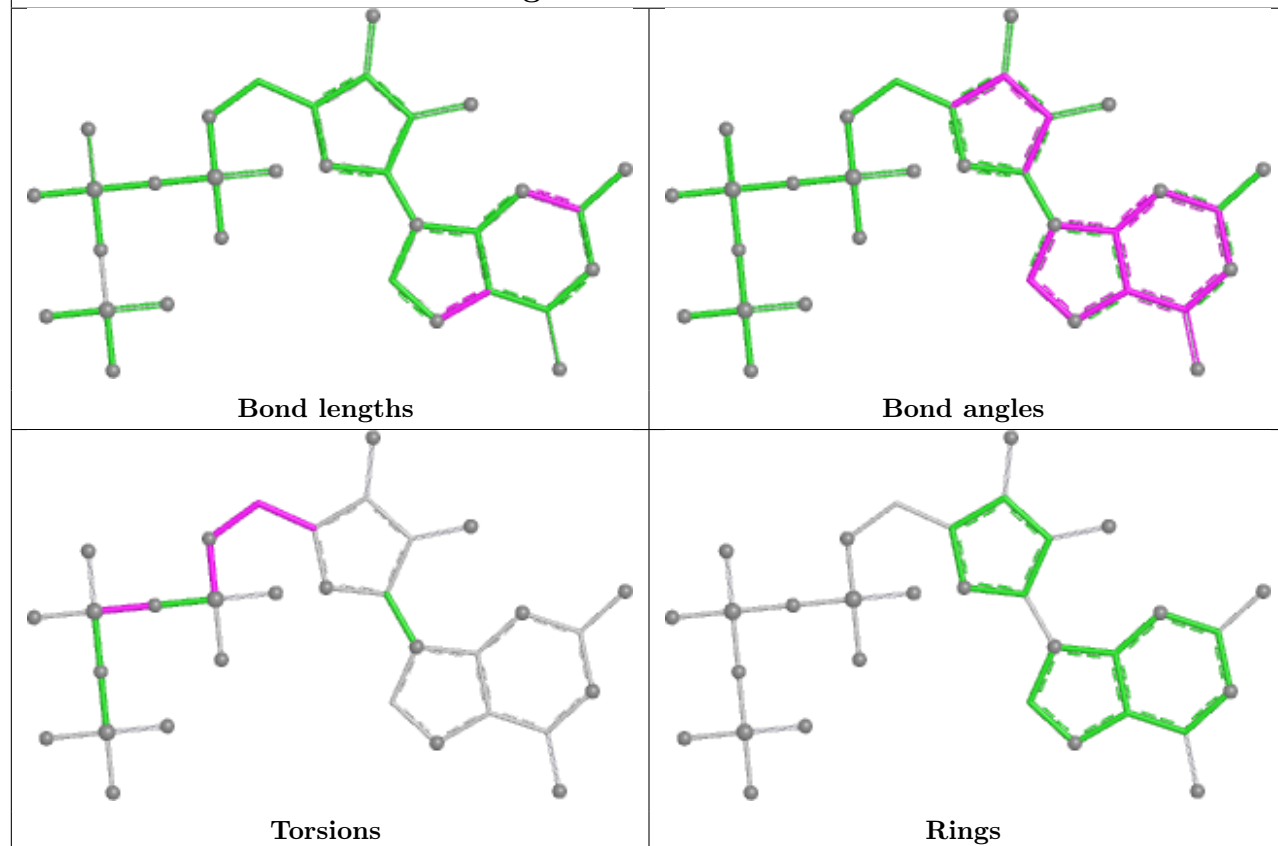


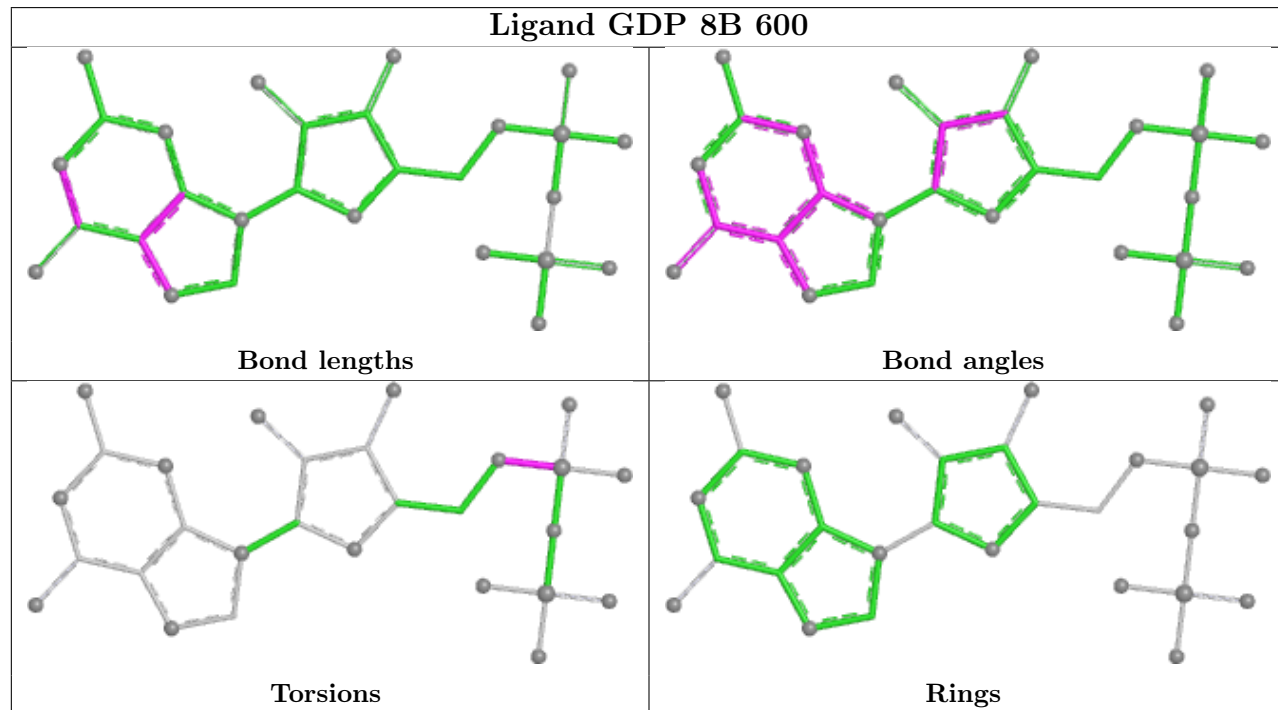
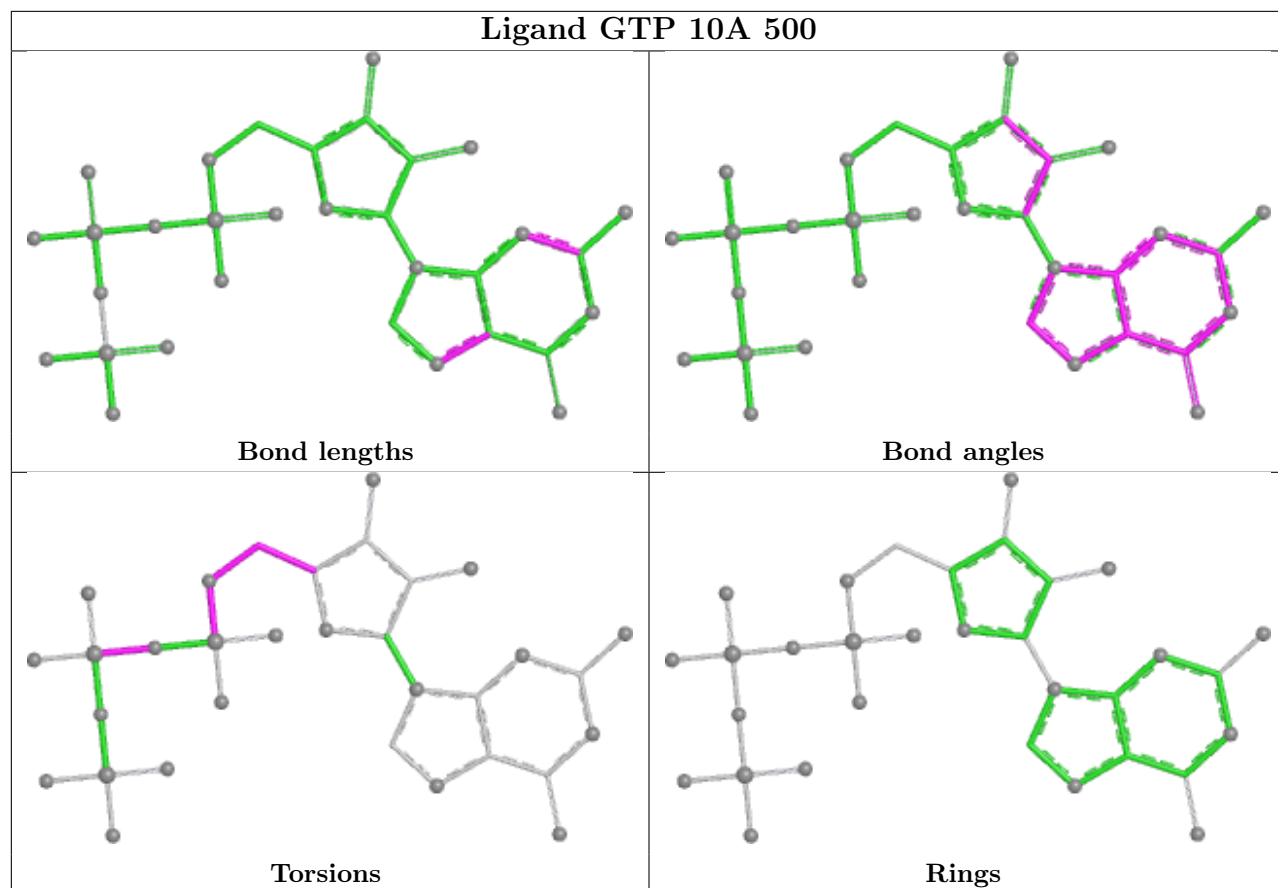


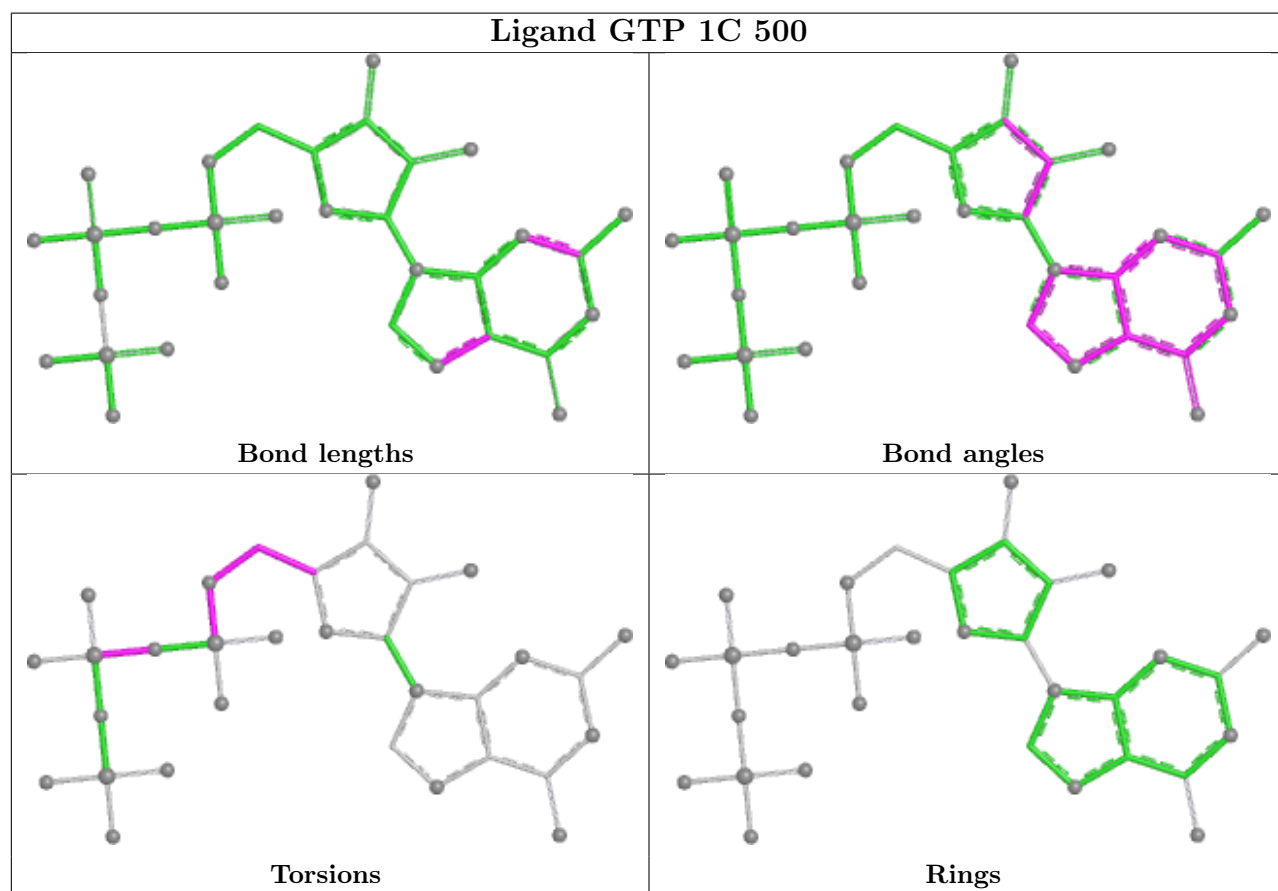
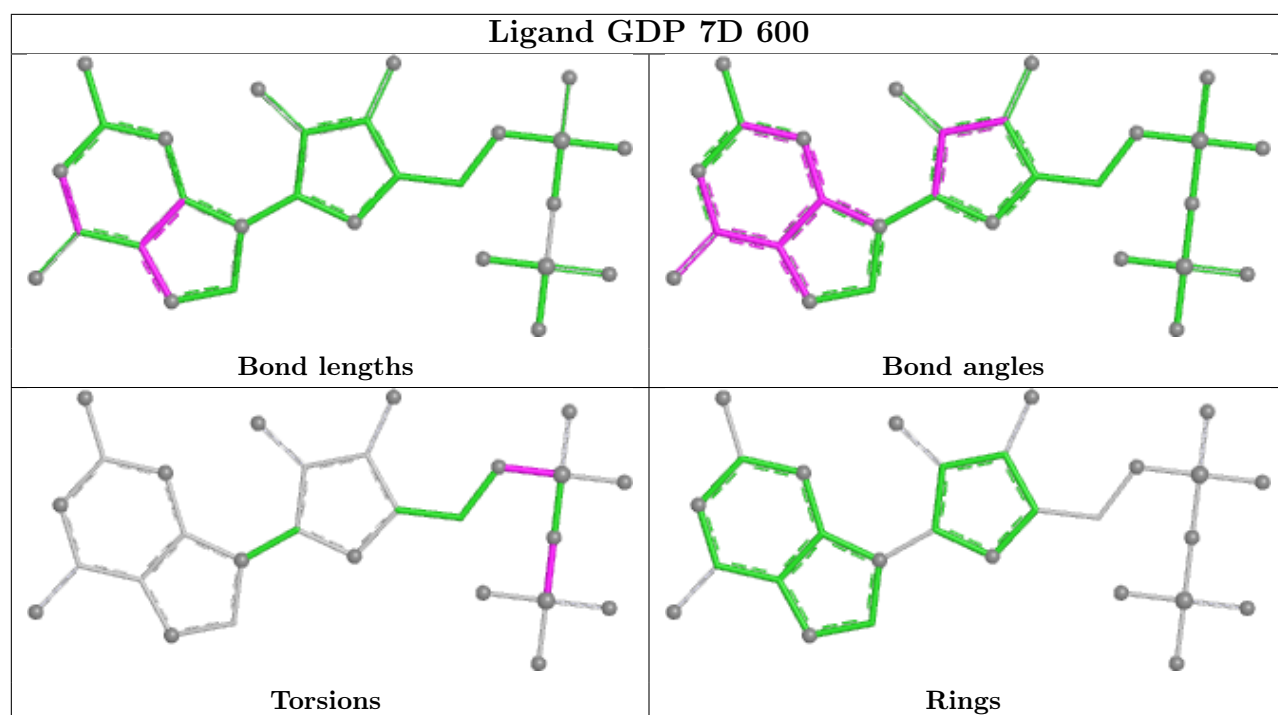
## Ligand GTP 10E 500



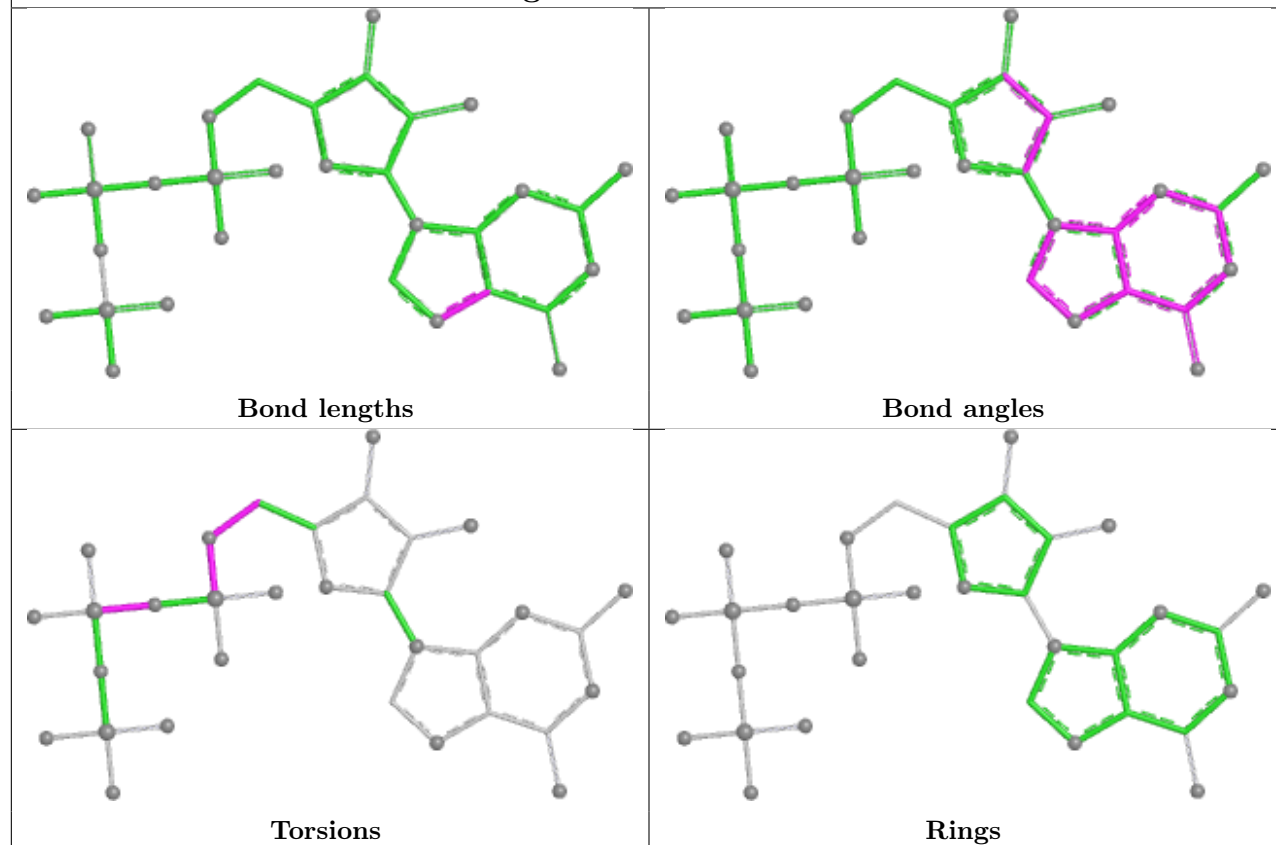
## Ligand GTP 1E 500



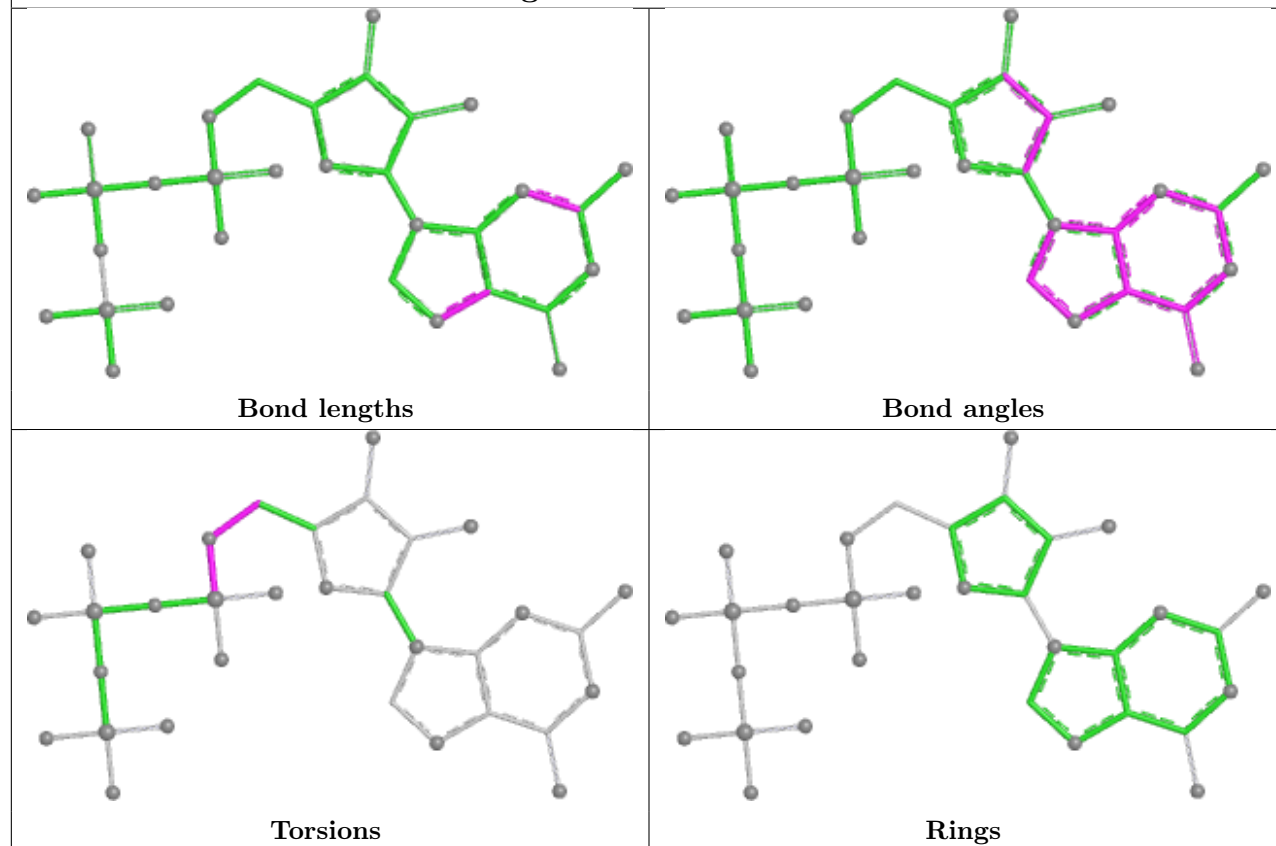




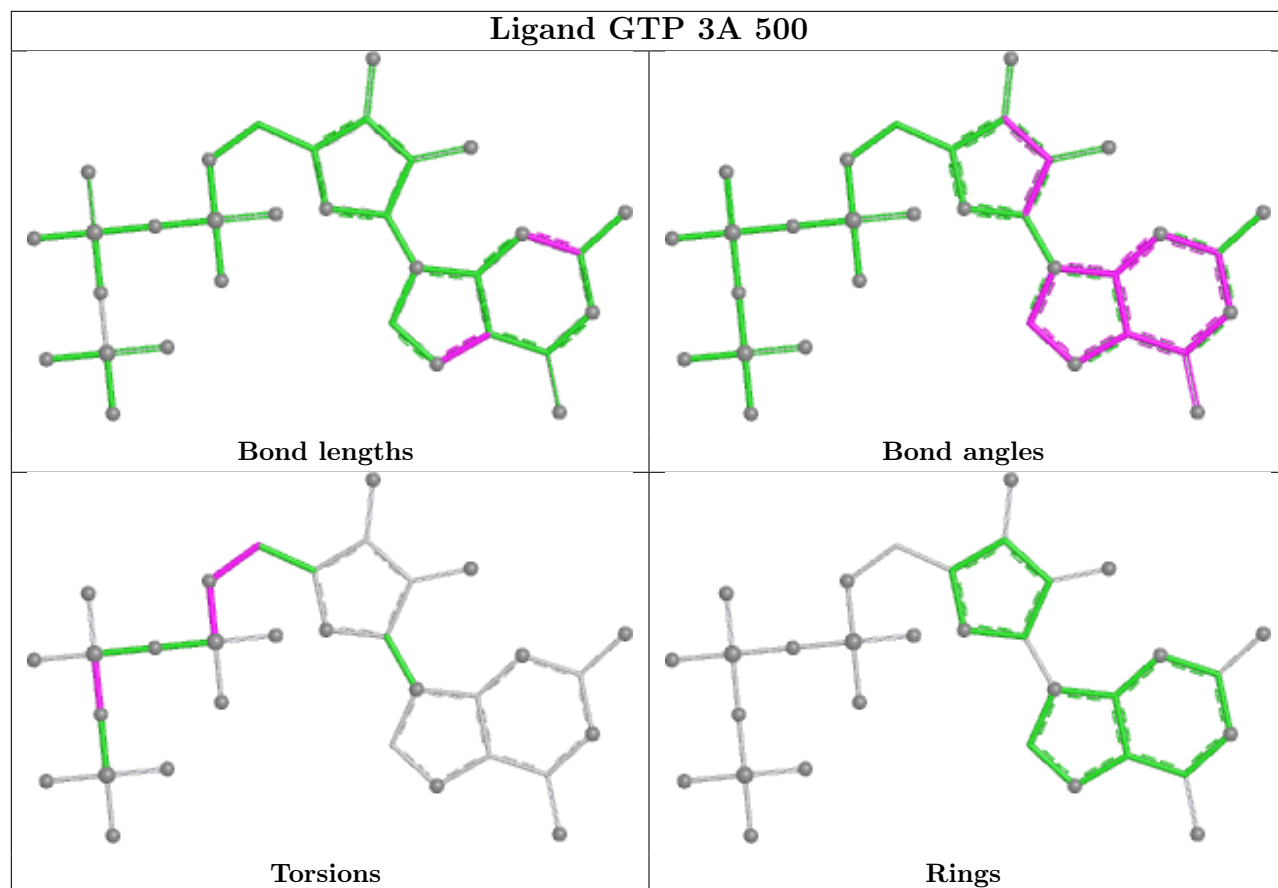
## Ligand GTP 5E 500



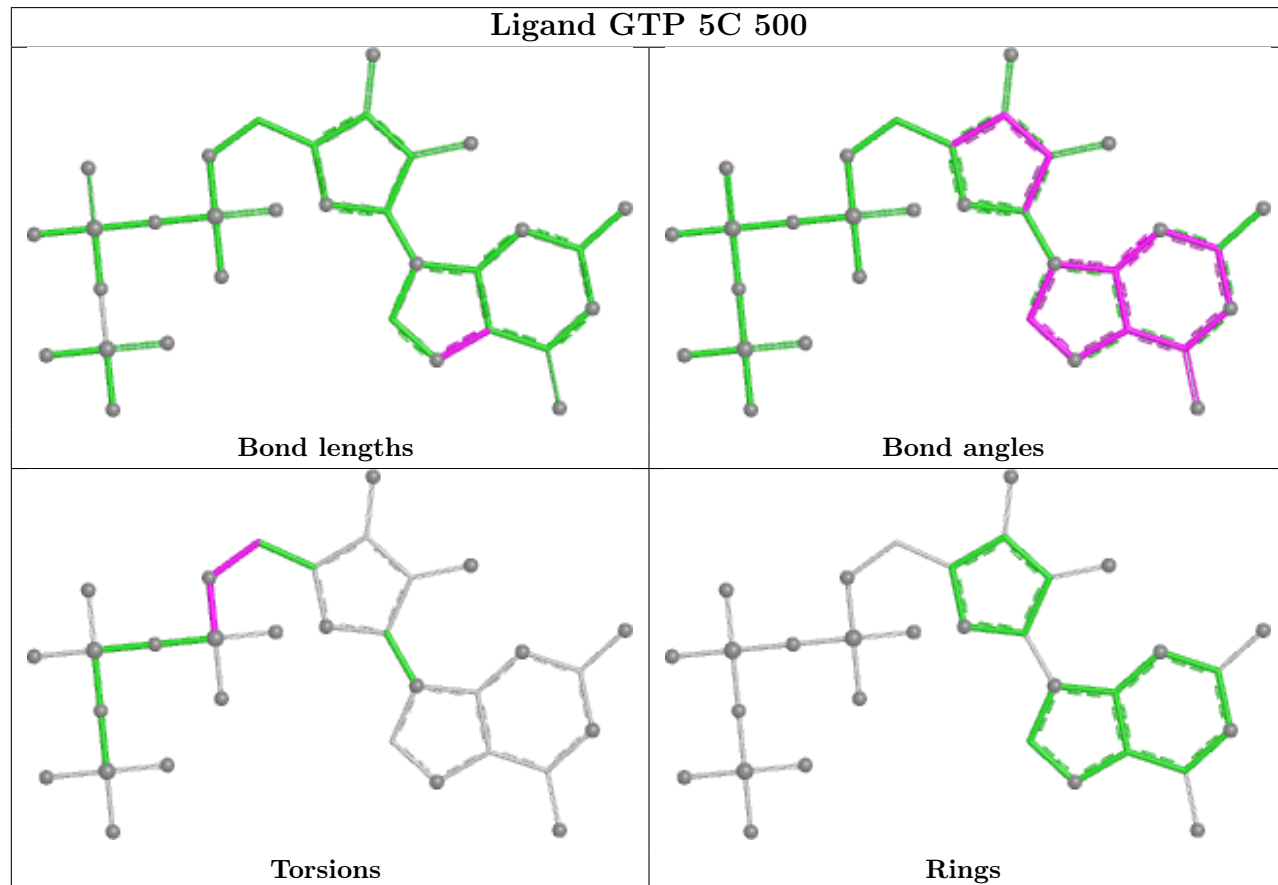
## Ligand GTP 7A 500

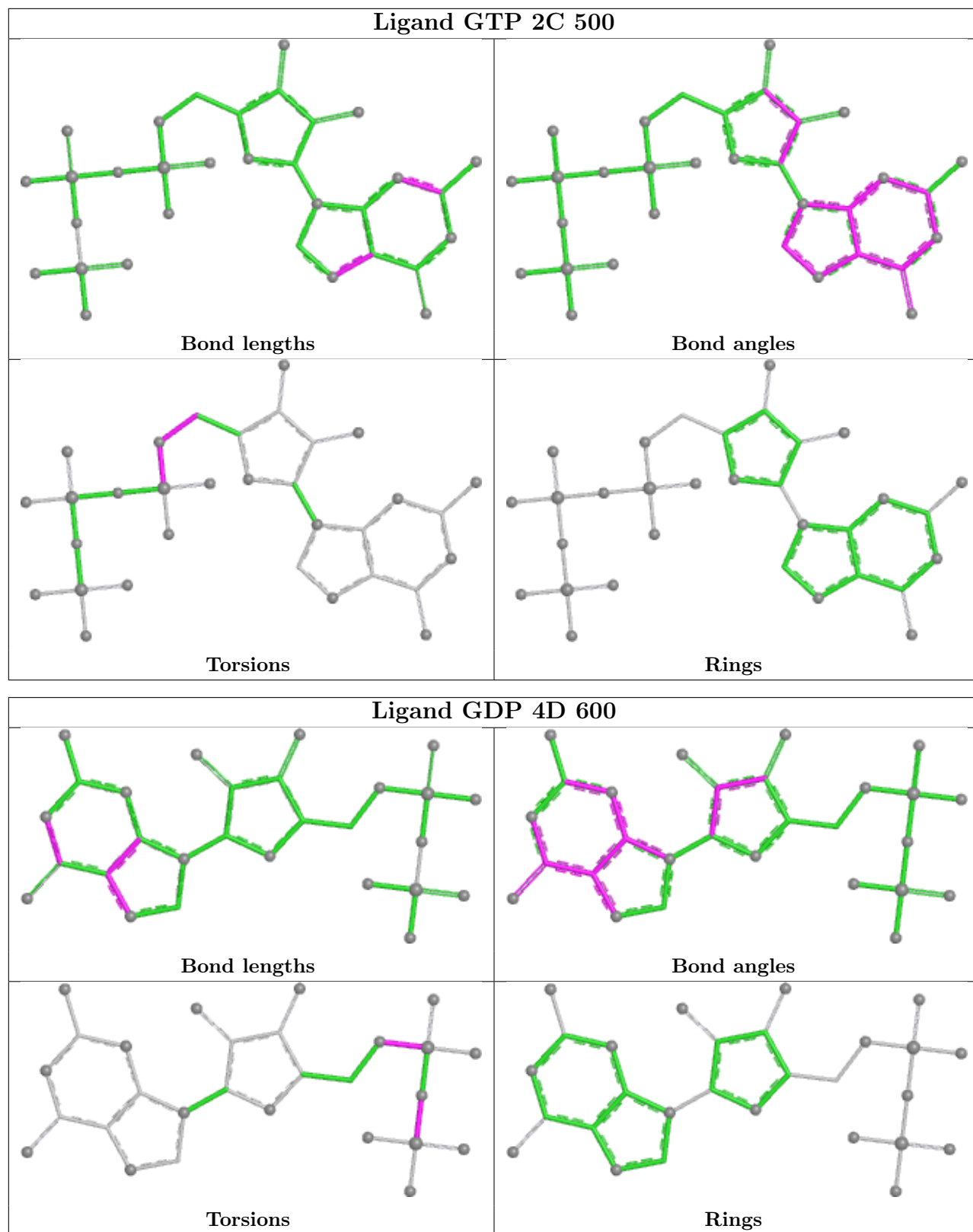


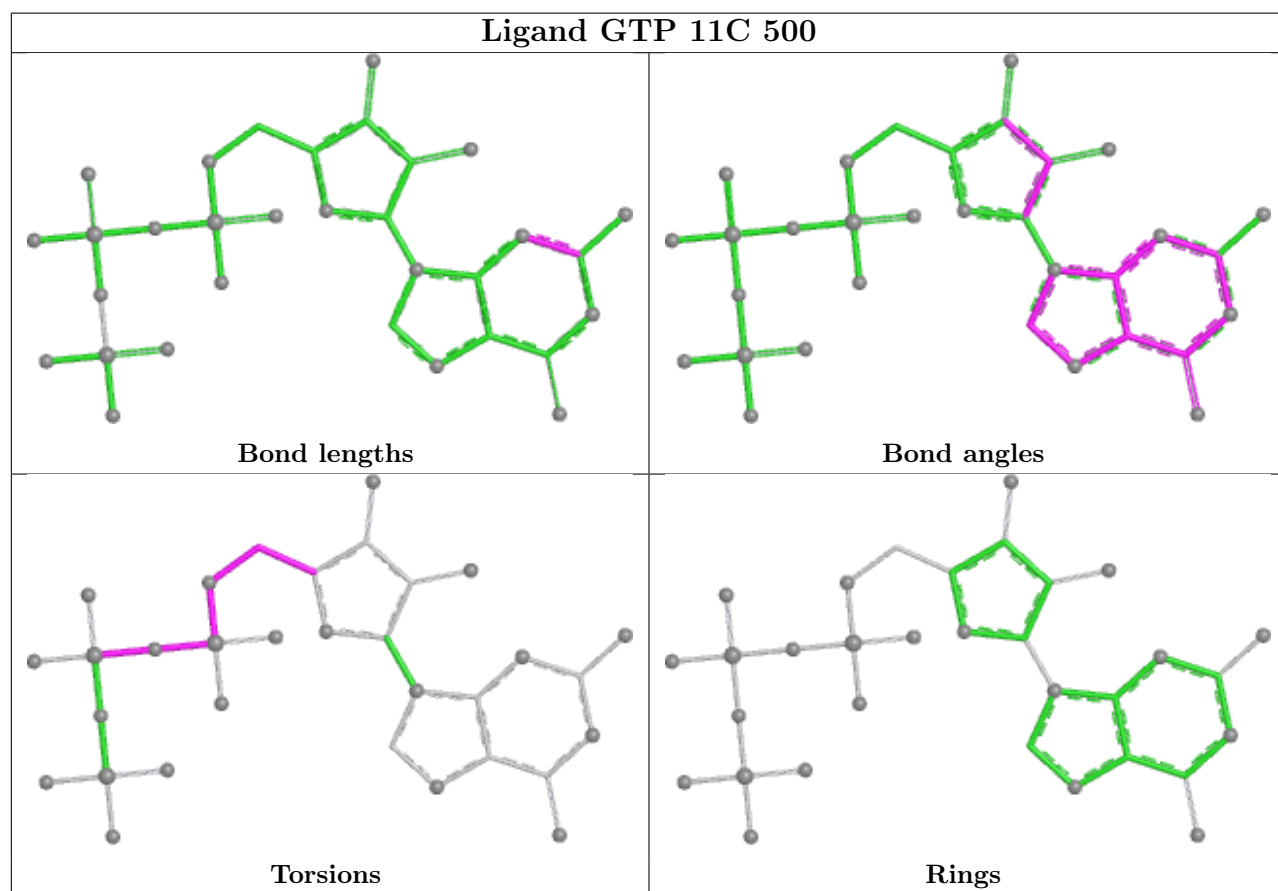
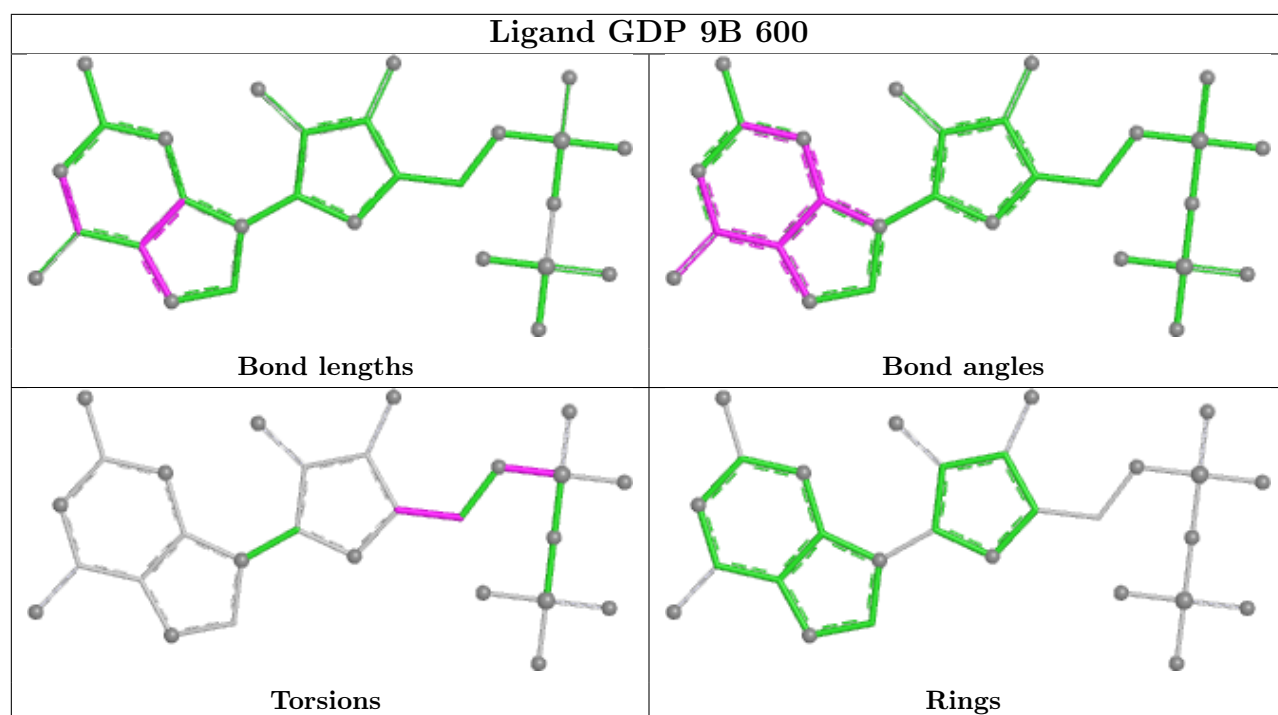
## Ligand GTP 3A 500



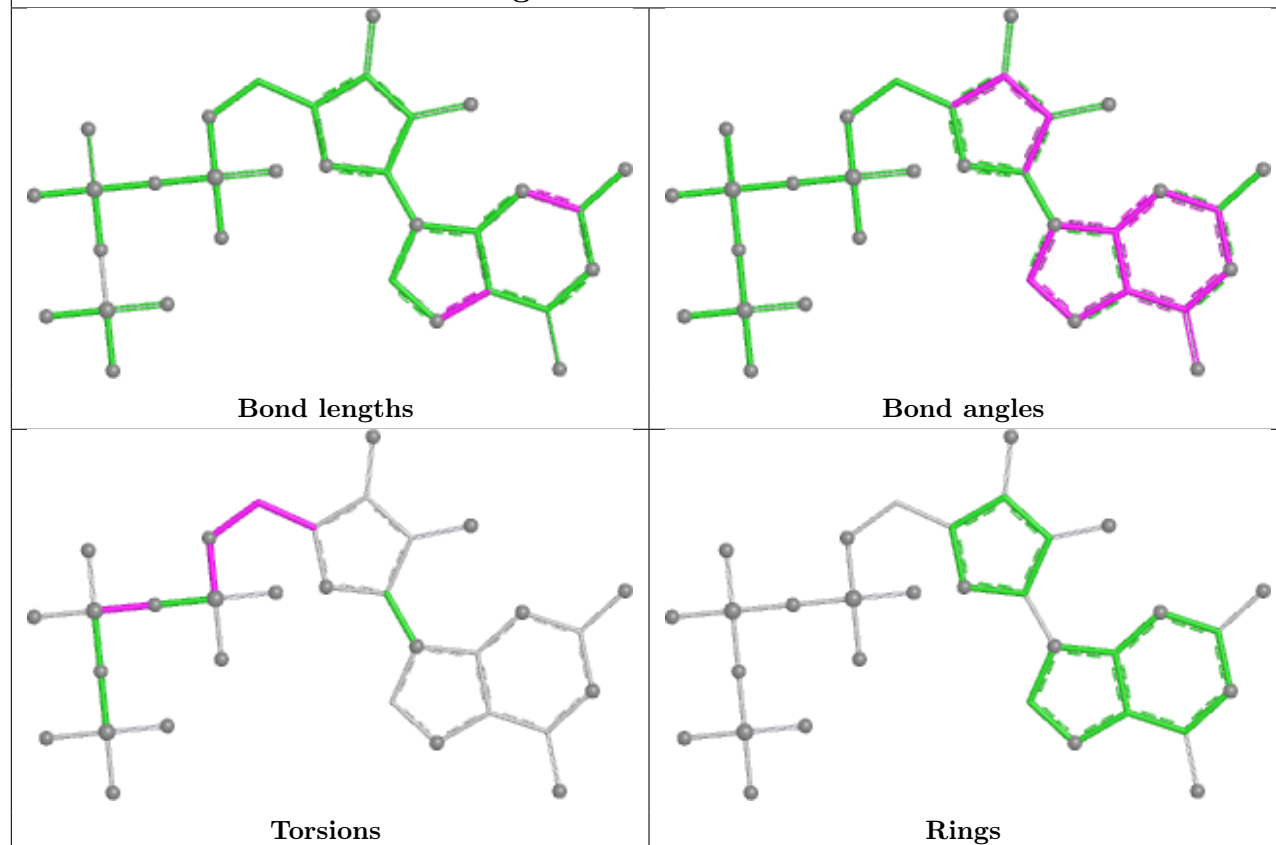
## Ligand GTP 5C 500



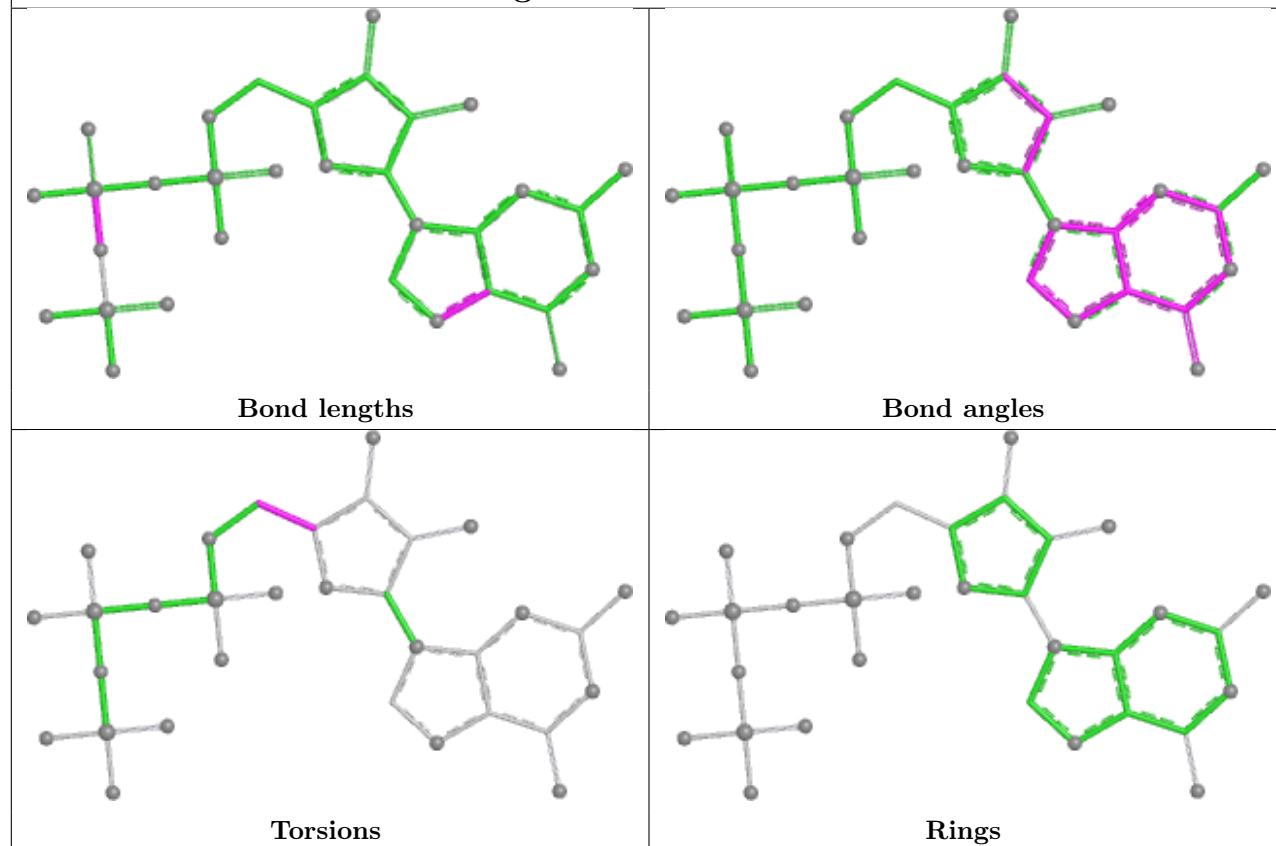


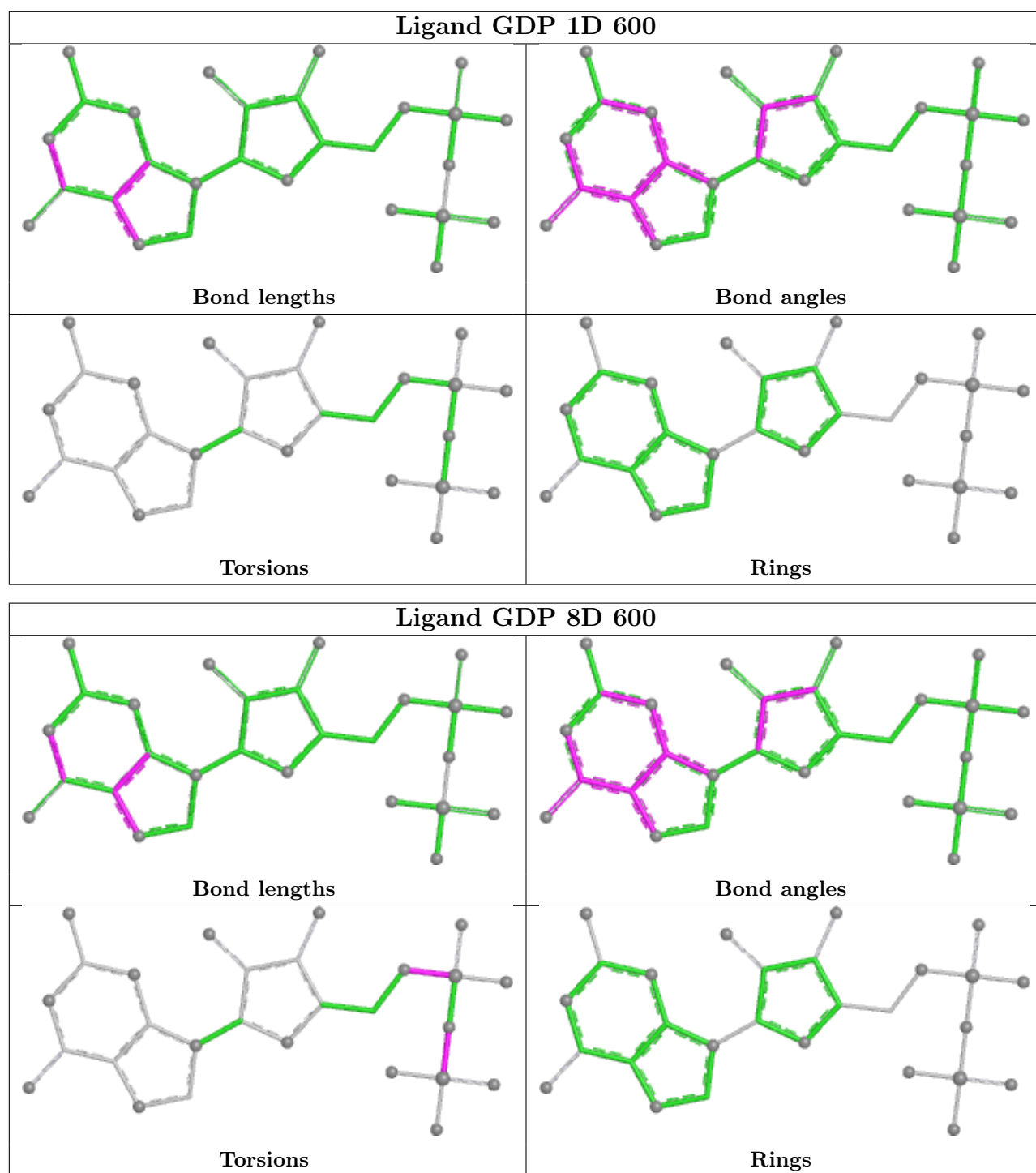


## Ligand GTP 10C 500

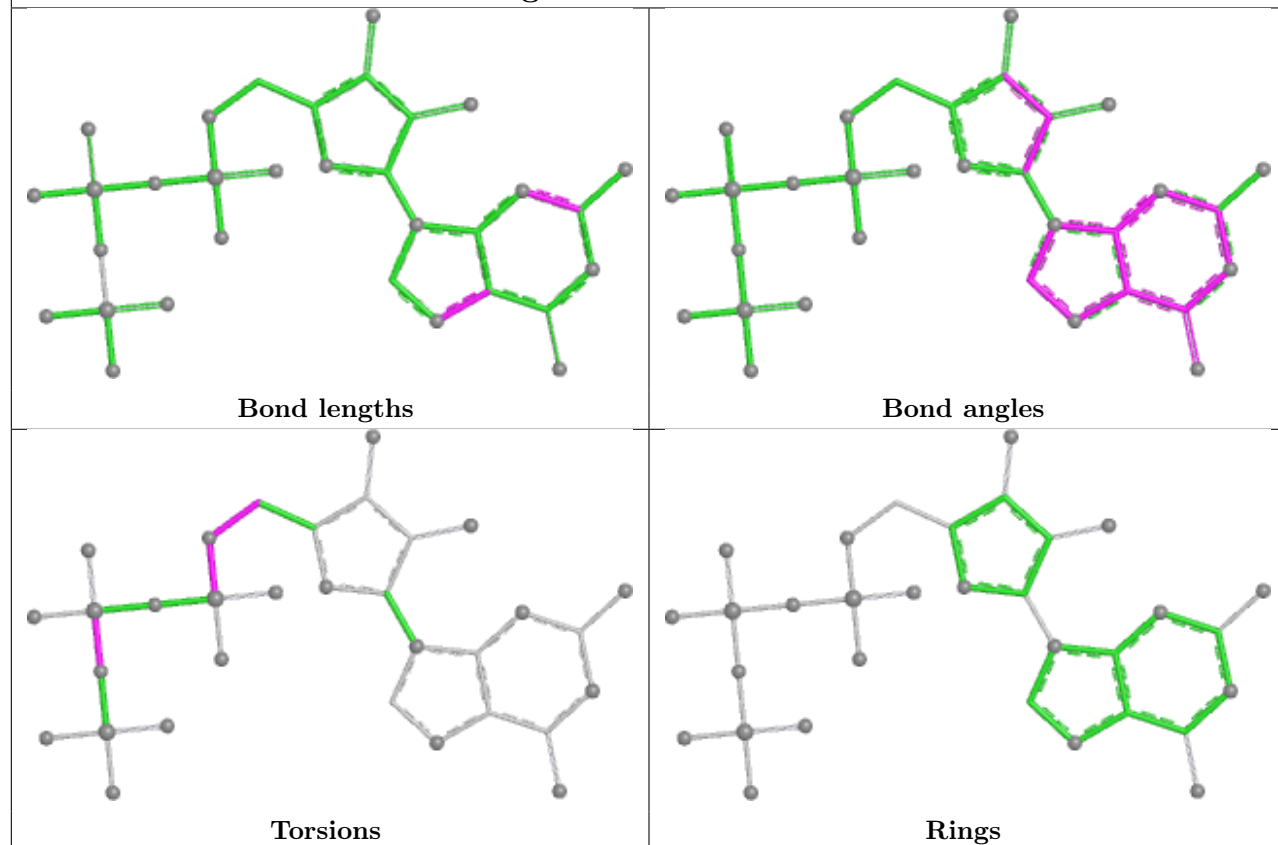


## Ligand GTP 12E 500

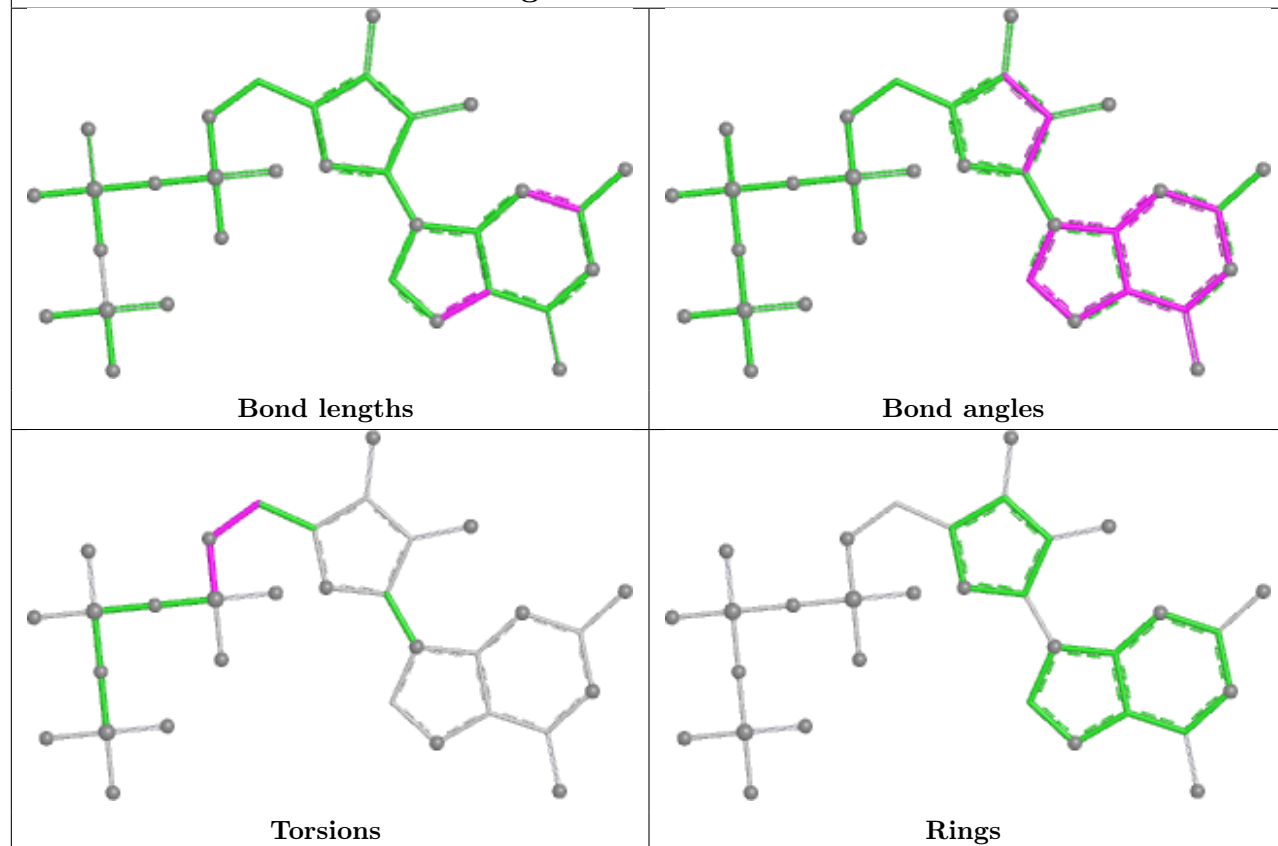




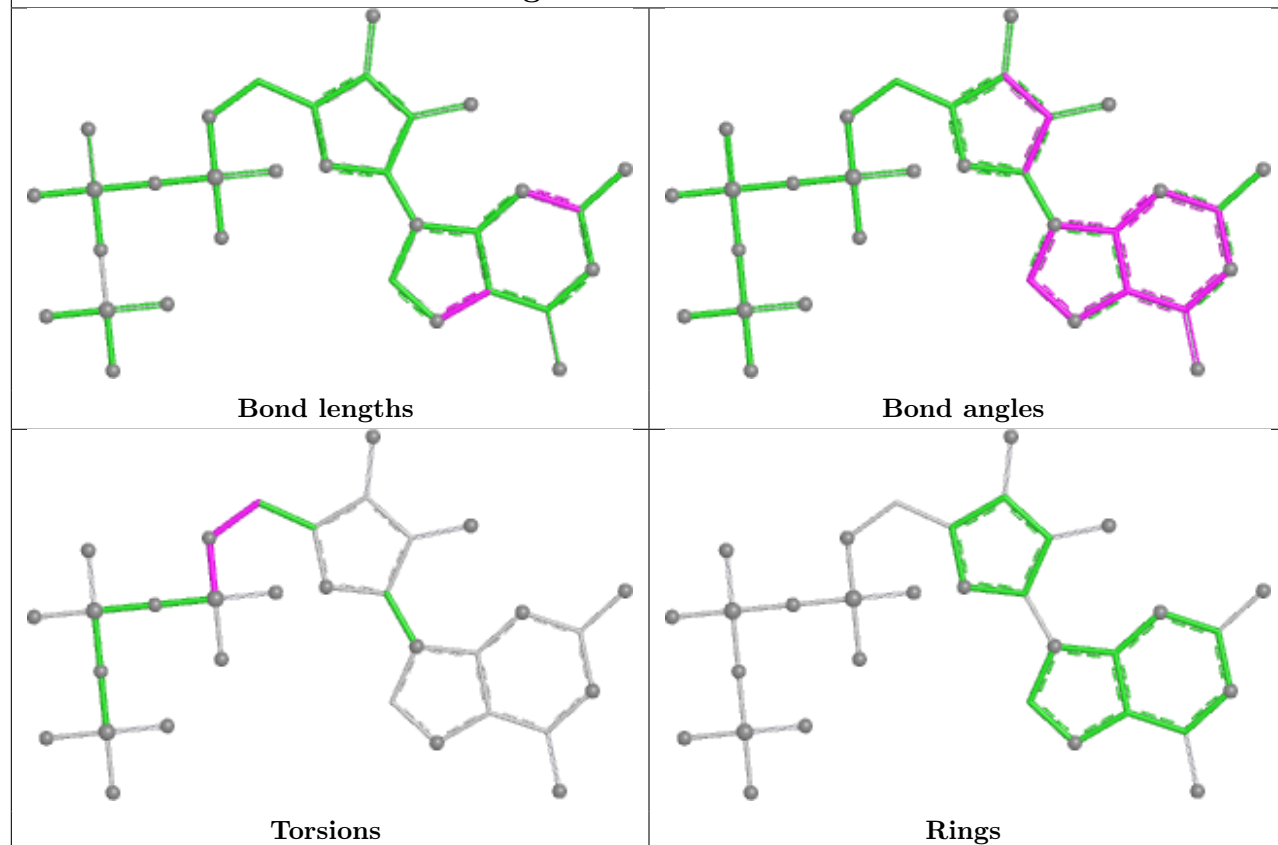
## Ligand GTP 3C 500



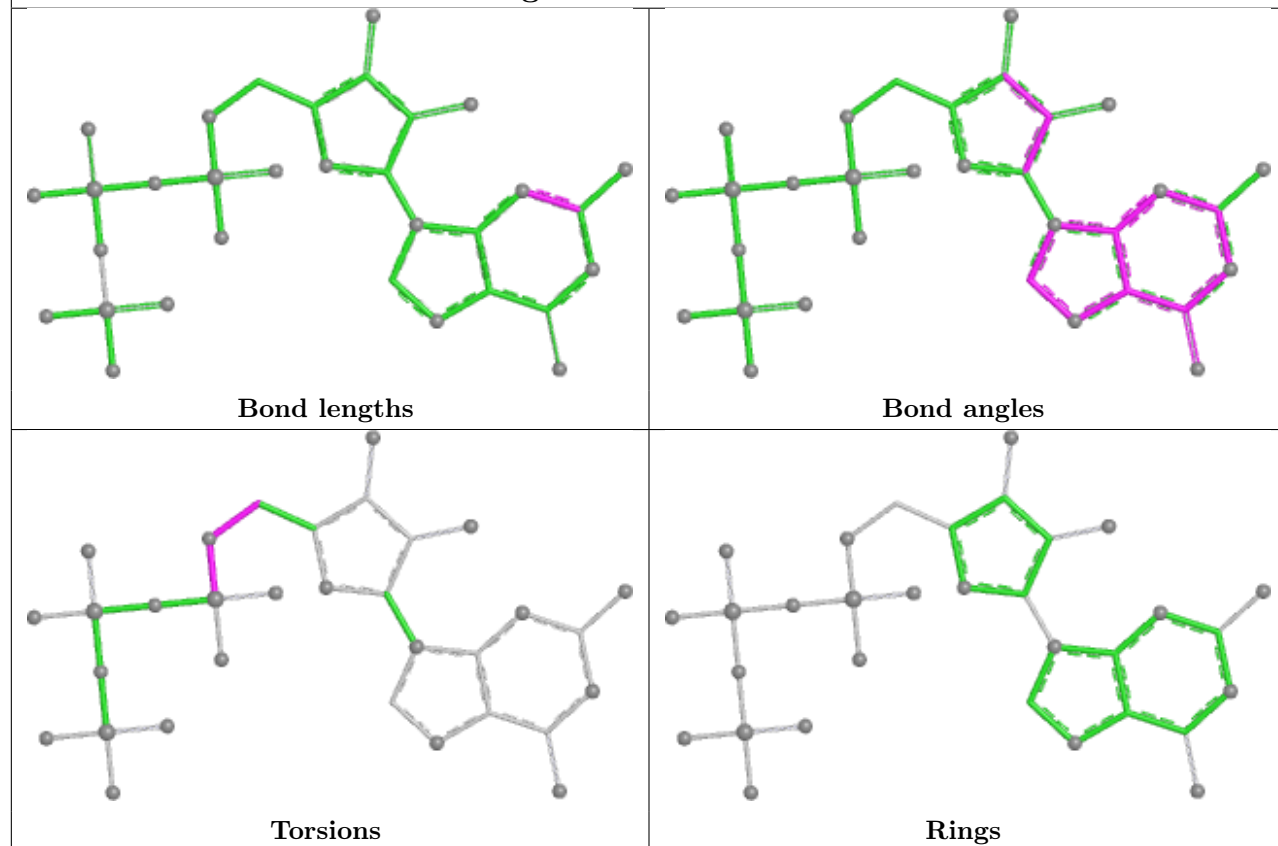
## Ligand GTP 6A 500



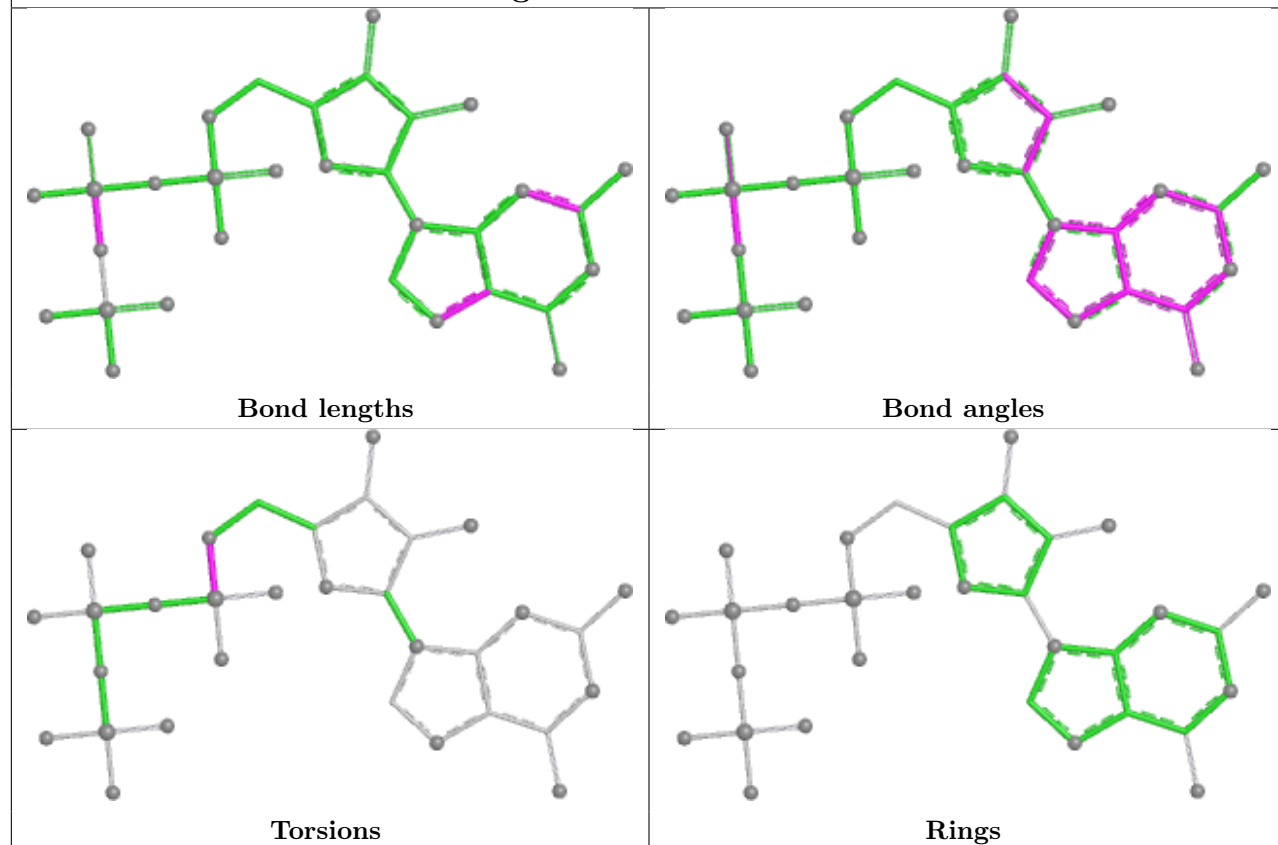
## Ligand GTP 2E 500



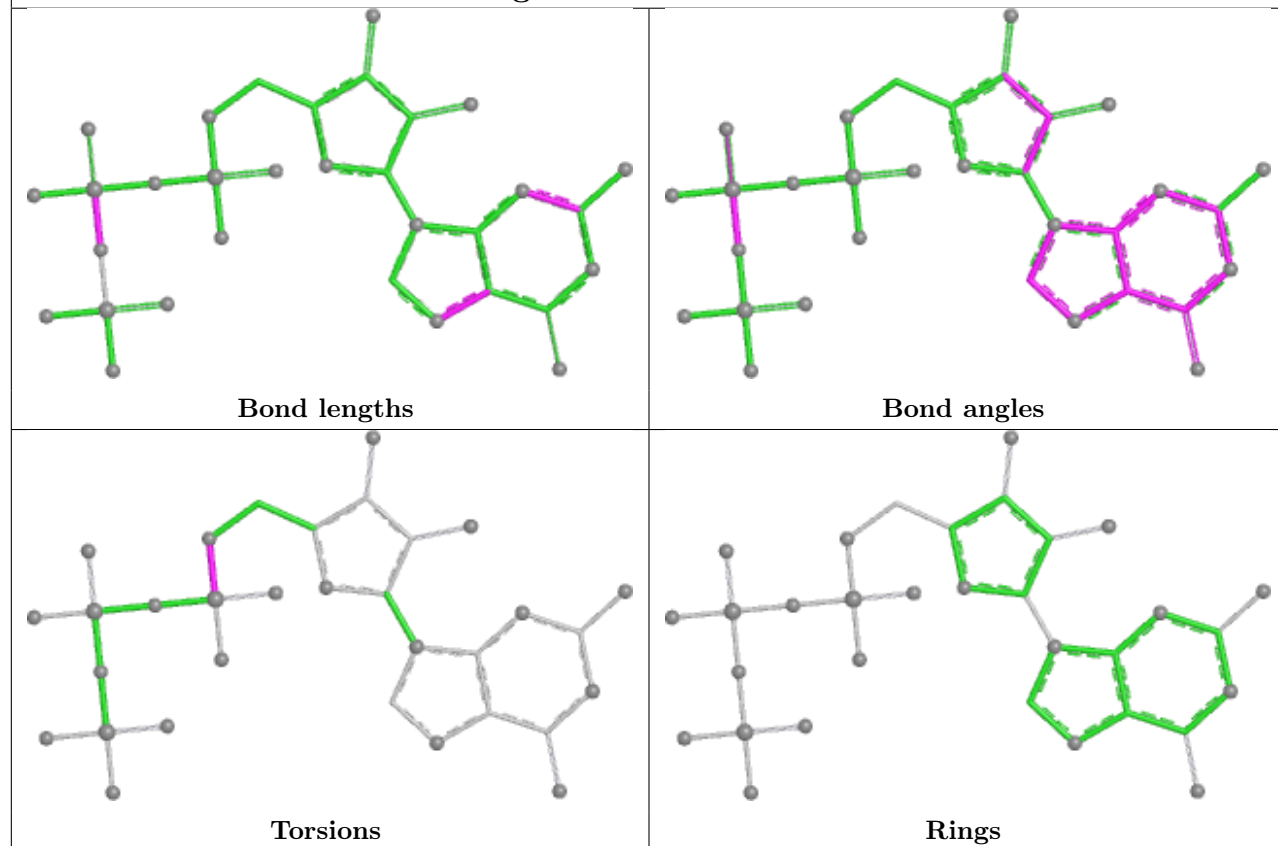
## Ligand GTP 6C 500



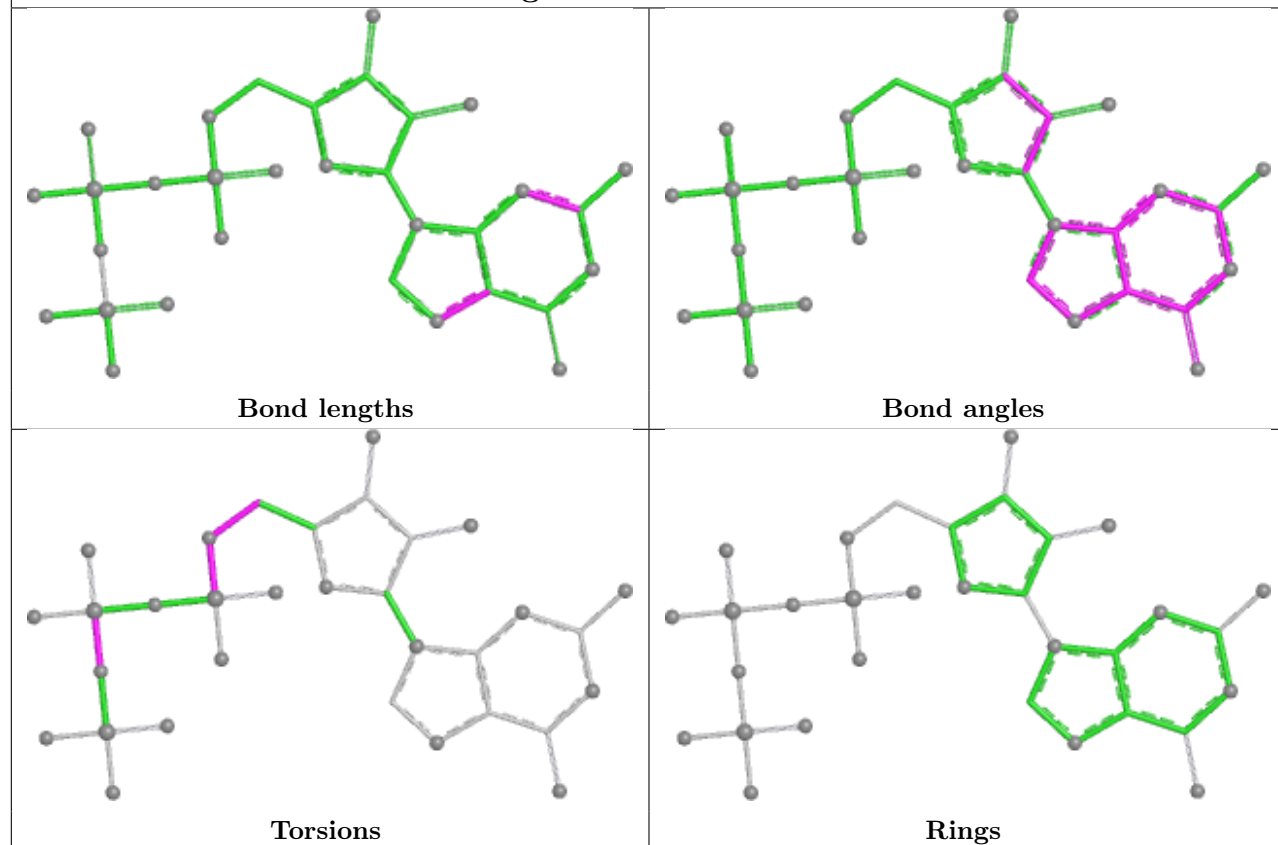
## Ligand GTP 12A 500



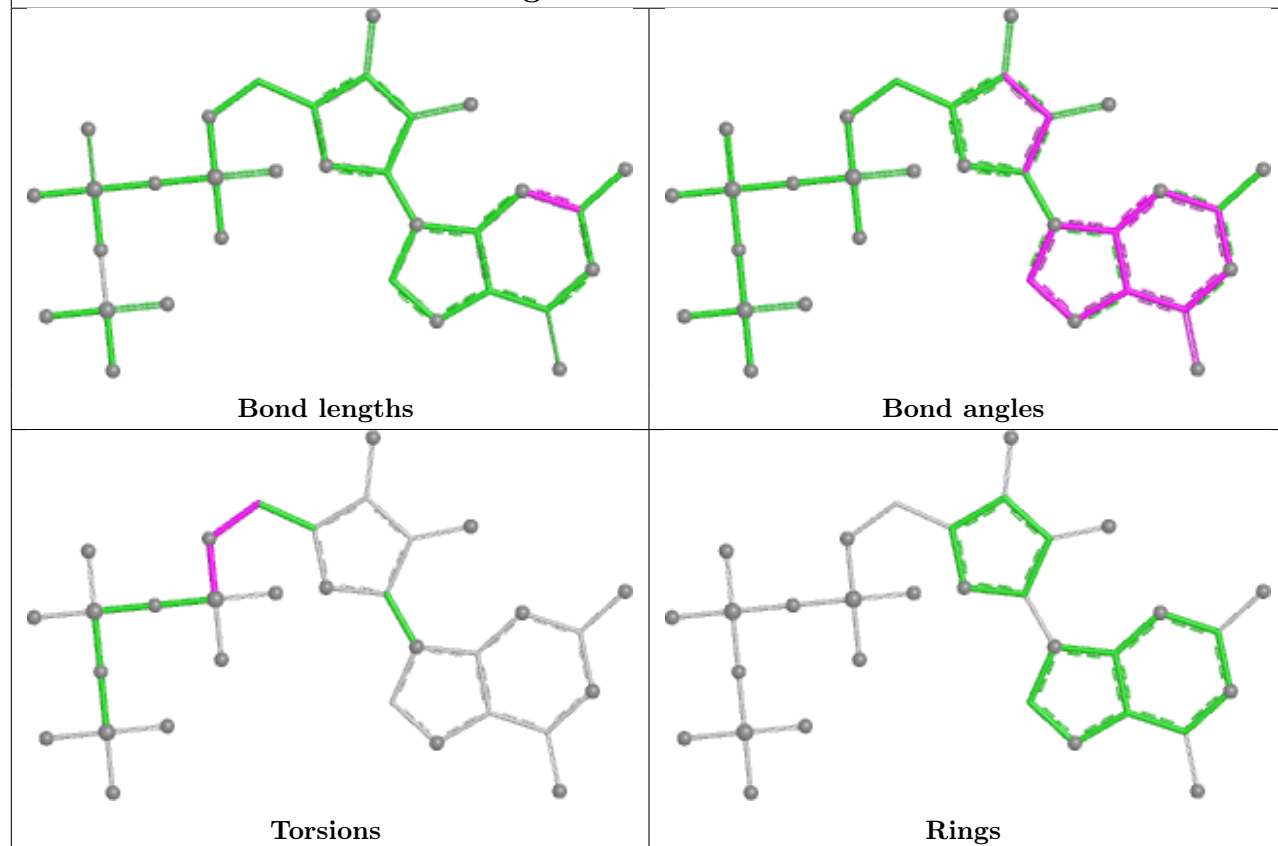
## Ligand GTP 12C 500

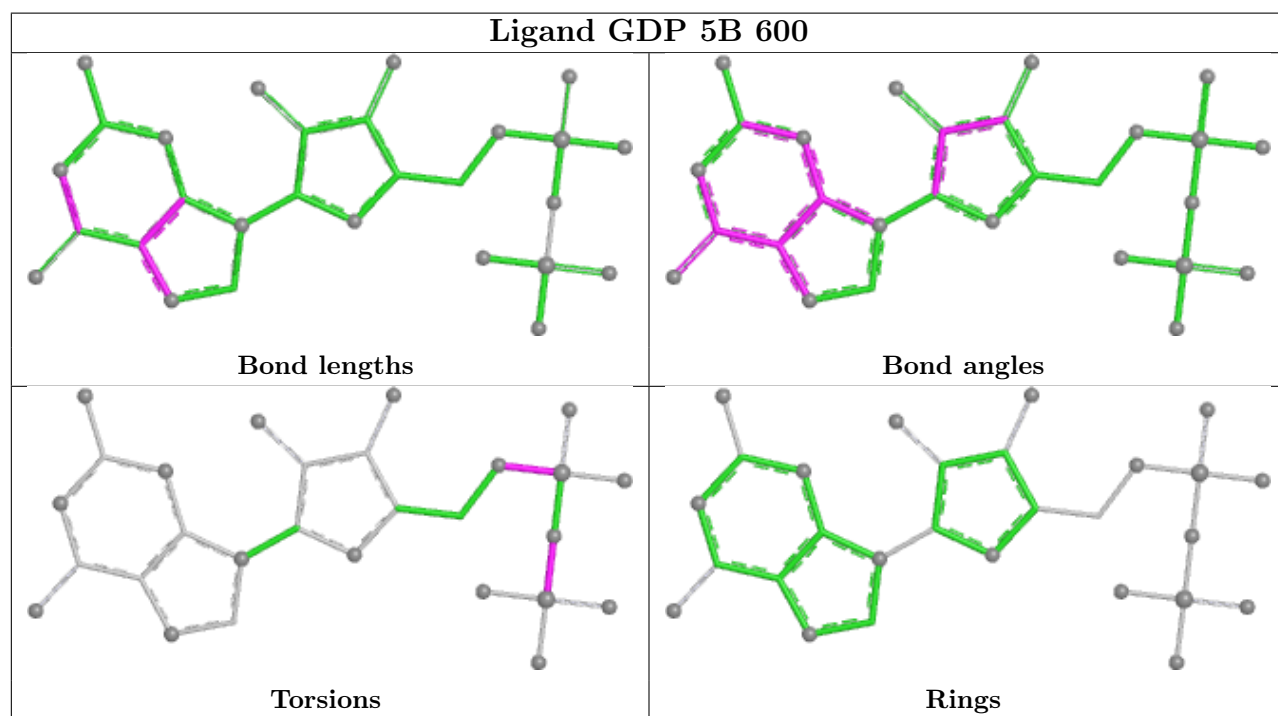
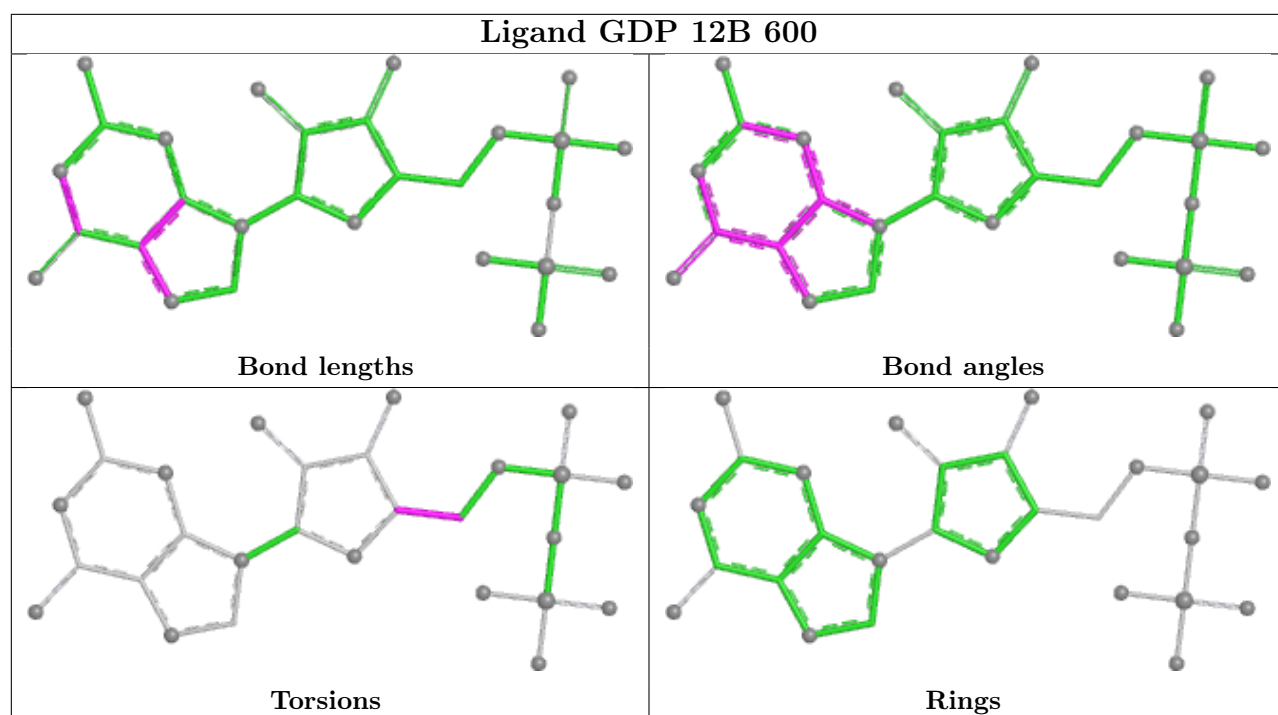


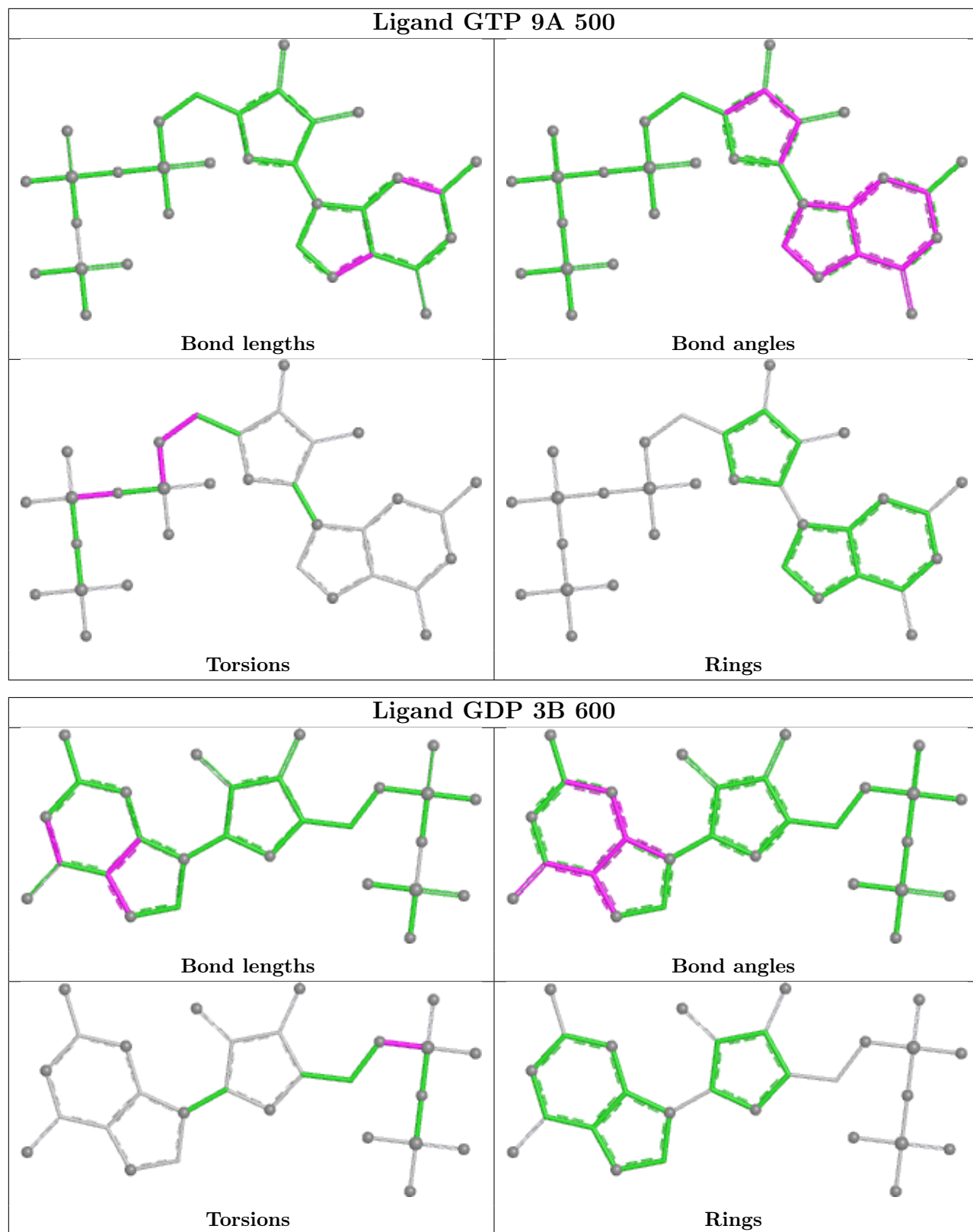
## Ligand GTP 4C 500

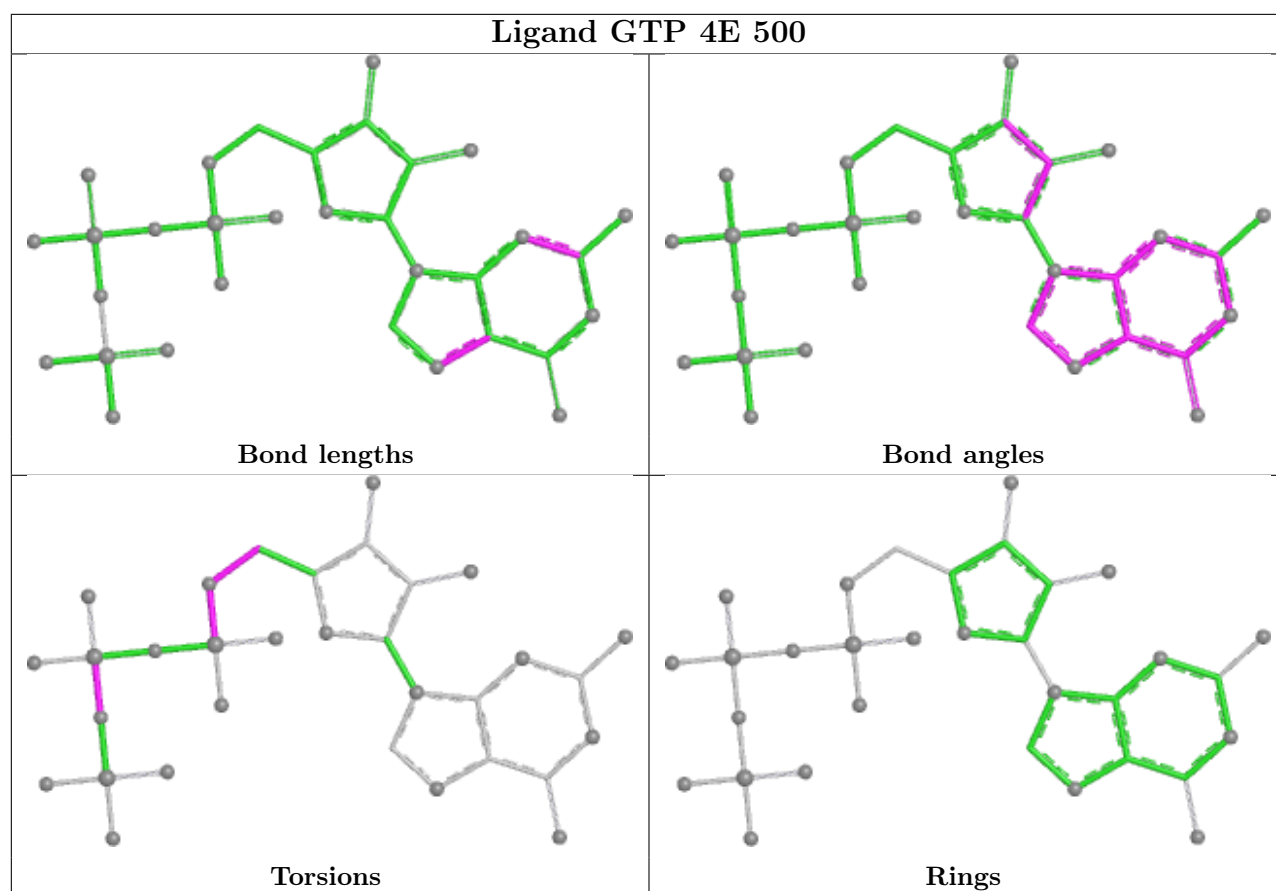


## Ligand GTP 6E 500









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

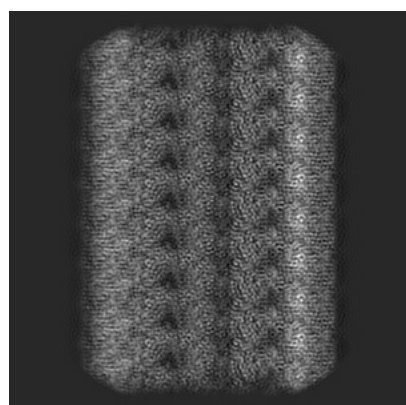
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14150. These allow visual inspection of the internal detail of the map and identification of artifacts.

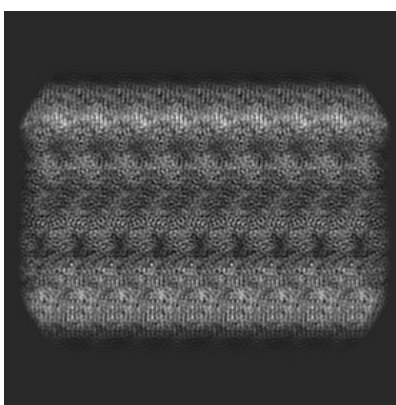
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

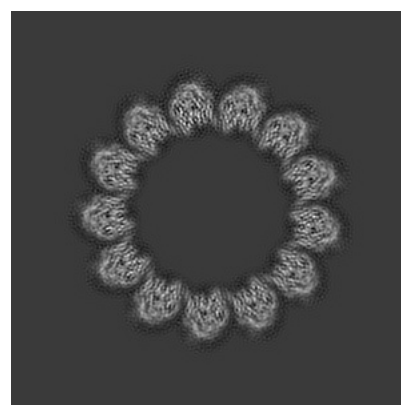
#### 6.1.1 Primary map



X



Y

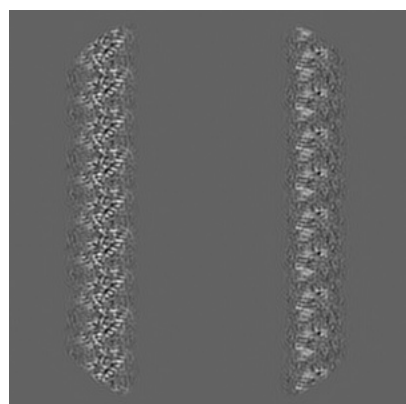


Z

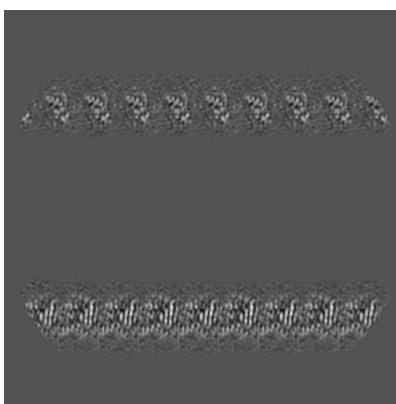
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

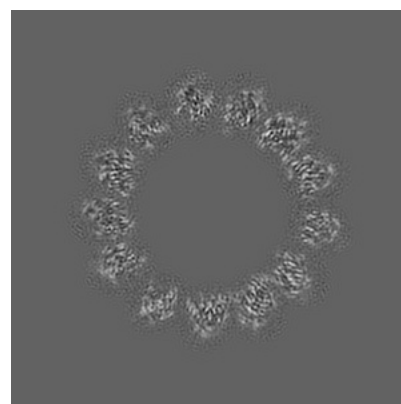
#### 6.2.1 Primary map



X Index: 196



Y Index: 196

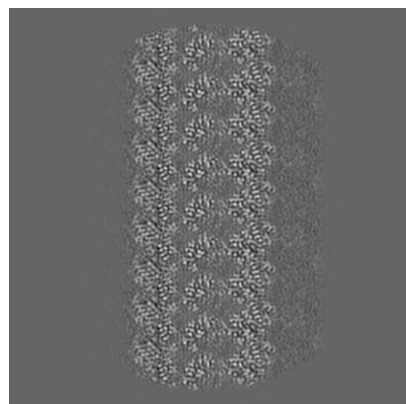


Z Index: 196

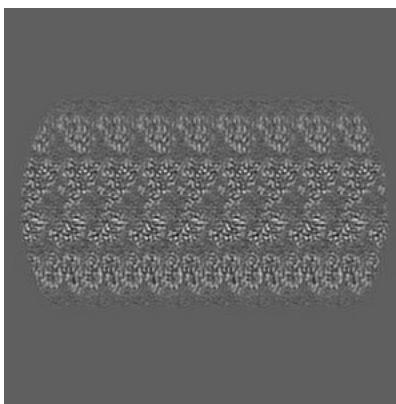
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

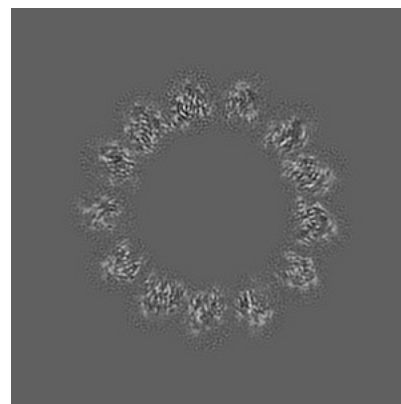
### 6.3.1 Primary map



X Index: 107



Y Index: 284

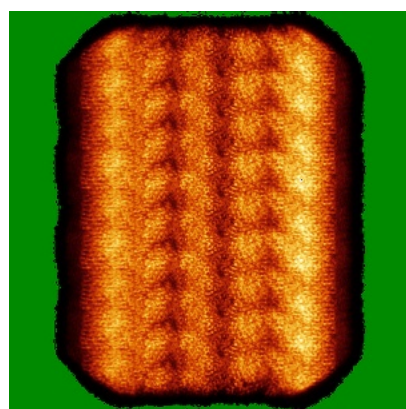


Z Index: 170

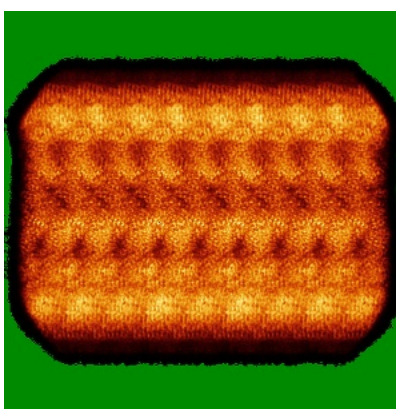
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

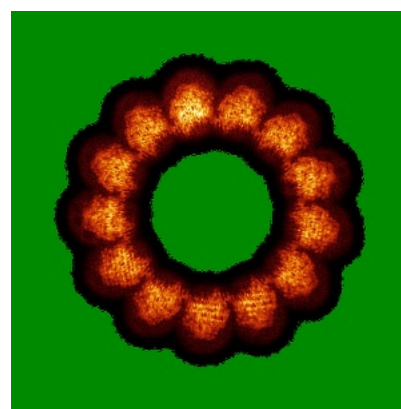
### 6.4.1 Primary map



X



Y

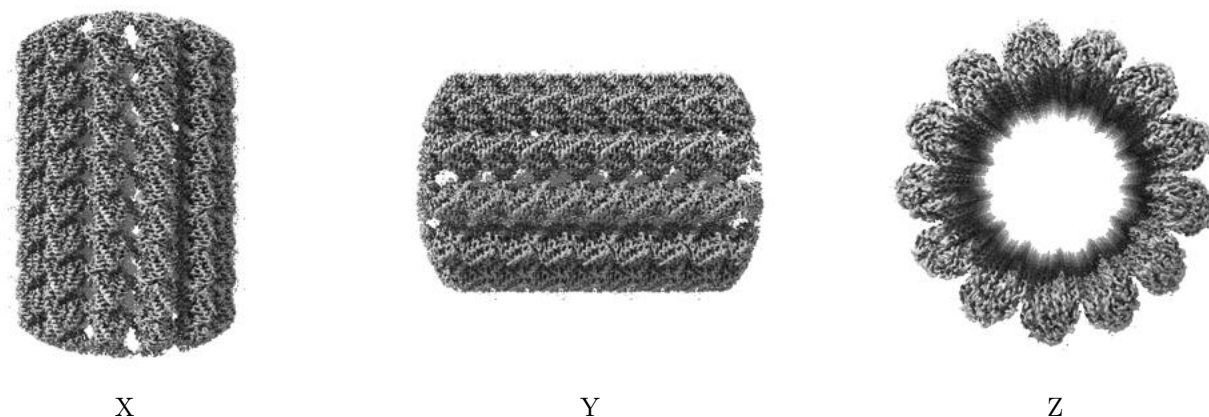


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.582. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

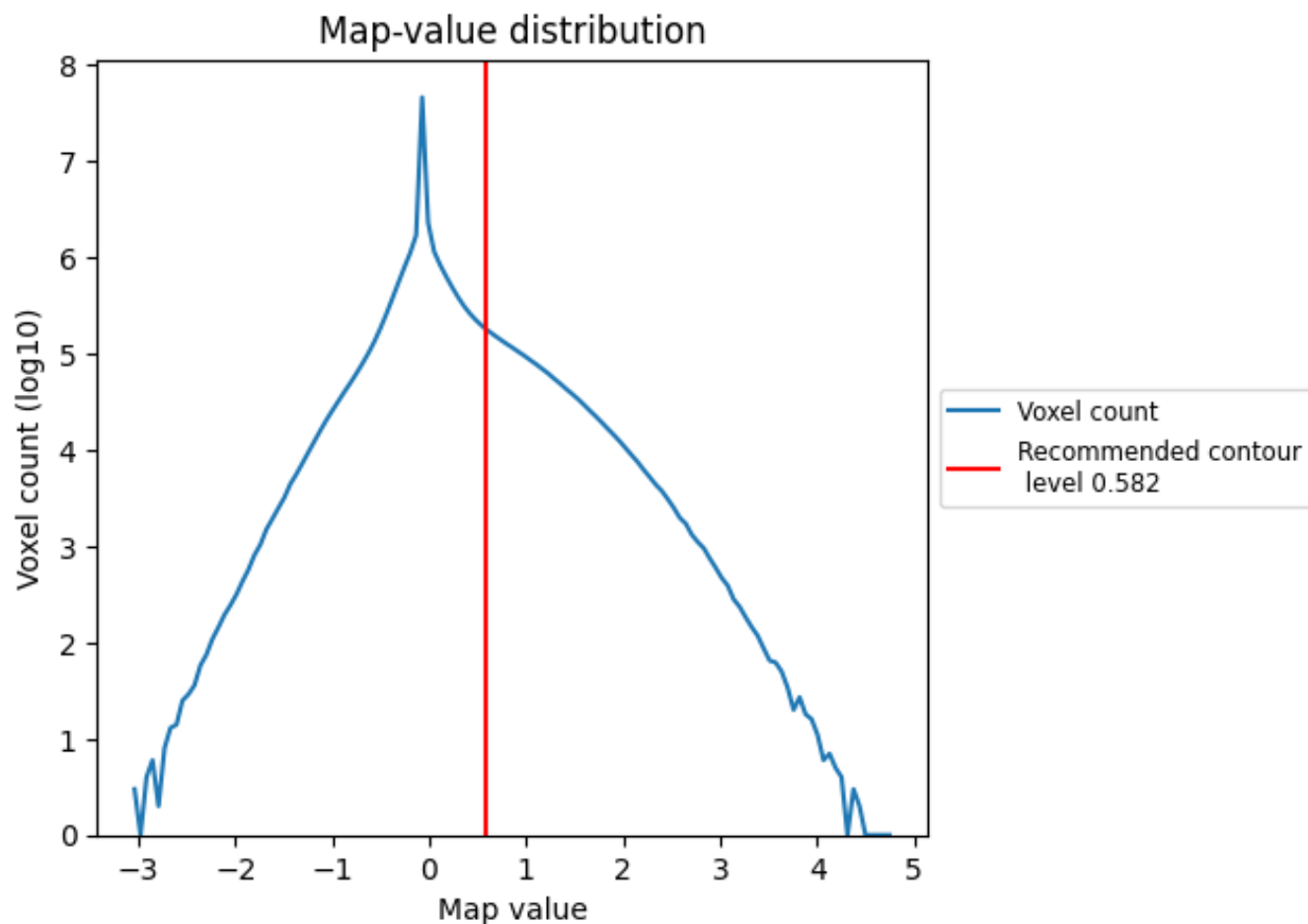
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

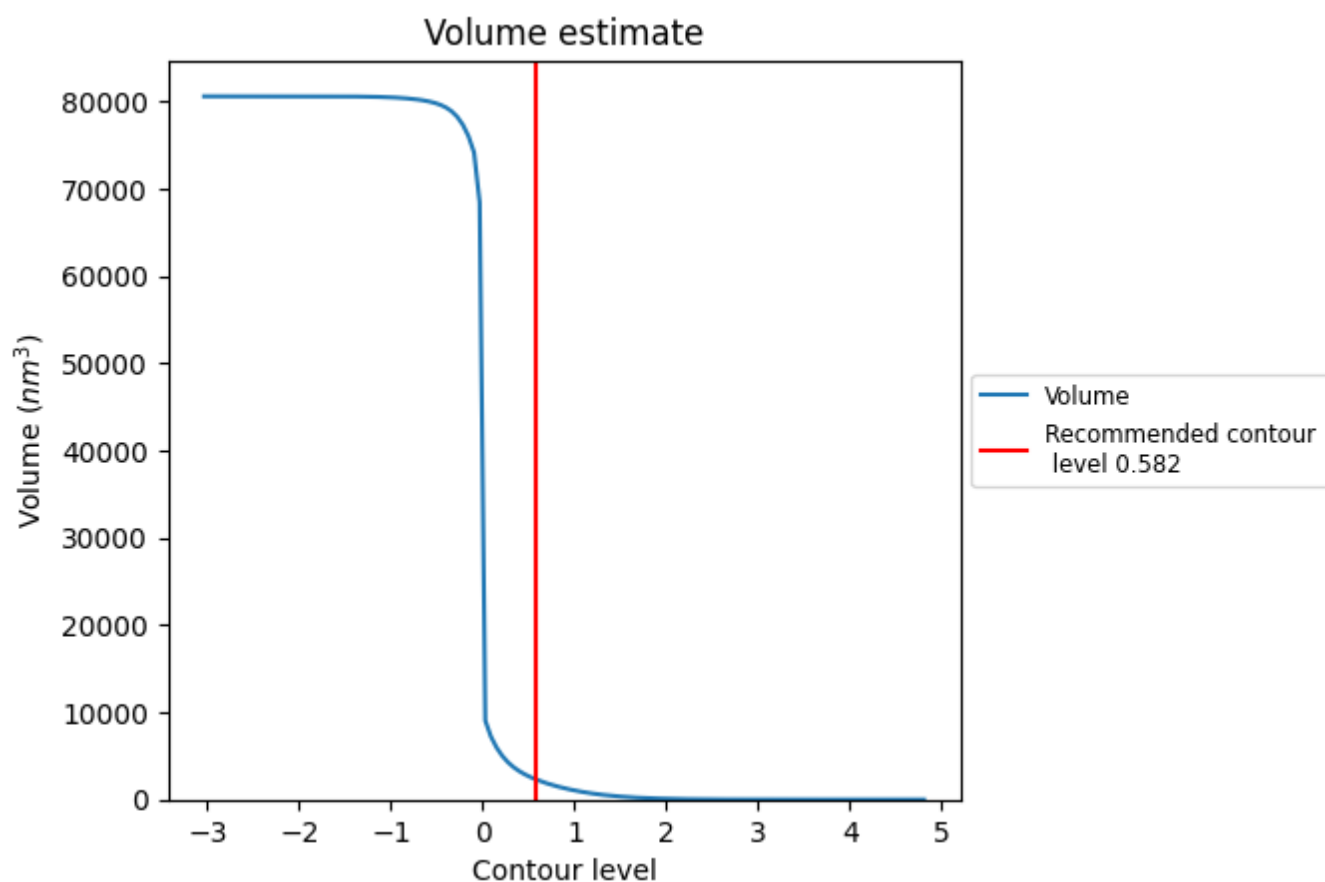
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

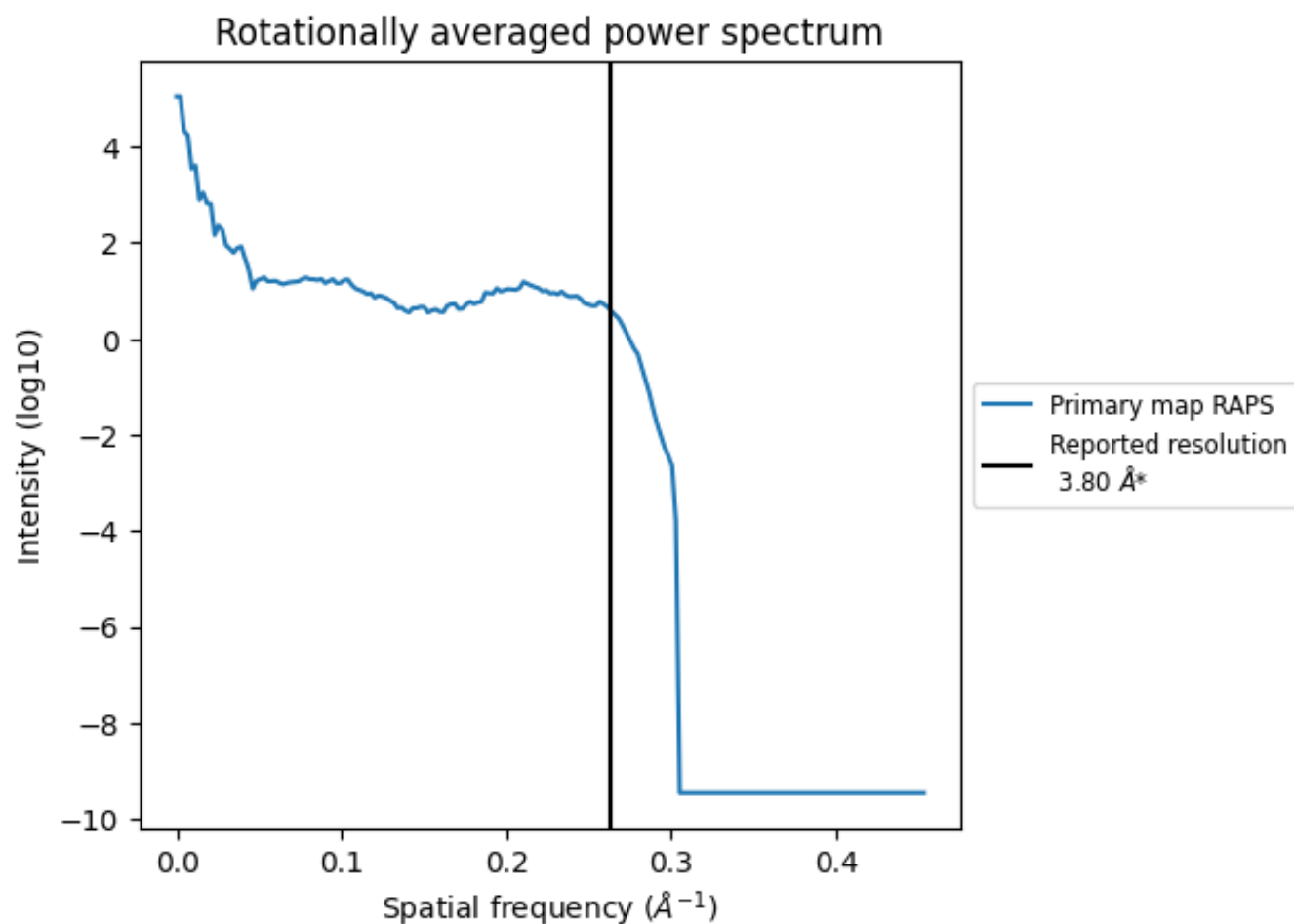
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2293 nm<sup>3</sup>; this corresponds to an approximate mass of 2072 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

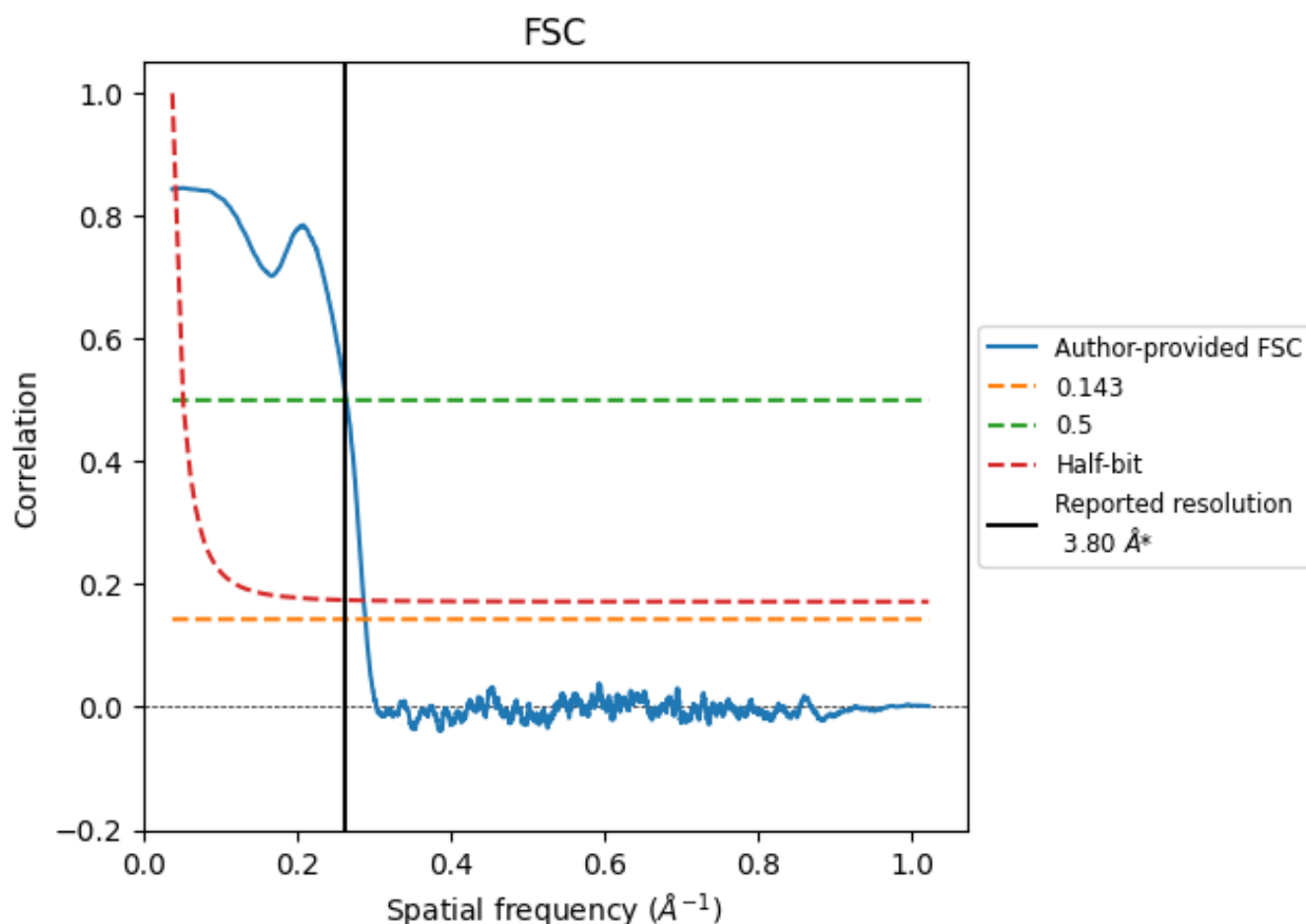


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

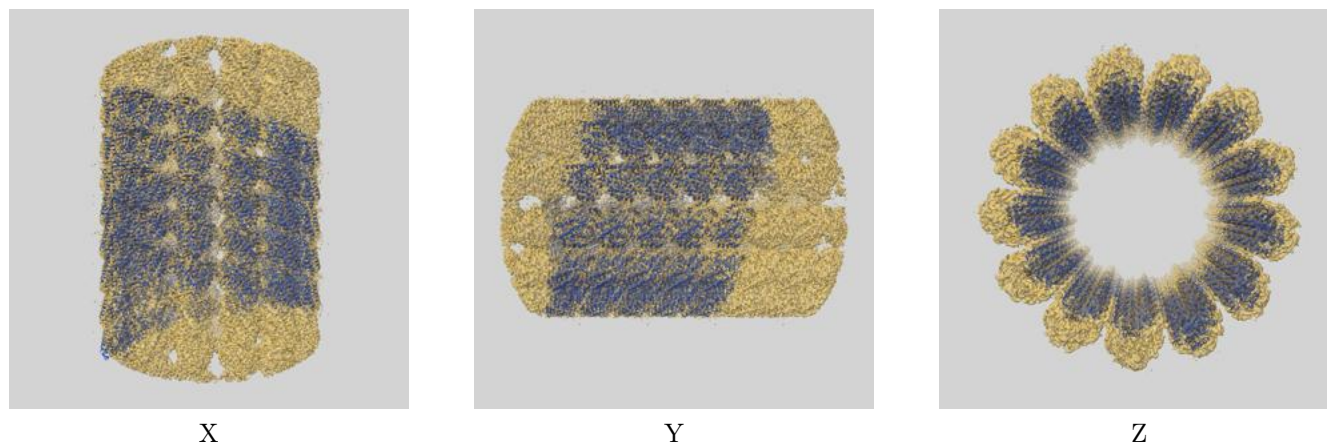
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | -                                  | 3.80 | -        |
| Author-provided FSC curve | 3.46                               | 3.78 | 3.48     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

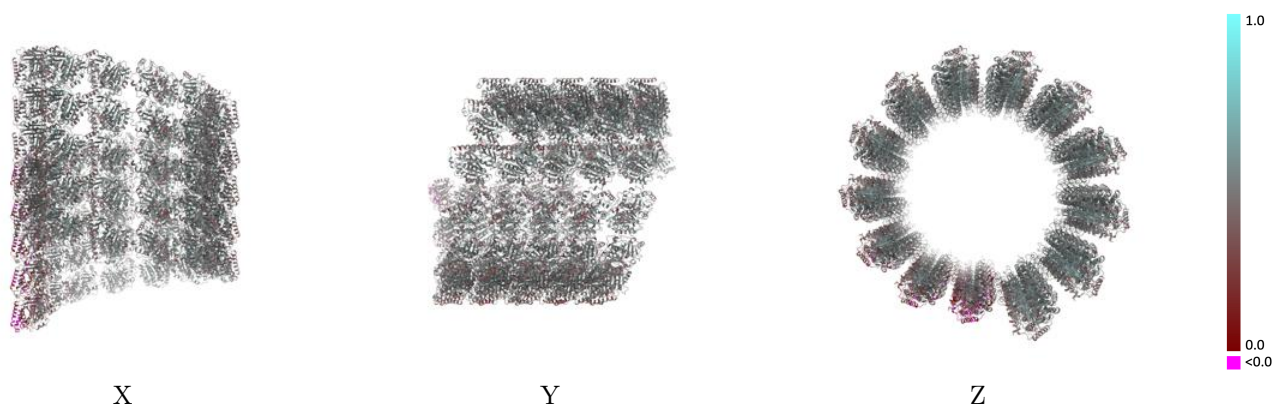
This section contains information regarding the fit between EMDB map EMD-14150 and PDB model 7QUP. Per-residue inclusion information can be found in section [3](#) on page [52](#).

### 9.1 Map-model overlay [i](#)



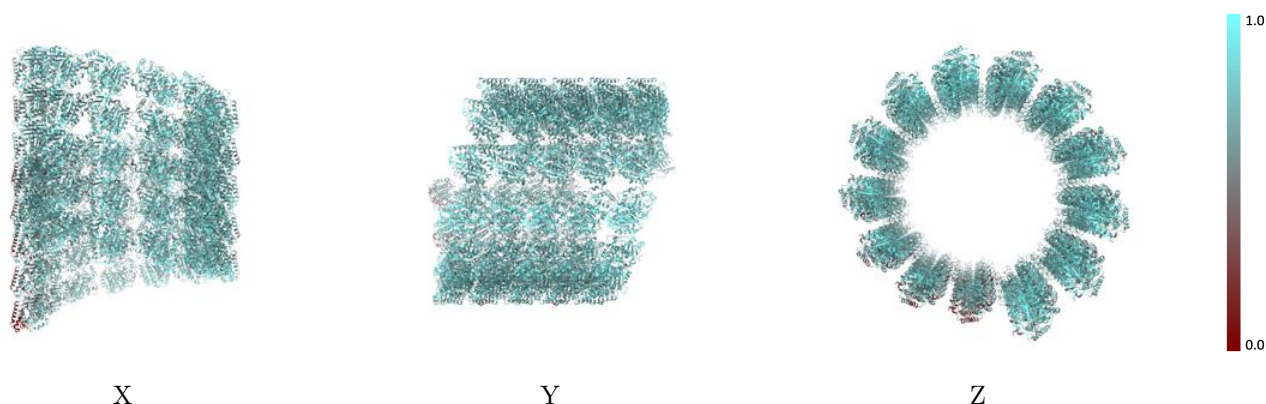
The images above show the 3D surface view of the map at the recommended contour level 0.582 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



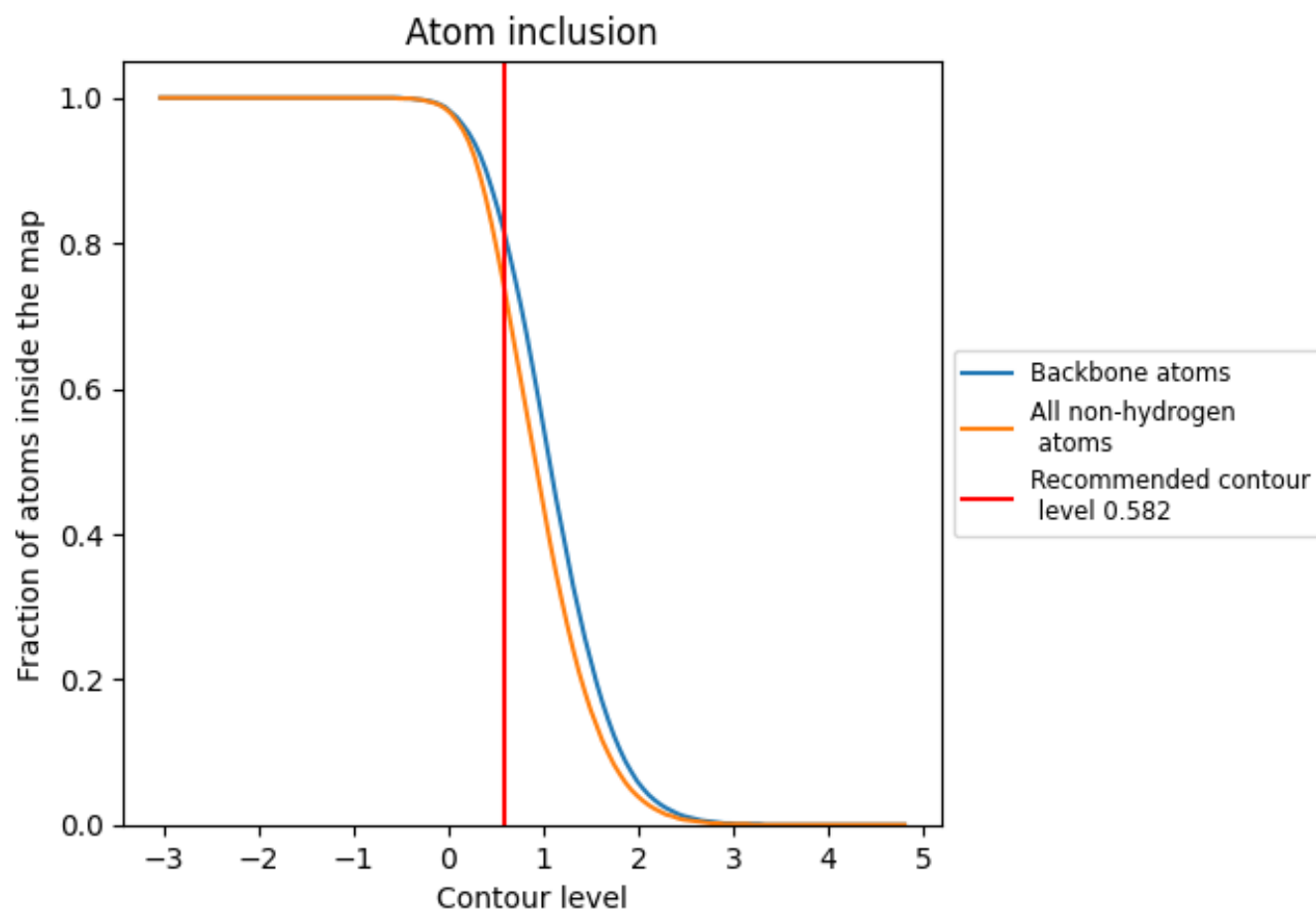
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.582).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.582) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7420   |  0.4600   |
| 10A   |  0.7530   |  0.4610   |
| 10B   |  0.7390   |  0.4610   |
| 10C   |  0.7560   |  0.4650   |
| 10D   |  0.7350   |  0.4620   |
| 10E   |  0.7380   |  0.4570   |
| 11A   |  0.7340   |  0.4390   |
| 11B   |  0.7330   |  0.4460   |
| 11C   |  0.7340   |  0.4400   |
| 11D   |  0.7290   |  0.4440   |
| 11E   |  0.7190   |  0.4350   |
| 12A   |  0.6760   |  0.4040   |
| 12B   |  0.6910   |  0.4180   |
| 12C   |  0.6850   |  0.4120   |
| 12D   |  0.6960  |  0.4210  |
| 12E   |  0.6300 |  0.3960 |
| 13A   |  0.5920 |  0.3290 |
| 13B   |  0.6470 |  0.3510 |
| 13C   |  0.6100 |  0.3460 |
| 13D   |  0.6310 |  0.3470 |
| 13E   |  0.5120 |  0.3050 |
| 1A    |  0.7350 |  0.4760 |
| 1B    |  0.7070 |  0.4690 |
| 1C    |  0.7450 |  0.4760 |
| 1D    |  0.7130 |  0.4710 |
| 1E    |  0.7470 |  0.4780 |
| 2A    |  0.7520 |  0.4880 |
| 2B    |  0.7340 |  0.4870 |
| 2C    |  0.7620 |  0.4920 |
| 2D    |  0.7370 |  0.4870 |
| 2E    |  0.7580 |  0.4890 |
| 3A    |  0.7630 |  0.4840 |
| 3B    |  0.7560 |  0.4840 |
| 3C    |  0.7680 |  0.4870 |
| 3D    |  0.7550 |  0.4820 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 3E    |  0.7570   |  0.4860   |
| 4A    |  0.7600   |  0.4830   |
| 4B    |  0.7640   |  0.4870   |
| 4C    |  0.7680   |  0.4890   |
| 4D    |  0.7660   |  0.4870   |
| 4E    |  0.7660   |  0.4870   |
| 5A    |  0.7660   |  0.4810   |
| 5B    |  0.7760   |  0.4840   |
| 5C    |  0.7610   |  0.4830   |
| 5D    |  0.7740   |  0.4850   |
| 5E    |  0.7600   |  0.4820   |
| 6A    |  0.7690   |  0.4780   |
| 6B    |  0.7740   |  0.4830   |
| 6C    |  0.7760   |  0.4790   |
| 6D    |  0.7760   |  0.4840   |
| 6E    |  0.7660   |  0.4800   |
| 7A    |  0.8250   |  0.4870   |
| 7B    |  0.8200  |  0.4890  |
| 7C    |  0.8190 |  0.4880 |
| 7D    |  0.8190 |  0.4880 |
| 7E    |  0.8210 |  0.4860 |
| 8A    |  0.7800 |  0.4750 |
| 8B    |  0.7650 |  0.4770 |
| 8C    |  0.7770 |  0.4740 |
| 8D    |  0.7620 |  0.4760 |
| 8E    |  0.7720 |  0.4730 |
| 9A    |  0.7680 |  0.4710 |
| 9B    |  0.7530 |  0.4730 |
| 9C    |  0.7700 |  0.4740 |
| 9D    |  0.7500 |  0.4730 |
| 9E    |  0.7600 |  0.4700 |