



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:04 PM UTC

PDB ID : 9YA2 / pdb\_00009ya2  
EMDB ID : EMD-72718  
Title : Cryo-EM structure of intraconoidal microtubule 1 (ICMT1) from *Toxoplasma gondii* (8-nm repeat)  
Authors : Zeng, J.; Zhang, R.  
Deposited on : 2025-09-15  
Resolution : 3.34 Å(reported)

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

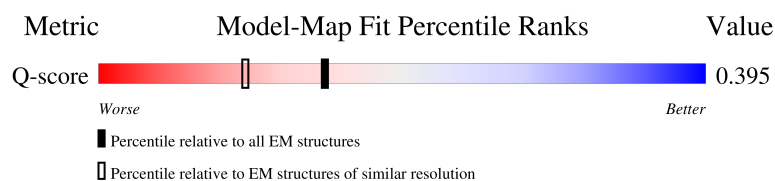
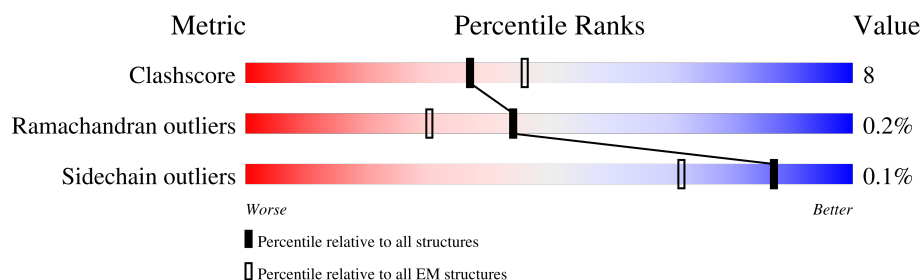
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.34 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.



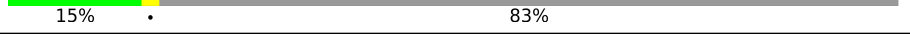
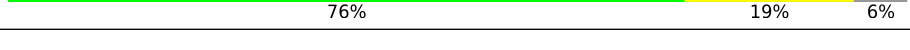
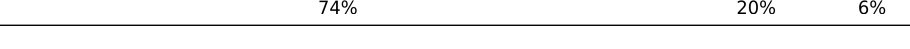
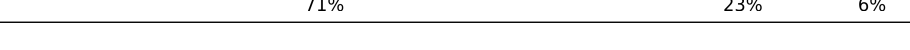
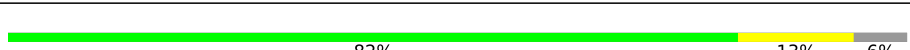
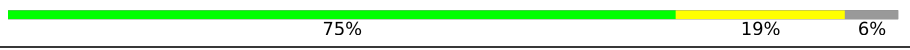
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14446 ( 2.84 - 3.84 )                                    |

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   | A     | 351    |                  |
| 1   | B     | 351    |                  |
| 1   | C     | 351    |                  |
| 1   | D     | 351    |                  |

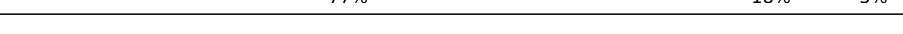
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 351    |    |
| 1   | F     | 351    |    |
| 1   | G     | 351    |    |
| 1   | H     | 351    |    |
| 1   | I     | 351    |    |
| 1   | J     | 351    |    |
| 1   | K     | 351    |    |
| 2   | A0    | 453    |    |
| 2   | A2    | 453    |    |
| 2   | A4    | 453    |    |
| 2   | A6    | 453    |    |
| 2   | A8    | 453    |  |
| 2   | B0    | 453    |  |
| 2   | B2    | 453    |  |
| 2   | B4    | 453    |  |
| 2   | B6    | 453    |  |
| 2   | B8    | 453    |  |
| 2   | C0    | 453    |  |
| 2   | C2    | 453    |  |
| 2   | C4    | 453    |  |
| 2   | C6    | 453    |  |
| 2   | C8    | 453    |  |
| 2   | D0    | 453    |  |
| 2   | D2    | 453    |  |
| 2   | D4    | 453    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | D6    | 453    |    |
| 2   | D8    | 453    |    |
| 2   | E0    | 453    |    |
| 2   | E2    | 453    |    |
| 2   | E4    | 453    |    |
| 2   | E6    | 453    |    |
| 2   | E8    | 453    |    |
| 2   | F0    | 453    |    |
| 3   | A1    | 449    |    |
| 3   | A3    | 449    |    |
| 3   | A5    | 449    |    |
| 3   | A7    | 449    |    |
| 3   | A9    | 449    |  |
| 3   | B1    | 449    |  |
| 3   | B3    | 449    |  |
| 3   | B5    | 449    |  |
| 3   | B7    | 449    |  |
| 3   | B9    | 449    |  |
| 3   | C1    | 449    |  |
| 3   | C3    | 449    |  |
| 3   | C5    | 449    |  |
| 3   | C7    | 449    |  |
| 3   | C9    | 449    |  |
| 3   | D1    | 449    |  |
| 3   | D3    | 449    |  |

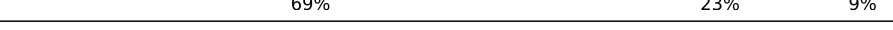
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | D5    | 449    |                  |
| 3   | D7    | 449    |                  |
| 3   | D9    | 449    |                  |
| 3   | E1    | 449    |                  |
| 3   | E3    | 449    |                  |
| 3   | E5    | 449    |                  |
| 3   | E7    | 449    |                  |
| 3   | E9    | 449    |                  |
| 3   | F1    | 449    |                  |
| 4   | L     | 1678   |                  |
| 4   | M     | 1678   |                  |
| 4   | N     | 1678   |                  |
| 4   | Q     | 1678   |                  |
| 4   | V     | 1678   |                  |
| 4   | W     | 1678   |                  |
| 5   | O     | 583    |                  |
| 5   | P     | 583    |                  |
| 6   | R     | 336    |                  |
| 6   | S     | 336    |                  |
| 6   | T     | 336    |                  |
| 6   | U     | 336    |                  |
| 7   | a     | 220    |                  |
| 7   | b     | 220    |                  |
| 7   | c     | 220    |                  |
| 7   | d     | 220    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 7   | e     | 220    |    |
| 7   | f     | 220    |    |
| 7   | g     | 220    |    |
| 7   | h     | 220    |    |
| 7   | i     | 220    |    |
| 7   | j     | 220    |    |
| 7   | m     | 220    |    |
| 7   | n     | 220    |    |
| 7   | o     | 220    |    |
| 7   | p     | 220    |    |
| 7   | q     | 220    |    |
| 7   | r     | 220    |   |
| 7   | s     | 220    |  |
| 7   | t     | 220    |  |
| 7   | u     | 220    |  |
| 7   | v     | 220    |  |
| 7   | w     | 220    |  |
| 7   | x     | 220    |  |
| 8   | k     | 189    |  |
| 8   | l     | 189    |  |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 231266 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 Microtubule associated protein SPM1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | A     | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 464   | 306 | 74 | 83 | 1 |         |       |
| 1   | B     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | C     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | D     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | E     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | F     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | G     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | H     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | I     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | J     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |
| 1   | K     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 311 | 75 | 84 | 1 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| A     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| B     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| C     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| D     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| E     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| F     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| G     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| H     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| I     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| J     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |
| K     | 93      | ARG      | PRO    | conflict | UNP A0A7J6K285 |

- Molecule 2 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | A2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | A4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | A6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | A8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | B0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | B2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | B4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | B6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | B8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | C0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | C2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | C4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | C6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | C8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | D0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | D2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | D4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | D6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | D8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E2    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E4    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E6    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | E8    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |
| 2   | F0    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2105 | 569 | 625 | 26 |         |       |

- Molecule 3 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | A1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A3    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A5    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A7    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | A9    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B3    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B5    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B7    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | B9    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |
| 3   | C1    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 569 | 641 | 27 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 3   | C3    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | C5    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | C7    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | C9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D3    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D5    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D7    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | D9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E3    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E5    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E7    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | E9    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |
| 3   | F1    | 426      | Total<br>3331 | C<br>2094 | N<br>569 | O<br>641 | S<br>27 | 0       | 0     |

- Molecule 4 is a protein called ICMAP2, TGME49\_224700.

| Mol | Chain | Residues | Atoms         |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 4   | L     | 162      | Total<br>1334 | C<br>868 | N<br>226 | O<br>231 | S<br>9 | 0       | 0     |
| 4   | M     | 162      | Total<br>1334 | C<br>868 | N<br>226 | O<br>231 | S<br>9 | 0       | 0     |
| 4   | N     | 162      | Total<br>1334 | C<br>868 | N<br>226 | O<br>231 | S<br>9 | 0       | 0     |
| 4   | Q     | 162      | Total<br>1334 | C<br>868 | N<br>226 | O<br>231 | S<br>9 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | V     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1334  | 868 | 226 | 231 | 9 |         |       |
| 4   | W     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1334  | 868 | 226 | 231 | 9 |         |       |

- Molecule 5 is a protein called TLAP3 (apical cap protein AC5), TGME49\_235380.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | O     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1736  | 1078 | 328 | 328 | 2 |         |       |
| 5   | P     | 219      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1736  | 1078 | 328 | 328 | 2 |         |       |

- Molecule 6 is a protein called TLAP4 (thioredoxin-like associated protein), TGME49\_201760.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | R     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 954   | 592 | 182 | 179 | 1 |         |       |
| 6   | S     | 22       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 182   | 112 | 38  | 31  | 1 |         |       |
| 6   | T     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 954   | 592 | 182 | 179 | 1 |         |       |
| 6   | U     | 91       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 772   | 480 | 144 | 148 |   |         |       |

- Molecule 7 is a protein called TRXL1, TGME49\_232410.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | a     | 161      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1289  | 824  | 224 | 236 | 5 |         |       |
| 7   | b     | 161      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1289  | 824  | 224 | 236 | 5 |         |       |
| 7   | c     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | d     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | e     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | f     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | g     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | h     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | i     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | j     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | m     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | n     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | o     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | p     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | q     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | r     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | s     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | t     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | u     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | v     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | w     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |
| 7   | x     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1608  | 1021 | 283 | 297 | 7 |         |       |

- Molecule 8 is a protein called TRXL2, TGME49\_225790.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | k     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1187  | 770 | 209 | 203 | 5 |         |       |
| 8   | l     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1187  | 770 | 209 | 203 | 5 |         |       |

There are 46 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| k     | 167     | SER      | -      | expression tag | UNP A0A7J6K232 |

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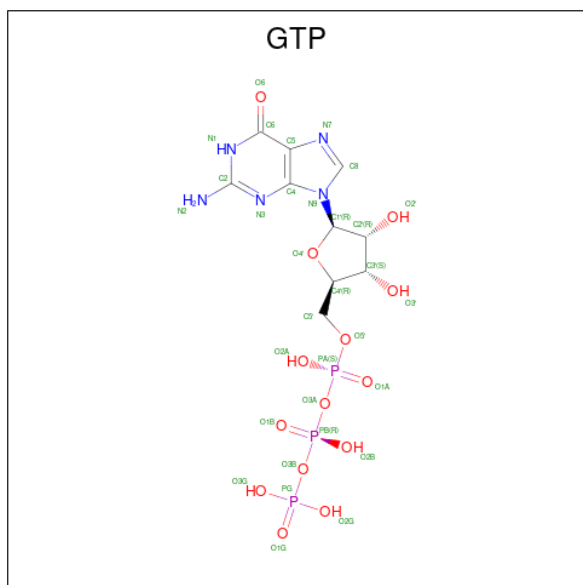
| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| k     | 168     | ALA      | -      | expression tag | UNP A0A7J6K232 |
| k     | 169     | GLN      | -      | expression tag | UNP A0A7J6K232 |
| k     | 170     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| k     | 171     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| k     | 172     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| k     | 173     | THR      | -      | expression tag | UNP A0A7J6K232 |
| k     | 174     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| k     | 175     | ASN      | -      | expression tag | UNP A0A7J6K232 |
| k     | 176     | ASP      | -      | expression tag | UNP A0A7J6K232 |
| k     | 177     | ALA      | -      | expression tag | UNP A0A7J6K232 |
| k     | 178     | THR      | -      | expression tag | UNP A0A7J6K232 |
| k     | 179     | ASP      | -      | expression tag | UNP A0A7J6K232 |
| k     | 180     | PRO      | -      | expression tag | UNP A0A7J6K232 |
| k     | 181     | TRP      | -      | expression tag | UNP A0A7J6K232 |
| k     | 182     | LYS      | -      | expression tag | UNP A0A7J6K232 |
| k     | 183     | LYS      | -      | expression tag | UNP A0A7J6K232 |
| k     | 184     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| k     | 185     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| k     | 186     | PRO      | -      | expression tag | UNP A0A7J6K232 |
| k     | 187     | GLN      | -      | expression tag | UNP A0A7J6K232 |
| k     | 188     | ASN      | -      | expression tag | UNP A0A7J6K232 |
| k     | 189     | VAL      | -      | expression tag | UNP A0A7J6K232 |
| l     | 167     | SER      | -      | expression tag | UNP A0A7J6K232 |
| l     | 168     | ALA      | -      | expression tag | UNP A0A7J6K232 |
| l     | 169     | GLN      | -      | expression tag | UNP A0A7J6K232 |
| l     | 170     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| l     | 171     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| l     | 172     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| l     | 173     | THR      | -      | expression tag | UNP A0A7J6K232 |
| l     | 174     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| l     | 175     | ASN      | -      | expression tag | UNP A0A7J6K232 |
| l     | 176     | ASP      | -      | expression tag | UNP A0A7J6K232 |
| l     | 177     | ALA      | -      | expression tag | UNP A0A7J6K232 |
| l     | 178     | THR      | -      | expression tag | UNP A0A7J6K232 |
| l     | 179     | ASP      | -      | expression tag | UNP A0A7J6K232 |
| l     | 180     | PRO      | -      | expression tag | UNP A0A7J6K232 |
| l     | 181     | TRP      | -      | expression tag | UNP A0A7J6K232 |
| l     | 182     | LYS      | -      | expression tag | UNP A0A7J6K232 |
| l     | 183     | LYS      | -      | expression tag | UNP A0A7J6K232 |
| l     | 184     | ARG      | -      | expression tag | UNP A0A7J6K232 |
| l     | 185     | LEU      | -      | expression tag | UNP A0A7J6K232 |
| l     | 186     | PRO      | -      | expression tag | UNP A0A7J6K232 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| 1     | 187     | GLN      | -      | expression tag | UNP A0A7J6K232 |
| 1     | 188     | ASN      | -      | expression tag | UNP A0A7J6K232 |
| 1     | 189     | VAL      | -      | expression tag | UNP A0A7J6K232 |

- Molecule 9 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 9   | A0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | A2    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | A4    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | A6    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | A8    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | B0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | B2    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | B4    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | B6    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 9   | B8    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | C0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | C3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | C4    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | C6    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | C8    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | D0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | D2    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | D4    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | D6    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | D8    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | E0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | E2    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | E4    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | E6    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | E8    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 9   | F0    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | A0    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 10  | A2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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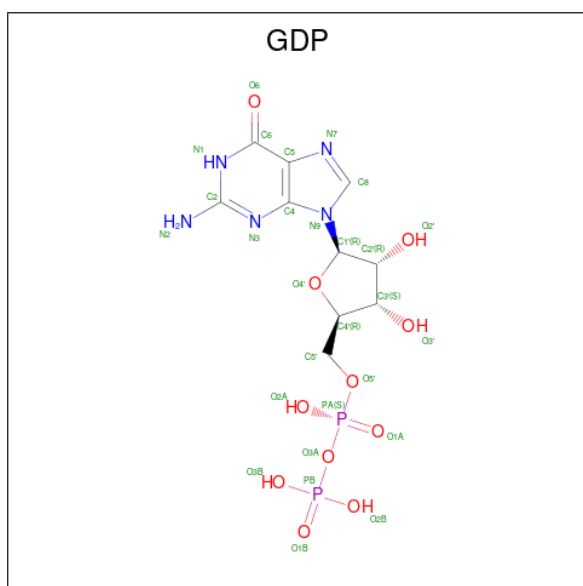
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 10  | A5    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | A7    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | A8    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | B0    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | B2    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | B4    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | B6    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | B8    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | C0    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | C2    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | C4    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | C6    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | C8    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | D0    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | D2    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | D4    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | D6    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | D8    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | E1    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | E2    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 10  | E4    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | E6    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 10  | E9    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 10  | F0    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 11  | A1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | A3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | A5    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | A7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | A9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | B1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | B3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | B5    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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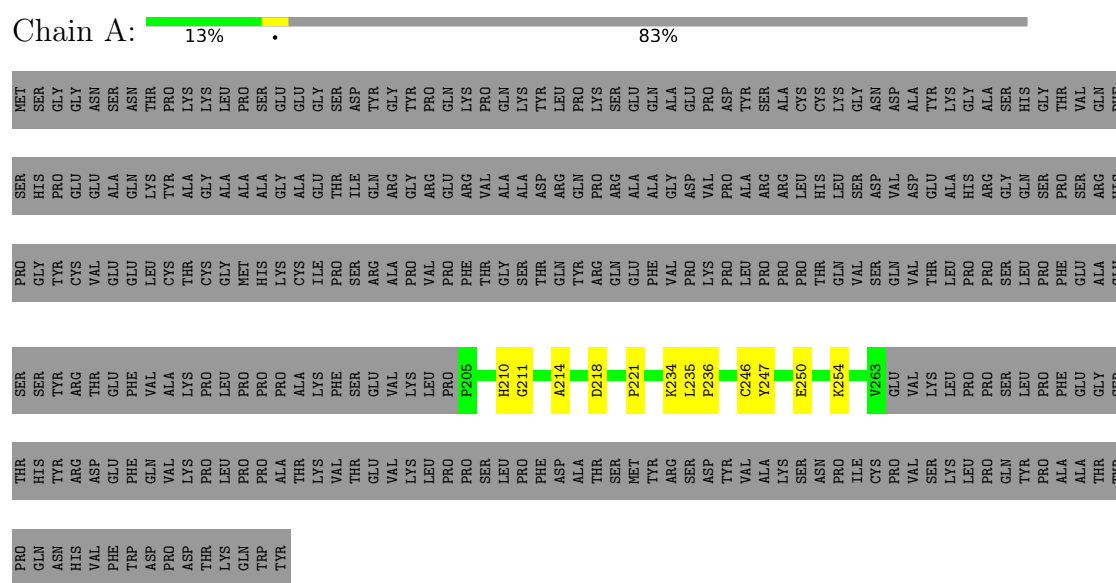
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 11  | B7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | B9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | C1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | C3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | C5    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | C7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | C9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | D1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | D3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | D5    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | D7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | D9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | E1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | E3    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | E5    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | E7    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | E9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 11  | F1    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

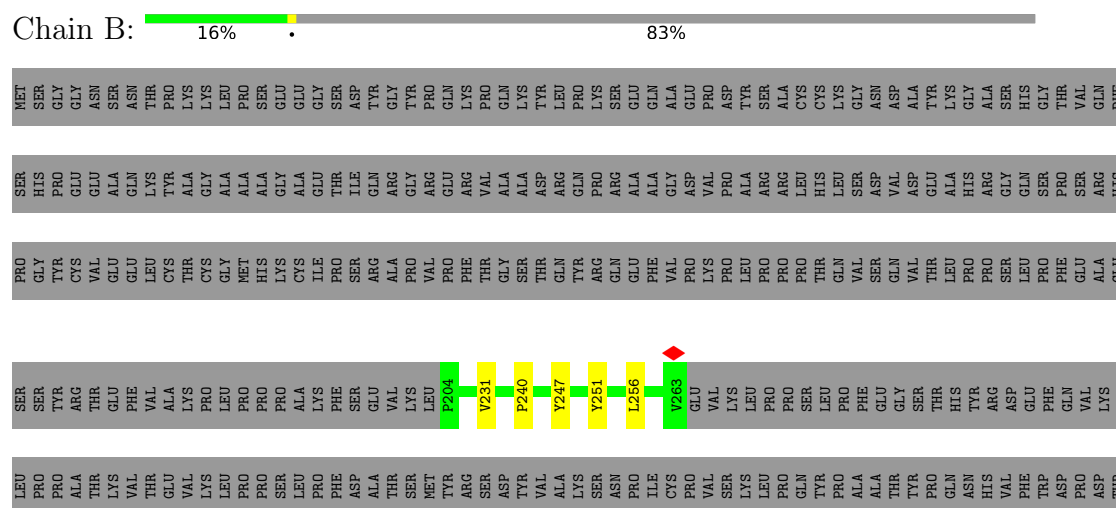
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

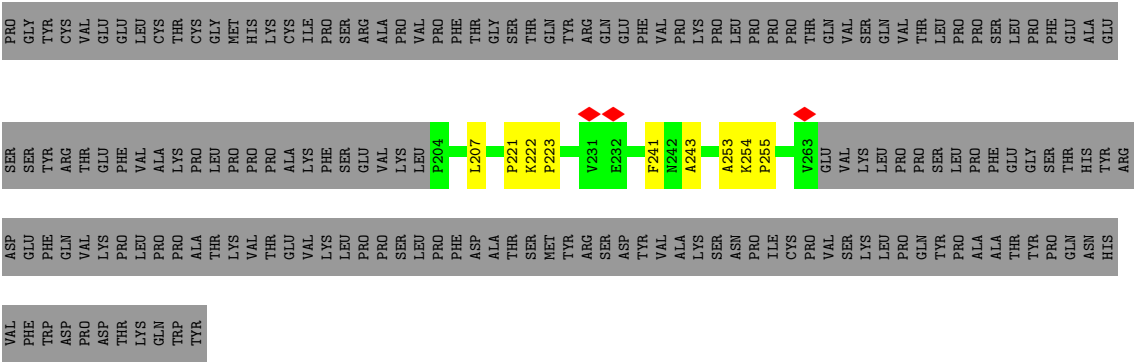
#### • Molecule 1: Microtubule associated protein SPM1



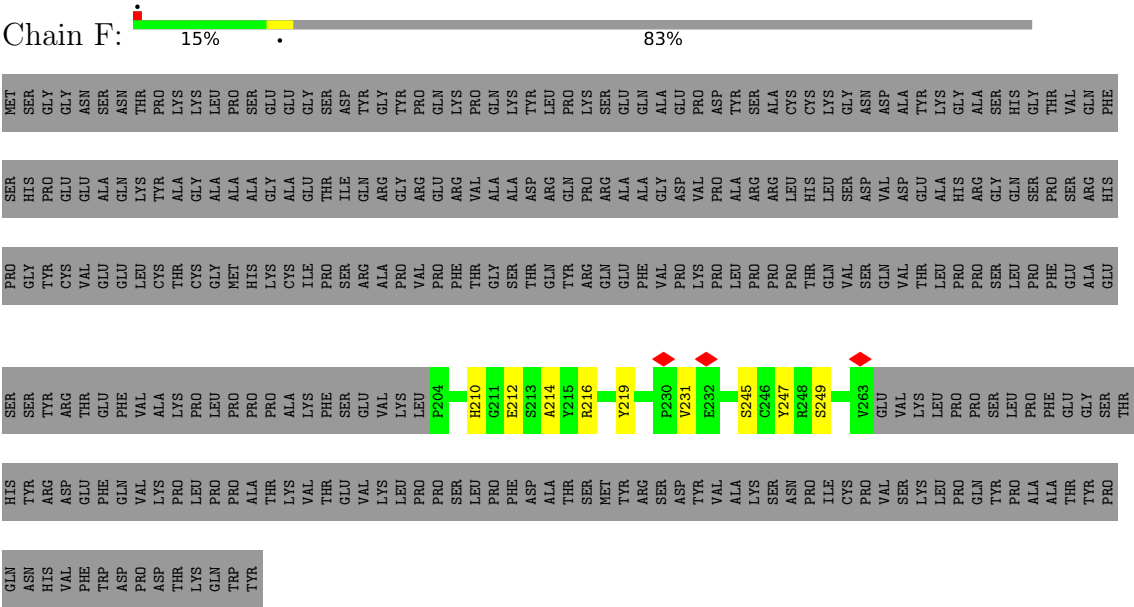
#### • Molecule 1: Microtubule associated protein SPM1



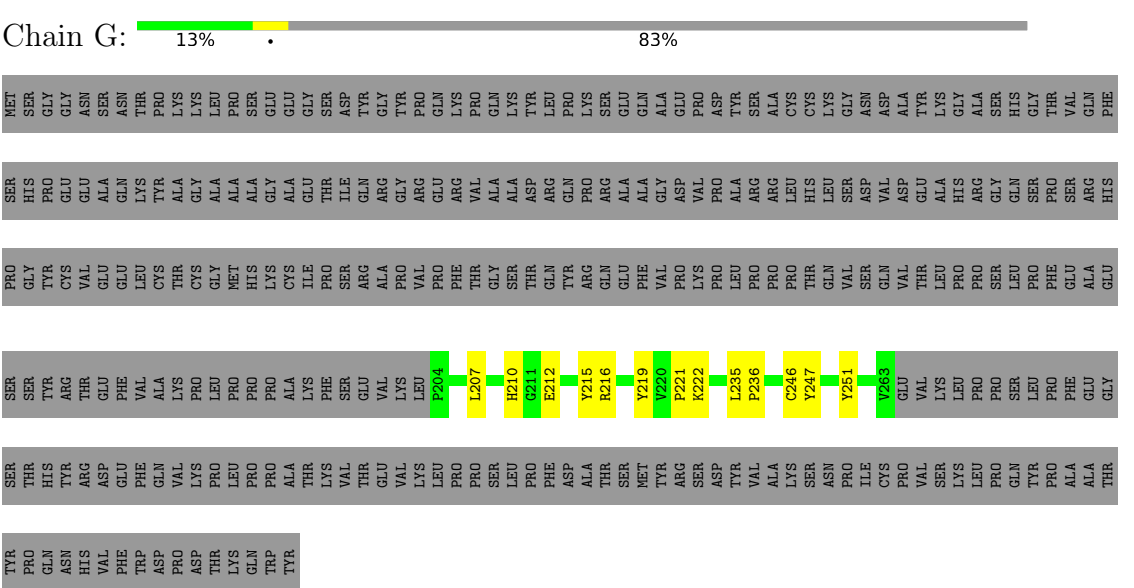
[illegible]



• Molecule 1: Microtubule associated protein SPM1



• Molecule 1: Microtubule associated protein SPM1





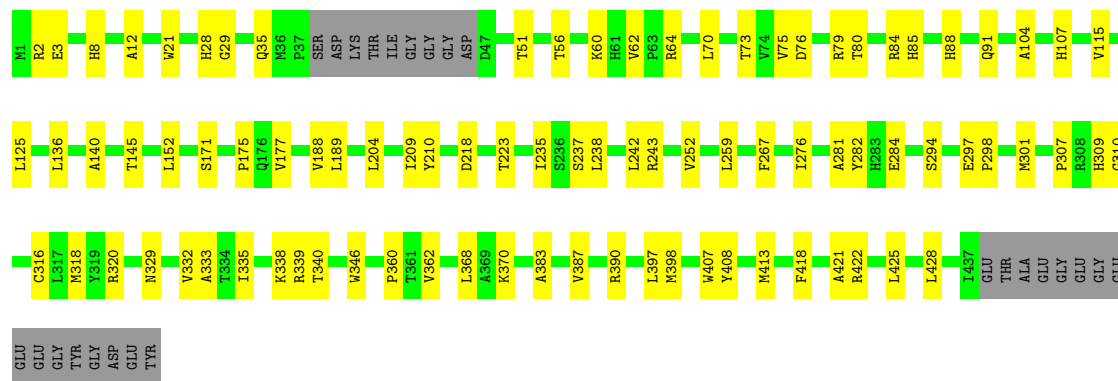






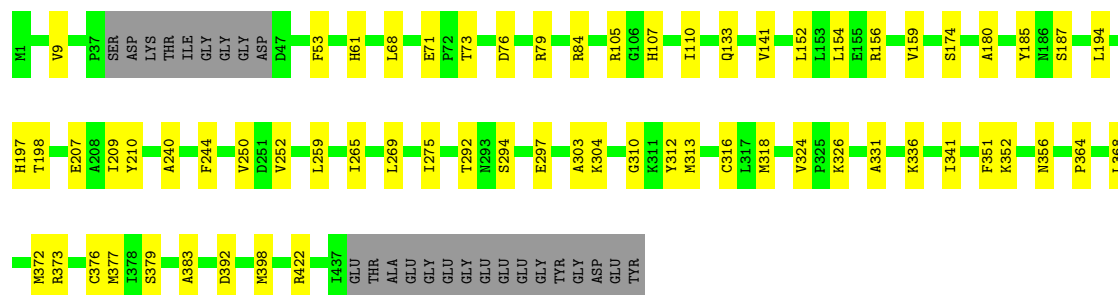
• Molecule 2: Tubulin alpha chain

Chain B0: 75% 19% 6%



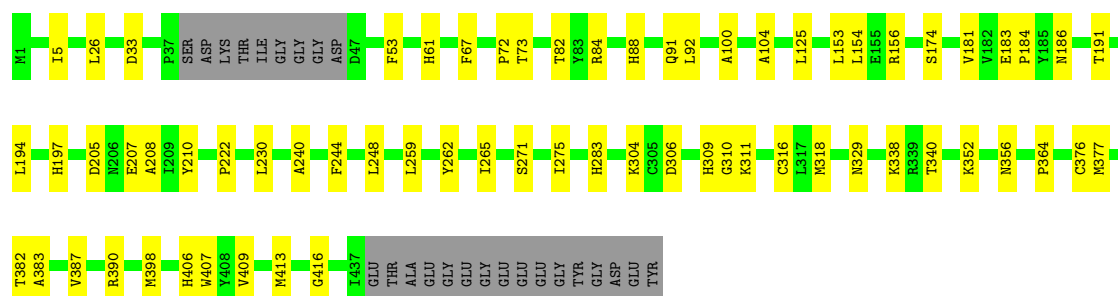
• Molecule 2: Tubulin alpha chain

Chain B2: 80% 14% 6%



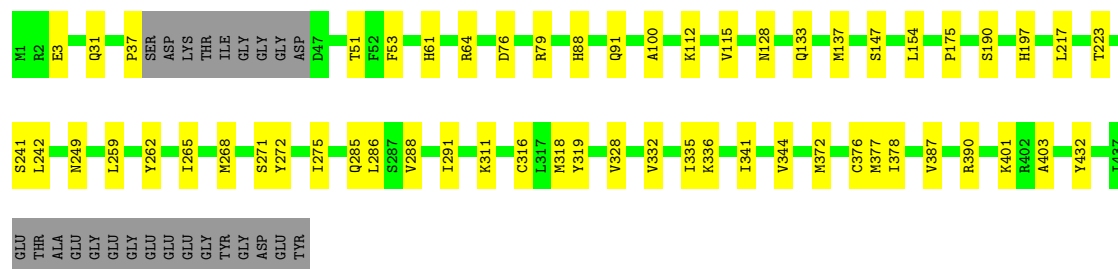
• Molecule 2: Tubulin alpha chain

Chain B4: 80% 15% 6%



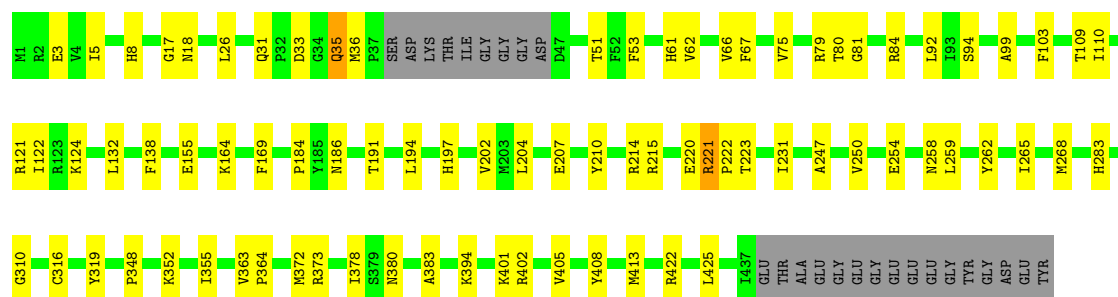
• Molecule 2: Tubulin alpha chain

Chain B6: 82% 13% 6%



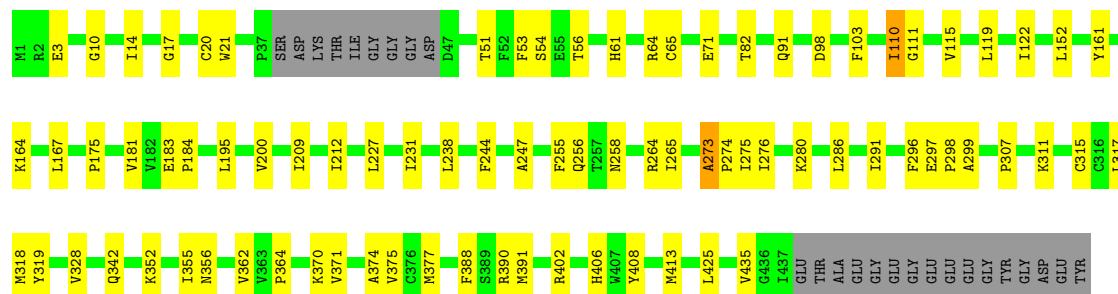
- Molecule 2: Tubulin alpha chain

Chain B8: 77% 17% 6%



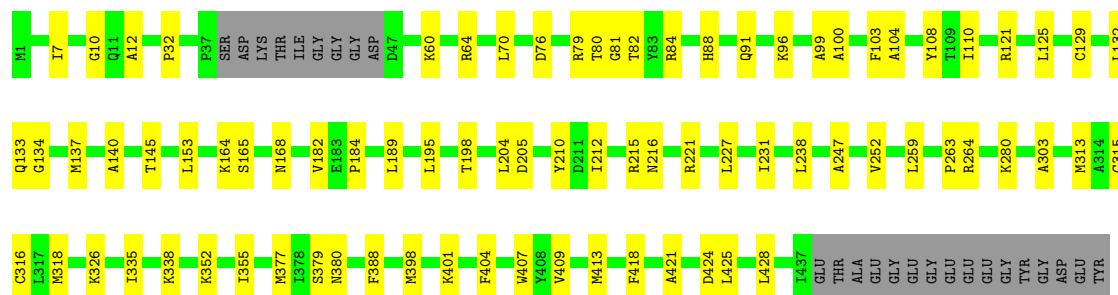
- Molecule 2: Tubulin alpha chain

Chain C0: 76% 18% 6%



- Molecule 2: Tubulin alpha chain

Chain C2: 77% 18% 6%



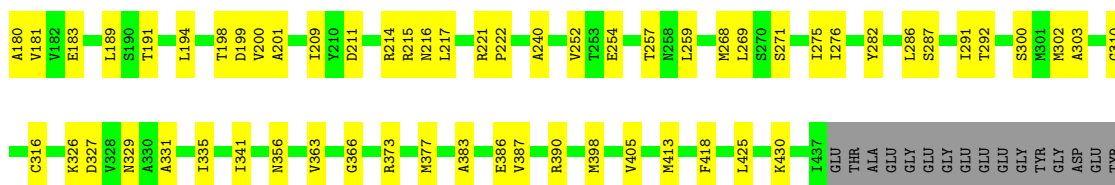
- Molecule 2: Tubulin alpha chain

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |   |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|---|
| H309 | H310 | H311 | H312 | H313 | H314 | H315 | H316 | H317 | H318 | H319 | H320 | H321 | H322 | H323 | H324 | H325 | H326 | H327 | H328 | H329 | H330 | H331 | H332 | H333 | H334 | H335 | H336 | H337 | H338 | H339 | H340 | H341 | H342 | H343 | H344 | H345 | H346 | H347 | H348 | H349 | H350 | H351 | H352 | H353 | H354 | H355 | H356 | H357 | H358 | H359 | H360 | H361 | H362 | H363 | H364 | H365 | H366 | H367 | H368 | H369 | H370 | H371 | H372 | H373 | H374 | H375 | H376 | H377 | H378 | H379 | H380 | H381 | H382 | H383 | H384 | H385 | H386 | H387 | H388 | H389 | H390 | H391 | H392 | H393 | H394 | H395 | H396 | H397 | H398 | H399 | H400 | H401 | H402 | H403 | H404 | H405 | H406 | H407 | H408 | H409 | H410 | H411 | H412 | H413 | H414 | H415 | H416 | H417 | H418 | H419 | H420 | H421 | H422 | H423 | H424 | H425 | H426 | H427 | H428 | H429 | H430 | H431 | H432 | H433 | H434 | H435 | H436 | H437 | H438 | H439 | H440 | H441 | H442 | H443 | H444 | H445 | H446 | H447 | H448 | H449 | H450 | H451 | H452 | H453 | H454 | H455 | H456 | H457 | H458 | H459 | H460 | H461 | H462 | H463 | H464 | H465 | H466 | H467 | H468 | H469 | H470 | H471 | H472 | H473 | H474 | H475 | H476 | H477 | H478 | H479 | H480 | H481 | H482 | H483 | H484 | H485 | H486 | H487 | H488 | H489 | H490 | H491 | H492 | H493 | H494 | H495 | H496 | H497 | H498 | H499 | H500 | H501 | H502 | H503 | H504 | H505 | H506 | H507 | H508 | H509 | H510 | H511 | H512 | H513 | H514 | H515 | H516 | H517 | H518 | H519 | H520 | H521 | H522 | H523 | H524 | H525 | H526 | H527 | H528 | H529 | H530 | H531 | H532 | H533 | H534 | H535 | H536 | H537 | H538 | H539 | H540 | H541 | H542 | H543 | H544 | H545 | H546 | H547 | H548 | H549 | H550 | H551 | H552 | H553 | H554 | H555 | H556 | H557 | H558 | H559 | H560 | H561 | H562 | H563 | H564 | H565 | H566 | H567 | H568 | H569 | H570 | H571 | H572 | H573 | H574 | H575 | H576 | H577 | H578 | H579 | H580 | H581 | H582 | H583 | H584 | H585 | H586 | H587 | H588 | H589 | H590 | H591 | H592 | H593 | H594 | H595 | H596 | H597 | H598 | H599 | H600 | H601 | H602 | H603 | H604 | H605 | H606 | H607 | H608 | H609 | H610 | H611 | H612 | H613 | H614 | H615 | H616 | H617 | H618 | H619 | H620 | H621 | H622 | H623 | H624 | H625 | H626 | H627 | H628 | H629 | H630 | H631 | H632 | H633 | H634 | H635 | H636 | H637 | H638 | H639 | H640 | H641 | H642 | H643 | H644 | H645 | H646 | H647 | H648 | H649 | H650 | H651 | H652 | H653 | H654 | H655 | H656 | H657 | H658 | H659 | H660 | H661 | H662 | H663 | H664 | H665 | H666 | H667 | H668 | H669 | H670 | H671 | H672 | H673 | H674 | H675 | H676 | H677 | H678 | H679 | H680 | H681 | H682 | H683 | H684 | H685 | H686 | H687 | H688 | H689 | H690 | H691 | H692 | H693 | H694 | H695 | H696 | H697 | H698 | H699 | H700 | H701 | H702 | H703 | H704 | H705 | H706 | H707 | H708 | H709 | H710 | H711 | H712 | H713 | H714 | H715 | H716 | H717 | H718 | H719 | H720 | H721 | H722 | H723 | H724 | H725 | H726 | H727 | H728 | H729 | H730 | H731 | H732 | H733 | H734 | H735 | H736 | H737 | H738 | H739 | H740 | H741 | H742 | H743 | H744 | H745 | H746 | H747 | H748 | H749 | H750 | H751 | H752 | H753 | H754 | H755 | H756 | H757 | H758 | H759 | H760 | H761 | H762 | H763 | H764 | H765 | H766 | H767 | H768 | H769 | H770 | H771 | H772 | H773 | H774 | H775 | H776 | H777 | H778 | H779 | H780 | H781 | H782 | H783 | H784 | H785 | H786 | H787 | H788 | H789 | H790 | H791 | H792 | H793 | H794 | H795 | H796 | H797 | H798 | H799 | H800 | H801 | H802 | H803 | H804 | H805 | H806 | H807 | H808 | H809 | H810 | H811 | H812 | H813 | H814 | H815 | H816 | H817 | H818 | H819 | H |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|---|

|      |      |      |      |
|------|------|------|------|
| ALA  | L286 | S165 | M1   |
|      | GLU  | L166 | R2   |
|      | GLY  | L167 | E3   |
|      | GLU  | T292 | L23  |
|      | GLU  | K302 | E27  |
|      | GLU  | K311 | P37  |
|      | GLY  | V182 | SER  |
|      | TYR  | V323 | ASP  |
|      | GLY  | V324 | LYS  |
|      | ASP  | K326 | THR  |
| GLU  | D327 | T198 | I1E  |
|      | V328 | V200 | GLY  |
|      | A331 | A201 | GLY  |
|      |      | V202 | GLY  |
|      | V203 | ASP  |      |
|      | D47  | D47  |      |
|      | K339 | V210 | T51  |
|      | Q342 | C213 | V66  |
|      | K346 | L217 | E71  |
|      | G350 | D218 | T80  |
| F351 | I219 |      |      |
| GLU  | K352 | E220 |      |
|      | T355 | R221 | R84  |
|      |      | L227 | H88  |
|      | K356 | P89  | E90  |
|      | T361 | V234 | Q91  |
|      | V371 | L238 | D98  |
|      | K372 | T239 | M101 |
|      | R373 | A240 | N102 |
|      | N380 | A247 | F103 |
|      | T384 | E254 | A104 |
| F388 | F255 | R105 |      |
| GLU  | L397 | Q256 | Y108 |
|      | K401 | T257 | T109 |
|      | F404 | L259 | L119 |
|      |      | V260 | I122 |
|      | Y408 | L265 | C129 |
|      | M413 | F267 | L132 |
|      | E417 | M268 | M137 |
|      | L425 | P274 | F138 |
|      | L437 | L275 | L154 |
|      | GLU  | L276 | V164 |
| THR  | K280 |      |      |

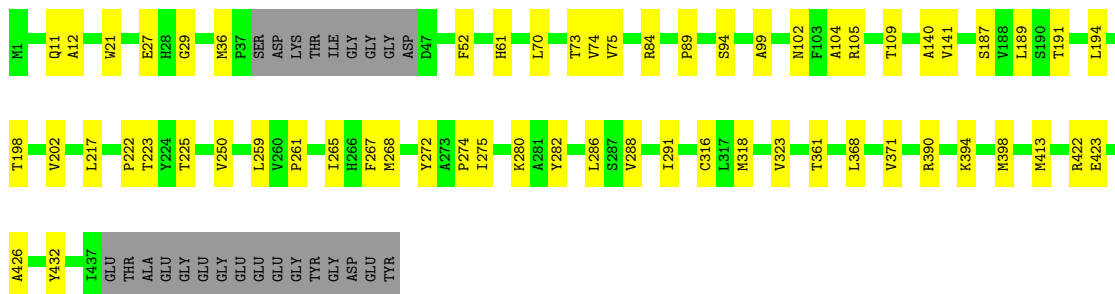
|     |     |      |      |      |
|-----|-----|------|------|------|
| TYR | GLY | C316 | A180 | M1   |
|     | ASP | V323 | V181 | R2   |
| TYR | GLU | V323 | V182 | E3   |
|     |     |      | E183 | V4   |
|     |     | T340 | M186 | G10  |
|     |     | I341 | S187 | I14  |
|     |     | I355 | L195 | H28  |
|     |     | V363 | T198 | C29  |
|     |     | G366 | D199 | I30  |
|     |     | M377 | V200 | P37  |
|     |     |      | A201 | SER  |
|     |     | R380 | N206 | ASP  |
|     |     | A383 | E207 | LYS  |
|     |     | F388 | A208 | THR  |
|     |     |      | I209 | ILE  |
|     |     |      | V210 | GLY  |
|     |     | F395 | I219 | GLY  |
|     |     | M398 | P222 | ASP  |
|     |     | V405 | T223 | D47  |
|     |     | H406 | V224 | T51  |
|     |     | A407 | L227 | L68  |
|     |     | V408 | L230 | F103 |
|     |     | M413 |      | A104 |
|     |     | E417 | A247 | G106 |
|     |     | F418 | F255 | H107 |
|     |     | S419 |      | Y108 |
|     |     | A420 | L259 | T109 |
|     |     | A421 | R264 | I110 |
|     |     | R422 | I265 | L119 |
|     |     |      |      | L123 |
|     |     | L425 | M268 |      |
|     |     | R430 | Y272 | L136 |
|     |     | D431 |      | V141 |
|     |     | V432 | I276 | T145 |
|     |     | E433 |      | L149 |
|     |     | E434 | E279 | L152 |
|     |     | I437 | K280 | L153 |
|     | GLU | THR  | M301 | L154 |
|     | ALA |      | K304 | E155 |
|     | GLU |      | C305 | R156 |
|     | GLY |      | D306 |      |
|     | GLU |      | G309 | D160 |
|     | GLU |      | H310 | Q176 |
|     | GLU |      | C310 | H177 |
|     | GLY |      | V213 |      |

|    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R1 | R2 | E3 | I7 | A12 | P37 | SER | ASP | LVS | THR | ILE | GLY | GLY | GLY | ASP | D47 | T51 | E71 | P72 | T73 | D76 | R79 | H88 | Q91 | D89 | A89 | A100 | M101 | H107 | V115 | I122 | R123 | Q133 | A140 | V141 | G144 | L152 | Y161 | K166 | L167 |
|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



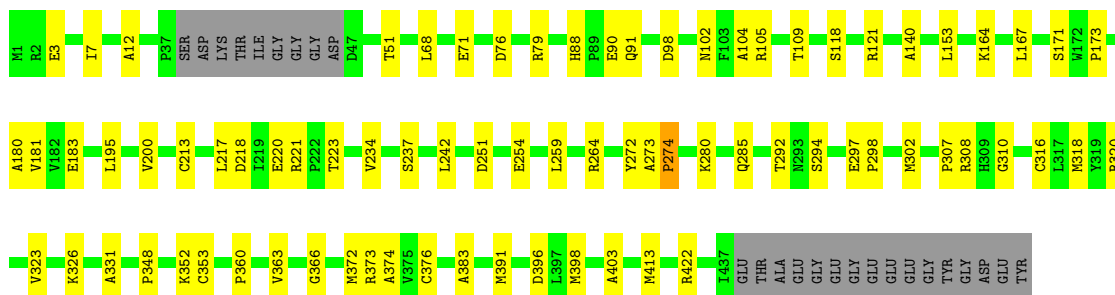
• Molecule 2: Tubulin alpha chain

Chain D2: 81% 13% 6%



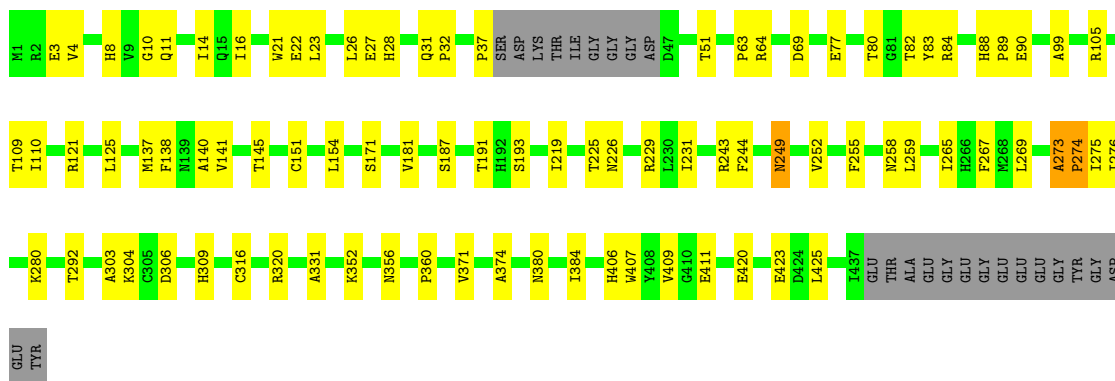
• Molecule 2: Tubulin alpha chain

Chain D4: 77% 17% 6%



• Molecule 2: Tubulin alpha chain

Chain D6: 75% 19% 6%



• Molecule 2: Tubulin alpha chain

|      |      |      |     |
|------|------|------|-----|
| K401 | F255 | D98  | M1  |
| M413 | L259 | A104 | R2  |
| E414 | L265 | R121 | E3  |
| G416 | H266 | L125 | V4  |
| L428 | F267 | F135 | I5  |
| E429 | M268 | M137 | S6  |
| A232 | A273 | F138 | I7  |
| I437 | P274 | M139 | H8  |
| GLU  | S277 | A140 | A12 |
| THR  | A278 | K164 | Q15 |
| ALA  | L286 | L167 | I16 |
| GLU  | R304 | S171 | E22 |
| GLY  | C305 | S174 | C25 |
| GLU  | D306 | P175 | H28 |
| GLU  | P307 | G176 | G29 |
| GLU  | G310 | V177 | I30 |
| GLU  | C316 | L195 | P37 |
| TYR  | L317 | V200 | SER |
| GLY  | K318 | M203 | ASP |
| ASP  | V319 | L204 | LVS |
| GLU  | R320 | D211 | THR |
| TYR  | K338 | R214 | I1E |
|      | R339 | L217 | GLY |
|      | T340 | E220 | GLY |
|      | P348 | R221 | GLY |
|      | K352 | T225 | ASP |
|      | N356 | M226 | ASP |
|      | Y357 | L227 | D47 |
|      | P360 | N228 | A48 |
|      | T361 | R229 | F53 |
|      | V362 | L230 | T56 |
|      | V363 | I231 | H61 |
|      | G366 | T235 | F67 |
|      | K370 | L238 | E71 |
|      | A374 | T239 | D76 |
|      | L378 | A240 | E77 |
|      | S379 | S241 | V78 |
|      | N380 | R242 | R79 |
|      | A383 | V250 | T80 |
|      |      |      | Y83 |
|      |      |      | H88 |
|      |      |      | E90 |
|      |      |      | Q91 |
|      |      |      | L92 |
|      |      |      | I93 |

|      |      |
|------|------|
| I437 | R1   |
| GLU  | R2   |
| THR  | H8   |
| ALA  | V9   |
| GLY  | G10  |
| GLU  | Q11  |
| GLY  | A12  |
| GLU  | G13  |
| GLU  | I14  |
| GLU  | Q15  |
| GLY  | W21  |
| TYR  | D33  |
| GLY  | K36  |
| ASP  | P37  |
| GLU  | SER  |
| GLU  | ASP  |
| GLU  | LYS  |
| GLU  | THR  |
| GLU  | TLE  |
| GLY  | GLY  |
| GLY  | GLY  |
| ASP  | D47  |
| ASP  | A48  |
|      | T51  |
|      | H61  |
|      | R64  |
|      | C65  |
|      | V66  |
|      | L70  |
|      | V74  |
|      | V75  |
|      | D76  |
|      | E77  |
|      | V78  |
|      | R79  |
|      | R105 |
|      | T109 |
|      | I110 |
|      | I122 |
|      | R123 |
|      | K124 |
|      | I125 |
|      | F138 |
|      | I139 |
|      | A140 |
|      | V141 |
|      | T145 |
|      | W172 |
|      | S178 |
|      | T179 |
|      | A180 |
|      | V181 |
|      | W182 |
|      | E183 |
|      | L189 |
|      | I219 |
|      | L238 |
|      | T239 |
|      | A240 |
|      | F244 |
|      | M258 |
|      | Y272 |
|      | A273 |
|      | P274 |
|      | T275 |
|      | I276 |
|      | L286 |
|      | K304 |
|      | M318 |
|      | Y319 |
|      | R320 |
|      | V328 |
|      | K352 |
|      | I355 |
|      | N356 |
|      | P360 |
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|      | R402 |
|      | W407 |
|      | M413 |
|      | E414 |
|      | E415 |

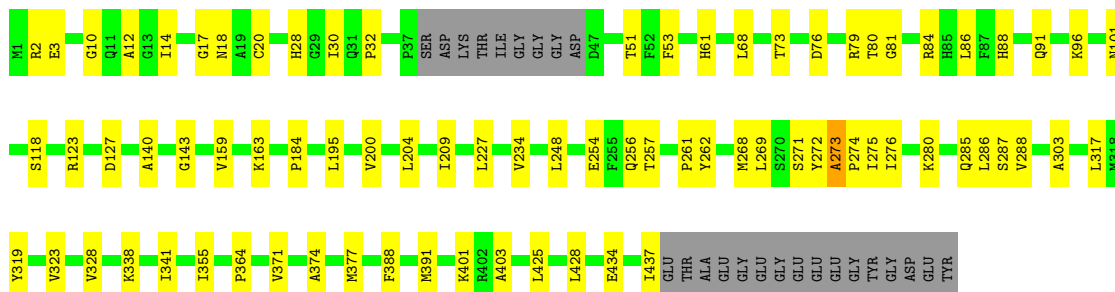
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| I378 | T198 | M1   |
| S379 | A201 | Q11  |
| N380 | D205 | N18  |
| M391 | Y210 | M36  |
| M413 | T223 | P37  |
| E417 | L230 | SR   |
| L428 | F244 | ASP  |
| I437 | F255 | LYS  |
| GLU  | L259 | THR  |
| THR  | I265 | ILE  |
| ALA  | M268 | GLY  |
| GLU  | S271 | GLY  |
| GLU  | Y272 | ASP  |
| GLY  | I276 | D47  |
| GLU  | L286 | A48  |
| GLU  | F296 | H61  |
| GLU  | E297 | L70  |
| GLU  | T298 | E71  |
| TYR  | A303 | V74  |
| GLY  | K311 | V75  |
| GLY  | Y312 | D76  |
| ASP  | M313 | R79  |
| GLU  | C316 | T82  |
| TYR  | L317 | S94  |
|      | R320 | D98  |
|      | K326 | A99  |
|      | L335 | A100 |
|      | K336 | N101 |
|      | T337 | R105 |
|      | K338 | L132 |
|      | V344 | C151 |
|      | N356 | E155 |
|      | P360 | K163 |
|      | M372 | K164 |
|      | M377 | A180 |
|      |      | E183 |
|      |      | P184 |
|      |      | V188 |
|      |      | L195 |

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| E207 | A208 | I209 | Y210 | L227 | F244 | A247 | R264 | I265 | H266 | F267 | A273 | P274 | K280 | A281 | Y282 | R320 | I355 | N356 | G363 | G366 | A374 | N380 | S381 | I384 | V387 | F388 | S389 | R390 | M398 | W407 | M413 | L425 | I437 | GLU  | THR  | ALA  | GLU  | GLU  |      |      |
| E207 | A208 | I209 | Y210 | L227 | F244 | A247 | R264 | I265 | H266 | F267 | A273 | P274 | K280 | A281 | Y282 | R320 | I355 | N356 | G363 | G366 | A374 | N380 | S381 | I384 | V387 | F388 | S389 | R390 | M398 | W407 | M413 | L425 | I437 | GLU  | THR  | ALA  | GLU  | GLU  |      |      |
| R1   | R2   | E3   | V9   | L26  | Q31  | P37  | SEN  | ASP  | LVS  | THR  | ILE  | GLY  | GLY  | ASP  | D47  | T51  | S54  | R64  | L68  | D69  | L70  | E71  | P72  | T73  | X86  | E97  | D98  | A99  | G111 | I114 | L119 | D120 | R121 | K124 | G144 | R156 | T191 | L195 | M203 | L204 |

GLY  
GLU  
GLU  
GLU  
GLY  
TYR  
GLY  
ASP  
GLU  
TYR

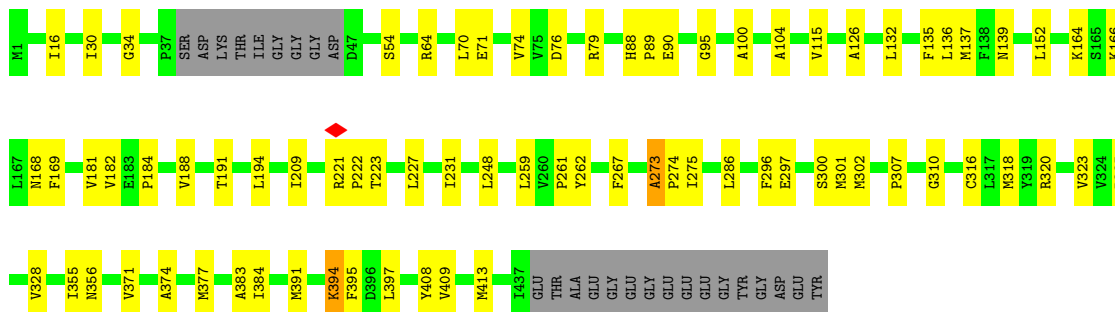
• Molecule 2: Tubulin alpha chain

Chain E6: 77% 17% 6%



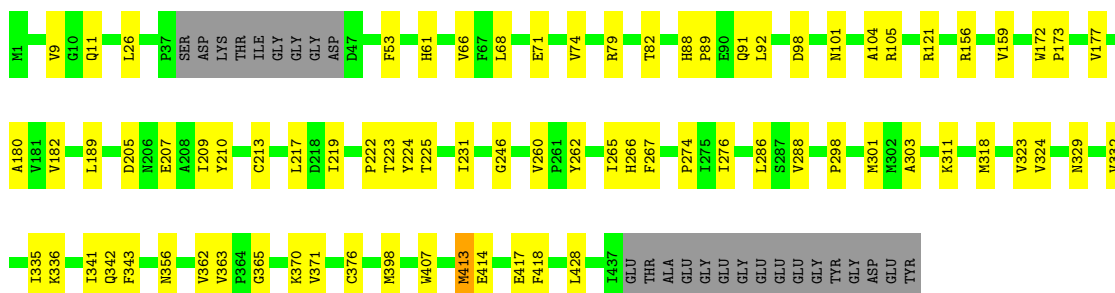
• Molecule 2: Tubulin alpha chain

Chain E8: 78% 16% 6%



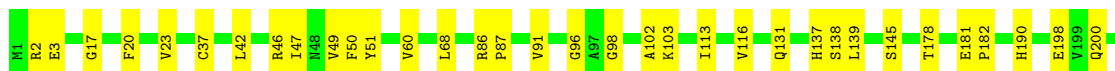
• Molecule 2: Tubulin alpha chain

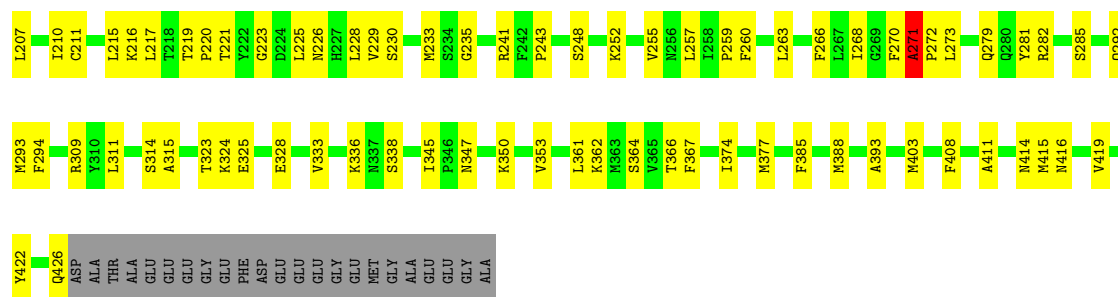
Chain F0: 77% 17% 6%



• Molecule 3: Tubulin beta chain

Chain A1: 71% 24% 5%





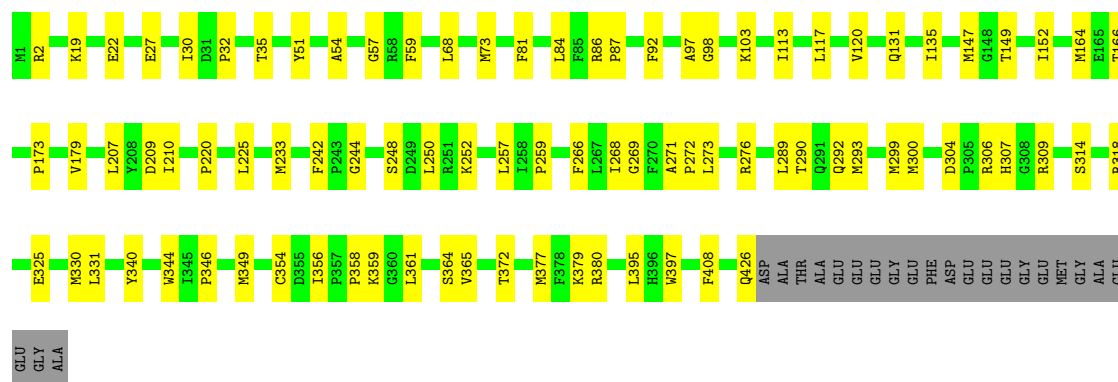
• Molecule 3: Tubulin beta chain

Chain A3: 72% 22% 5%



• Molecule 3: Tubulin beta chain

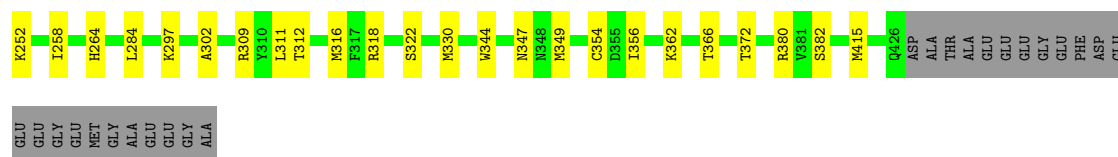
Chain A5: 76% 19% 5%



• Molecule 3: Tubulin beta chain

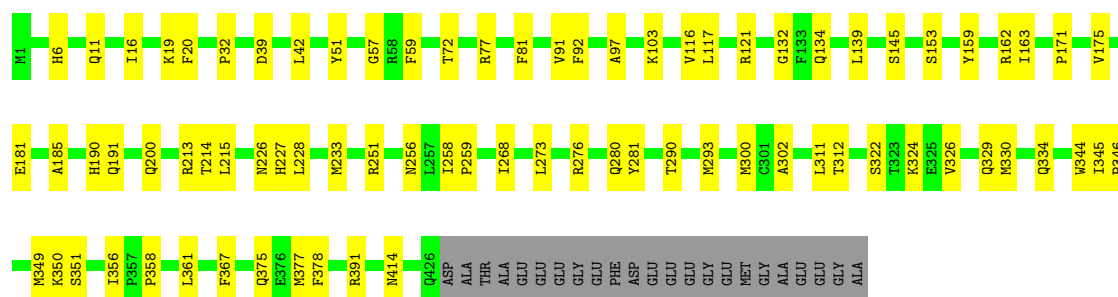
Chain A7: 82% 13% 5%





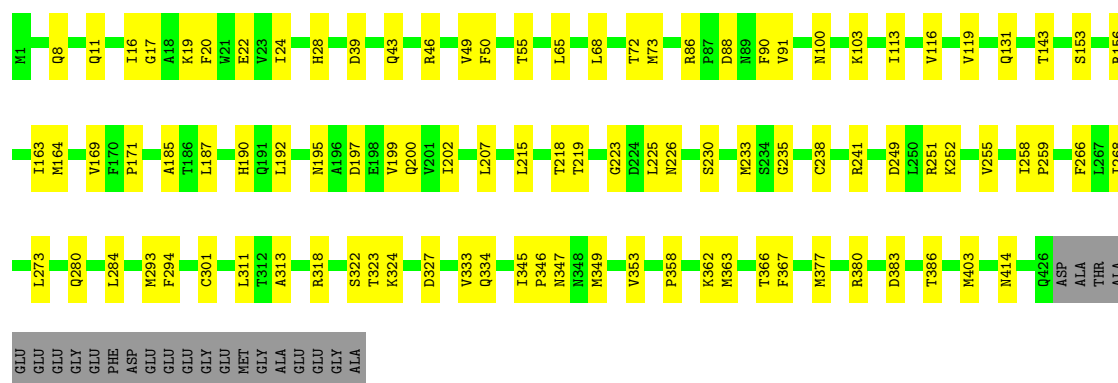
• Molecule 3: Tubulin beta chain

Chain A9: 77% 18% 5%



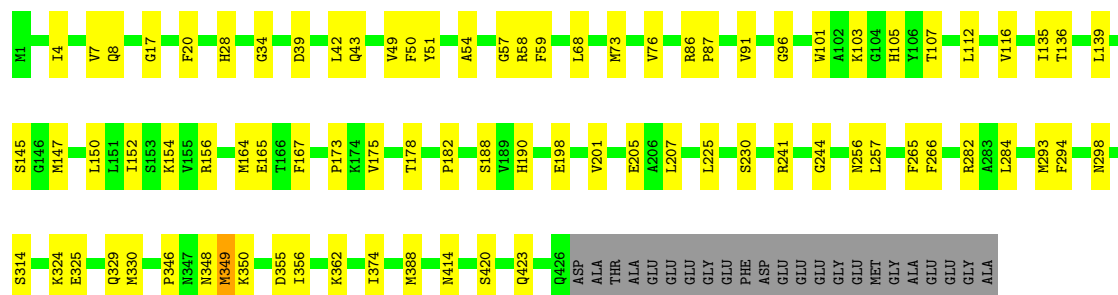
• Molecule 3: Tubulin beta chain

Chain B1: 73% 21% 5%



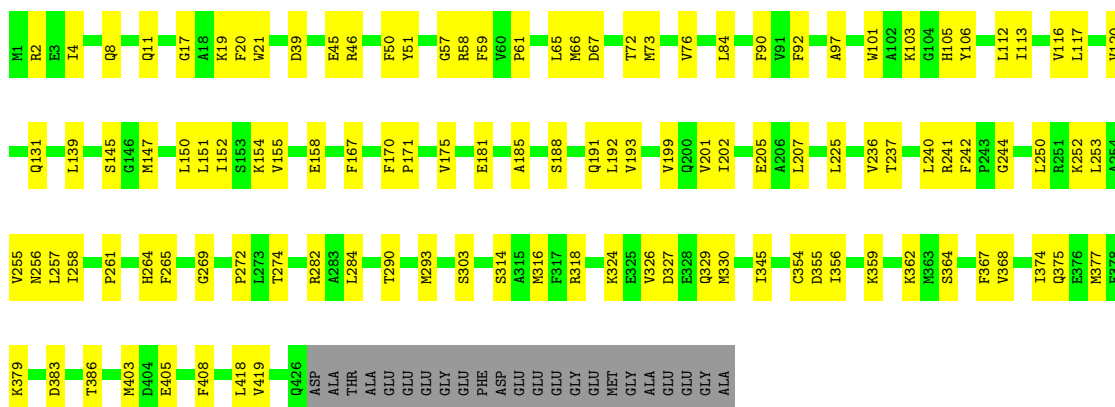
• Molecule 3: Tubulin beta chain

Chain B3: 77% 18% 5%



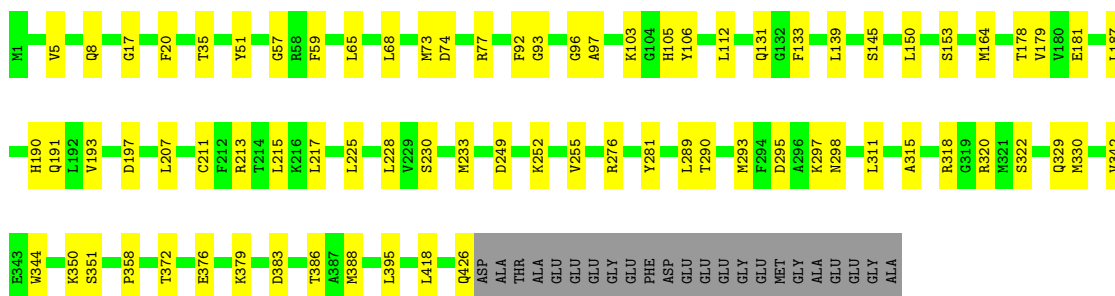
• Molecule 3: Tubulin beta chain

Chain B5: 69% 25% 5%



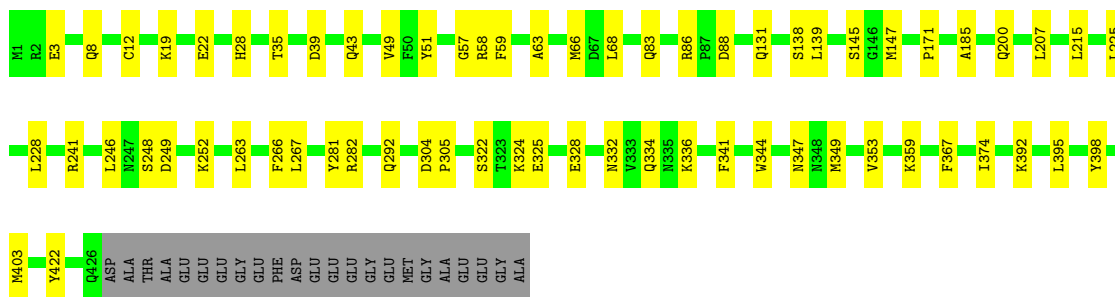
- Molecule 3: Tubulin beta chain

Chain B7: 78% 17% 5%



- Molecule 3: Tubulin beta chain

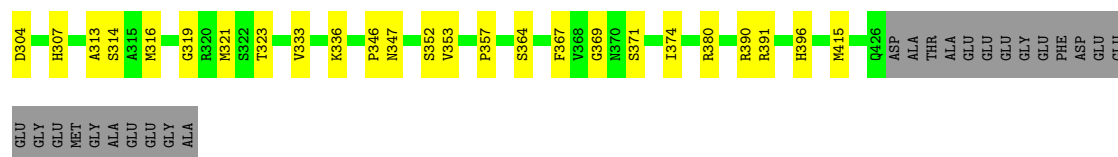
Chain B9: 80% 14% 5%



- Molecule 3: Tubulin beta chain

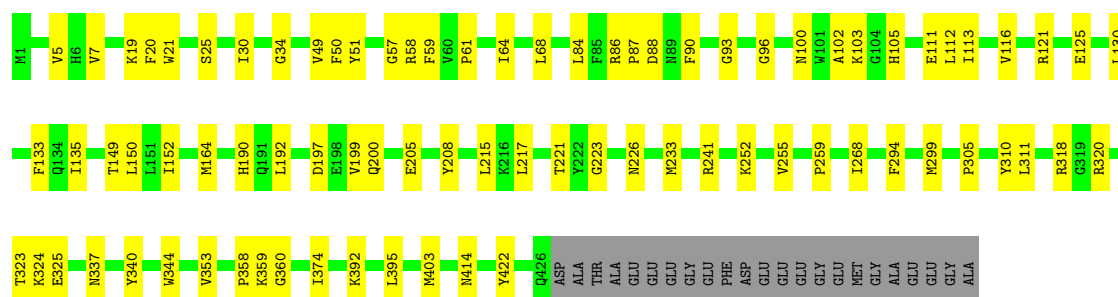
Chain C1: 74% 20% 5%





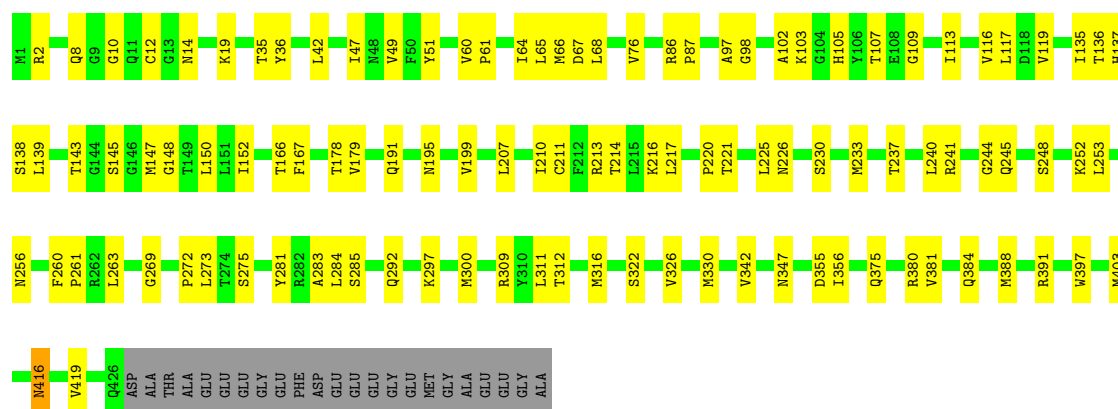
- Molecule 3: Tubulin beta chain

Chain C3: 77% 18% 5%



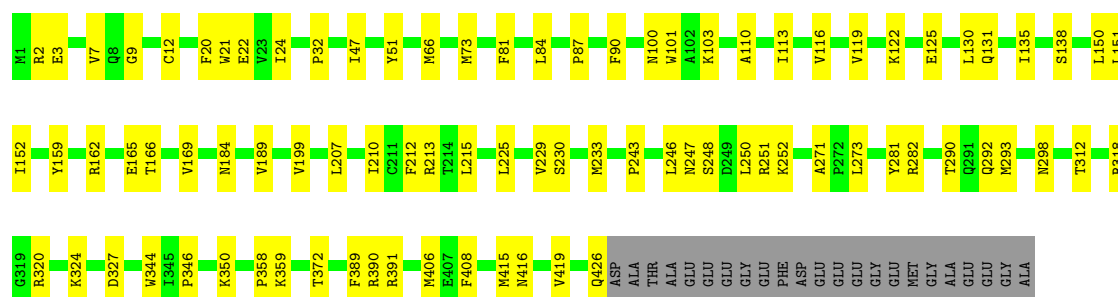
- Molecule 3: Tubulin beta chain

Chain C5: 71% 24% 5%



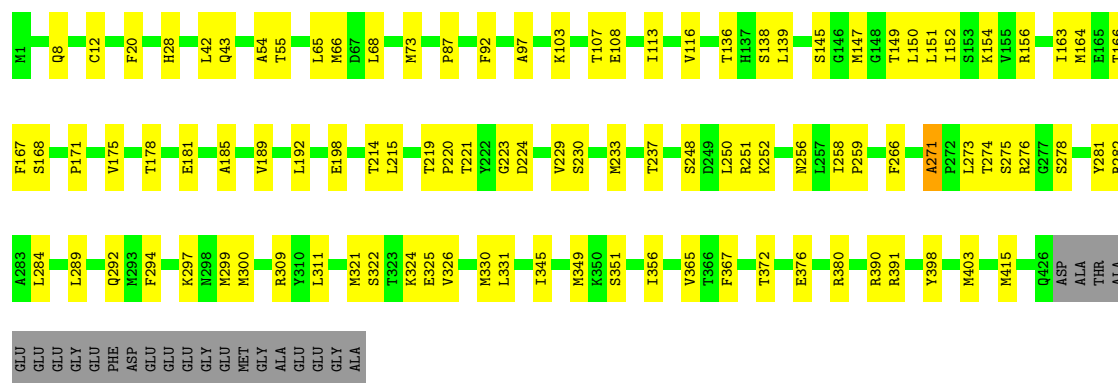
- Molecule 3: Tubulin beta chain

Chain C7: 76% 19% 5%



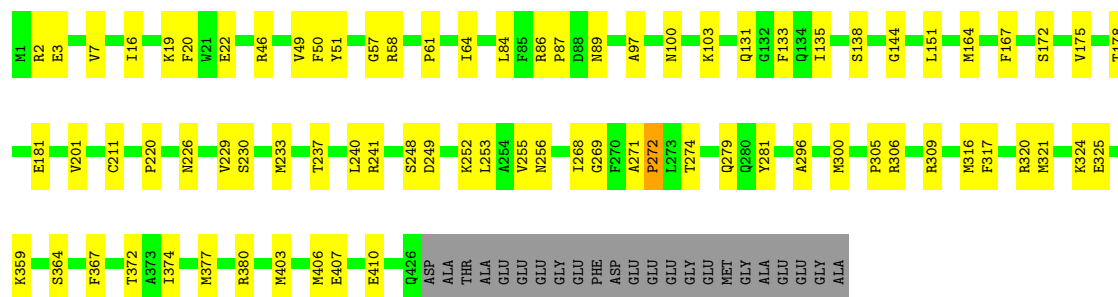
- Molecule 3: Tubulin beta chain

Chain C9:  72% 22% 5%



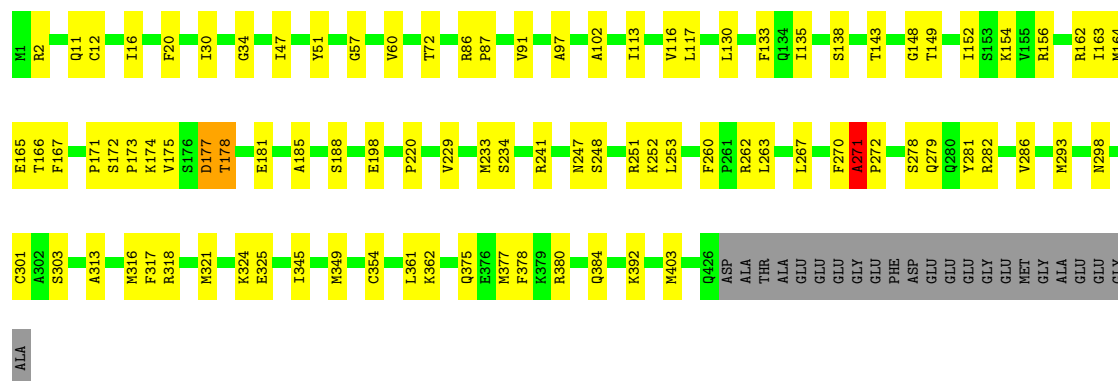
• Molecule 3: Tubulin beta chain

Chain D1:  77% 17% 5%



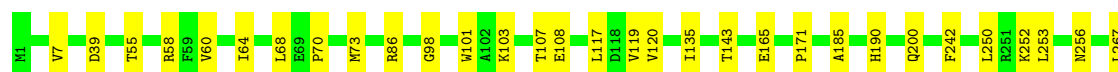
• Molecule 3: Tubulin beta chain

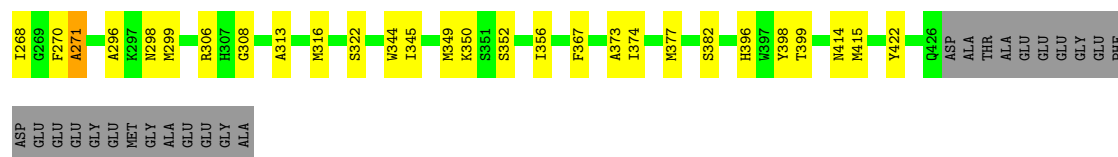
Chain D3:  74% 20% 5%



• Molecule 3: Tubulin beta chain

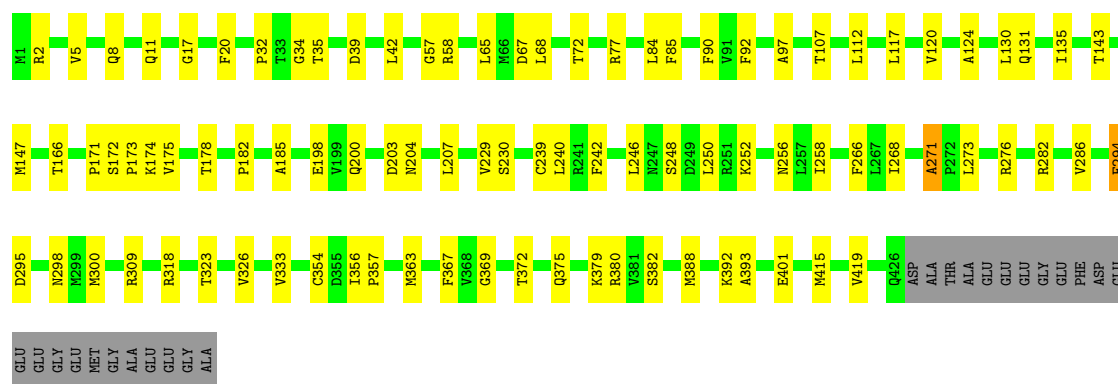
Chain D5:  82% 13% 5%





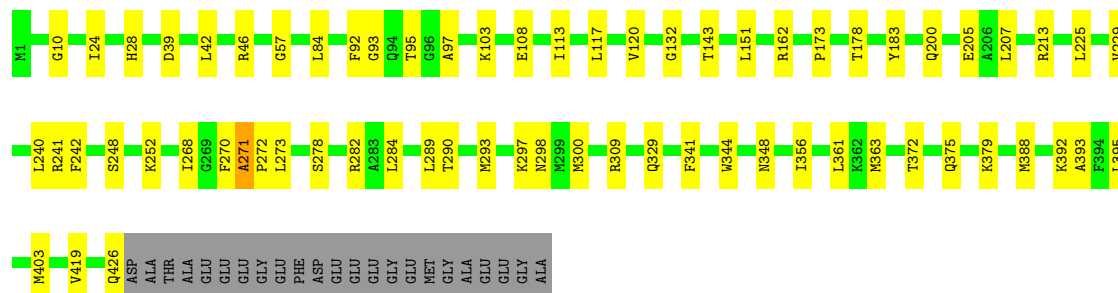
• Molecule 3: Tubulin beta chain

Chain D7: 75% 20% 5%



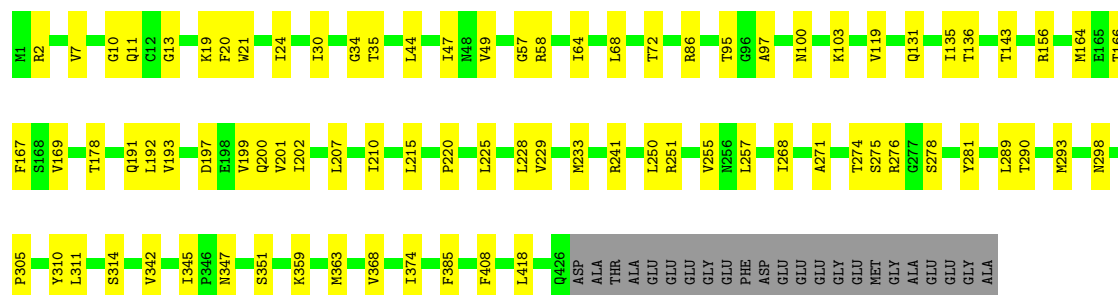
• Molecule 3: Tubulin beta chain

Chain D9: 80% 15% 5%



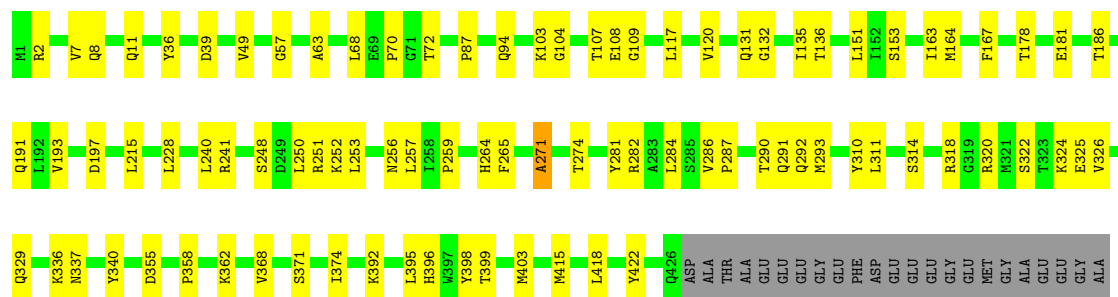
• Molecule 3: Tubulin beta chain

Chain E1: 76% 18% 5%



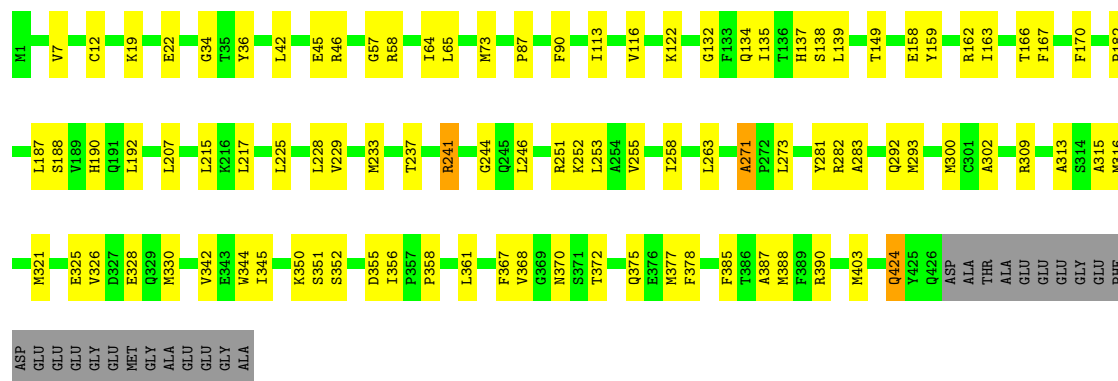
• Molecule 3: Tubulin beta chain

Chain E3: 75% 20% 5%



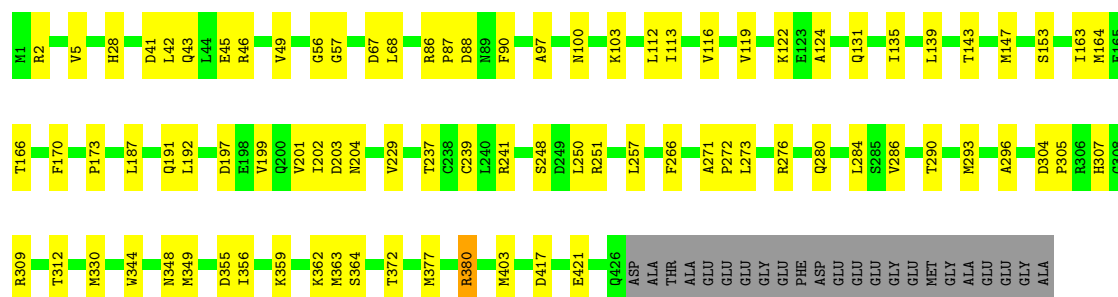
• Molecule 3: Tubulin beta chain

Chain E5: 73% 21% 5%



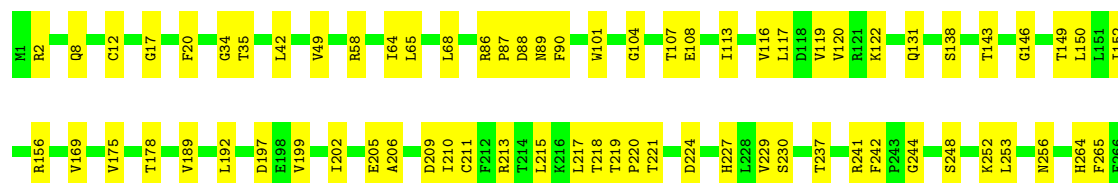
• Molecule 3: Tubulin beta chain

Chain E7: 76% 19% 5%



• Molecule 3: Tubulin beta chain

Chain E9: 71% 23% 5%





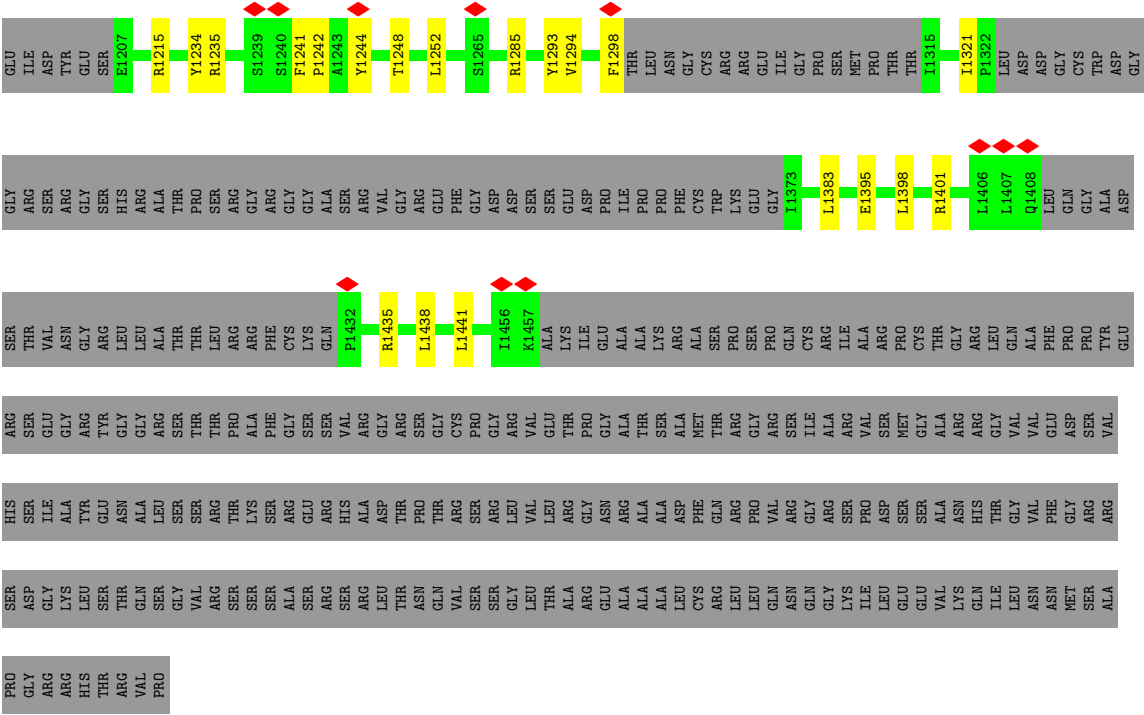




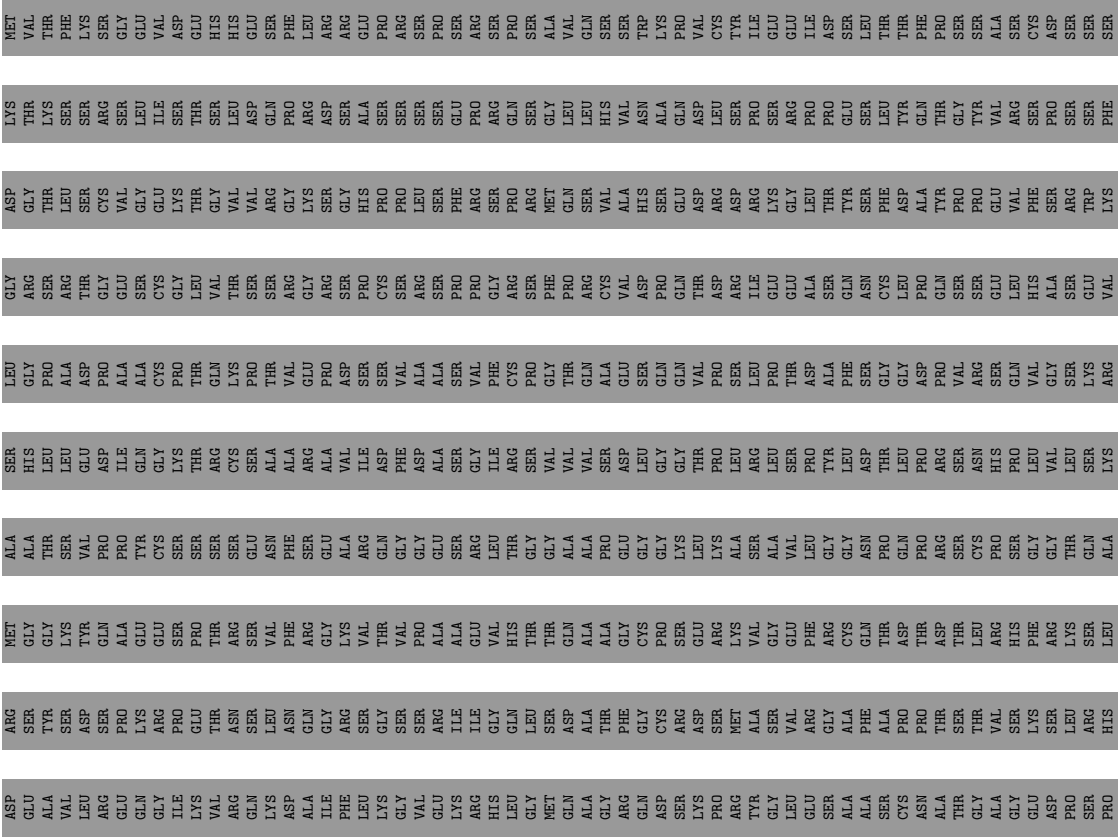








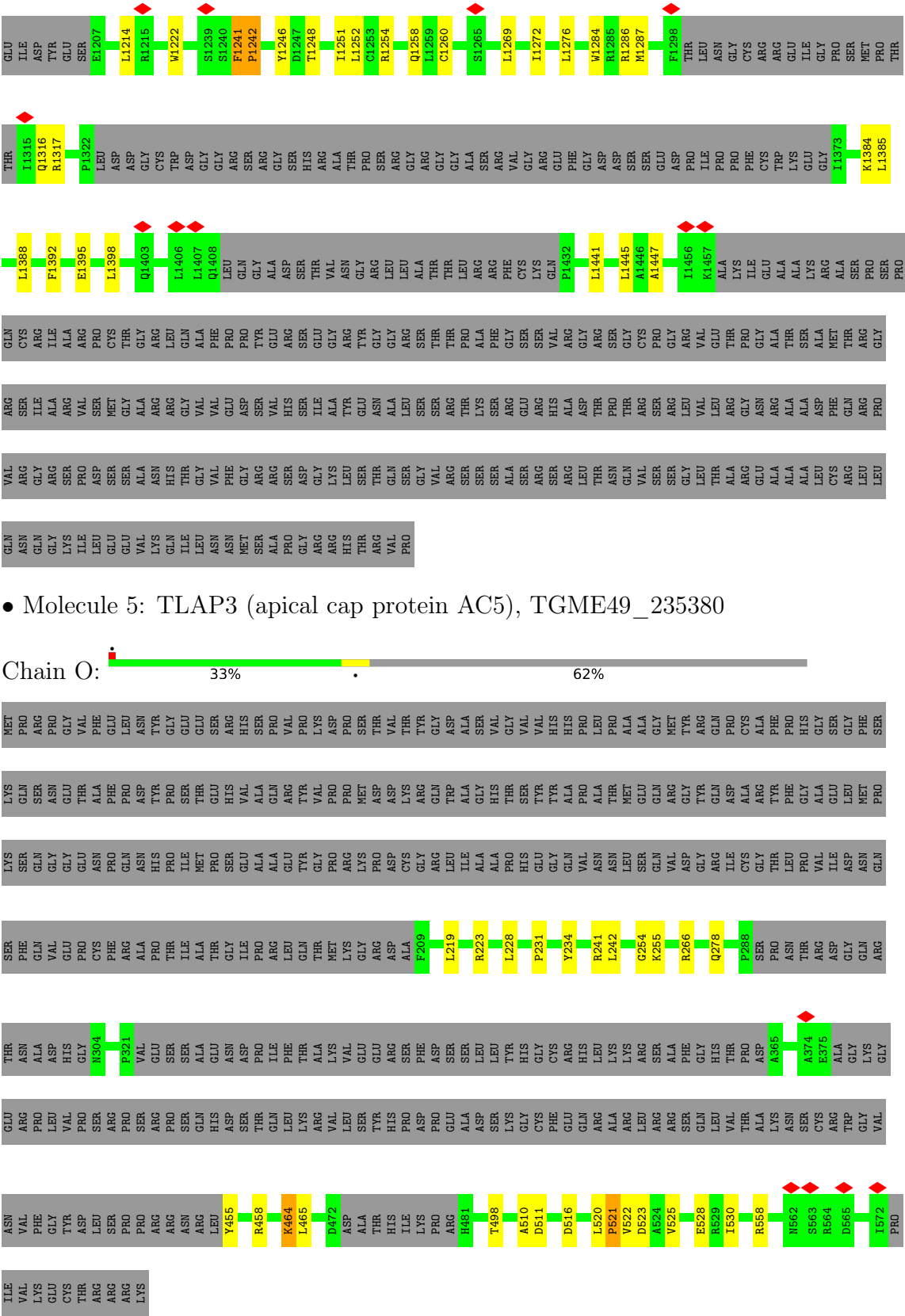
● Molecule 4: ICMAP2, TGME49\_224700

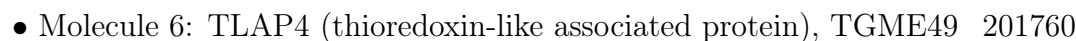
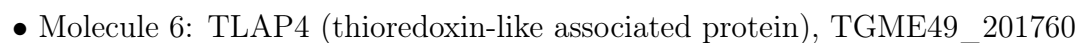


● Molecule 4: ICMAP2, TGME49 224700





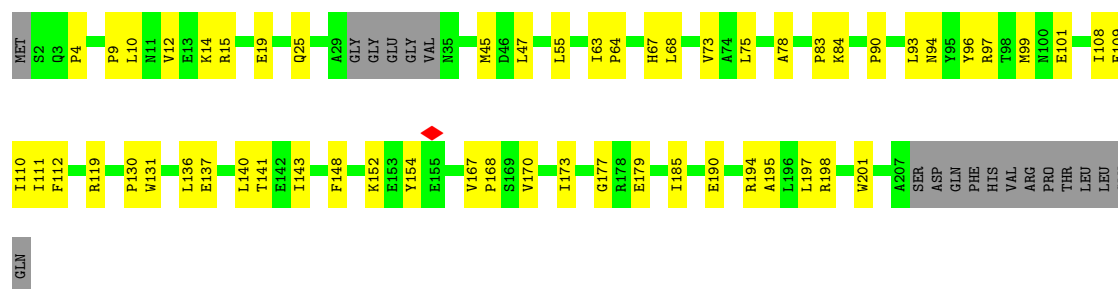






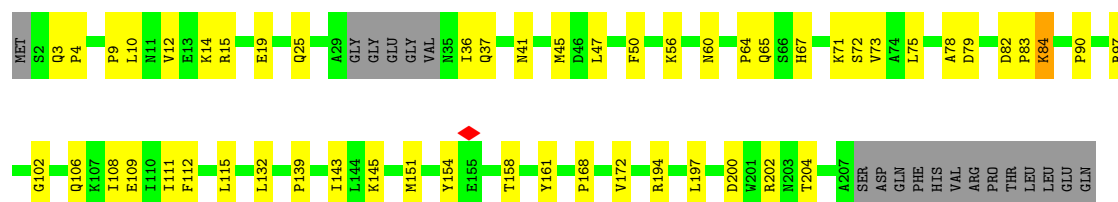


Chain e: 



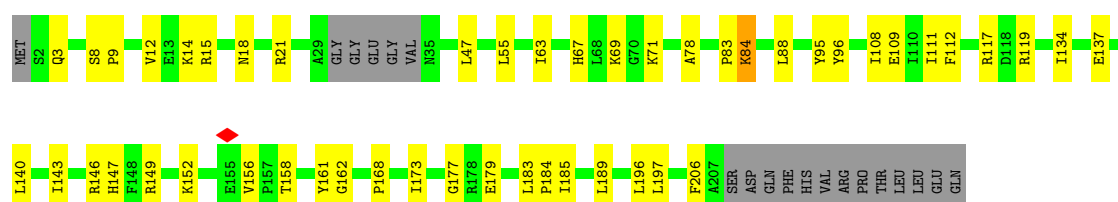
• Molecule 7: TRXL1, TGME49\_232410

Chain f: 



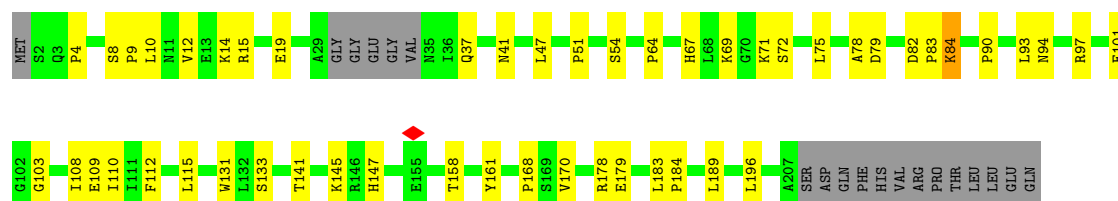
• Molecule 7: TRXL1, TGME49\_232410

Chain g: 



• Molecule 7: TRXL1, TGME49\_232410

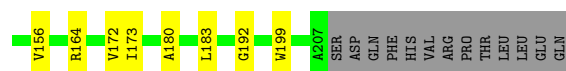
Chain h: 



• Molecule 7: TRXL1, TGME49\_232410

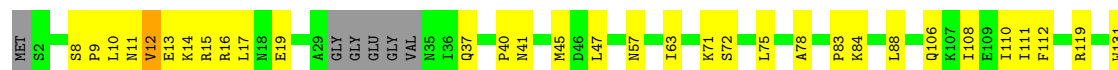
Chain i: 





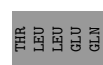
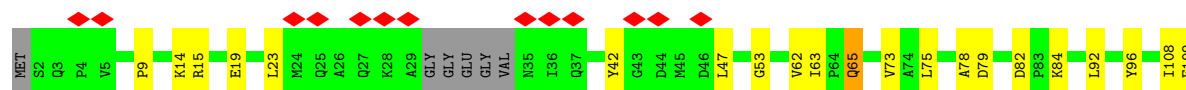
- Molecule 7: TRXL1, TGME49\_232410

Chain j: 70% 21% 9%



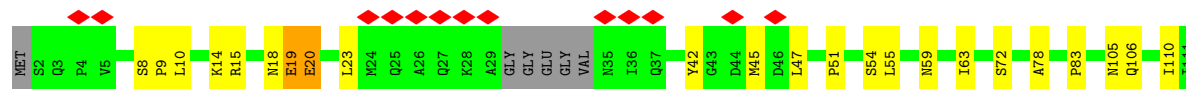
- Molecule 7: TRXL1, TGME49\_232410

Chain m: 6% 68% 23% 9%



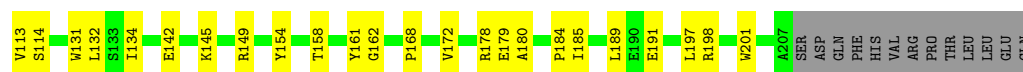
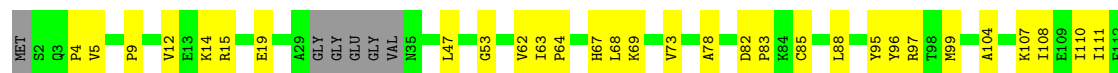
- Molecule 7: TRXL1, TGME49\_232410

Chain n: 6% 70% 20% 9%



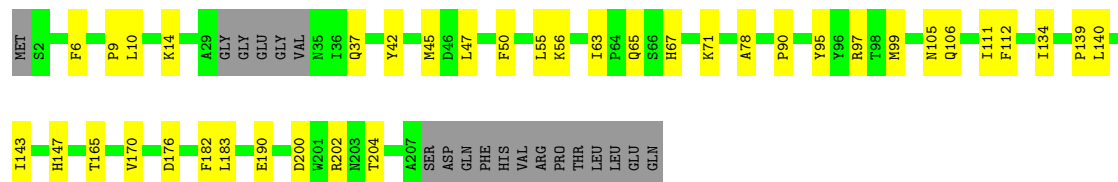
- Molecule 7: TRXL1, TGME49\_232410

Chain o: 67% 25% 9%



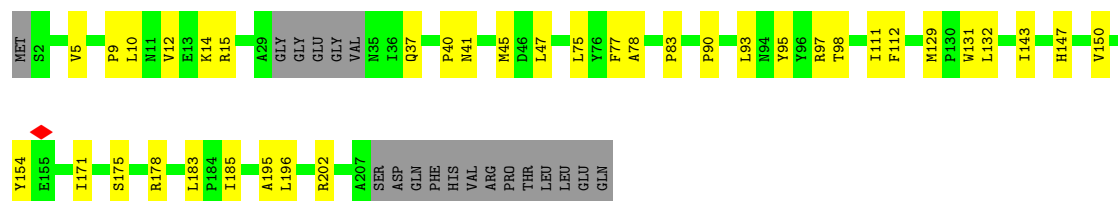
- Molecule 7: TRXL1, TGME49\_232410

Chain p:  74% 17% 9%



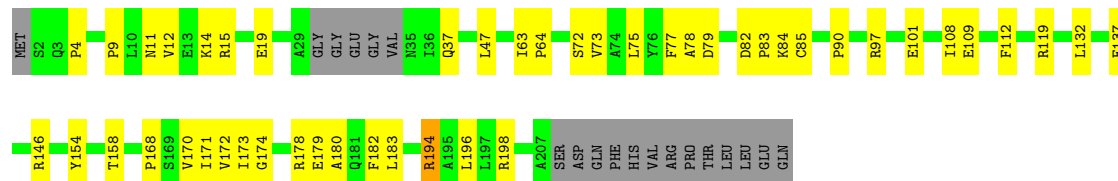
- Molecule 7: TRXL1, TGME49\_232410

Chain q:  75% 17% 9%



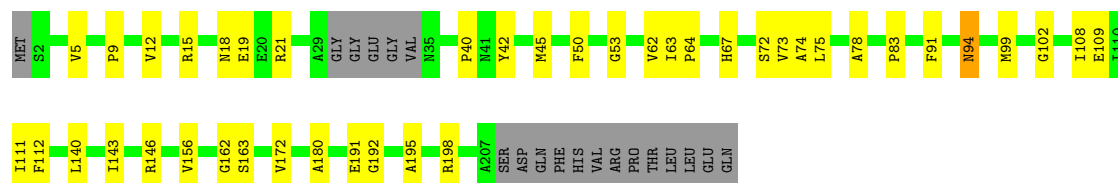
- Molecule 7: TRXL1, TGME49\_232410

Chain r:  70% 21% 9%



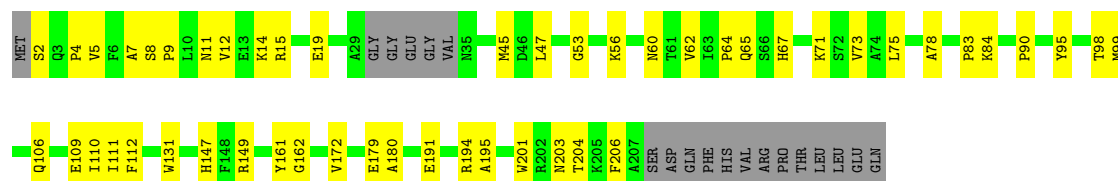
- Molecule 7: TRXL1, TGME49\_232410

Chain s:  72% 19% 9%



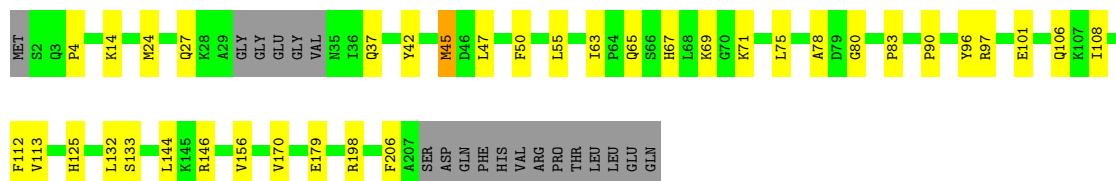
- Molecule 7: TRXL1, TGME49\_232410

Chain t:  69% 23% 9%



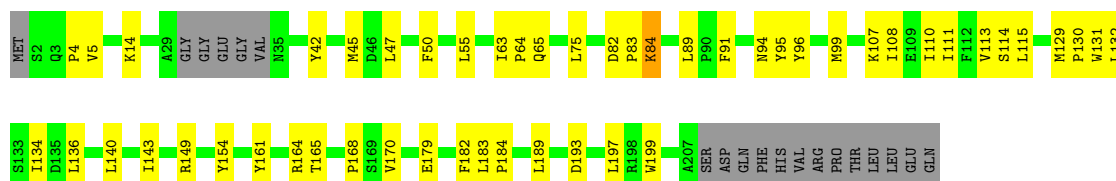
- Molecule 7: TRXL1, TGME49\_232410

Chain u: 



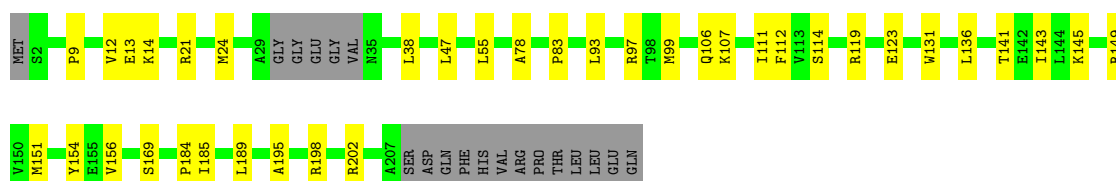
- Molecule 7: TRXL1, TGME49\_232410

Chain v: 



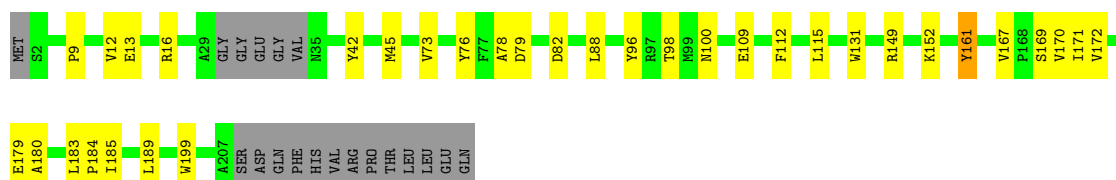
- Molecule 7: TRXL1, TGME49\_232410

Chain w: 



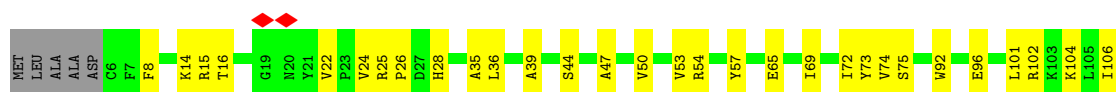
- Molecule 7: TRXL1, TGME49\_232410

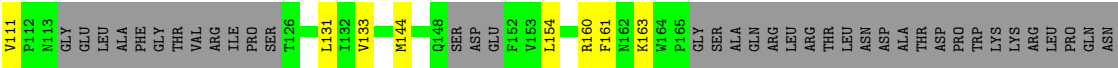
Chain x: 



- Molecule 8: TRXL2, TGME49\_225790

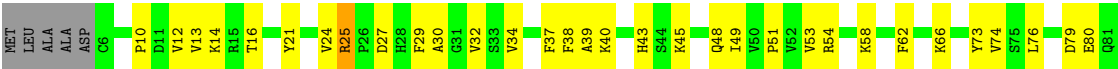
Chain k: 





VAL

• Molecule 8: TRXL2, TGME49\_225790



PRO  
TRP  
LYS  
LYS  
ARG  
LEU  
PRO  
GLN  
ASN  
VAL

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 57592                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 5000                                    | Depositor |
| Maximum defocus (nm)                 | 25000                                   | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 2.205                                   | Depositor |
| Minimum map value                    | -0.068                                  | Depositor |
| Average map value                    | 0.021                                   | Depositor |
| Map value standard deviation         | 0.096                                   | Depositor |
| Recommended contour level            | 0.05                                    | Depositor |
| Map size (Å)                         | 536.0, 536.0, 536.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.34, 1.34, 1.34                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.24         | 0/483         | 0.60        | 0/667         |
| 1   | B     | 0.23         | 0/491         | 0.60        | 0/679         |
| 1   | C     | 0.27         | 0/491         | 0.86        | 2/679 (0.3%)  |
| 1   | D     | 0.31         | 0/491         | 0.90        | 1/679 (0.1%)  |
| 1   | E     | 0.28         | 0/491         | 0.61        | 0/679         |
| 1   | F     | 0.25         | 0/491         | 0.59        | 0/679         |
| 1   | G     | 0.24         | 0/491         | 0.55        | 0/679         |
| 1   | H     | 0.29         | 0/491         | 0.65        | 0/679         |
| 1   | I     | 0.29         | 0/491         | 0.67        | 0/679         |
| 1   | J     | 0.24         | 0/491         | 0.60        | 0/679         |
| 1   | K     | 0.24         | 0/491         | 0.60        | 0/679         |
| 2   | A0    | 0.25         | 0/3398        | 0.61        | 4/4606 (0.1%) |
| 2   | A2    | 0.26         | 0/3398        | 0.64        | 0/4606        |
| 2   | A4    | 0.26         | 0/3398        | 0.66        | 0/4606        |
| 2   | A6    | 0.26         | 0/3398        | 0.64        | 2/4606 (0.0%) |
| 2   | A8    | 0.24         | 0/3398        | 0.53        | 0/4606        |
| 2   | B0    | 0.22         | 0/3398        | 0.54        | 0/4606        |
| 2   | B2    | 0.23         | 0/3398        | 0.52        | 1/4606 (0.0%) |
| 2   | B4    | 0.22         | 0/3398        | 0.52        | 0/4606        |
| 2   | B6    | 0.23         | 0/3398        | 0.51        | 0/4606        |
| 2   | B8    | 0.27         | 1/3398 (0.0%) | 0.54        | 1/4606 (0.0%) |
| 2   | C0    | 0.22         | 0/3398        | 0.57        | 0/4606        |
| 2   | C2    | 0.26         | 0/3398        | 0.63        | 2/4606 (0.0%) |
| 2   | C4    | 0.24         | 0/3398        | 0.66        | 1/4606 (0.0%) |
| 2   | C6    | 0.26         | 0/3398        | 0.63        | 2/4606 (0.0%) |
| 2   | C8    | 0.25         | 0/3398        | 0.58        | 0/4606        |
| 2   | D0    | 0.26         | 0/3398        | 0.60        | 1/4606 (0.0%) |
| 2   | D2    | 0.25         | 0/3398        | 0.58        | 0/4606        |
| 2   | D4    | 0.27         | 0/3398        | 0.62        | 0/4606        |
| 2   | D6    | 0.26         | 0/3398        | 0.58        | 0/4606        |
| 2   | D8    | 0.27         | 0/3398        | 0.61        | 0/4606        |
| 2   | E0    | 0.22         | 0/3398        | 0.54        | 0/4606        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 2   | E2    | 0.25         | 0/3398        | 0.61        | 0/4606        |
| 2   | E4    | 0.23         | 0/3398        | 0.60        | 1/4606 (0.0%) |
| 2   | E6    | 0.24         | 0/3398        | 0.61        | 2/4606 (0.0%) |
| 2   | E8    | 0.24         | 0/3398        | 0.59        | 3/4606 (0.1%) |
| 2   | F0    | 0.25         | 0/3398        | 0.59        | 1/4606 (0.0%) |
| 3   | A1    | 0.27         | 0/3404        | 0.70        | 5/4606 (0.1%) |
| 3   | A3    | 0.24         | 0/3404        | 0.62        | 1/4606 (0.0%) |
| 3   | A5    | 0.25         | 0/3404        | 0.65        | 4/4606 (0.1%) |
| 3   | A7    | 0.21         | 0/3404        | 0.54        | 2/4606 (0.0%) |
| 3   | A9    | 0.23         | 0/3404        | 0.56        | 0/4606        |
| 3   | B1    | 0.23         | 0/3404        | 0.59        | 0/4606        |
| 3   | B3    | 0.25         | 0/3404        | 0.62        | 4/4606 (0.1%) |
| 3   | B5    | 0.26         | 0/3404        | 0.63        | 0/4606        |
| 3   | B7    | 0.25         | 0/3404        | 0.60        | 0/4606        |
| 3   | B9    | 0.23         | 0/3404        | 0.59        | 0/4606        |
| 3   | C1    | 0.27         | 0/3404        | 0.68        | 0/4606        |
| 3   | C3    | 0.24         | 0/3404        | 0.63        | 1/4606 (0.0%) |
| 3   | C5    | 0.26         | 0/3404        | 0.68        | 2/4606 (0.0%) |
| 3   | C7    | 0.24         | 0/3404        | 0.63        | 1/4606 (0.0%) |
| 3   | C9    | 0.27         | 0/3404        | 0.64        | 0/4606        |
| 3   | D1    | 0.25         | 0/3404        | 0.62        | 0/4606        |
| 3   | D3    | 0.26         | 0/3404        | 0.62        | 5/4606 (0.1%) |
| 3   | D5    | 0.24         | 0/3404        | 0.61        | 3/4606 (0.1%) |
| 3   | D7    | 0.24         | 0/3404        | 0.60        | 1/4606 (0.0%) |
| 3   | D9    | 0.26         | 0/3404        | 0.64        | 2/4606 (0.0%) |
| 3   | E1    | 0.26         | 0/3404        | 0.64        | 1/4606 (0.0%) |
| 3   | E3    | 0.24         | 0/3404        | 0.58        | 0/4606        |
| 3   | E5    | 0.26         | 1/3404 (0.0%) | 0.60        | 0/4606        |
| 3   | E7    | 0.26         | 0/3404        | 0.63        | 1/4606 (0.0%) |
| 3   | E9    | 0.24         | 0/3404        | 0.63        | 4/4606 (0.1%) |
| 3   | F1    | 0.25         | 0/3404        | 0.69        | 2/4606 (0.0%) |
| 4   | L     | 0.23         | 0/1364        | 0.68        | 0/1841        |
| 4   | M     | 0.23         | 0/1364        | 0.68        | 0/1841        |
| 4   | N     | 0.22         | 0/1364        | 0.64        | 0/1841        |
| 4   | Q     | 0.24         | 0/1364        | 0.69        | 0/1841        |
| 4   | V     | 0.27         | 0/1364        | 0.67        | 0/1841        |
| 4   | W     | 0.23         | 0/1364        | 0.66        | 0/1841        |
| 5   | O     | 0.28         | 0/1768        | 0.81        | 5/2392 (0.2%) |
| 5   | P     | 0.30         | 0/1768        | 0.82        | 0/2392        |
| 6   | R     | 0.32         | 0/982         | 0.78        | 1/1332 (0.1%) |
| 6   | S     | 0.26         | 0/186         | 0.67        | 0/251         |
| 6   | T     | 0.31         | 0/982         | 0.79        | 0/1332        |
| 6   | U     | 0.27         | 0/796         | 0.67        | 0/1081        |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 7   | a     | 0.30         | 0/1321          | 0.79        | 2/1788 (0.1%)    |
| 7   | b     | 0.28         | 0/1321          | 0.71        | 1/1788 (0.1%)    |
| 7   | c     | 0.27         | 0/1645          | 0.69        | 2/2225 (0.1%)    |
| 7   | d     | 0.26         | 0/1645          | 0.63        | 1/2225 (0.0%)    |
| 7   | e     | 0.26         | 0/1645          | 0.61        | 0/2225           |
| 7   | f     | 0.29         | 0/1645          | 0.71        | 1/2225 (0.0%)    |
| 7   | g     | 0.32         | 0/1645          | 0.63        | 1/2225 (0.0%)    |
| 7   | h     | 0.28         | 0/1645          | 0.66        | 1/2225 (0.0%)    |
| 7   | i     | 0.27         | 0/1645          | 0.68        | 2/2225 (0.1%)    |
| 7   | j     | 0.28         | 0/1645          | 0.71        | 4/2225 (0.2%)    |
| 7   | m     | 0.26         | 0/1645          | 0.64        | 1/2225 (0.0%)    |
| 7   | n     | 0.28         | 0/1645          | 0.70        | 4/2225 (0.2%)    |
| 7   | o     | 0.26         | 0/1645          | 0.60        | 0/2225           |
| 7   | p     | 0.29         | 0/1645          | 0.65        | 0/2225           |
| 7   | q     | 0.25         | 0/1645          | 0.56        | 0/2225           |
| 7   | r     | 0.27         | 0/1645          | 0.64        | 1/2225 (0.0%)    |
| 7   | s     | 0.27         | 0/1645          | 0.65        | 2/2225 (0.1%)    |
| 7   | t     | 0.26         | 0/1645          | 0.62        | 1/2225 (0.0%)    |
| 7   | u     | 0.28         | 0/1645          | 0.69        | 1/2225 (0.0%)    |
| 7   | v     | 0.27         | 0/1645          | 0.63        | 1/2225 (0.0%)    |
| 7   | w     | 0.24         | 0/1645          | 0.61        | 0/2225           |
| 7   | x     | 0.27         | 0/1645          | 0.63        | 0/2225           |
| 8   | k     | 0.26         | 0/1218          | 0.64        | 0/1646           |
| 8   | l     | 0.33         | 0/1218          | 0.88        | 0/1646           |
| All | All   | 0.25         | 2/234889 (0.0%) | 0.63        | 95/318163 (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 |
|-----|-------|---------------------|---------------------|
| 1   | D     | 0                   | 2                   |
| 2   | A2    | 0                   | 1                   |
| 2   | A6    | 0                   | 1                   |
| 2   | B0    | 0                   | 1                   |
| 2   | C0    | 0                   | 1                   |
| 2   | C4    | 0                   | 2                   |
| 2   | C8    | 0                   | 1                   |
| 2   | D2    | 0                   | 1                   |
| 2   | D4    | 0                   | 2                   |
| 2   | D6    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | D8    | 0                   | 1                   |
| 2   | E4    | 0                   | 2                   |
| 2   | E6    | 0                   | 1                   |
| 2   | E8    | 0                   | 2                   |
| 3   | A1    | 0                   | 2                   |
| 3   | A3    | 0                   | 1                   |
| 3   | A5    | 0                   | 1                   |
| 3   | B3    | 0                   | 1                   |
| 3   | C1    | 0                   | 1                   |
| 3   | C5    | 0                   | 2                   |
| 3   | C7    | 0                   | 1                   |
| 3   | C9    | 0                   | 1                   |
| 3   | D1    | 0                   | 1                   |
| 3   | D3    | 0                   | 1                   |
| 3   | D5    | 0                   | 2                   |
| 3   | D7    | 0                   | 2                   |
| 3   | D9    | 0                   | 1                   |
| 3   | E1    | 0                   | 1                   |
| 3   | E3    | 0                   | 1                   |
| 3   | E5    | 0                   | 3                   |
| 3   | E7    | 0                   | 2                   |
| 3   | E9    | 0                   | 1                   |
| 3   | F1    | 0                   | 2                   |
| 4   | L     | 0                   | 1                   |
| 4   | M     | 0                   | 1                   |
| 4   | N     | 0                   | 1                   |
| 4   | Q     | 0                   | 1                   |
| 4   | V     | 0                   | 1                   |
| 4   | W     | 0                   | 1                   |
| 5   | P     | 0                   | 3                   |
| 6   | R     | 0                   | 2                   |
| 6   | T     | 0                   | 1                   |
| 7   | a     | 0                   | 1                   |
| 7   | b     | 0                   | 1                   |
| 7   | p     | 0                   | 1                   |
| 7   | x     | 0                   | 1                   |
| 8   | l     | 0                   | 2                   |
| All | All   | 0                   | 64                  |

All (2) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B8    | 35  | GLN  | C-N   | 5.96  | 1.42        | 1.33     |
| 3   | E5    | 241 | ARG  | C-N   | -5.21 | 1.26        | 1.33     |

All (95) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 253 | ALA  | CA-C-N   | 9.24  | 154.31      | 121.59   |
| 1   | C     | 253 | ALA  | C-N-CA   | 9.24  | 154.31      | 121.59   |
| 3   | B3    | 349 | MET  | CB-CG-SD | -9.05 | 85.56       | 112.70   |
| 5   | O     | 498 | THR  | CA-C-N   | 8.80  | 138.34      | 121.54   |
| 5   | O     | 498 | THR  | C-N-CA   | 8.80  | 138.34      | 121.54   |
| 6   | R     | 174 | ARG  | CG-CD-NE | -8.51 | 93.28       | 112.00   |
| 3   | D3    | 270 | PHE  | CA-C-N   | -7.97 | 114.96      | 122.37   |
| 3   | D3    | 270 | PHE  | C-N-CA   | -7.97 | 114.96      | 122.37   |
| 3   | C3    | 360 | GLY  | N-CA-C   | -7.47 | 105.58      | 113.58   |
| 3   | D3    | 271 | ALA  | N-CA-C   | 6.95  | 118.76      | 108.76   |
| 2   | D0    | 141 | VAL  | N-CA-C   | -6.91 | 106.76      | 113.53   |
| 7   | i     | 192 | GLY  | CA-C-N   | 6.79  | 133.20      | 122.61   |
| 7   | i     | 192 | GLY  | C-N-CA   | 6.79  | 133.20      | 122.61   |
| 3   | A1    | 270 | PHE  | CA-C-N   | -6.74 | 115.41      | 122.28   |
| 3   | A1    | 270 | PHE  | C-N-CA   | -6.74 | 115.41      | 122.28   |
| 2   | C4    | 182 | VAL  | N-CA-C   | -6.56 | 106.12      | 112.29   |
| 3   | F1    | 285 | SER  | CA-C-N   | 6.55  | 124.36      | 120.24   |
| 3   | F1    | 285 | SER  | C-N-CA   | 6.55  | 124.36      | 120.24   |
| 7   | n     | 19  | GLU  | CB-CA-C  | 6.54  | 120.69      | 109.24   |
| 2   | C2    | 182 | VAL  | CA-C-N   | 6.42  | 129.06      | 120.58   |
| 2   | C2    | 182 | VAL  | C-N-CA   | 6.42  | 129.06      | 120.58   |
| 3   | A1    | 285 | SER  | CA-C-N   | 6.41  | 124.28      | 120.24   |
| 3   | A1    | 285 | SER  | C-N-CA   | 6.41  | 124.28      | 120.24   |
| 3   | A5    | 30  | ILE  | CA-C-N   | 6.41  | 130.41      | 120.68   |
| 3   | A5    | 30  | ILE  | C-N-CA   | 6.41  | 130.41      | 120.68   |
| 3   | D5    | 270 | PHE  | CA-C-N   | -6.36 | 115.79      | 122.28   |
| 3   | D5    | 270 | PHE  | C-N-CA   | -6.36 | 115.79      | 122.28   |
| 5   | O     | 464 | LYS  | CA-CB-CG | 6.34  | 126.77      | 114.10   |
| 7   | v     | 84  | LYS  | CA-CB-CG | 6.17  | 126.43      | 114.10   |
| 3   | C5    | 285 | SER  | CA-C-N   | 6.16  | 124.12      | 120.24   |
| 3   | C5    | 285 | SER  | C-N-CA   | 6.16  | 124.12      | 120.24   |
| 7   | j     | 12  | VAL  | CA-C-N   | -6.15 | 110.83      | 121.66   |
| 7   | j     | 12  | VAL  | C-N-CA   | -6.15 | 110.83      | 121.66   |
| 7   | j     | 84  | LYS  | CA-CB-CG | 6.09  | 126.29      | 114.10   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | A0    | 50  | ASN  | CA-C-N   | 6.01  | 137.09      | 126.45   |
| 2   | A0    | 50  | ASN  | C-N-CA   | 6.01  | 137.09      | 126.45   |
| 7   | h     | 84  | LYS  | CA-CB-CG | 6.00  | 126.11      | 114.10   |
| 2   | E4    | 413 | MET  | CB-CG-SD | -5.88 | 95.07       | 112.70   |
| 3   | D9    | 270 | PHE  | CA-C-N   | -5.77 | 115.77      | 122.00   |
| 3   | D9    | 270 | PHE  | C-N-CA   | -5.77 | 115.77      | 122.00   |
| 3   | E9    | 107 | THR  | CA-C-N   | 5.77  | 132.56      | 121.54   |
| 3   | E9    | 107 | THR  | C-N-CA   | 5.77  | 132.56      | 121.54   |
| 7   | u     | 45  | MET  | CB-CG-SD | 5.73  | 129.89      | 112.70   |
| 3   | A1    | 271 | ALA  | N-CA-C   | 5.72  | 119.60      | 110.73   |
| 3   | D5    | 271 | ALA  | N-CA-C   | 5.71  | 119.58      | 110.73   |
| 7   | g     | 84  | LYS  | CA-CB-CG | 5.69  | 125.47      | 114.10   |
| 2   | B8    | 221 | ARG  | CB-CG-CD | 5.67  | 124.33      | 111.30   |
| 2   | E6    | 159 | VAL  | N-CA-C   | -5.52 | 108.12      | 113.53   |
| 7   | c     | 191 | GLU  | CA-CB-CG | 5.51  | 125.12      | 114.10   |
| 3   | B3    | 349 | MET  | CA-CB-CG | 5.48  | 125.06      | 114.10   |
| 3   | C7    | 350 | LYS  | CB-CG-CD | 5.44  | 123.82      | 111.30   |
| 7   | t     | 84  | LYS  | CA-CB-CG | 5.44  | 124.98      | 114.10   |
| 2   | A6    | 178 | SER  | CA-C-N   | 5.43  | 130.06      | 122.08   |
| 2   | A6    | 178 | SER  | C-N-CA   | 5.43  | 130.06      | 122.08   |
| 3   | B3    | 54  | ALA  | CA-C-N   | 5.42  | 131.07      | 122.61   |
| 3   | B3    | 54  | ALA  | C-N-CA   | 5.42  | 131.07      | 122.61   |
| 2   | B2    | 209 | ILE  | N-CA-C   | -5.41 | 107.09      | 113.42   |
| 7   | s     | 192 | GLY  | CA-C-N   | 5.39  | 131.84      | 121.54   |
| 7   | s     | 192 | GLY  | C-N-CA   | 5.39  | 131.84      | 121.54   |
| 7   | a     | 152 | LYS  | CA-C-N   | 5.38  | 131.81      | 121.54   |
| 7   | a     | 152 | LYS  | C-N-CA   | 5.38  | 131.81      | 121.54   |
| 2   | E8    | 182 | VAL  | CA-C-N   | 5.37  | 127.67      | 120.58   |
| 2   | E8    | 182 | VAL  | C-N-CA   | 5.37  | 127.67      | 120.58   |
| 7   | b     | 84  | LYS  | CA-CB-CG | 5.36  | 124.82      | 114.10   |
| 7   | m     | 84  | LYS  | CA-CB-CG | 5.35  | 124.80      | 114.10   |
| 7   | n     | 19  | GLU  | CA-CB-CG | 5.33  | 124.76      | 114.10   |
| 2   | A0    | 114 | ILE  | N-CA-C   | -5.33 | 107.64      | 112.96   |
| 2   | C6    | 217 | LEU  | CA-C-N   | 5.31  | 132.72      | 123.91   |
| 2   | C6    | 217 | LEU  | C-N-CA   | 5.31  | 132.72      | 123.91   |
| 2   | E8    | 394 | LYS  | CB-CG-CD | -5.29 | 99.14       | 111.30   |
| 3   | E9    | 88  | ASP  | N-CA-C   | -5.27 | 107.86      | 114.56   |
| 3   | D3    | 177 | ASP  | CA-C-N   | 5.25  | 131.57      | 121.54   |
| 3   | D3    | 177 | ASP  | C-N-CA   | 5.25  | 131.57      | 121.54   |
| 1   | D     | 243 | ALA  | N-CA-C   | -5.23 | 101.77      | 109.62   |
| 7   | n     | 20  | GLU  | N-CA-CB  | 5.21  | 117.77      | 110.12   |
| 7   | c     | 19  | GLU  | N-CA-CB  | 5.20  | 118.88      | 110.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | n     | 19  | GLU  | N-CA-CB  | -5.20 | 102.88      | 110.47   |
| 3   | E1    | 276 | ARG  | CB-CG-CD | -5.18 | 99.38       | 111.30   |
| 3   | D7    | 392 | LYS  | CB-CG-CD | 5.17  | 123.20      | 111.30   |
| 7   | d     | 191 | GLU  | CA-CB-CG | 5.15  | 124.40      | 114.10   |
| 2   | F0    | 413 | MET  | CB-CG-SD | 5.14  | 128.13      | 112.70   |
| 3   | E7    | 56  | GLY  | N-CA-C   | -5.12 | 107.92      | 114.37   |
| 3   | E9    | 108 | GLU  | CA-CB-CG | 5.12  | 124.34      | 114.10   |
| 7   | f     | 84  | LYS  | CA-CB-CG | 5.11  | 124.32      | 114.10   |
| 3   | A7    | 54  | ALA  | CA-C-N   | 5.10  | 130.57      | 122.61   |
| 3   | A7    | 54  | ALA  | C-N-CA   | 5.10  | 130.57      | 122.61   |
| 2   | E6    | 256 | GLN  | CA-CB-CG | 5.09  | 124.28      | 114.10   |
| 7   | r     | 194 | ARG  | CA-CB-CG | 5.06  | 124.22      | 114.10   |
| 5   | O     | 510 | ALA  | CA-C-N   | 5.04  | 131.17      | 121.54   |
| 5   | O     | 510 | ALA  | C-N-CA   | 5.04  | 131.17      | 121.54   |
| 7   | j     | 13  | GLU  | CA-CB-CG | 5.04  | 124.17      | 114.10   |
| 3   | A3    | 200 | GLN  | CA-CB-CG | 5.02  | 124.14      | 114.10   |
| 2   | A0    | 415 | GLU  | CA-CB-CG | 5.00  | 124.11      | 114.10   |
| 3   | A5    | 54  | ALA  | CA-C-N   | 5.00  | 131.09      | 121.54   |
| 3   | A5    | 54  | ALA  | C-N-CA   | 5.00  | 131.09      | 121.54   |

There are no chirality outliers.

All (64) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | A1    | 137 | HIS  | Peptide   |
| 3   | A1    | 271 | ALA  | Peptide   |
| 2   | A2    | 373 | ARG  | Sidechain |
| 3   | A3    | 200 | GLN  | Peptide   |
| 3   | A5    | 271 | ALA  | Peptide   |
| 2   | A6    | 99  | ALA  | Peptide   |
| 2   | B0    | 284 | GLU  | Peptide   |
| 3   | B3    | 348 | ASN  | Peptide   |
| 2   | C0    | 273 | ALA  | Peptide   |
| 3   | C1    | 271 | ALA  | Peptide   |
| 2   | C4    | 273 | ALA  | Peptide   |
| 2   | C4    | 304 | LYS  | Peptide   |
| 3   | C5    | 107 | THR  | Peptide   |
| 3   | C5    | 137 | HIS  | Peptide   |
| 3   | C7    | 271 | ALA  | Peptide   |
| 2   | C8    | 279 | GLU  | Peptide   |
| 3   | C9    | 271 | ALA  | Peptide   |
| 1   | D     | 217 | THR  | Peptide   |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | D     | 242  | ASN  | Peptide   |
| 3   | D1    | 271  | ALA  | Peptide   |
| 2   | D2    | 109  | THR  | Peptide   |
| 3   | D3    | 271  | ALA  | Peptide   |
| 2   | D4    | 109  | THR  | Peptide   |
| 2   | D4    | 273  | ALA  | Peptide   |
| 3   | D5    | 107  | THR  | Peptide   |
| 3   | D5    | 271  | ALA  | Peptide   |
| 2   | D6    | 273  | ALA  | Peptide   |
| 3   | D7    | 271  | ALA  | Peptide   |
| 3   | D7    | 294  | PHE  | Peptide   |
| 2   | D8    | 273  | ALA  | Peptide   |
| 3   | D9    | 271  | ALA  | Peptide   |
| 3   | E1    | 271  | ALA  | Peptide   |
| 3   | E3    | 271  | ALA  | Peptide   |
| 2   | E4    | 156  | ARG  | Sidechain |
| 2   | E4    | 273  | ALA  | Peptide   |
| 3   | E5    | 137  | HIS  | Peptide   |
| 3   | E5    | 271  | ALA  | Peptide   |
| 3   | E5    | 424  | GLN  | Peptide   |
| 2   | E6    | 273  | ALA  | Peptide   |
| 3   | E7    | 271  | ALA  | Peptide   |
| 3   | E7    | 380  | ARG  | Sidechain |
| 2   | E8    | 262  | TYR  | Peptide   |
| 2   | E8    | 273  | ALA  | Peptide   |
| 3   | E9    | 271  | ALA  | Peptide   |
| 3   | F1    | 260  | PHE  | Peptide   |
| 3   | F1    | 271  | ALA  | Peptide   |
| 4   | L     | 1241 | PHE  | Peptide   |
| 4   | M     | 1241 | PHE  | Peptide   |
| 4   | N     | 1241 | PHE  | Peptide   |
| 5   | P     | 468  | ASN  | Peptide   |
| 5   | P     | 532  | ARG  | Sidechain |
| 5   | P     | 558  | ARG  | Sidechain |
| 4   | Q     | 1241 | PHE  | Peptide   |
| 6   | R     | 174  | ARG  | Peptide   |
| 6   | R     | 87   | TYR  | Peptide   |
| 6   | T     | 87   | TYR  | Peptide   |
| 4   | V     | 1241 | PHE  | Peptide   |
| 4   | W     | 1241 | PHE  | Peptide   |
| 7   | a     | 128  | HIS  | Peptide   |
| 7   | b     | 154  | TYR  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 8   | l     | 25  | ARG  | Sidechain |
| 8   | l     | 66  | LYS  | Peptide   |
| 7   | p     | 97  | ARG  | Sidechain |
| 7   | x     | 161 | TYR  | Peptide   |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 464   | 0        | 469      | 10      | 0            |
| 1   | B     | 471   | 0        | 476      | 4       | 0            |
| 1   | C     | 471   | 0        | 475      | 12      | 0            |
| 1   | D     | 471   | 0        | 476      | 19      | 0            |
| 1   | E     | 471   | 0        | 476      | 9       | 0            |
| 1   | F     | 471   | 0        | 476      | 7       | 0            |
| 1   | G     | 471   | 0        | 476      | 10      | 0            |
| 1   | H     | 471   | 0        | 476      | 9       | 0            |
| 1   | I     | 471   | 0        | 476      | 13      | 0            |
| 1   | J     | 471   | 0        | 476      | 12      | 0            |
| 1   | K     | 471   | 0        | 476      | 5       | 0            |
| 2   | A0    | 3325  | 0        | 3252     | 58      | 0            |
| 2   | A2    | 3325  | 0        | 3252     | 66      | 0            |
| 2   | A4    | 3325  | 0        | 3252     | 68      | 0            |
| 2   | A6    | 3325  | 0        | 3252     | 45      | 0            |
| 2   | A8    | 3325  | 0        | 3251     | 49      | 0            |
| 2   | B0    | 3325  | 0        | 3252     | 61      | 0            |
| 2   | B2    | 3325  | 0        | 3252     | 40      | 0            |
| 2   | B4    | 3325  | 0        | 3252     | 46      | 0            |
| 2   | B6    | 3325  | 0        | 3252     | 36      | 0            |
| 2   | B8    | 3325  | 0        | 3251     | 59      | 0            |
| 2   | C0    | 3325  | 0        | 3252     | 53      | 0            |
| 2   | C2    | 3325  | 0        | 3252     | 54      | 0            |
| 2   | C4    | 3325  | 0        | 3252     | 52      | 0            |
| 2   | C6    | 3325  | 0        | 3252     | 64      | 0            |
| 2   | C8    | 3325  | 0        | 3252     | 61      | 0            |
| 2   | D0    | 3325  | 0        | 3252     | 54      | 0            |
| 2   | D2    | 3325  | 0        | 3252     | 40      | 0            |
| 2   | D4    | 3325  | 0        | 3252     | 53      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D6    | 3325  | 0        | 3252     | 63      | 0            |
| 2   | D8    | 3325  | 0        | 3252     | 66      | 0            |
| 2   | E0    | 3325  | 0        | 3252     | 42      | 0            |
| 2   | E2    | 3325  | 0        | 3252     | 42      | 0            |
| 2   | E4    | 3325  | 0        | 3252     | 35      | 0            |
| 2   | E6    | 3325  | 0        | 3252     | 47      | 0            |
| 2   | E8    | 3325  | 0        | 3252     | 43      | 0            |
| 2   | F0    | 3325  | 0        | 3252     | 52      | 0            |
| 3   | A1    | 3331  | 0        | 3207     | 77      | 0            |
| 3   | A3    | 3331  | 0        | 3209     | 74      | 0            |
| 3   | A5    | 3331  | 0        | 3207     | 59      | 0            |
| 3   | A7    | 3331  | 0        | 3207     | 37      | 0            |
| 3   | A9    | 3331  | 0        | 3207     | 55      | 0            |
| 3   | B1    | 3331  | 0        | 3209     | 65      | 0            |
| 3   | B3    | 3331  | 0        | 3207     | 55      | 0            |
| 3   | B5    | 3331  | 0        | 3207     | 75      | 0            |
| 3   | B7    | 3331  | 0        | 3209     | 53      | 0            |
| 3   | B9    | 3331  | 0        | 3209     | 40      | 0            |
| 3   | C1    | 3331  | 0        | 3209     | 60      | 0            |
| 3   | C3    | 3331  | 0        | 3207     | 52      | 0            |
| 3   | C5    | 3331  | 0        | 3209     | 73      | 0            |
| 3   | C7    | 3331  | 0        | 3209     | 58      | 0            |
| 3   | C9    | 3331  | 0        | 3209     | 73      | 0            |
| 3   | D1    | 3331  | 0        | 3209     | 54      | 0            |
| 3   | D3    | 3331  | 0        | 3207     | 65      | 0            |
| 3   | D5    | 3331  | 0        | 3207     | 33      | 0            |
| 3   | D7    | 3331  | 0        | 3207     | 57      | 0            |
| 3   | D9    | 3331  | 0        | 3207     | 39      | 0            |
| 3   | E1    | 3331  | 0        | 3207     | 53      | 0            |
| 3   | E3    | 3331  | 0        | 3209     | 59      | 0            |
| 3   | E5    | 3331  | 0        | 3207     | 59      | 0            |
| 3   | E7    | 3331  | 0        | 3207     | 57      | 0            |
| 3   | E9    | 3331  | 0        | 3206     | 70      | 0            |
| 3   | F1    | 3331  | 0        | 3207     | 63      | 0            |
| 4   | L     | 1334  | 0        | 1345     | 15      | 0            |
| 4   | M     | 1334  | 0        | 1345     | 17      | 0            |
| 4   | N     | 1334  | 0        | 1345     | 11      | 0            |
| 4   | Q     | 1334  | 0        | 1345     | 15      | 0            |
| 4   | V     | 1334  | 0        | 1345     | 17      | 0            |
| 4   | W     | 1334  | 0        | 1345     | 18      | 0            |
| 5   | O     | 1736  | 0        | 1725     | 22      | 0            |
| 5   | P     | 1736  | 0        | 1725     | 45      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | R     | 954   | 0        | 899      | 23      | 0            |
| 6   | S     | 182   | 0        | 183      | 1       | 0            |
| 6   | T     | 954   | 0        | 899      | 21      | 0            |
| 6   | U     | 772   | 0        | 716      | 14      | 0            |
| 7   | a     | 1289  | 0        | 1274     | 29      | 0            |
| 7   | b     | 1289  | 0        | 1274     | 31      | 0            |
| 7   | c     | 1608  | 0        | 1590     | 36      | 0            |
| 7   | d     | 1608  | 0        | 1590     | 35      | 0            |
| 7   | e     | 1608  | 0        | 1590     | 42      | 0            |
| 7   | f     | 1608  | 0        | 1590     | 39      | 0            |
| 7   | g     | 1608  | 0        | 1590     | 32      | 0            |
| 7   | h     | 1608  | 0        | 1590     | 40      | 0            |
| 7   | i     | 1608  | 0        | 1590     | 26      | 0            |
| 7   | j     | 1608  | 0        | 1590     | 29      | 0            |
| 7   | m     | 1608  | 0        | 1590     | 35      | 0            |
| 7   | n     | 1608  | 0        | 1590     | 35      | 0            |
| 7   | o     | 1608  | 0        | 1590     | 38      | 0            |
| 7   | p     | 1608  | 0        | 1590     | 28      | 0            |
| 7   | q     | 1608  | 0        | 1590     | 27      | 0            |
| 7   | r     | 1608  | 0        | 1590     | 32      | 0            |
| 7   | s     | 1608  | 0        | 1590     | 31      | 0            |
| 7   | t     | 1608  | 0        | 1590     | 31      | 0            |
| 7   | u     | 1608  | 0        | 1590     | 26      | 0            |
| 7   | v     | 1608  | 0        | 1590     | 34      | 0            |
| 7   | w     | 1608  | 0        | 1590     | 26      | 0            |
| 7   | x     | 1608  | 0        | 1590     | 20      | 0            |
| 8   | k     | 1187  | 0        | 1180     | 26      | 0            |
| 8   | l     | 1187  | 0        | 1180     | 29      | 0            |
| 9   | A0    | 32    | 0        | 12       | 0       | 0            |
| 9   | A2    | 32    | 0        | 12       | 0       | 0            |
| 9   | A4    | 32    | 0        | 12       | 0       | 0            |
| 9   | A6    | 32    | 0        | 12       | 0       | 0            |
| 9   | A8    | 32    | 0        | 12       | 0       | 0            |
| 9   | B0    | 32    | 0        | 12       | 0       | 0            |
| 9   | B2    | 32    | 0        | 12       | 0       | 0            |
| 9   | B4    | 32    | 0        | 12       | 0       | 0            |
| 9   | B6    | 32    | 0        | 12       | 0       | 0            |
| 9   | B8    | 32    | 0        | 12       | 0       | 0            |
| 9   | C0    | 32    | 0        | 12       | 0       | 0            |
| 9   | C3    | 32    | 0        | 12       | 0       | 0            |
| 9   | C4    | 32    | 0        | 12       | 0       | 0            |
| 9   | C6    | 32    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | C8    | 32    | 0        | 12       | 0       | 0            |
| 9   | D0    | 32    | 0        | 12       | 0       | 0            |
| 9   | D2    | 32    | 0        | 12       | 0       | 0            |
| 9   | D4    | 32    | 0        | 12       | 0       | 0            |
| 9   | D6    | 32    | 0        | 12       | 0       | 0            |
| 9   | D8    | 32    | 0        | 12       | 0       | 0            |
| 9   | E0    | 32    | 0        | 12       | 0       | 0            |
| 9   | E2    | 32    | 0        | 12       | 0       | 0            |
| 9   | E4    | 32    | 0        | 12       | 1       | 0            |
| 9   | E6    | 32    | 0        | 12       | 0       | 0            |
| 9   | E8    | 32    | 0        | 12       | 0       | 0            |
| 9   | F0    | 32    | 0        | 12       | 0       | 0            |
| 10  | A0    | 1     | 0        | 0        | 0       | 0            |
| 10  | A2    | 1     | 0        | 0        | 0       | 0            |
| 10  | A5    | 1     | 0        | 0        | 0       | 0            |
| 10  | A7    | 1     | 0        | 0        | 0       | 0            |
| 10  | A8    | 1     | 0        | 0        | 0       | 0            |
| 10  | B0    | 1     | 0        | 0        | 0       | 0            |
| 10  | B2    | 1     | 0        | 0        | 0       | 0            |
| 10  | B4    | 1     | 0        | 0        | 0       | 0            |
| 10  | B6    | 1     | 0        | 0        | 0       | 0            |
| 10  | B8    | 1     | 0        | 0        | 0       | 0            |
| 10  | C0    | 1     | 0        | 0        | 0       | 0            |
| 10  | C2    | 1     | 0        | 0        | 0       | 0            |
| 10  | C4    | 1     | 0        | 0        | 0       | 0            |
| 10  | C6    | 1     | 0        | 0        | 0       | 0            |
| 10  | C8    | 1     | 0        | 0        | 0       | 0            |
| 10  | D0    | 1     | 0        | 0        | 0       | 0            |
| 10  | D2    | 1     | 0        | 0        | 0       | 0            |
| 10  | D4    | 1     | 0        | 0        | 0       | 0            |
| 10  | D6    | 1     | 0        | 0        | 0       | 0            |
| 10  | D8    | 1     | 0        | 0        | 0       | 0            |
| 10  | E1    | 1     | 0        | 0        | 0       | 0            |
| 10  | E2    | 1     | 0        | 0        | 0       | 0            |
| 10  | E4    | 1     | 0        | 0        | 0       | 0            |
| 10  | E6    | 1     | 0        | 0        | 0       | 0            |
| 10  | E9    | 1     | 0        | 0        | 0       | 0            |
| 10  | F0    | 1     | 0        | 0        | 0       | 0            |
| 11  | A1    | 28    | 0        | 12       | 1       | 0            |
| 11  | A3    | 28    | 0        | 12       | 0       | 0            |
| 11  | A5    | 28    | 0        | 12       | 0       | 0            |
| 11  | A7    | 28    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 11  | A9    | 28     | 0        | 12       | 0       | 0            |
| 11  | B1    | 28     | 0        | 12       | 0       | 0            |
| 11  | B3    | 28     | 0        | 12       | 1       | 0            |
| 11  | B5    | 28     | 0        | 12       | 0       | 0            |
| 11  | B7    | 28     | 0        | 12       | 0       | 0            |
| 11  | B9    | 28     | 0        | 12       | 0       | 0            |
| 11  | C1    | 28     | 0        | 12       | 0       | 0            |
| 11  | C3    | 28     | 0        | 12       | 0       | 0            |
| 11  | C5    | 28     | 0        | 12       | 0       | 0            |
| 11  | C7    | 28     | 0        | 12       | 0       | 0            |
| 11  | C9    | 28     | 0        | 12       | 0       | 0            |
| 11  | D1    | 28     | 0        | 12       | 0       | 0            |
| 11  | D3    | 28     | 0        | 12       | 0       | 0            |
| 11  | D5    | 28     | 0        | 12       | 0       | 0            |
| 11  | D7    | 28     | 0        | 12       | 0       | 0            |
| 11  | D9    | 28     | 0        | 12       | 0       | 0            |
| 11  | E1    | 28     | 0        | 12       | 0       | 0            |
| 11  | E3    | 28     | 0        | 12       | 0       | 0            |
| 11  | E5    | 28     | 0        | 12       | 2       | 0            |
| 11  | E7    | 28     | 0        | 12       | 1       | 0            |
| 11  | E9    | 28     | 0        | 12       | 0       | 0            |
| 11  | F1    | 28     | 0        | 12       | 0       | 0            |
| All | All   | 231266 | 0        | 224728   | 3480    | 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 8.

All (3480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A3:258:ILE:HD12 | 3:A3:264:HIS:HB3  | 1.57                     | 0.86              |
| 1:D:245:SER:O     | 1:D:249:SER:HB3   | 1.77                     | 0.84              |
| 2:B4:407:TRP:HE1  | 3:B5:258:ILE:HG23 | 1.42                     | 0.83              |
| 3:D3:130:LEU:HB3  | 3:D3:162:ARG:HE   | 1.46                     | 0.80              |
| 7:h:12:VAL:HG12   | 7:h:15:ARG:HH21   | 1.45                     | 0.80              |
| 1:I:245:SER:O     | 1:I:249:SER:HB3   | 1.82                     | 0.80              |
| 7:t:2:SER:HA      | 7:t:11:ASN:HD21   | 1.47                     | 0.79              |
| 7:w:14:LYS:HD3    | 7:w:47:LEU:HD23   | 1.67                     | 0.77              |
| 2:B6:268:MET:HE2  | 2:B6:378:ILE:HG22 | 1.67                     | 0.77              |
| 2:D0:221:ARG:HH12 | 7:p:190:GLU:HB2   | 1.47                     | 0.76              |
| 2:A4:2:ARG:HH12   | 5:O:266:ARG:HH12  | 1.34                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:f:71:LYS:HD3    | 7:f:109:GLU:HG2   | 1.66                     | 0.76              |
| 3:C1:390:ARG:HH22 | 3:C1:391:ARG:HH21 | 1.34                     | 0.76              |
| 2:A0:3:GLU:HA     | 2:A0:51:THR:HA    | 1.69                     | 0.75              |
| 2:A2:212:ILE:HD12 | 2:A2:215:ARG:HH12 | 1.52                     | 0.75              |
| 2:A6:178:SER:HB2  | 3:A7:347:ASN:HD22 | 1.51                     | 0.75              |
| 3:D3:377:MET:HA   | 3:D3:380:ARG:HB2  | 1.67                     | 0.75              |
| 3:C1:6:HIS:HB3    | 3:C1:63:ALA:HA    | 1.67                     | 0.75              |
| 7:a:79:ASP:HB2    | 7:a:82:ASP:HB2    | 1.68                     | 0.75              |
| 3:B1:8:GLN:HE22   | 3:B1:17:GLY:HA3   | 1.53                     | 0.74              |
| 3:D3:102:ALA:HB2  | 3:D3:403:MET:HE2  | 1.67                     | 0.74              |
| 2:D6:274:PRO:HG3  | 2:D6:374:ALA:HA   | 1.69                     | 0.74              |
| 2:A2:133:GLN:HE22 | 2:A2:253:THR:HG23 | 1.52                     | 0.74              |
| 4:M:1231:ALA:HB1  | 4:M:1235:ARG:HH12 | 1.52                     | 0.74              |
| 4:Q:1398:LEU:HB2  | 4:Q:1401:ARG:HH21 | 1.53                     | 0.74              |
| 3:E5:57:GLY:HA3   | 7:u:83:PRO:HB2    | 1.69                     | 0.74              |
| 1:G:247:TYR:O     | 1:G:251:TYR:HB2   | 1.86                     | 0.74              |
| 7:e:84:LYS:HB3    | 7:e:168:PRO:HD3   | 1.69                     | 0.74              |
| 3:C5:230:SER:HA   | 3:C5:233:MET:HG2  | 1.71                     | 0.73              |
| 2:D6:258:ASN:HD22 | 2:D6:352:LYS:HD3  | 1.53                     | 0.73              |
| 8:l:14:LYS:HZ1    | 8:l:83:PHE:HZ     | 1.37                     | 0.73              |
| 2:A2:133:GLN:HE21 | 2:A2:252:VAL:HB   | 1.54                     | 0.73              |
| 7:a:115:LEU:HD21  | 7:a:145:LYS:HZ3   | 1.52                     | 0.73              |
| 2:B8:202:VAL:HA   | 2:B8:268:MET:HB2  | 1.71                     | 0.73              |
| 3:A7:242:PHE:HB3  | 3:A7:356:ILE:HD13 | 1.70                     | 0.72              |
| 5:P:211:GLN:HA    | 5:P:216:GLN:HE22  | 1.55                     | 0.72              |
| 2:D2:222:PRO:HD2  | 3:D3:324:LYS:HD2  | 1.71                     | 0.72              |
| 7:i:14:LYS:HE3    | 7:i:45:MET:HG2    | 1.71                     | 0.72              |
| 3:B7:35:THR:HG22  | 7:g:83:PRO:HG3    | 1.70                     | 0.72              |
| 7:m:14:LYS:HB2    | 7:m:47:LEU:HD22   | 1.70                     | 0.72              |
| 3:D9:375:GLN:HB2  | 3:D9:419:VAL:HG13 | 1.72                     | 0.72              |
| 2:D4:234:VAL:HG21 | 2:D4:302:MET:HE1  | 1.72                     | 0.71              |
| 7:n:63:ILE:HD11   | 7:n:132:LEU:HD21  | 1.71                     | 0.71              |
| 3:B5:258:ILE:HD12 | 3:B5:264:HIS:HB3  | 1.71                     | 0.71              |
| 3:A5:395:LEU:HD21 | 3:A5:408:PHE:HE2  | 1.55                     | 0.71              |
| 2:B8:31:GLN:HE21  | 2:B8:33:ASP:HB3   | 1.55                     | 0.71              |
| 3:E9:218:THR:HG23 | 6:T:174:ARG:HH22  | 1.54                     | 0.71              |
| 7:e:94:ASN:HA     | 7:e:97:ARG:HE     | 1.56                     | 0.71              |
| 7:c:11:ASN:HA     | 7:c:14:LYS:HG2    | 1.73                     | 0.71              |
| 3:A5:2:ARG:HB3    | 3:A5:131:GLN:HB2  | 1.73                     | 0.70              |
| 3:C7:2:ARG:HB3    | 3:C7:131:GLN:HB2  | 1.73                     | 0.70              |
| 2:C0:274:PRO:HG3  | 2:C0:374:ALA:HA   | 1.72                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B1:131:GLN:HE22 | 3:B1:249:ASP:HB3  | 1.56                     | 0.70              |
| 3:C9:178:THR:HB   | 3:C9:181:GLU:HG3  | 1.73                     | 0.70              |
| 3:C1:66:MET:HE1   | 3:C1:151:LEU:HD22 | 1.74                     | 0.70              |
| 2:C4:31:GLN:HE21  | 2:C4:35:GLN:HB2   | 1.56                     | 0.70              |
| 2:D0:3:GLU:HA     | 2:D0:51:THR:HA    | 1.73                     | 0.70              |
| 3:E1:257:LEU:HD21 | 3:E1:314:SER:HB2  | 1.72                     | 0.70              |
| 2:C0:258:ASN:HB3  | 2:C0:352:LYS:HG3  | 1.72                     | 0.70              |
| 3:D7:295:ASP:H    | 3:D7:298:ASN:HD21 | 1.37                     | 0.70              |
| 7:j:57:ASN:HD22   | 7:j:63:ILE:HD11   | 1.56                     | 0.70              |
| 3:C1:19:LYS:HA    | 3:C1:22:GLU:HG3   | 1.74                     | 0.70              |
| 2:A6:387:VAL:HA   | 2:A6:390:ARG:HH12 | 1.56                     | 0.70              |
| 3:C1:6:HIS:CD2    | 3:C1:21:TRP:HE1   | 2.10                     | 0.70              |
| 3:E9:361:LEU:HA   | 6:U:105:HIS:HE1   | 1.55                     | 0.70              |
| 2:A6:285:GLN:HB2  | 2:B0:56:THR:HA    | 1.73                     | 0.69              |
| 3:A5:377:MET:HA   | 3:A5:380:ARG:HE   | 1.56                     | 0.69              |
| 2:D0:286:LEU:HB3  | 2:D0:291:ILE:HD11 | 1.75                     | 0.69              |
| 3:B5:405:GLU:HG3  | 4:M:1234:TYR:HE2  | 1.56                     | 0.69              |
| 2:F0:71:GLU:HB3   | 2:F0:98:ASP:HB2   | 1.73                     | 0.69              |
| 3:C7:281:TYR:HD2  | 3:D1:87:PRO:HD3   | 1.58                     | 0.69              |
| 3:D7:11:GLN:HG3   | 3:D7:72:THR:HG21  | 1.75                     | 0.69              |
| 3:B5:152:ILE:HG22 | 3:B5:191:GLN:HE22 | 1.57                     | 0.69              |
| 7:h:93:LEU:HB3    | 7:h:97:ARG:HH21   | 1.57                     | 0.69              |
| 2:E2:76:ASP:HA    | 2:E2:79:ARG:HD2   | 1.74                     | 0.69              |
| 3:E3:11:GLN:HG3   | 3:E3:72:THR:HG21  | 1.74                     | 0.69              |
| 3:E9:2:ARG:HB3    | 3:E9:131:GLN:HB2  | 1.72                     | 0.69              |
| 2:C2:316:CYS:HA   | 2:C2:352:LYS:HB2  | 1.73                     | 0.68              |
| 2:E4:195:LEU:HD21 | 2:E4:264:ARG:HH21 | 1.58                     | 0.68              |
| 3:F1:248:SER:HA   | 3:F1:252:LYS:HD2  | 1.76                     | 0.68              |
| 7:p:14:LYS:HG3    | 7:p:47:LEU:HB3    | 1.74                     | 0.68              |
| 3:D9:248:SER:HA   | 3:D9:252:LYS:HG3  | 1.76                     | 0.68              |
| 7:x:73:VAL:HG12   | 7:x:109:GLU:HB3   | 1.74                     | 0.68              |
| 2:F0:180:ALA:HA   | 3:F1:256:ASN:HD21 | 1.58                     | 0.68              |
| 2:A2:121:ARG:HE   | 2:A2:124:LYS:HD3  | 1.59                     | 0.68              |
| 2:A6:71:GLU:HB2   | 2:A6:98:ASP:HB3   | 1.73                     | 0.68              |
| 7:e:10:LEU:HG     | 7:e:143:ILE:HG12  | 1.76                     | 0.68              |
| 3:E5:215:LEU:HB3  | 3:E5:217:LEU:HD13 | 1.75                     | 0.68              |
| 3:E7:135:ILE:HB   | 3:E7:166:THR:HG22 | 1.76                     | 0.68              |
| 7:b:153:GLU:H     | 7:b:164:ARG:HH12  | 1.41                     | 0.68              |
| 3:A3:293:MET:HA   | 3:A3:298:ASN:HD21 | 1.59                     | 0.68              |
| 3:C9:248:SER:HA   | 3:C9:252:LYS:HD3  | 1.75                     | 0.68              |
| 2:C6:234:VAL:HG21 | 2:C6:302:MET:HE1  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B6:272:TYR:HB3  | 2:B6:275:ILE:HD11 | 1.75                     | 0.67              |
| 2:C2:70:LEU:HD12  | 2:C2:99:ALA:HB2   | 1.77                     | 0.67              |
| 2:C6:203:MET:HE1  | 2:C6:267:PHE:HB3  | 1.75                     | 0.67              |
| 2:E2:244:PHE:HA   | 5:P:558:ARG:HG3   | 1.76                     | 0.67              |
| 2:E2:101:ASN:HD22 | 3:E3:256:ASN:HD21 | 1.39                     | 0.67              |
| 2:E4:54:SER:HB3   | 2:E4:64:ARG:HE    | 1.59                     | 0.67              |
| 2:A0:123:ARG:HH21 | 2:A0:124:LYS:HD2  | 1.60                     | 0.67              |
| 2:B2:152:LEU:HG   | 2:B2:156:ARG:HH22 | 1.59                     | 0.67              |
| 7:b:172:VAL:HG13  | 7:b:180:ALA:HB3   | 1.77                     | 0.67              |
| 2:A0:288:VAL:HG21 | 2:A0:327:ASP:HB3  | 1.75                     | 0.67              |
| 3:A3:334:GLN:HE22 | 3:A3:347:ASN:HA   | 1.58                     | 0.67              |
| 7:r:73:VAL:HA     | 7:r:109:GLU:O     | 1.94                     | 0.67              |
| 3:A1:211:CYS:HA   | 3:A1:215:LEU:HB2  | 1.77                     | 0.67              |
| 3:D3:220:PRO:HD2  | 2:D4:326:LYS:HD3  | 1.77                     | 0.67              |
| 3:D9:293:MET:HA   | 3:D9:298:ASN:HD22 | 1.59                     | 0.67              |
| 2:F0:365:GLY:HA3  | 6:T:127:ARG:HH11  | 1.59                     | 0.67              |
| 2:D6:292:THR:HG21 | 2:D6:331:ALA:HB1  | 1.76                     | 0.67              |
| 7:e:14:LYS:HZ1    | 7:e:45:MET:HB3    | 1.60                     | 0.66              |
| 2:A2:219:ILE:HG13 | 7:b:198:ARG:HH22  | 1.59                     | 0.66              |
| 7:c:63:ILE:HD11   | 7:c:132:LEU:HD21  | 1.75                     | 0.66              |
| 2:B0:259:LEU:HD21 | 2:B0:316:CYS:HB2  | 1.75                     | 0.66              |
| 2:D6:105:ARG:HH21 | 2:D6:110:ILE:HD13 | 1.60                     | 0.66              |
| 4:M:1374:ARG:HE   | 4:M:1377:VAL:HG23 | 1.61                     | 0.66              |
| 2:E0:272:TYR:HB3  | 2:E0:275:ILE:HD11 | 1.77                     | 0.66              |
| 3:B5:326:VAL:HG12 | 3:B5:330:MET:HE2  | 1.78                     | 0.66              |
| 3:B7:74:ASP:HA    | 3:B7:77:ARG:HD3   | 1.77                     | 0.66              |
| 2:C2:88:HIS:HB3   | 2:C2:91:GLN:HG2   | 1.77                     | 0.66              |
| 3:D1:317:PHE:HB3  | 3:D1:321:MET:HE3  | 1.77                     | 0.66              |
| 7:d:9:PRO:HB2     | 7:d:143:ILE:HG23  | 1.77                     | 0.66              |
| 7:u:24:MET:HB2    | 7:u:27:GLN:HE21   | 1.61                     | 0.66              |
| 7:w:112:PHE:HB2   | 7:w:131:TRP:HE1   | 1.60                     | 0.66              |
| 3:A1:314:SER:HA   | 3:A1:350:LYS:HB3  | 1.77                     | 0.66              |
| 3:E9:390:ARG:HE   | 3:E9:391:ARG:HG3  | 1.60                     | 0.66              |
| 2:B6:88:HIS:HB3   | 2:B6:91:GLN:HG2   | 1.76                     | 0.66              |
| 7:i:10:LEU:HD12   | 7:i:143:ILE:HG22  | 1.78                     | 0.66              |
| 2:A6:223:THR:HG22 | 3:A7:322:SER:HA   | 1.76                     | 0.66              |
| 3:D1:19:LYS:HG2   | 3:D1:22:GLU:HG3   | 1.78                     | 0.66              |
| 3:A1:98:GLY:H     | 3:A1:103:LYS:HD3  | 1.59                     | 0.65              |
| 3:E1:34:GLY:HA3   | 3:E1:58:ARG:HE    | 1.60                     | 0.65              |
| 3:D7:229:VAL:HA   | 3:D7:300:MET:HE1  | 1.78                     | 0.65              |
| 3:C7:20:PHE:HB2   | 3:C7:233:MET:HG3  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E6:184:PRO:HA   | 2:E6:391:MET:HE1  | 1.78                     | 0.65              |
| 5:O:464:LYS:HD2   | 5:O:465:LEU:H     | 1.61                     | 0.65              |
| 2:A6:57:GLY:HA2   | 5:P:254:GLY:H     | 1.62                     | 0.65              |
| 3:B3:139:LEU:HA   | 3:B3:145:SER:HB3  | 1.79                     | 0.65              |
| 3:B5:303:SER:HB3  | 3:B5:377:MET:HE3  | 1.76                     | 0.65              |
| 3:C5:381:VAL:HA   | 3:C5:384:GLN:HE21 | 1.62                     | 0.65              |
| 2:D0:271:SER:HB3  | 2:D0:377:MET:HB3  | 1.77                     | 0.65              |
| 2:E2:188:VAL:HG23 | 2:E2:391:MET:HE2  | 1.77                     | 0.65              |
| 1:F:212:GLU:HG3   | 1:F:216:ARG:HG3   | 1.79                     | 0.65              |
| 8:l:45:LYS:HA     | 8:l:48:GLN:HG2    | 1.78                     | 0.65              |
| 7:q:9:PRO:HB2     | 7:q:143:ILE:HG23  | 1.78                     | 0.65              |
| 1:A:214:ALA:O     | 1:A:218:ASP:HB2   | 1.96                     | 0.65              |
| 3:E1:215:LEU:HD22 | 5:P:570:ASN:HD21  | 1.61                     | 0.65              |
| 3:B9:139:LEU:HA   | 3:B9:145:SER:HB3  | 1.77                     | 0.65              |
| 3:A9:153:SER:HB3  | 3:A9:191:GLN:HE22 | 1.61                     | 0.65              |
| 7:f:9:PRO:HB2     | 7:f:143:ILE:HG23  | 1.77                     | 0.65              |
| 2:A6:208:ALA:HB2  | 2:A6:304:LYS:HG2  | 1.79                     | 0.65              |
| 7:e:194:ARG:HH12  | 7:e:198:ARG:HH21  | 1.43                     | 0.65              |
| 2:B4:318:MET:HB2  | 2:B4:376:CYS:HB3  | 1.78                     | 0.65              |
| 2:B8:109:THR:HG22 | 2:B8:110:ILE:HG23 | 1.77                     | 0.65              |
| 3:D9:309:ARG:H    | 3:D9:372:THR:HG22 | 1.62                     | 0.65              |
| 7:p:9:PRO:HB2     | 7:p:143:ILE:HG23  | 1.78                     | 0.65              |
| 2:D6:3:GLU:HA     | 2:D6:51:THR:HA    | 1.79                     | 0.64              |
| 7:d:171:ILE:HD13  | 7:d:182:PHE:HD1   | 1.62                     | 0.64              |
| 3:A3:164:MET:HB3  | 3:A3:197:ASP:H    | 1.61                     | 0.64              |
| 3:C3:190:HIS:HB2  | 3:C3:414:ASN:HD21 | 1.62                     | 0.64              |
| 3:D3:260:PHE:HB2  | 3:D3:263:LEU:HD12 | 1.79                     | 0.64              |
| 3:A1:207:LEU:HB3  | 3:A1:225:LEU:HD22 | 1.79                     | 0.64              |
| 2:C2:335:ILE:HA   | 2:C2:338:LYS:HZ2  | 1.63                     | 0.64              |
| 2:A0:391:MET:HG3  | 2:A0:394:LYS:HD2  | 1.79                     | 0.64              |
| 2:A4:176:GLN:HB2  | 3:A5:331:LEU:HD11 | 1.79                     | 0.64              |
| 3:C5:139:LEU:HA   | 3:C5:145:SER:HB3  | 1.79                     | 0.64              |
| 2:D4:274:PRO:HG2  | 2:D4:374:ALA:HA   | 1.80                     | 0.64              |
| 3:E7:304:ASP:HB3  | 3:E7:307:HIS:CE1  | 2.33                     | 0.64              |
| 2:C8:105:ARG:HH12 | 3:C9:251:ARG:HD3  | 1.62                     | 0.64              |
| 3:D1:133:PHE:HB2  | 3:D1:164:MET:HG3  | 1.80                     | 0.64              |
| 2:C2:100:ALA:HA   | 3:C3:252:LYS:HG3  | 1.79                     | 0.64              |
| 3:E7:67:ASP:HA    | 3:E7:143:THR:HG21 | 1.78                     | 0.64              |
| 7:d:170:VAL:HG12  | 7:d:185:ILE:HD11  | 1.80                     | 0.64              |
| 7:h:158:THR:HB    | 7:h:161:TYR:HB2   | 1.78                     | 0.64              |
| 7:m:112:PHE:HB2   | 7:m:131:TRP:HE1   | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:p:14:LYS:HE2    | 7:p:45:MET:HG3    | 1.79                     | 0.64              |
| 2:A4:194:LEU:HB3  | 2:A4:267:PHE:HE1  | 1.63                     | 0.64              |
| 2:C0:184:PRO:HA   | 2:C0:391:MET:HE1  | 1.80                     | 0.64              |
| 2:E4:320:ARG:HB3  | 2:E4:374:ALA:HB3  | 1.79                     | 0.64              |
| 2:A8:407:TRP:HE1  | 3:A9:258:ILE:HB   | 1.63                     | 0.63              |
| 3:B9:51:TYR:HB3   | 3:B9:59:PHE:HB3   | 1.79                     | 0.63              |
| 3:C9:103:LYS:HA   | 3:C9:107:THR:HB   | 1.79                     | 0.63              |
| 1:D:208:PRO:HB2   | 7:t:162:GLY:HA2   | 1.80                     | 0.63              |
| 8:l:25:ARG:HD2    | 7:n:20:GLU:HG3    | 1.80                     | 0.63              |
| 2:A0:332:VAL:HG13 | 2:A0:351:PHE:HD2  | 1.63                     | 0.63              |
| 3:B9:35:THR:HG22  | 7:h:83:PRO:HG3    | 1.79                     | 0.63              |
| 3:B9:325:GLU:HA   | 3:B9:328:GLU:HG3  | 1.80                     | 0.63              |
| 3:C5:102:ALA:HB2  | 3:C5:403:MET:HE2  | 1.78                     | 0.63              |
| 2:C8:417:GLU:HA   | 2:C8:420:GLU:HG2  | 1.80                     | 0.63              |
| 2:A4:384:ILE:HG12 | 2:A4:432:TYR:CZ   | 2.34                     | 0.63              |
| 3:A3:91:VAL:HG21  | 3:A3:116:VAL:HG12 | 1.80                     | 0.63              |
| 2:B4:174:SER:HB3  | 2:B4:205:ASP:HB3  | 1.79                     | 0.63              |
| 2:E0:76:ASP:HA    | 2:E0:79:ARG:HG3   | 1.80                     | 0.63              |
| 2:E0:402:ARG:HH12 | 2:E0:415:GLU:HG3  | 1.63                     | 0.63              |
| 7:h:14:LYS:HB2    | 7:h:47:LEU:HD12   | 1.81                     | 0.63              |
| 7:o:149:ARG:HD2   | 7:o:161:TYR:HB3   | 1.81                     | 0.63              |
| 7:r:9:PRO:HA      | 7:r:12:VAL:HG22   | 1.80                     | 0.63              |
| 3:B9:66:MET:HB3   | 3:B9:147:MET:HE1  | 1.81                     | 0.63              |
| 2:C6:210:TYR:HB3  | 3:C7:324:LYS:HZ3  | 1.64                     | 0.63              |
| 2:D0:7:ILE:HD11   | 2:D0:122:ILE:HD11 | 1.80                     | 0.63              |
| 3:D9:132:GLY:HA2  | 3:D9:162:ARG:HB3  | 1.81                     | 0.63              |
| 2:B8:75:VAL:HG13  | 2:B8:92:LEU:HD12  | 1.81                     | 0.63              |
| 2:C0:265:ILE:HD11 | 2:C0:435:VAL:HG21 | 1.80                     | 0.63              |
| 2:A4:310:GLY:HA3  | 2:A4:383:ALA:HB2  | 1.81                     | 0.63              |
| 2:E8:273:ALA:HA   | 2:E8:275:ILE:HG12 | 1.81                     | 0.63              |
| 7:i:9:PRO:HB2     | 7:i:143:ILE:HG23  | 1.81                     | 0.63              |
| 7:p:14:LYS:HE3    | 7:p:47:LEU:HD22   | 1.80                     | 0.63              |
| 3:B5:150:LEU:HD23 | 3:B5:154:LYS:HZ2  | 1.64                     | 0.62              |
| 3:C5:260:PHE:HB2  | 3:C5:263:LEU:HD23 | 1.80                     | 0.62              |
| 1:D:256:LEU:HD12  | 1:D:257:PRO:HD2   | 1.81                     | 0.62              |
| 2:D4:398:MET:HE3  | 3:D5:345:ILE:HG23 | 1.81                     | 0.62              |
| 3:C1:267:LEU:HD13 | 3:C1:371:SER:HB3  | 1.81                     | 0.62              |
| 2:E0:78:VAL:HA    | 1:F:247:TYR:HE2   | 1.65                     | 0.62              |
| 2:B2:364:PRO:HG2  | 1:E:254:LYS:HE3   | 1.81                     | 0.62              |
| 4:V:1285:ARG:HE   | 4:V:1289:ARG:HH12 | 1.47                     | 0.62              |
| 7:h:9:PRO:HA      | 7:h:12:VAL:HG22   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:w:151:MET:HE1   | 7:w:156:VAL:HG12  | 1.80                     | 0.62              |
| 3:A1:260:PHE:HB2  | 3:A1:263:LEU:HD23 | 1.80                     | 0.62              |
| 3:C7:320:ARG:HH22 | 1:J:211:GLY:HA2   | 1.63                     | 0.62              |
| 2:B0:223:THR:HG22 | 3:B1:322:SER:HA   | 1.82                     | 0.62              |
| 3:C9:276:ARG:HD3  | 5:P:499:ASP:HA    | 1.81                     | 0.62              |
| 3:A5:242:PHE:HB3  | 3:A5:356:ILE:HD13 | 1.80                     | 0.62              |
| 2:B0:73:THR:HA    | 3:B1:46:ARG:HH21  | 1.64                     | 0.62              |
| 3:B1:200:GLN:HG2  | 3:B1:268:ILE:HD11 | 1.82                     | 0.62              |
| 2:B8:220:GLU:HG2  | 2:B8:221:ARG:HG2  | 1.82                     | 0.62              |
| 2:C6:276:ILE:HD12 | 2:C6:281:ALA:HA   | 1.80                     | 0.62              |
| 2:D8:414:GLU:HG2  | 2:D8:416:GLY:H    | 1.65                     | 0.62              |
| 3:E5:166:THR:HG21 | 3:E5:192:LEU:HD11 | 1.82                     | 0.62              |
| 2:E8:54:SER:HA    | 2:E8:64:ARG:HH21  | 1.65                     | 0.62              |
| 2:A0:271:SER:HB2  | 2:A0:377:MET:HG2  | 1.80                     | 0.62              |
| 2:B8:408:TYR:HB3  | 2:B8:413:MET:HE2  | 1.79                     | 0.62              |
| 3:C1:281:TYR:HE1  | 3:C5:87:PRO:HD3   | 1.65                     | 0.62              |
| 2:E6:273:ALA:HA   | 2:E6:275:ILE:HG12 | 1.82                     | 0.62              |
| 7:g:88:LEU:HD11   | 7:g:185:ILE:HD13  | 1.82                     | 0.62              |
| 7:v:5:VAL:HG21    | 7:v:161:TYR:HE1   | 1.64                     | 0.62              |
| 2:A4:338:LYS:HE3  | 2:A4:340:THR:HB   | 1.82                     | 0.62              |
| 3:A5:330:MET:HE2  | 3:A5:349:MET:HE3  | 1.81                     | 0.62              |
| 3:A7:22:GLU:HB2   | 3:A7:81:PHE:HD2   | 1.63                     | 0.62              |
| 3:B5:327:ASP:HA   | 3:B5:330:MET:HE3  | 1.82                     | 0.62              |
| 3:C3:100:ASN:HB3  | 3:C3:103:LYS:HG2  | 1.80                     | 0.62              |
| 4:N:1271:SER:HA   | 4:N:1274:MET:HE2  | 1.80                     | 0.62              |
| 7:d:172:VAL:HG23  | 7:d:180:ALA:HB3   | 1.82                     | 0.62              |
| 7:f:25:GLN:HE22   | 7:f:36:ILE:HG21   | 1.64                     | 0.62              |
| 7:i:115:LEU:HD13  | 7:i:145:LYS:HE2   | 1.82                     | 0.62              |
| 2:B0:338:LYS:HZ2  | 2:B0:340:THR:H    | 1.47                     | 0.62              |
| 3:E3:337:ASN:HB2  | 3:E3:340:TYR:HD2  | 1.65                     | 0.62              |
| 3:E7:257:LEU:HD23 | 3:E7:312:THR:HG23 | 1.81                     | 0.62              |
| 2:A8:259:LEU:HD21 | 2:A8:316:CYS:HB2  | 1.81                     | 0.62              |
| 2:C8:405:VAL:HG13 | 2:C8:418:PHE:HE2  | 1.65                     | 0.62              |
| 3:D1:7:VAL:HB     | 3:D1:135:ILE:HG12 | 1.82                     | 0.62              |
| 3:D5:313:ALA:HB3  | 3:D5:349:MET:HG2  | 1.82                     | 0.62              |
| 2:E2:272:TYR:HB3  | 2:E2:275:ILE:HD11 | 1.82                     | 0.62              |
| 3:E3:318:ARG:HD2  | 3:E3:358:PRO:HD3  | 1.80                     | 0.62              |
| 2:A0:280:LYS:HZ1  | 2:A4:90:GLU:HG3   | 1.64                     | 0.61              |
| 3:B5:101:TRP:HE1  | 3:B5:188:SER:HB2  | 1.65                     | 0.61              |
| 3:E3:2:ARG:HB3    | 3:E3:131:GLN:HB2  | 1.82                     | 0.61              |
| 3:E3:136:THR:HG22 | 3:E3:167:PHE:HB2  | 1.80                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F1:30:ILE:HG13  | 3:F1:51:TYR:HE1   | 1.65                     | 0.61              |
| 3:C5:98:GLY:HA2   | 2:C6:254:GLU:HG2  | 1.82                     | 0.61              |
| 3:C9:271:ALA:HB1  | 3:C9:292:GLN:HB3  | 1.83                     | 0.61              |
| 3:D7:248:SER:HA   | 3:D7:252:LYS:HD3  | 1.83                     | 0.61              |
| 7:q:90:PRO:HA     | 7:q:93:LEU:HD12   | 1.83                     | 0.61              |
| 2:A0:200:VAL:HG11 | 2:A0:255:PHE:HE2  | 1.66                     | 0.61              |
| 3:A3:207:LEU:HB3  | 3:A3:225:LEU:HG   | 1.82                     | 0.61              |
| 2:A4:298:PRO:HG2  | 2:A4:308:ARG:HH11 | 1.64                     | 0.61              |
| 3:A9:227:HIS:HD2  | 5:P:312:ILE:HG23  | 1.66                     | 0.61              |
| 2:A0:135:PHE:HB2  | 2:A0:166:LYS:HG2  | 1.82                     | 0.61              |
| 3:A3:308:GLY:HA3  | 3:A3:373:ALA:HB2  | 1.82                     | 0.61              |
| 2:E0:320:ARG:HH21 | 2:E0:360:PRO:HA   | 1.66                     | 0.61              |
| 3:E5:187:LEU:HD12 | 3:E5:190:HIS:HE1  | 1.65                     | 0.61              |
| 3:E5:207:LEU:HB3  | 3:E5:225:LEU:HD11 | 1.83                     | 0.61              |
| 7:b:178:ARG:HH12  | 7:b:180:ALA:HB2   | 1.65                     | 0.61              |
| 8:l:27:ASP:HB2    | 8:l:30:ALA:HB3    | 1.83                     | 0.61              |
| 3:A1:257:LEU:HD11 | 3:A1:314:SER:HB3  | 1.82                     | 0.61              |
| 3:A7:318:ARG:HA   | 3:A7:354:CYS:HB2  | 1.82                     | 0.61              |
| 3:E5:65:LEU:HB3   | 3:E5:73:MET:HE1   | 1.82                     | 0.61              |
| 4:M:1254:ARG:HH21 | 4:M:1266:ALA:HB1  | 1.65                     | 0.61              |
| 2:A0:210:TYR:CE2  | 3:A1:324:LYS:HE3  | 2.36                     | 0.61              |
| 2:C2:81:GLY:HA2   | 1:I:216:ARG:HD3   | 1.81                     | 0.61              |
| 3:E3:274:THR:HB   | 3:E3:282:ARG:HH11 | 1.66                     | 0.61              |
| 2:E8:181:VAL:HB   | 3:E9:256:ASN:HB2  | 1.83                     | 0.61              |
| 7:f:14:LYS:HD3    | 7:f:47:LEU:HB2    | 1.82                     | 0.61              |
| 7:g:149:ARG:HH22  | 7:g:162:GLY:H     | 1.47                     | 0.61              |
| 7:j:16:ARG:HE     | 7:j:17:LEU:HD22   | 1.66                     | 0.61              |
| 8:l:45:LYS:HZ2    | 8:l:129:PRO:HD2   | 1.65                     | 0.61              |
| 3:A3:165:GLU:HG2  | 3:A3:200:GLN:HE22 | 1.65                     | 0.61              |
| 2:D2:84:ARG:HH21  | 7:o:197:LEU:HD21  | 1.66                     | 0.61              |
| 3:D3:60:VAL:HG21  | 3:D3:86:ARG:HG3   | 1.81                     | 0.61              |
| 2:E4:244:PHE:HB2  | 2:E4:356:ASN:HD21 | 1.66                     | 0.61              |
| 2:B8:214:ARG:HE   | 2:B8:215:ARG:HG3  | 1.66                     | 0.61              |
| 3:D9:10:GLY:HA2   | 3:D9:143:THR:HG23 | 1.83                     | 0.61              |
| 3:E7:45:GLU:HG2   | 3:E7:46:ARG:HG2   | 1.81                     | 0.61              |
| 3:E9:342:VAL:HG22 | 3:E9:344:TRP:H    | 1.66                     | 0.61              |
| 2:D0:133:GLN:HB3  | 2:D0:252:VAL:HG11 | 1.83                     | 0.60              |
| 7:i:10:LEU:HD11   | 7:i:144:LEU:HD12  | 1.81                     | 0.60              |
| 2:D0:405:VAL:HG13 | 2:D0:418:PHE:HE2  | 1.66                     | 0.60              |
| 3:D1:178:THR:HB   | 3:D1:181:GLU:HG3  | 1.82                     | 0.60              |
| 2:D4:213:CYS:HA   | 2:D4:217:LEU:HD13 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:l:106:ILE:HG13  | 8:l:111:VAL:HB    | 1.83                     | 0.60              |
| 3:A9:311:LEU:HD23 | 3:A9:312:THR:HG23 | 1.84                     | 0.60              |
| 2:C2:64:ARG:HG3   | 2:C2:125:LEU:HD21 | 1.82                     | 0.60              |
| 3:C7:248:SER:HA   | 3:C7:252:LYS:HD3  | 1.82                     | 0.60              |
| 3:E3:57:GLY:HA3   | 7:t:83:PRO:HB2    | 1.84                     | 0.60              |
| 3:F1:276:ARG:HB3  | 6:T:97:LEU:HD22   | 1.83                     | 0.60              |
| 2:A0:364:PRO:HB2  | 5:O:242:LEU:HB2   | 1.83                     | 0.60              |
| 2:A8:78:VAL:HA    | 1:C:247:TYR:HE1   | 1.67                     | 0.60              |
| 2:C4:112:LYS:HA   | 2:C4:115:VAL:HG12 | 1.82                     | 0.60              |
| 2:C6:286:LEU:HD13 | 2:C6:371:VAL:HG13 | 1.82                     | 0.60              |
| 2:E8:104:ALA:HB2  | 2:E8:413:MET:HG2  | 1.83                     | 0.60              |
| 2:C6:71:GLU:HB3   | 2:C6:98:ASP:HB3   | 1.83                     | 0.60              |
| 2:D8:239:THR:HA   | 2:D8:242:LEU:HD23 | 1.84                     | 0.60              |
| 3:B1:187:LEU:HD13 | 3:B1:403:MET:HE1  | 1.83                     | 0.60              |
| 2:C8:105:ARG:HE   | 2:C8:110:ILE:HG13 | 1.66                     | 0.60              |
| 3:D1:320:ARG:HH22 | 1:K:217:THR:HG21  | 1.67                     | 0.60              |
| 3:E7:204:ASN:HD21 | 11:E7:501:GDP:H1' | 1.66                     | 0.60              |
| 2:B0:237:SER:HA   | 2:B0:320:ARG:HD2  | 1.84                     | 0.60              |
| 3:C3:192:LEU:HD21 | 3:C3:199:VAL:HG21 | 1.83                     | 0.60              |
| 3:C5:253:LEU:HD11 | 3:C5:316:MET:HE1  | 1.82                     | 0.60              |
| 2:C8:313:MET:HE3  | 2:C8:380:ASN:HB3  | 1.82                     | 0.60              |
| 7:f:10:LEU:HD22   | 7:f:47:LEU:HD11   | 1.83                     | 0.60              |
| 7:g:14:LYS:HD2    | 7:g:47:LEU:HB2    | 1.83                     | 0.60              |
| 7:g:78:ALA:HB3    | 7:g:112:PHE:HE1   | 1.67                     | 0.60              |
| 3:B3:175:VAL:HG21 | 2:B4:329:ASN:HB3  | 1.84                     | 0.60              |
| 3:B7:290:THR:HG21 | 3:B7:329:GLN:HG2  | 1.82                     | 0.60              |
| 2:D6:181:VAL:HG12 | 3:D7:256:ASN:HD22 | 1.67                     | 0.60              |
| 3:E5:7:VAL:HB     | 3:E5:135:ILE:HG13 | 1.83                     | 0.60              |
| 3:E9:35:THR:HG22  | 7:w:83:PRO:HG3    | 1.84                     | 0.60              |
| 2:F0:66:VAL:HG23  | 2:F0:91:GLN:HB2   | 1.84                     | 0.60              |
| 7:c:10:LEU:HD13   | 7:c:147:HIS:HB2   | 1.84                     | 0.60              |
| 7:r:172:VAL:HG23  | 7:r:180:ALA:HB3   | 1.83                     | 0.60              |
| 3:B3:173:PRO:HD2  | 3:B3:205:GLU:HG2  | 1.82                     | 0.60              |
| 3:C9:113:ILE:HA   | 3:C9:116:VAL:HG12 | 1.84                     | 0.60              |
| 3:E1:49:VAL:HG11  | 3:E1:241:ARG:HG2  | 1.84                     | 0.60              |
| 7:b:158:THR:HB    | 7:b:159:TYR:HD1   | 1.65                     | 0.60              |
| 7:c:113:VAL:HG22  | 7:c:134:ILE:HD12  | 1.84                     | 0.60              |
| 7:p:42:TYR:HA     | 7:p:45:MET:HB2    | 1.83                     | 0.60              |
| 7:t:4:PRO:HG3     | 7:t:179:GLU:HB2   | 1.83                     | 0.60              |
| 3:A9:375:GLN:HA   | 3:A9:378:PHE:HD2  | 1.67                     | 0.60              |
| 3:E5:321:MET:HE1  | 3:E5:326:VAL:HB   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:M:1236:HIS:HB3  | 4:M:1249:THR:HG21 | 1.84                     | 0.60              |
| 3:C1:257:LEU:HD21 | 3:C1:314:SER:HB2  | 1.84                     | 0.59              |
| 4:L:1271:SER:HA   | 4:L:1274:MET:HE2  | 1.82                     | 0.59              |
| 2:A4:31:GLN:HE22  | 7:a:104:ALA:HB2   | 1.67                     | 0.59              |
| 2:B0:422:ARG:HH22 | 2:B0:425:LEU:HD22 | 1.66                     | 0.59              |
| 2:E4:71:GLU:HB3   | 2:E4:98:ASP:HB2   | 1.83                     | 0.59              |
| 2:F0:105:ARG:HH22 | 3:F1:251:ARG:HG2  | 1.67                     | 0.59              |
| 7:t:191:GLU:HB2   | 7:t:195:ALA:HB2   | 1.83                     | 0.59              |
| 2:A4:213:CYS:HA   | 2:A4:217:LEU:HD13 | 1.82                     | 0.59              |
| 3:B1:19:LYS:HD2   | 3:B1:226:ASN:HB2  | 1.85                     | 0.59              |
| 3:B1:377:MET:HA   | 3:B1:380:ARG:HE   | 1.66                     | 0.59              |
| 2:B4:262:TYR:HD1  | 2:B4:265:ILE:HD11 | 1.67                     | 0.59              |
| 3:B5:193:VAL:HG21 | 3:B5:418:LEU:HD21 | 1.84                     | 0.59              |
| 3:C9:73:MET:HE1   | 3:C9:92:PHE:HA    | 1.84                     | 0.59              |
| 5:P:517:ALA:H     | 5:P:521:PRO:HD2   | 1.66                     | 0.59              |
| 3:B1:91:VAL:HG11  | 3:B1:116:VAL:HG12 | 1.83                     | 0.59              |
| 3:B5:139:LEU:HA   | 3:B5:145:SER:HB3  | 1.84                     | 0.59              |
| 3:C5:135:ILE:HG12 | 3:C5:152:ILE:HD11 | 1.83                     | 0.59              |
| 3:E5:385:PHE:HA   | 3:E5:388:MET:HE2  | 1.84                     | 0.59              |
| 3:E9:361:LEU:HA   | 6:U:105:HIS:CE1   | 2.38                     | 0.59              |
| 7:v:149:ARG:HE    | 7:v:164:ARG:HB2   | 1.67                     | 0.59              |
| 3:B5:242:PHE:HB3  | 3:B5:356:ILE:HD13 | 1.85                     | 0.59              |
| 3:C7:119:VAL:HG13 | 3:C7:122:LYS:HE3  | 1.84                     | 0.59              |
| 2:D2:286:LEU:HD13 | 2:D2:371:VAL:HG13 | 1.85                     | 0.59              |
| 2:D6:16:ILE:HD11  | 2:D6:231:ILE:HB   | 1.84                     | 0.59              |
| 2:E0:244:PHE:HB2  | 2:E0:356:ASN:HD21 | 1.66                     | 0.59              |
| 7:f:14:LYS:HB2    | 7:f:47:LEU:HD12   | 1.85                     | 0.59              |
| 3:A9:57:GLY:HA3   | 7:c:83:PRO:HB2    | 1.83                     | 0.59              |
| 2:B4:398:MET:HE2  | 3:B5:345:ILE:HG23 | 1.83                     | 0.59              |
| 2:B8:3:GLU:HA     | 2:B8:51:THR:HA    | 1.85                     | 0.59              |
| 3:C5:237:THR:HG23 | 3:C5:240:LEU:HD13 | 1.84                     | 0.59              |
| 3:F1:271:ALA:HB1  | 3:F1:292:GLN:HG2  | 1.83                     | 0.59              |
| 7:w:151:MET:HE3   | 7:w:154:TYR:HA    | 1.85                     | 0.59              |
| 1:A:247:TYR:HE2   | 2:A4:78:VAL:HA    | 1.68                     | 0.59              |
| 2:C4:320:ARG:HH11 | 2:C4:360:PRO:HA   | 1.67                     | 0.59              |
| 3:C9:175:VAL:HG11 | 2:D0:329:ASN:HA   | 1.84                     | 0.59              |
| 3:E3:284:LEU:HB3  | 3:E3:362:LYS:HE3  | 1.84                     | 0.59              |
| 3:E5:45:GLU:HG2   | 3:E5:46:ARG:HG2   | 1.85                     | 0.59              |
| 2:E6:204:LEU:HD12 | 2:E6:209:ILE:HD11 | 1.83                     | 0.59              |
| 2:A6:102:ASN:HB3  | 2:A6:105:ARG:HG3  | 1.85                     | 0.59              |
| 3:B3:136:THR:HG22 | 3:B3:167:PHE:HB2  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B3:198:GLU:HG2  | 3:B3:266:PHE:HE2  | 1.66                     | 0.59              |
| 2:C2:137:MET:HB2  | 2:C2:168:ASN:HA   | 1.85                     | 0.59              |
| 2:D4:91:GLN:HG2   | 2:D4:121:ARG:HE   | 1.67                     | 0.59              |
| 2:E4:26:LEU:HD11  | 1:H:254:LYS:HG2   | 1.85                     | 0.59              |
| 2:F0:104:ALA:HB2  | 2:F0:413:MET:HG2  | 1.84                     | 0.59              |
| 2:A0:178:SER:HB3  | 3:A1:347:ASN:HD22 | 1.66                     | 0.59              |
| 2:B8:222:PRO:HD2  | 3:B9:324:LYS:HB2  | 1.83                     | 0.59              |
| 3:C1:272:PRO:HG3  | 3:C1:364:SER:HA   | 1.85                     | 0.59              |
| 3:C5:416:ASN:C    | 3:C5:416:ASN:HD22 | 2.07                     | 0.59              |
| 2:C6:311:LYS:HA   | 2:C6:342:GLN:HE22 | 1.68                     | 0.59              |
| 2:D4:3:GLU:HA     | 2:D4:51:THR:HA    | 1.85                     | 0.59              |
| 3:D7:375:GLN:HB2  | 3:D7:419:VAL:HG13 | 1.84                     | 0.59              |
| 2:E4:119:LEU:HD11 | 2:E4:156:ARG:HG3  | 1.85                     | 0.59              |
| 3:F1:7:VAL:HG22   | 3:F1:64:ILE:HB    | 1.83                     | 0.59              |
| 7:a:152:LYS:HA    | 7:a:164:ARG:HH21  | 1.68                     | 0.59              |
| 8:k:106:ILE:HG23  | 8:k:111:VAL:HB    | 1.85                     | 0.59              |
| 3:B7:51:TYR:HB3   | 3:B7:59:PHE:HB3   | 1.85                     | 0.59              |
| 3:C5:391:ARG:HD3  | 2:C6:346:TRP:HB3  | 1.84                     | 0.59              |
| 3:E1:210:ILE:HD11 | 3:E1:298:ASN:HA   | 1.84                     | 0.59              |
| 2:E4:210:TYR:HE1  | 2:E4:227:LEU:HD11 | 1.68                     | 0.59              |
| 3:E5:134:GLN:HE21 | 3:E5:167:PHE:HE2  | 1.49                     | 0.59              |
| 7:h:94:ASN:HA     | 7:h:97:ARG:HE     | 1.68                     | 0.59              |
| 7:h:184:PRO:HG3   | 7:h:189:LEU:HD23  | 1.85                     | 0.59              |
| 7:s:63:ILE:HB     | 7:s:67:HIS:ND1    | 2.17                     | 0.59              |
| 3:A3:102:ALA:HB2  | 3:A3:403:MET:HE2  | 1.83                     | 0.58              |
| 2:B0:177:VAL:HG21 | 3:B1:327:ASP:HB3  | 1.85                     | 0.58              |
| 2:C6:80:THR:HA    | 2:C6:84:ARG:HE    | 1.68                     | 0.58              |
| 3:A5:257:LEU:HD11 | 3:A5:314:SER:HB2  | 1.84                     | 0.58              |
| 2:B0:398:MET:HE1  | 3:B1:345:ILE:HG12 | 1.84                     | 0.58              |
| 3:D7:200:GLN:HG2  | 3:D7:268:ILE:HD12 | 1.86                     | 0.58              |
| 7:p:95:TYR:O      | 7:p:99:MET:HB3    | 2.03                     | 0.58              |
| 7:r:11:ASN:HB3    | 7:r:15:ARG:HH12   | 1.68                     | 0.58              |
| 7:t:5:VAL:HG11    | 7:t:149:ARG:HD3   | 1.85                     | 0.58              |
| 3:A9:51:TYR:HB3   | 3:A9:59:PHE:HB3   | 1.85                     | 0.58              |
| 3:A9:358:PRO:HG2  | 3:A9:361:LEU:HB2  | 1.84                     | 0.58              |
| 2:B8:319:TYR:HB2  | 2:B8:355:ILE:HG22 | 1.84                     | 0.58              |
| 3:F1:217:LEU:HA   | 6:R:174:ARG:HH12  | 1.68                     | 0.58              |
| 3:F1:356:ILE:HD12 | 6:T:113:TRP:HB3   | 1.85                     | 0.58              |
| 3:F1:358:PRO:HG2  | 3:F1:361:LEU:HB2  | 1.86                     | 0.58              |
| 7:j:119:ARG:HH12  | 7:j:136:LEU:HB3   | 1.67                     | 0.58              |
| 2:A4:269:LEU:HG   | 2:A4:301:MET:HE2  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:204:LEU:HD12 | 2:B0:209:ILE:HD11 | 1.84                     | 0.58              |
| 2:B4:244:PHE:HB2  | 2:B4:356:ASN:HD21 | 1.68                     | 0.58              |
| 3:E7:192:LEU:HD21 | 3:E7:199:VAL:HG21 | 1.85                     | 0.58              |
| 7:b:153:GLU:HA    | 7:b:164:ARG:HH22  | 1.68                     | 0.58              |
| 7:c:64:PRO:HD2    | 7:c:67:HIS:CD2    | 2.38                     | 0.58              |
| 3:A7:2:ARG:HB3    | 3:A7:131:GLN:HB2  | 1.85                     | 0.58              |
| 2:C4:187:SER:HB3  | 2:C4:391:MET:HE3  | 1.85                     | 0.58              |
| 2:E4:280:LYS:HZ3  | 2:E8:89:PRO:HB2   | 1.68                     | 0.58              |
| 3:E7:68:LEU:HD22  | 3:E7:97:ALA:HB2   | 1.86                     | 0.58              |
| 3:E9:101:TRP:H    | 3:E9:398:TYR:HE1  | 1.52                     | 0.58              |
| 3:E9:284:LEU:HD13 | 3:E9:363:MET:HG2  | 1.85                     | 0.58              |
| 1:F:231:VAL:HG21  | 5:P:561:VAL:H     | 1.67                     | 0.58              |
| 4:N:1285:ARG:HH22 | 4:N:1295:ILE:H    | 1.50                     | 0.58              |
| 7:m:78:ALA:HB3    | 7:m:112:PHE:HE1   | 1.69                     | 0.58              |
| 3:A3:281:TYR:HD1  | 3:A7:87:PRO:HD3   | 1.67                     | 0.58              |
| 3:B3:34:GLY:HA3   | 3:B3:58:ARG:HB2   | 1.86                     | 0.58              |
| 2:E2:320:ARG:HH12 | 2:E2:360:PRO:HA   | 1.67                     | 0.58              |
| 6:S:170:GLU:CD    | 6:S:171:ASP:H     | 2.12                     | 0.58              |
| 7:e:9:PRO:HA      | 7:e:12:VAL:HG22   | 1.86                     | 0.58              |
| 7:v:183:LEU:HD11  | 7:v:199:TRP:HB2   | 1.85                     | 0.58              |
| 3:A5:304:ASP:HB3  | 3:A5:307:HIS:CE1  | 2.38                     | 0.58              |
| 2:C6:138:PHE:HE1  | 2:C6:169:PHE:HD1  | 1.51                     | 0.58              |
| 2:C8:224:TYR:HA   | 2:C8:227:LEU:HD12 | 1.86                     | 0.58              |
| 3:E1:68:LEU:HD22  | 3:E1:97:ALA:HB2   | 1.86                     | 0.58              |
| 2:F0:207:GLU:HA   | 2:F0:210:TYR:HB2  | 1.84                     | 0.58              |
| 2:B2:265:ILE:HG21 | 2:B2:313:MET:HE1  | 1.85                     | 0.58              |
| 3:B3:282:ARG:HH12 | 3:B3:284:LEU:HB2  | 1.68                     | 0.58              |
| 2:B6:217:LEU:HD11 | 2:B6:275:ILE:HG22 | 1.86                     | 0.58              |
| 2:B8:53:PHE:HB3   | 2:B8:61:HIS:HB3   | 1.86                     | 0.58              |
| 3:D7:135:ILE:HB   | 3:D7:166:THR:HG22 | 1.86                     | 0.58              |
| 2:E6:3:GLU:HA     | 2:E6:51:THR:HA    | 1.86                     | 0.58              |
| 7:s:72:SER:HB3    | 7:s:108:ILE:HG22  | 1.86                     | 0.58              |
| 7:v:42:TYR:HA     | 7:v:45:MET:HG3    | 1.86                     | 0.58              |
| 3:A3:320:ARG:HH21 | 6:R:78:GLU:HB3    | 1.69                     | 0.58              |
| 3:C5:68:LEU:HD12  | 3:C5:97:ALA:HB2   | 1.86                     | 0.58              |
| 3:C5:178:THR:HA   | 2:C6:258:ASN:HD21 | 1.68                     | 0.58              |
| 2:E0:64:ARG:HG2   | 2:E0:125:LEU:HD22 | 1.85                     | 0.58              |
| 2:E0:398:MET:HG2  | 3:E1:345:ILE:HG22 | 1.84                     | 0.58              |
| 2:A0:222:PRO:O    | 3:A1:324:LYS:HD3  | 2.03                     | 0.58              |
| 2:A2:195:LEU:HD21 | 2:A2:264:ARG:HH22 | 1.69                     | 0.58              |
| 2:A8:225:THR:HG21 | 1:C:250:GLU:HG3   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A0:398:MET:HE1  | 3:A1:345:ILE:HG12 | 1.85                     | 0.57              |
| 3:A1:182:PRO:HG2  | 3:A1:388:MET:HE1  | 1.86                     | 0.57              |
| 3:C5:220:PRO:HG2  | 2:C6:326:LYS:HG3  | 1.85                     | 0.57              |
| 2:C8:3:GLU:HA     | 2:C8:51:THR:HA    | 1.86                     | 0.57              |
| 2:D0:209:ILE:HG13 | 2:D0:302:MET:HG2  | 1.86                     | 0.57              |
| 3:F1:257:LEU:HD21 | 3:F1:314:SER:HB2  | 1.86                     | 0.57              |
| 6:U:117:THR:O     | 6:U:121:TYR:HB2   | 2.04                     | 0.57              |
| 7:a:123:GLU:HA    | 7:a:126:ARG:HB2   | 1.85                     | 0.57              |
| 7:n:42:TYR:HA     | 7:n:45:MET:HE1    | 1.84                     | 0.57              |
| 2:B4:259:LEU:HD11 | 2:B4:316:CYS:HB2  | 1.86                     | 0.57              |
| 3:B7:139:LEU:HA   | 3:B7:145:SER:HB3  | 1.86                     | 0.57              |
| 3:C7:189:VAL:HG21 | 3:C7:415:MET:HE2  | 1.85                     | 0.57              |
| 2:C8:176:GLN:HB3  | 3:C9:331:LEU:HD11 | 1.86                     | 0.57              |
| 3:E1:156:ARG:HE   | 3:E1:164:MET:HE2  | 1.69                     | 0.57              |
| 7:c:10:LEU:HD12   | 7:c:143:ILE:HG12  | 1.85                     | 0.57              |
| 7:x:115:LEU:HD12  | 7:x:167:VAL:HG11  | 1.86                     | 0.57              |
| 3:A3:399:THR:HA   | 3:A3:403:MET:HB2  | 1.85                     | 0.57              |
| 2:D4:102:ASN:HB3  | 2:D4:105:ARG:HB2  | 1.86                     | 0.57              |
| 7:e:9:PRO:HB2     | 7:e:143:ILE:HG13  | 1.85                     | 0.57              |
| 7:r:119:ARG:HH21  | 7:r:137:GLU:HG2   | 1.68                     | 0.57              |
| 7:u:24:MET:HA     | 7:u:27:GLN:HG3    | 1.85                     | 0.57              |
| 2:A4:57:GLY:HA2   | 5:O:254:GLY:HA3   | 1.86                     | 0.57              |
| 2:C6:199:ASP:HB3  | 2:C6:256:GLN:HE22 | 1.70                     | 0.57              |
| 2:C6:311:LYS:HD2  | 2:C6:342:GLN:HE22 | 1.68                     | 0.57              |
| 3:C9:330:MET:HB3  | 3:C9:349:MET:HG3  | 1.85                     | 0.57              |
| 3:F1:207:LEU:HB3  | 3:F1:225:LEU:HD12 | 1.87                     | 0.57              |
| 3:A5:220:PRO:HD2  | 2:A6:326:LYS:HE2  | 1.86                     | 0.57              |
| 2:B8:138:PHE:HD1  | 2:B8:169:PHE:HB2  | 1.70                     | 0.57              |
| 3:C3:318:ARG:HE   | 3:C3:358:PRO:HD3  | 1.69                     | 0.57              |
| 2:C4:34:GLY:HA3   | 2:C4:60:LYS:HD2   | 1.86                     | 0.57              |
| 2:C6:119:LEU:HD23 | 2:C6:122:ILE:HD12 | 1.85                     | 0.57              |
| 2:D4:218:ASP:HB3  | 7:r:194:ARG:HH22  | 1.68                     | 0.57              |
| 2:D4:320:ARG:HH21 | 2:D4:360:PRO:HA   | 1.70                     | 0.57              |
| 3:E1:220:PRO:HD2  | 2:E2:326:LYS:HD3  | 1.85                     | 0.57              |
| 7:e:93:LEU:HB3    | 7:e:97:ARG:HH21   | 1.69                     | 0.57              |
| 8:k:101:LEU:HA    | 8:k:104:LYS:HD2   | 1.87                     | 0.57              |
| 3:A1:60:VAL:HG11  | 3:A1:86:ARG:HB2   | 1.87                     | 0.57              |
| 2:A2:70:LEU:HD12  | 2:A2:99:ALA:HB2   | 1.87                     | 0.57              |
| 2:B2:71:GLU:HB3   | 2:B2:73:THR:HG22  | 1.86                     | 0.57              |
| 2:B4:222:PRO:HD2  | 3:B5:324:LYS:HG2  | 1.86                     | 0.57              |
| 2:C0:238:LEU:HD13 | 2:C0:318:MET:HE1  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C6:177:VAL:HG11 | 2:C6:210:TYR:HE2  | 1.69                     | 0.57              |
| 2:C8:259:LEU:HD21 | 2:C8:316:CYS:HB2  | 1.86                     | 0.57              |
| 2:D4:140:ALA:HA   | 2:D4:171:SER:HB3  | 1.86                     | 0.57              |
| 2:D6:320:ARG:HB3  | 2:D6:374:ALA:HB3  | 1.86                     | 0.57              |
| 3:E9:113:ILE:HA   | 3:E9:116:VAL:HG12 | 1.86                     | 0.57              |
| 7:a:143:ILE:HD12  | 7:a:146:ARG:HD2   | 1.87                     | 0.57              |
| 7:u:97:ARG:O      | 7:u:101:GLU:HB2   | 2.03                     | 0.57              |
| 2:D2:11:GLN:HA    | 2:D2:74:VAL:HG11  | 1.86                     | 0.57              |
| 2:E0:178:SER:HB2  | 3:E1:347:ASN:HD22 | 1.70                     | 0.57              |
| 2:F0:205:ASP:HB2  | 2:F0:303:ALA:HA   | 1.86                     | 0.57              |
| 7:o:99:MET:HE3    | 7:o:107:LYS:HE3   | 1.86                     | 0.57              |
| 2:B6:318:MET:HB2  | 2:B6:376:CYS:HB3  | 1.86                     | 0.57              |
| 3:B9:200:GLN:HB3  | 3:B9:266:PHE:HB2  | 1.87                     | 0.57              |
| 2:D4:167:LEU:HA   | 2:D4:200:VAL:HB   | 1.87                     | 0.57              |
| 3:E1:44:LEU:HG    | 3:E1:47:ILE:HD12  | 1.86                     | 0.57              |
| 7:e:14:LYS:HE2    | 7:e:47:LEU:HD22   | 1.87                     | 0.57              |
| 3:A1:219:THR:HA   | 2:A2:326:LYS:HD2  | 1.86                     | 0.57              |
| 3:B7:215:LEU:HD21 | 5:P:371:ARG:HH22  | 1.69                     | 0.57              |
| 3:C5:179:VAL:HG13 | 2:C6:350:GLY:HA3  | 1.87                     | 0.57              |
| 3:D3:11:GLN:HA    | 3:D3:72:THR:HG21  | 1.86                     | 0.57              |
| 3:E9:215:LEU:HD11 | 6:U:102:LEU:HD11  | 1.85                     | 0.57              |
| 4:W:1395:GLU:HA   | 4:W:1398:LEU:HG   | 1.86                     | 0.57              |
| 7:r:9:PRO:HD3     | 7:r:146:ARG:HD2   | 1.86                     | 0.57              |
| 2:A0:188:VAL:HG13 | 2:A0:425:LEU:HD12 | 1.87                     | 0.57              |
| 2:B0:3:GLU:HA     | 2:B0:51:THR:HA    | 1.86                     | 0.57              |
| 3:B1:163:ILE:HD11 | 3:B1:251:ARG:HE   | 1.68                     | 0.57              |
| 3:B5:274:THR:HG22 | 3:B5:282:ARG:HE   | 1.69                     | 0.57              |
| 3:B9:359:LYS:HB3  | 1:G:207:LEU:HD23  | 1.85                     | 0.57              |
| 2:D8:220:GLU:HG2  | 2:D8:221:ARG:HG2  | 1.87                     | 0.57              |
| 2:A4:292:THR:HG21 | 2:A4:331:ALA:HB1  | 1.87                     | 0.56              |
| 3:B5:11:GLN:HA    | 3:B5:72:THR:HG21  | 1.85                     | 0.56              |
| 3:B5:253:LEU:HD21 | 3:B5:368:VAL:HG11 | 1.86                     | 0.56              |
| 3:C9:28:HIS:HA    | 3:C9:43:GLN:HG2   | 1.87                     | 0.56              |
| 2:D0:180:ALA:HB3  | 2:D0:183:GLU:HB2  | 1.86                     | 0.56              |
| 3:D3:271:ALA:HB2  | 3:D3:298:ASN:HD21 | 1.68                     | 0.56              |
| 3:E3:257:LEU:HD21 | 3:E3:314:SER:HB2  | 1.87                     | 0.56              |
| 2:E6:17:GLY:HA2   | 2:E6:20:CYS:HB2   | 1.87                     | 0.56              |
| 3:E7:237:THR:HG23 | 3:E7:241:ARG:HE   | 1.70                     | 0.56              |
| 7:c:55:LEU:HB3    | 7:c:132:LEU:HD23  | 1.87                     | 0.56              |
| 7:i:15:ARG:O      | 7:i:19:GLU:HG2    | 2.04                     | 0.56              |
| 8:k:57:TYR:HA     | 8:k:69:ILE:HD11   | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:r:4:PRO:HG3     | 7:r:179:GLU:HB2   | 1.86                     | 0.56              |
| 3:A5:268:ILE:H    | 3:A5:299:MET:HE1  | 1.71                     | 0.56              |
| 3:A5:276:ARG:HH22 | 5:P:288:PRO:HG3   | 1.70                     | 0.56              |
| 3:B1:8:GLN:HB2    | 3:B1:65:LEU:HA    | 1.87                     | 0.56              |
| 2:B2:294:SER:HA   | 2:B2:297:GLU:HG3  | 1.87                     | 0.56              |
| 2:B8:207:GLU:HA   | 2:B8:210:TYR:HB2  | 1.87                     | 0.56              |
| 3:C7:22:GLU:HA    | 3:C7:81:PHE:HD2   | 1.70                     | 0.56              |
| 3:C9:259:PRO:HG2  | 3:C9:311:LEU:HD23 | 1.88                     | 0.56              |
| 2:D2:250:VAL:HG11 | 2:D2:318:MET:HE1  | 1.87                     | 0.56              |
| 2:D4:12:ALA:HB3   | 2:D4:140:ALA:HB2  | 1.87                     | 0.56              |
| 2:D6:267:PHE:HB3  | 2:D6:384:ILE:HD13 | 1.87                     | 0.56              |
| 1:F:245:SER:O     | 1:F:249:SER:HB3   | 2.05                     | 0.56              |
| 3:A1:323:THR:HG22 | 3:A1:353:VAL:HG21 | 1.87                     | 0.56              |
| 3:A1:416:ASN:HA   | 3:A1:419:VAL:HG22 | 1.86                     | 0.56              |
| 3:A3:199:VAL:HG23 | 3:A3:264:HIS:CE1  | 2.41                     | 0.56              |
| 3:B1:218:THR:HG23 | 3:B1:219:THR:HG23 | 1.86                     | 0.56              |
| 2:B2:207:GLU:HG3  | 2:B2:304:LYS:HE3  | 1.87                     | 0.56              |
| 3:C1:323:THR:HG22 | 3:C1:353:VAL:HG21 | 1.85                     | 0.56              |
| 2:C2:80:THR:HA    | 2:C2:84:ARG:HE    | 1.70                     | 0.56              |
| 3:C3:49:VAL:HG11  | 3:C3:241:ARG:HG2  | 1.87                     | 0.56              |
| 2:D6:11:GLN:HE22  | 3:D7:246:LEU:HA   | 1.70                     | 0.56              |
| 2:E2:48:ALA:HB2   | 5:P:558:ARG:HD2   | 1.87                     | 0.56              |
| 3:E7:284:LEU:HD22 | 3:E7:362:LYS:HE2  | 1.87                     | 0.56              |
| 4:L:1241:PHE:CD2  | 4:L:1242:PRO:HD3  | 2.41                     | 0.56              |
| 7:b:199:TRP:HD1   | 7:b:201:TRP:HE3   | 1.54                     | 0.56              |
| 7:o:154:TYR:HE1   | 7:o:158:THR:HG22  | 1.71                     | 0.56              |
| 7:t:75:LEU:HD23   | 7:t:111:ILE:HB    | 1.85                     | 0.56              |
| 7:u:97:ARG:HH12   | 7:w:149:ARG:HH22  | 1.54                     | 0.56              |
| 3:A1:272:PRO:HG3  | 3:A1:364:SER:HA   | 1.88                     | 0.56              |
| 2:A2:417:GLU:HA   | 2:A2:420:GLU:HG2  | 1.88                     | 0.56              |
| 3:B1:39:ASP:HA    | 7:d:90:PRO:HG3    | 1.87                     | 0.56              |
| 3:C7:100:ASN:HB3  | 3:C7:103:LYS:HD3  | 1.88                     | 0.56              |
| 2:D0:189:LEU:HD13 | 2:D0:413:MET:HE1  | 1.86                     | 0.56              |
| 3:D9:57:GLY:HA3   | 7:r:83:PRO:HB2    | 1.86                     | 0.56              |
| 2:E6:2:ARG:HG2    | 2:E6:51:THR:HG22  | 1.86                     | 0.56              |
| 7:d:10:LEU:HD21   | 7:d:144:LEU:HD12  | 1.87                     | 0.56              |
| 7:w:195:ALA:HA    | 7:w:198:ARG:HG3   | 1.86                     | 0.56              |
| 3:A5:248:SER:HA   | 3:A5:252:LYS:HD2  | 1.88                     | 0.56              |
| 2:A6:407:TRP:HZ2  | 3:A7:258:ILE:HB   | 1.68                     | 0.56              |
| 2:B4:104:ALA:HB2  | 2:B4:413:MET:HE2  | 1.85                     | 0.56              |
| 2:B4:240:ALA:HB1  | 2:B4:356:ASN:HD22 | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C5:98:GLY:H     | 3:C5:103:LYS:HD2  | 1.69                     | 0.56              |
| 2:E2:271:SER:HB3  | 2:E2:377:MET:HB3  | 1.86                     | 0.56              |
| 3:E5:87:PRO:HA    | 3:E5:90:PHE:HD2   | 1.69                     | 0.56              |
| 2:E6:88:HIS:HB3   | 2:E6:91:GLN:HB2   | 1.87                     | 0.56              |
| 3:F1:217:LEU:HA   | 6:R:174:ARG:HH22  | 1.69                     | 0.56              |
| 7:u:113:VAL:HG21  | 7:u:144:LEU:HD11  | 1.87                     | 0.56              |
| 7:x:115:LEU:HD13  | 7:x:152:LYS:HG3   | 1.87                     | 0.56              |
| 1:A:214:ALA:O     | 1:A:218:ASP:CB    | 2.54                     | 0.56              |
| 3:B1:249:ASP:H    | 3:B1:252:LYS:HB3  | 1.71                     | 0.56              |
| 3:B7:178:THR:HG23 | 3:B7:181:GLU:HG3  | 1.86                     | 0.56              |
| 3:C1:221:THR:HG23 | 3:C1:223:GLY:H    | 1.70                     | 0.56              |
| 3:C5:12:CYS:HB3   | 3:C5:138:SER:HB3  | 1.87                     | 0.56              |
| 2:D2:75:VAL:HG11  | 2:D2:94:SER:HB2   | 1.87                     | 0.56              |
| 2:D4:104:ALA:HB2  | 2:D4:413:MET:HE2  | 1.88                     | 0.56              |
| 3:D5:98:GLY:H     | 3:D5:103:LYS:HD2  | 1.71                     | 0.56              |
| 2:E2:265:ILE:HG21 | 2:E2:313:MET:HE1  | 1.87                     | 0.56              |
| 2:B2:244:PHE:HB2  | 2:B2:356:ASN:HD21 | 1.71                     | 0.56              |
| 3:C5:66:MET:HE1   | 3:C5:148:GLY:HA2  | 1.87                     | 0.56              |
| 2:E8:301:MET:HE1  | 2:E8:307:PRO:HD3  | 1.88                     | 0.56              |
| 7:c:72:SER:HB3    | 7:c:108:ILE:HG22  | 1.88                     | 0.56              |
| 7:n:14:LYS:HB2    | 7:n:47:LEU:HD22   | 1.86                     | 0.56              |
| 3:A5:259:PRO:HB3  | 3:A5:344:TRP:HH2  | 1.71                     | 0.56              |
| 2:A8:219:ILE:HG12 | 7:e:198:ARG:HH22  | 1.71                     | 0.56              |
| 2:C6:326:LYS:HE2  | 5:P:458:ARG:HH12  | 1.70                     | 0.56              |
| 2:D8:338:LYS:HE3  | 2:D8:340:THR:HG22 | 1.88                     | 0.56              |
| 2:E6:323:VAL:HG23 | 2:E6:355:ILE:HG23 | 1.87                     | 0.56              |
| 3:E9:390:ARG:HH21 | 3:E9:391:ARG:HD2  | 1.70                     | 0.56              |
| 8:l:10:PRO:HG2    | 8:l:12:VAL:HG22   | 1.88                     | 0.56              |
| 2:A8:417:GLU:HA   | 2:A8:420:GLU:HG2  | 1.88                     | 0.56              |
| 3:C7:230:SER:HA   | 3:C7:233:MET:HG2  | 1.87                     | 0.56              |
| 3:E9:113:ILE:HD13 | 3:E9:150:LEU:HG   | 1.87                     | 0.56              |
| 1:H:247:TYR:O     | 1:H:251:TYR:HB2   | 2.05                     | 0.56              |
| 7:e:110:ILE:HB    | 7:e:131:TRP:CG    | 2.41                     | 0.56              |
| 7:m:15:ARG:O      | 7:m:19:GLU:HB3    | 2.06                     | 0.56              |
| 2:B8:18:ASN:HB3   | 1:G:219:TYR:HE2   | 1.71                     | 0.56              |
| 3:B9:246:LEU:HB2  | 3:B9:353:VAL:H    | 1.71                     | 0.56              |
| 1:D:215:TYR:HD1   | 2:D8:22:GLU:HB3   | 1.69                     | 0.56              |
| 3:D1:406:MET:HE3  | 3:D1:410:GLU:HB2  | 1.87                     | 0.56              |
| 3:D3:117:LEU:HD21 | 3:D3:154:LYS:HB3  | 1.87                     | 0.56              |
| 2:D8:370:LYS:HG2  | 7:t:203:ASN:HD21  | 1.69                     | 0.56              |
| 2:E6:319:TYR:HB3  | 2:E6:323:VAL:HG21 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E9:217:LEU:HD21 | 3:E9:276:ARG:HD2  | 1.87                     | 0.56              |
| 5:P:216:GLN:HA    | 5:P:219:LEU:HG    | 1.88                     | 0.56              |
| 7:g:12:VAL:HG12   | 7:g:15:ARG:HH22   | 1.71                     | 0.56              |
| 7:j:9:PRO:HB2     | 7:j:143:ILE:HG23  | 1.87                     | 0.56              |
| 2:A2:308:ARG:HA   | 2:A2:342:GLN:HE22 | 1.71                     | 0.55              |
| 3:A3:8:GLN:HB2    | 3:A3:65:LEU:HA    | 1.87                     | 0.55              |
| 3:B3:49:VAL:HG21  | 3:B3:241:ARG:HG2  | 1.89                     | 0.55              |
| 3:B7:320:ARG:HH22 | 1:G:246:CYS:HA    | 1.72                     | 0.55              |
| 3:A5:209:ASP:HB3  | 3:A5:210:ILE:HD12 | 1.88                     | 0.55              |
| 3:A7:311:LEU:HD23 | 3:A7:312:THR:HG23 | 1.88                     | 0.55              |
| 3:D1:97:ALA:HA    | 3:D1:103:LYS:HE3  | 1.89                     | 0.55              |
| 2:D4:403:ALA:HB2  | 3:D5:344:TRP:HZ3  | 1.69                     | 0.55              |
| 3:D7:34:GLY:HA3   | 3:D7:58:ARG:HG3   | 1.87                     | 0.55              |
| 3:E1:193:VAL:HG21 | 3:E1:418:LEU:HD21 | 1.88                     | 0.55              |
| 3:E9:189:VAL:HA   | 3:E9:192:LEU:HB3  | 1.88                     | 0.55              |
| 7:b:155:GLU:HA    | 7:b:159:TYR:CZ    | 2.42                     | 0.55              |
| 8:l:32:VAL:HA     | 8:l:163:LYS:HZ2   | 1.72                     | 0.55              |
| 8:l:76:LEU:HA     | 8:l:102:ARG:HH22  | 1.71                     | 0.55              |
| 7:w:99:MET:HE3    | 7:w:107:LYS:HD2   | 1.87                     | 0.55              |
| 2:B2:76:ASP:HA    | 2:B2:79:ARG:HE    | 1.71                     | 0.55              |
| 2:B4:183:GLU:HA   | 2:B4:186:ASN:HB2  | 1.88                     | 0.55              |
| 3:C3:86:ARG:HD2   | 3:C3:88:ASP:HB2   | 1.88                     | 0.55              |
| 2:D0:211:ASP:HA   | 2:D0:214:ARG:HG2  | 1.88                     | 0.55              |
| 3:D3:173:PRO:HG2  | 3:D3:380:ARG:HB3  | 1.87                     | 0.55              |
| 2:D4:220:GLU:HG2  | 2:D4:221:ARG:HG3  | 1.88                     | 0.55              |
| 2:E8:139:ASN:HD21 | 2:E8:168:ASN:HD21 | 1.52                     | 0.55              |
| 3:A5:290:THR:HA   | 3:A5:293:MET:HE2  | 1.87                     | 0.55              |
| 3:B9:58:ARG:HH12  | 3:B9:83:GLN:HE22  | 1.55                     | 0.55              |
| 2:C0:364:PRO:HB2  | 1:I:254:LYS:HE2   | 1.88                     | 0.55              |
| 3:C7:87:PRO:HA    | 3:C7:90:PHE:HD2   | 1.71                     | 0.55              |
| 2:D0:254:GLU:HA   | 2:D0:257:THR:HG22 | 1.88                     | 0.55              |
| 2:D4:180:ALA:HB3  | 2:D4:183:GLU:HB2  | 1.88                     | 0.55              |
| 3:E3:186:THR:HG22 | 3:E3:415:MET:HE1  | 1.88                     | 0.55              |
| 3:E9:68:LEU:HD12  | 3:E9:143:THR:HG22 | 1.88                     | 0.55              |
| 7:m:75:LEU:HD13   | 7:m:173:ILE:HG13  | 1.88                     | 0.55              |
| 3:A5:135:ILE:HB   | 3:A5:166:THR:HG22 | 1.88                     | 0.55              |
| 3:A9:6:HIS:HD2    | 3:A9:134:GLN:HG3  | 1.71                     | 0.55              |
| 3:B7:97:ALA:HA    | 3:B7:103:LYS:HE2  | 1.89                     | 0.55              |
| 2:D6:90:GLU:HG2   | 2:D6:121:ARG:HD2  | 1.88                     | 0.55              |
| 3:F1:44:LEU:HD12  | 3:F1:47:ILE:HD13  | 1.87                     | 0.55              |
| 7:g:67:HIS:CE1    | 7:i:20:GLU:HG3    | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A6:140:ALA:HA   | 2:A6:171:SER:HB3  | 1.87                     | 0.55              |
| 2:B4:153:LEU:HA   | 2:B4:156:ARG:HG2  | 1.88                     | 0.55              |
| 2:C2:7:ILE:HG21   | 2:C2:153:LEU:HD21 | 1.87                     | 0.55              |
| 2:C4:288:VAL:HG11 | 2:C4:323:VAL:HG13 | 1.88                     | 0.55              |
| 3:C7:243:PRO:HA   | 3:C7:247:ASN:HD21 | 1.72                     | 0.55              |
| 2:C8:323:VAL:HG13 | 2:C8:355:ILE:HG23 | 1.88                     | 0.55              |
| 3:C9:309:ARG:H    | 3:C9:372:THR:HB   | 1.71                     | 0.55              |
| 3:D5:64:ILE:HD12  | 3:D5:119:VAL:HG12 | 1.89                     | 0.55              |
| 2:D8:5:ILE:HD12   | 2:D8:125:LEU:HG   | 1.88                     | 0.55              |
| 2:E2:71:GLU:HB3   | 2:E2:98:ASP:HB3   | 1.89                     | 0.55              |
| 3:E7:280:GLN:HE22 | 3:F1:58:ARG:HD2   | 1.72                     | 0.55              |
| 2:B6:403:ALA:HB2  | 3:B7:344:TRP:HZ3  | 1.72                     | 0.55              |
| 3:C1:6:HIS:CE1    | 3:C1:8:GLN:HE21   | 2.23                     | 0.55              |
| 2:C4:204:LEU:HD22 | 2:C4:231:ILE:HD12 | 1.88                     | 0.55              |
| 2:C8:247:ALA:HB3  | 2:C8:355:ILE:HB   | 1.88                     | 0.55              |
| 2:C8:272:TYR:HB3  | 2:C8:275:ILE:HD11 | 1.89                     | 0.55              |
| 3:D1:138:SER:HB3  | 3:D1:144:GLY:HA3  | 1.88                     | 0.55              |
| 2:D4:167:LEU:HG   | 2:D4:200:VAL:HG11 | 1.89                     | 0.55              |
| 3:D5:396:HIS:HA   | 3:D5:399:THR:HG22 | 1.87                     | 0.55              |
| 2:D8:104:ALA:HB2  | 2:D8:413:MET:HE2  | 1.89                     | 0.55              |
| 3:E3:193:VAL:HA   | 3:E3:264:HIS:HE1  | 1.71                     | 0.55              |
| 6:R:79:THR:HG22   | 6:R:82:ARG:HG2    | 1.88                     | 0.55              |
| 7:i:183:LEU:HD11  | 7:i:199:TRP:HB2   | 1.87                     | 0.55              |
| 3:B3:51:TYR:HB3   | 3:B3:59:PHE:HB3   | 1.87                     | 0.55              |
| 2:B8:191:THR:HA   | 2:B8:194:LEU:HG   | 1.89                     | 0.55              |
| 7:e:4:PRO:HG3     | 7:e:179:GLU:HB2   | 1.88                     | 0.55              |
| 7:h:183:LEU:HD23  | 7:h:196:LEU:HA    | 1.88                     | 0.55              |
| 2:A4:79:ARG:HH22  | 2:A4:94:SER:HB2   | 1.72                     | 0.55              |
| 2:A6:2:ARG:HH21   | 2:A6:242:LEU:HD12 | 1.71                     | 0.55              |
| 3:C1:173:PRO:HG3  | 3:C1:380:ARG:HD2  | 1.88                     | 0.55              |
| 2:C6:413:MET:HE2  | 2:C6:417:GLU:HB2  | 1.89                     | 0.55              |
| 4:N:1274:MET:HG3  | 4:N:1275:LEU:HD12 | 1.88                     | 0.55              |
| 7:e:148:PHE:HZ    | 7:e:173:ILE:HD13  | 1.72                     | 0.55              |
| 7:w:55:LEU:HD22   | 7:w:111:ILE:HG12  | 1.88                     | 0.55              |
| 3:A3:101:TRP:HE3  | 3:A3:403:MET:HE1  | 1.72                     | 0.55              |
| 2:B0:104:ALA:HB2  | 2:B0:413:MET:HE2  | 1.87                     | 0.55              |
| 3:A1:17:GLY:HA2   | 3:A1:20:PHE:HB3   | 1.89                     | 0.54              |
| 3:A3:215:LEU:HD21 | 3:A3:273:LEU:HD22 | 1.90                     | 0.54              |
| 2:E2:105:ARG:HH22 | 3:E3:251:ARG:HD3  | 1.71                     | 0.54              |
| 3:E5:7:VAL:HG22   | 3:E5:64:ILE:HB    | 1.89                     | 0.54              |
| 3:E5:229:VAL:HG12 | 3:E5:233:MET:HE2  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:284:LEU:HD21 | 3:E7:363:MET:HB2  | 1.89                     | 0.54              |
| 7:g:55:LEU:HD21   | 7:g:111:ILE:HD13  | 1.89                     | 0.54              |
| 3:A1:223:GLY:HA2  | 3:A1:226:ASN:HD22 | 1.72                     | 0.54              |
| 2:A2:195:LEU:HD13 | 2:A2:428:LEU:HD12 | 1.89                     | 0.54              |
| 3:A7:230:SER:HA   | 3:A7:233:MET:HB2  | 1.90                     | 0.54              |
| 2:A8:221:ARG:HD2  | 7:e:190:GLU:HB3   | 1.88                     | 0.54              |
| 3:B1:16:ILE:HA    | 3:B1:226:ASN:HB3  | 1.89                     | 0.54              |
| 3:B5:207:LEU:HB3  | 3:B5:225:LEU:HG   | 1.88                     | 0.54              |
| 2:C6:88:HIS:HB3   | 2:C6:91:GLN:HG2   | 1.89                     | 0.54              |
| 7:e:15:ARG:O      | 7:e:19:GLU:HG3    | 2.07                     | 0.54              |
| 7:j:9:PRO:HA      | 7:j:12:VAL:HG22   | 1.89                     | 0.54              |
| 3:A1:91:VAL:HG21  | 3:A1:116:VAL:HG12 | 1.89                     | 0.54              |
| 2:A2:346:TRP:HH2  | 2:A2:436:GLY:HA2  | 1.72                     | 0.54              |
| 2:A4:75:VAL:HA    | 2:A4:78:VAL:HG12  | 1.90                     | 0.54              |
| 3:A7:330:MET:HB3  | 3:A7:349:MET:HE1  | 1.89                     | 0.54              |
| 2:B2:240:ALA:HB1  | 2:B2:356:ASN:HD22 | 1.72                     | 0.54              |
| 2:B8:81:GLY:HA3   | 1:G:215:TYR:HE2   | 1.71                     | 0.54              |
| 2:E6:73:THR:HA    | 3:E7:46:ARG:HH22  | 1.72                     | 0.54              |
| 6:R:58:LEU:HA     | 6:R:61:TRP:HD1    | 1.73                     | 0.54              |
| 3:C1:333:VAL:HG22 | 3:C1:336:LYS:HE2  | 1.89                     | 0.54              |
| 2:D0:181:VAL:HG12 | 3:D1:256:ASN:HB2  | 1.88                     | 0.54              |
| 3:D3:248:SER:HA   | 3:D3:252:LYS:HG3  | 1.89                     | 0.54              |
| 2:F0:298:PRO:HA   | 2:F0:301:MET:HE1  | 1.90                     | 0.54              |
| 4:W:1252:LEU:HD21 | 4:W:1441:LEU:HB3  | 1.89                     | 0.54              |
| 2:A8:214:ARG:HH12 | 3:A9:324:LYS:HG2  | 1.72                     | 0.54              |
| 3:B5:290:THR:HG21 | 3:B5:329:GLN:HB3  | 1.89                     | 0.54              |
| 3:B5:359:LYS:HB3  | 1:E:207:LEU:HD22  | 1.89                     | 0.54              |
| 2:D4:71:GLU:HG3   | 2:D4:98:ASP:HB2   | 1.90                     | 0.54              |
| 3:D7:42:LEU:HD13  | 3:D7:356:ILE:HG12 | 1.89                     | 0.54              |
| 3:D7:67:ASP:HA    | 3:D7:143:THR:HG21 | 1.90                     | 0.54              |
| 3:E7:42:LEU:HD13  | 3:E7:356:ILE:HD11 | 1.89                     | 0.54              |
| 7:u:78:ALA:HB3    | 7:u:112:PHE:HE1   | 1.72                     | 0.54              |
| 2:A2:72:PRO:HD2   | 3:A3:2:ARG:HH11   | 1.72                     | 0.54              |
| 3:A5:207:LEU:HD13 | 3:A5:225:LEU:HB3  | 1.89                     | 0.54              |
| 2:B0:218:ASP:HB3  | 7:f:194:ARG:HH22  | 1.72                     | 0.54              |
| 2:C2:12:ALA:HB3   | 2:C2:140:ALA:HB2  | 1.89                     | 0.54              |
| 2:C4:55:GLU:HG3   | 2:C4:57:GLY:H     | 1.71                     | 0.54              |
| 3:C7:73:MET:HE3   | 3:C7:90:PHE:HD1   | 1.73                     | 0.54              |
| 2:C8:107:HIS:HD2  | 2:C8:152:LEU:HB2  | 1.71                     | 0.54              |
| 3:D3:375:GLN:HA   | 3:D3:378:PHE:HB2  | 1.90                     | 0.54              |
| 2:D8:362:VAL:HB   | 2:D8:370:LYS:HD2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:274:PRO:HB2  | 2:E0:276:ILE:HG13 | 1.89                     | 0.54              |
| 3:E9:276:ARG:HA   | 3:E9:279:GLN:HE21 | 1.73                     | 0.54              |
| 1:F:210:HIS:NE2   | 7:v:154:TYR:HB2   | 2.22                     | 0.54              |
| 3:F1:172:SER:HB2  | 3:F1:204:ASN:H    | 1.73                     | 0.54              |
| 1:B:256:LEU:HD11  | 2:D2:29:GLY:HA2   | 1.90                     | 0.54              |
| 3:B5:253:LEU:HD11 | 3:B5:368:VAL:HG21 | 1.88                     | 0.54              |
| 2:B6:3:GLU:HA     | 2:B6:51:THR:HA    | 1.89                     | 0.54              |
| 3:C1:6:HIS:HE1    | 3:C1:8:GLN:HE21   | 1.55                     | 0.54              |
| 2:C4:166:LYS:HD2  | 2:C4:198:THR:HA   | 1.89                     | 0.54              |
| 3:C5:49:VAL:HG11  | 3:C5:241:ARG:HG2  | 1.89                     | 0.54              |
| 2:C6:3:GLU:OE2    | 2:C6:129:CYS:HB3  | 2.08                     | 0.54              |
| 5:P:312:ILE:HA    | 5:P:315:LEU:HB2   | 1.89                     | 0.54              |
| 7:e:73:VAL:HA     | 7:e:109:GLU:O     | 2.08                     | 0.54              |
| 7:e:140:LEU:HA    | 7:e:143:ILE:HG22  | 1.90                     | 0.54              |
| 7:w:78:ALA:HB3    | 7:w:112:PHE:HE1   | 1.73                     | 0.54              |
| 2:A0:269:LEU:HD23 | 2:A0:303:ALA:HB3  | 1.90                     | 0.54              |
| 2:B4:88:HIS:HB3   | 2:B4:91:GLN:HG3   | 1.89                     | 0.54              |
| 3:B7:388:MET:HE3  | 2:B8:348:PRO:HD2  | 1.89                     | 0.54              |
| 2:B8:26:LEU:HD21  | 2:B8:363:VAL:HG12 | 1.89                     | 0.54              |
| 2:C2:132:LEU:HG   | 2:C2:164:LYS:HE2  | 1.90                     | 0.54              |
| 7:w:9:PRO:HA      | 7:w:12:VAL:HG22   | 1.89                     | 0.54              |
| 3:A1:207:LEU:HD23 | 3:A1:210:ILE:HD11 | 1.90                     | 0.54              |
| 2:C0:297:GLU:HG3  | 2:C0:299:ALA:H    | 1.72                     | 0.54              |
| 3:C3:51:TYR:HB3   | 3:C3:59:PHE:HB3   | 1.89                     | 0.54              |
| 3:D1:58:ARG:HH21  | 3:D1:84:LEU:HA    | 1.72                     | 0.54              |
| 2:D2:12:ALA:HB3   | 2:D2:140:ALA:HB2  | 1.90                     | 0.54              |
| 3:E3:2:ARG:HD2    | 3:E3:240:LEU:HD23 | 1.90                     | 0.54              |
| 3:E5:113:ILE:HA   | 3:E5:116:VAL:HG12 | 1.90                     | 0.54              |
| 7:i:48:ILE:HD11   | 7:i:65:GLN:HG2    | 1.89                     | 0.54              |
| 7:i:75:LEU:HG     | 7:i:173:ILE:HG13  | 1.90                     | 0.54              |
| 7:r:73:VAL:HG12   | 7:r:109:GLU:HB3   | 1.88                     | 0.54              |
| 3:C3:200:GLN:HG3  | 3:C3:268:ILE:HD11 | 1.90                     | 0.54              |
| 3:E1:44:LEU:HD22  | 7:s:91:PHE:HE2    | 1.73                     | 0.54              |
| 7:h:97:ARG:HH22   | 7:j:160:GLY:HA3   | 1.73                     | 0.54              |
| 7:j:15:ARG:O      | 7:j:19:GLU:HG3    | 2.08                     | 0.54              |
| 3:A1:333:VAL:HA   | 3:A1:336:LYS:HG2  | 1.90                     | 0.53              |
| 2:A4:51:THR:HG21  | 2:A4:243:ARG:HB2  | 1.90                     | 0.53              |
| 3:A7:7:VAL:HG13   | 3:A7:66:MET:HE1   | 1.91                     | 0.53              |
| 2:D4:298:PRO:HG2  | 2:D4:308:ARG:HE   | 1.73                     | 0.53              |
| 3:D9:229:VAL:HA   | 3:D9:300:MET:HE1  | 1.88                     | 0.53              |
| 2:E4:3:GLU:HA     | 2:E4:51:THR:HA    | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E5:358:PRO:HG2  | 3:E5:361:LEU:HB2  | 1.88                     | 0.53              |
| 11:E5:501:GDP:H8  | 2:E6:248:LEU:HD21 | 1.73                     | 0.53              |
| 7:c:9:PRO:HA      | 7:c:12:VAL:HG22   | 1.90                     | 0.53              |
| 7:g:119:ARG:HH22  | 7:g:137:GLU:HB3   | 1.72                     | 0.53              |
| 7:o:68:LEU:HD23   | 7:o:73:VAL:HG21   | 1.91                     | 0.53              |
| 7:s:172:VAL:HG23  | 7:s:180:ALA:HB3   | 1.89                     | 0.53              |
| 2:A0:247:ALA:HB3  | 2:A0:355:ILE:HB   | 1.90                     | 0.53              |
| 2:B4:271:SER:HB2  | 2:B4:377:MET:HB3  | 1.91                     | 0.53              |
| 3:B5:201:VAL:HG21 | 3:B5:374:ILE:HD11 | 1.90                     | 0.53              |
| 2:C8:14:ILE:HD11  | 2:C8:68:LEU:H     | 1.71                     | 0.53              |
| 2:D2:288:VAL:HA   | 2:D2:291:ILE:HG22 | 1.90                     | 0.53              |
| 3:E3:164:MET:HB3  | 3:E3:197:ASP:H    | 1.73                     | 0.53              |
| 3:E5:19:LYS:HD2   | 3:E5:22:GLU:HG3   | 1.90                     | 0.53              |
| 3:E5:387:ALA:HA   | 3:E5:390:ARG:HE   | 1.72                     | 0.53              |
| 3:E7:57:GLY:N     | 7:v:84:LYS:HZ3    | 2.06                     | 0.53              |
| 3:E9:253:LEU:HD21 | 3:E9:368:VAL:HG21 | 1.91                     | 0.53              |
| 7:c:53:GLY:HA2    | 7:c:62:VAL:HG21   | 1.90                     | 0.53              |
| 7:m:191:GLU:HB2   | 7:m:195:ALA:HB2   | 1.91                     | 0.53              |
| 3:A1:68:LEU:HB3   | 3:A1:96:GLY:HA2   | 1.91                     | 0.53              |
| 7:c:78:ALA:HB3    | 7:c:112:PHE:HE1   | 1.72                     | 0.53              |
| 7:h:78:ALA:HB3    | 7:h:112:PHE:HE1   | 1.73                     | 0.53              |
| 7:q:75:LEU:HD23   | 7:q:111:ILE:HB    | 1.90                     | 0.53              |
| 3:B7:311:LEU:HD12 | 3:B7:342:VAL:HG11 | 1.89                     | 0.53              |
| 3:C5:68:LEU:HD21  | 3:C5:109:GLY:HA2  | 1.91                     | 0.53              |
| 3:D1:296:ALA:H    | 3:D1:306:ARG:HH12 | 1.56                     | 0.53              |
| 2:D6:191:THR:HG21 | 2:D6:425:LEU:HD12 | 1.89                     | 0.53              |
| 3:E5:293:MET:HE3  | 3:E5:367:PHE:HB2  | 1.88                     | 0.53              |
| 3:F1:284:LEU:HD23 | 3:F1:362:LYS:HG2  | 1.90                     | 0.53              |
| 7:d:72:SER:HB3    | 7:d:108:ILE:HG22  | 1.90                     | 0.53              |
| 7:d:171:ILE:HD11  | 7:d:179:GLU:HG2   | 1.90                     | 0.53              |
| 7:f:172:VAL:HG11  | 7:f:204:THR:HG21  | 1.89                     | 0.53              |
| 7:r:78:ALA:HB3    | 7:r:112:PHE:HE1   | 1.74                     | 0.53              |
| 2:A0:102:ASN:HB3  | 2:A0:105:ARG:HB2  | 1.91                     | 0.53              |
| 2:A4:397:LEU:HD11 | 3:A5:346:PRO:HD3  | 1.89                     | 0.53              |
| 2:B2:84:ARG:HH21  | 7:e:197:LEU:HD21  | 1.73                     | 0.53              |
| 2:D2:191:THR:HA   | 2:D2:194:LEU:HB3  | 1.90                     | 0.53              |
| 3:D3:174:LYS:HG3  | 3:D3:175:VAL:HG22 | 1.91                     | 0.53              |
| 2:D4:195:LEU:HD21 | 2:D4:264:ARG:HH21 | 1.74                     | 0.53              |
| 3:E1:215:LEU:HD11 | 3:E1:228:LEU:HD21 | 1.91                     | 0.53              |
| 3:E1:274:THR:HG22 | 3:E1:275:SER:H    | 1.73                     | 0.53              |
| 3:E3:49:VAL:HG21  | 3:E3:241:ARG:HG2  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:o:14:LYS:HG3    | 7:o:47:LEU:HB2    | 1.91                     | 0.53              |
| 7:s:9:PRO:HA      | 7:s:12:VAL:HG22   | 1.91                     | 0.53              |
| 7:v:113:VAL:HG12  | 7:v:134:ILE:HB    | 1.89                     | 0.53              |
| 2:A0:177:VAL:HG11 | 2:A0:210:TYR:HE1  | 1.74                     | 0.53              |
| 2:A6:265:ILE:HG22 | 2:A6:380:ASN:HD21 | 1.74                     | 0.53              |
| 2:B2:9:VAL:HG12   | 2:B2:68:LEU:HB2   | 1.91                     | 0.53              |
| 2:B8:364:PRO:HG2  | 1:G:222:LYS:HB3   | 1.90                     | 0.53              |
| 2:C0:328:VAL:HG11 | 2:C0:355:ILE:HD11 | 1.91                     | 0.53              |
| 2:C4:240:ALA:HB2  | 2:C4:320:ARG:HH21 | 1.74                     | 0.53              |
| 2:C4:310:GLY:HA3  | 2:C4:383:ALA:HB2  | 1.90                     | 0.53              |
| 3:C5:221:THR:HG21 | 5:P:460:HIS:HB2   | 1.91                     | 0.53              |
| 2:D2:217:LEU:HD21 | 2:D2:368:LEU:HD23 | 1.90                     | 0.53              |
| 2:E6:401:LYS:HZ1  | 3:E7:344:TRP:CD1  | 2.27                     | 0.53              |
| 2:E8:137:MET:HB3  | 2:E8:168:ASN:HA   | 1.91                     | 0.53              |
| 7:x:172:VAL:HG23  | 7:x:180:ALA:HB3   | 1.89                     | 0.53              |
| 2:A4:99:ALA:HB2   | 2:A4:110:ILE:HD11 | 1.91                     | 0.53              |
| 2:A6:53:PHE:HB3   | 2:A6:61:HIS:HB3   | 1.89                     | 0.53              |
| 2:A8:102:ASN:HB2  | 2:A8:105:ARG:HB3  | 1.90                     | 0.53              |
| 3:B3:57:GLY:HA3   | 7:e:83:PRO:HB2    | 1.90                     | 0.53              |
| 3:B3:91:VAL:HG21  | 3:B3:116:VAL:HG22 | 1.90                     | 0.53              |
| 2:B8:5:ILE:HG12   | 2:B8:132:LEU:HD11 | 1.90                     | 0.53              |
| 2:C2:238:LEU:HD13 | 2:C2:318:MET:HE1  | 1.90                     | 0.53              |
| 2:C2:404:PHE:HD1  | 2:C2:407:TRP:HH2  | 1.56                     | 0.53              |
| 3:C3:359:LYS:NZ   | 1:I:207:LEU:HB3   | 2.24                     | 0.53              |
| 2:C6:185:TYR:HB3  | 2:C6:408:TYR:HE2  | 1.73                     | 0.53              |
| 2:E2:296:PHE:HE2  | 2:E2:317:LEU:HD21 | 1.73                     | 0.53              |
| 7:b:100:ASN:HD21  | 7:b:106:GLN:HG3   | 1.74                     | 0.53              |
| 2:A4:53:PHE:HB3   | 2:A4:61:HIS:HB3   | 1.90                     | 0.53              |
| 3:C3:221:THR:HG23 | 3:C3:223:GLY:H    | 1.73                     | 0.53              |
| 3:D7:242:PHE:HB3  | 3:D7:356:ILE:HD13 | 1.89                     | 0.53              |
| 2:E2:259:LEU:HD11 | 2:E2:268:MET:HE1  | 1.89                     | 0.53              |
| 1:G:221:PRO:HG3   | 7:h:101:GLU:HB3   | 1.90                     | 0.53              |
| 8:k:160:ARG:HA    | 8:k:163:LYS:HE2   | 1.91                     | 0.53              |
| 7:u:96:TYR:HA     | 7:u:108:ILE:HD11  | 1.91                     | 0.53              |
| 2:A0:274:PRO:HD3  | 2:A0:374:ALA:HA   | 1.91                     | 0.53              |
| 2:A2:259:LEU:HD13 | 2:A2:268:MET:HG2  | 1.91                     | 0.53              |
| 3:B5:57:GLY:HA3   | 7:f:83:PRO:HB2    | 1.91                     | 0.53              |
| 2:B6:319:TYR:HE1  | 2:B6:328:VAL:HG13 | 1.74                     | 0.53              |
| 2:C6:371:VAL:HG12 | 2:C6:373:ARG:H    | 1.74                     | 0.53              |
| 2:D0:76:ASP:HA    | 2:D0:79:ARG:HE    | 1.74                     | 0.53              |
| 3:D1:172:SER:HB2  | 3:D1:175:VAL:HB   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D5:308:GLY:HA3  | 3:D5:373:ALA:HB2  | 1.91                     | 0.53              |
| 2:D6:252:VAL:HA   | 2:D6:255:PHE:HD2  | 1.74                     | 0.53              |
| 3:E1:20:PHE:HB2   | 3:E1:233:MET:HE3  | 1.90                     | 0.53              |
| 2:F0:398:MET:HG3  | 3:F1:345:ILE:HD13 | 1.90                     | 0.53              |
| 7:f:84:LYS:HB2    | 7:f:168:PRO:HD3   | 1.91                     | 0.53              |
| 7:n:78:ALA:HB3    | 7:n:112:PHE:HE1   | 1.74                     | 0.53              |
| 7:x:112:PHE:HB2   | 7:x:131:TRP:HE1   | 1.73                     | 0.53              |
| 2:A6:178:SER:HB3  | 2:A6:183:GLU:HG2  | 1.90                     | 0.53              |
| 2:C0:200:VAL:HG23 | 2:C0:256:GLN:HG3  | 1.91                     | 0.53              |
| 3:C1:113:ILE:HA   | 3:C1:116:VAL:HG12 | 1.90                     | 0.53              |
| 3:C1:178:THR:H    | 2:C2:352:LYS:HD2  | 1.74                     | 0.53              |
| 2:C4:51:THR:HG21  | 2:C4:243:ARG:HG2  | 1.91                     | 0.53              |
| 1:D:240:PRO:HG2   | 7:s:163:SER:HB2   | 1.91                     | 0.53              |
| 3:D3:178:THR:HG23 | 3:D3:181:GLU:HG3  | 1.90                     | 0.53              |
| 2:D4:396:ASP:HB3  | 2:D4:422:ARG:HH12 | 1.74                     | 0.53              |
| 3:D7:309:ARG:H    | 3:D7:372:THR:HG22 | 1.72                     | 0.53              |
| 3:E1:169:VAL:HG12 | 3:E1:202:ILE:HB   | 1.90                     | 0.53              |
| 2:F0:407:TRP:HZ2  | 3:F1:258:ILE:HD11 | 1.73                     | 0.53              |
| 3:F1:102:ALA:HB2  | 3:F1:403:MET:HE2  | 1.91                     | 0.53              |
| 4:N:1432:PRO:HD2  | 4:N:1435:ARG:HH21 | 1.74                     | 0.53              |
| 5:P:242:LEU:HD12  | 5:P:243:PRO:HD2   | 1.90                     | 0.53              |
| 7:h:72:SER:HB3    | 7:h:108:ILE:HG22  | 1.91                     | 0.53              |
| 7:r:183:LEU:HD13  | 7:r:196:LEU:HA    | 1.91                     | 0.53              |
| 2:A0:174:SER:HB3  | 2:A0:207:GLU:HG3  | 1.92                     | 0.52              |
| 3:A1:259:PRO:HG2  | 3:A1:311:LEU:HD23 | 1.90                     | 0.52              |
| 3:A3:54:ALA:HB3   | 3:A3:58:ARG:HB3   | 1.89                     | 0.52              |
| 3:B1:301:CYS:HB3  | 3:B1:377:MET:HE1  | 1.91                     | 0.52              |
| 3:B5:244:GLY:HA2  | 3:B5:355:ASP:HB2  | 1.91                     | 0.52              |
| 2:C0:175:PRO:HB3  | 2:C0:390:ARG:HD3  | 1.90                     | 0.52              |
| 2:D2:70:LEU:HD12  | 2:D2:99:ALA:HB2   | 1.90                     | 0.52              |
| 3:D5:165:GLU:HG3  | 3:D5:250:LEU:HD22 | 1.91                     | 0.52              |
| 3:E3:163:ILE:HD13 | 3:E3:250:LEU:HG   | 1.91                     | 0.52              |
| 3:F1:49:VAL:HG11  | 3:F1:241:ARG:HG2  | 1.91                     | 0.52              |
| 4:Q:1294:VAL:HG23 | 4:Q:1321:ILE:HD13 | 1.91                     | 0.52              |
| 7:p:63:ILE:HB     | 7:p:67:HIS:HD2    | 1.74                     | 0.52              |
| 3:A3:5:VAL:HB     | 3:A3:133:PHE:HD1  | 1.74                     | 0.52              |
| 3:A5:35:THR:HG22  | 7:a:83:PRO:HG3    | 1.91                     | 0.52              |
| 2:A6:238:LEU:HD11 | 2:A6:378:ILE:HD11 | 1.92                     | 0.52              |
| 3:A9:32:PRO:HB3   | 3:A9:81:PHE:HA    | 1.90                     | 0.52              |
| 3:B1:164:MET:HB3  | 3:B1:197:ASP:H    | 1.75                     | 0.52              |
| 2:B6:88:HIS:HB3   | 2:B6:91:GLN:HE21  | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:12:ALA:HB3   | 2:E0:140:ALA:HB2  | 1.90                     | 0.52              |
| 2:E6:76:ASP:HA    | 2:E6:79:ARG:HD2   | 1.92                     | 0.52              |
| 7:e:75:LEU:HD23   | 7:e:111:ILE:HB    | 1.91                     | 0.52              |
| 7:x:183:LEU:HD11  | 7:x:199:TRP:HB2   | 1.91                     | 0.52              |
| 3:A9:190:HIS:HB2  | 3:A9:414:ASN:HB3  | 1.89                     | 0.52              |
| 2:B0:136:LEU:HD13 | 2:B0:235:ILE:HD11 | 1.91                     | 0.52              |
| 2:C2:247:ALA:HB3  | 2:C2:355:ILE:HB   | 1.90                     | 0.52              |
| 2:D2:223:THR:HG23 | 2:D2:225:THR:H    | 1.73                     | 0.52              |
| 3:D9:272:PRO:HG2  | 3:D9:361:LEU:HD13 | 1.92                     | 0.52              |
| 1:E:254:LYS:HD2   | 1:E:255:PRO:HD2   | 1.90                     | 0.52              |
| 3:E7:2:ARG:HB3    | 3:E7:131:GLN:HB2  | 1.92                     | 0.52              |
| 3:E7:272:PRO:HG3  | 3:E7:364:SER:HA   | 1.91                     | 0.52              |
| 3:F1:28:HIS:HD1   | 3:F1:47:ILE:HD12  | 1.73                     | 0.52              |
| 4:V:1257:TYR:HD1  | 4:V:1283:LEU:HD11 | 1.75                     | 0.52              |
| 7:d:9:PRO:HA      | 7:d:12:VAL:HG22   | 1.90                     | 0.52              |
| 7:q:15:ARG:HG2    | 7:q:45:MET:HE1    | 1.92                     | 0.52              |
| 7:v:99:MET:HE2    | 7:v:107:LYS:HD2   | 1.90                     | 0.52              |
| 3:A1:139:LEU:HA   | 3:A1:145:SER:HB2  | 1.92                     | 0.52              |
| 3:C3:87:PRO:HA    | 3:C3:90:PHE:HD2   | 1.74                     | 0.52              |
| 3:C3:337:ASN:HB2  | 3:C3:340:TYR:HB2  | 1.91                     | 0.52              |
| 2:D2:102:ASN:HB2  | 2:D2:105:ARG:HB3  | 1.91                     | 0.52              |
| 3:D9:200:GLN:HG2  | 3:D9:268:ILE:HD12 | 1.91                     | 0.52              |
| 3:E5:271:ALA:HA   | 3:E5:273:LEU:HD13 | 1.92                     | 0.52              |
| 7:s:78:ALA:HB3    | 7:s:112:PHE:HE1   | 1.75                     | 0.52              |
| 3:A1:3:GLU:HA     | 3:A1:49:VAL:HA    | 1.91                     | 0.52              |
| 2:B0:339:ARG:NH2  | 4:Q:1234:TYR:HB3  | 2.24                     | 0.52              |
| 2:B2:141:VAL:HG12 | 2:B2:187:SER:HA   | 1.92                     | 0.52              |
| 2:B2:392:ASP:HA   | 2:B2:422:ARG:HH12 | 1.74                     | 0.52              |
| 3:B5:51:TYR:HB3   | 3:B5:59:PHE:HB3   | 1.90                     | 0.52              |
| 3:C5:248:SER:HA   | 3:C5:252:LYS:HD2  | 1.91                     | 0.52              |
| 3:C7:12:CYS:HB2   | 3:C7:138:SER:HB3  | 1.91                     | 0.52              |
| 2:C8:206:ASN:HB3  | 2:C8:210:TYR:CZ   | 2.45                     | 0.52              |
| 2:D0:107:HIS:HD2  | 2:D0:152:LEU:HB2  | 1.74                     | 0.52              |
| 2:E6:28:HIS:HB2   | 2:E6:30:ILE:HG12  | 1.92                     | 0.52              |
| 3:E7:131:GLN:HE22 | 3:E7:250:LEU:HB2  | 1.74                     | 0.52              |
| 2:E8:100:ALA:HA   | 3:E9:252:LYS:HG3  | 1.92                     | 0.52              |
| 2:E8:132:LEU:HB2  | 2:E8:164:LYS:HZ1  | 1.75                     | 0.52              |
| 3:E9:217:LEU:HB2  | 3:E9:220:PRO:HD3  | 1.91                     | 0.52              |
| 4:N:1250:ALA:HB1  | 4:N:1254:ARG:HH12 | 1.74                     | 0.52              |
| 7:n:184:PRO:HD2   | 7:n:195:ALA:HB1   | 1.90                     | 0.52              |
| 7:p:134:ILE:HD13  | 7:p:140:LEU:HD22  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:t:14:LYS:HD3    | 7:t:47:LEU:HD13   | 1.91                     | 0.52              |
| 2:A2:364:PRO:HB2  | 5:P:242:LEU:HB3   | 1.92                     | 0.52              |
| 2:A8:221:ARG:HG3  | 3:A9:322:SER:HB2  | 1.91                     | 0.52              |
| 3:B1:171:PRO:HG2  | 3:B1:185:ALA:HB2  | 1.91                     | 0.52              |
| 3:B1:313:ALA:HB3  | 3:B1:349:MET:HB3  | 1.91                     | 0.52              |
| 3:B3:178:THR:HG21 | 11:B3:501:GDP:H5' | 1.92                     | 0.52              |
| 2:B8:31:GLN:HE22  | 2:B8:35:GLN:H     | 1.58                     | 0.52              |
| 1:C:240:PRO:HG3   | 7:e:154:TYR:CG    | 2.45                     | 0.52              |
| 3:C1:86:ARG:HD2   | 3:C1:88:ASP:HB2   | 1.91                     | 0.52              |
| 2:D2:222:PRO:HG2  | 3:D3:324:LYS:HZ1  | 1.74                     | 0.52              |
| 2:E4:121:ARG:HH21 | 2:E4:124:LYS:HG2  | 1.73                     | 0.52              |
| 3:E7:330:MET:HG3  | 3:E7:349:MET:HG3  | 1.91                     | 0.52              |
| 3:E9:104:GLY:HA3  | 3:E9:146:GLY:HA3  | 1.92                     | 0.52              |
| 2:F0:223:THR:HG23 | 2:F0:225:THR:HG22 | 1.90                     | 0.52              |
| 1:J:255:PRO:HG3   | 7:m:178:ARG:HH22  | 1.75                     | 0.52              |
| 5:P:309:SER:HB2   | 5:P:312:ILE:HG22  | 1.91                     | 0.52              |
| 6:R:64:PRO:HB3    | 6:R:72:PRO:HG3    | 1.92                     | 0.52              |
| 7:a:153:GLU:H     | 7:a:164:ARG:HE    | 1.56                     | 0.52              |
| 8:k:25:ARG:HH12   | 7:m:23:LEU:HD12   | 1.73                     | 0.52              |
| 7:o:5:VAL:HG11    | 7:o:149:ARG:HD3   | 1.91                     | 0.52              |
| 3:A5:244:GLY:HA3  | 3:A5:354:CYS:HA   | 1.91                     | 0.52              |
| 2:C2:195:LEU:HD13 | 2:C2:264:ARG:HH22 | 1.75                     | 0.52              |
| 2:C6:259:LEU:HD21 | 2:C6:268:MET:HG2  | 1.92                     | 0.52              |
| 2:C8:123:ARG:HH22 | 2:C8:160:ASP:HB3  | 1.75                     | 0.52              |
| 3:C9:326:VAL:HG22 | 3:C9:351:SER:HB2  | 1.90                     | 0.52              |
| 3:D5:242:PHE:HB3  | 3:D5:356:ILE:HG13 | 1.92                     | 0.52              |
| 3:D7:2:ARG:HH21   | 3:D7:240:LEU:HD12 | 1.75                     | 0.52              |
| 3:D9:271:ALA:HA   | 3:D9:273:LEU:HG   | 1.91                     | 0.52              |
| 8:k:15:ARG:HH21   | 8:k:16:THR:HG22   | 1.75                     | 0.52              |
| 2:A2:12:ALA:HB3   | 2:A2:140:ALA:HB2  | 1.92                     | 0.52              |
| 2:A8:195:LEU:HD21 | 2:A8:428:LEU:HD12 | 1.92                     | 0.52              |
| 2:B4:191:THR:HA   | 2:B4:194:LEU:HG   | 1.92                     | 0.52              |
| 3:B7:8:GLN:HB2    | 3:B7:65:LEU:HA    | 1.92                     | 0.52              |
| 3:B7:68:LEU:HB3   | 3:B7:96:GLY:HA2   | 1.92                     | 0.52              |
| 3:B9:68:LEU:HD21  | 3:B9:147:MET:HG3  | 1.92                     | 0.52              |
| 3:C1:124:ALA:HB1  | 3:C1:130:LEU:HD13 | 1.90                     | 0.52              |
| 3:C7:320:ARG:NH2  | 1:J:212:GLU:H     | 2.08                     | 0.52              |
| 3:C9:166:THR:HG21 | 3:C9:192:LEU:HD11 | 1.91                     | 0.52              |
| 3:D1:309:ARG:H    | 3:D1:372:THR:HB   | 1.75                     | 0.52              |
| 3:E9:116:VAL:HA   | 3:E9:119:VAL:HG12 | 1.91                     | 0.52              |
| 2:F0:311:LYS:HD3  | 2:F0:342:GLN:HG2  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:212:GLU:OE1   | 1:I:216:ARG:HB2   | 2.10                     | 0.52              |
| 8:l:73:TYR:HB2    | 8:l:92:TRP:HE1    | 1.75                     | 0.52              |
| 3:A5:22:GLU:HG2   | 3:A5:81:PHE:CD2   | 2.45                     | 0.52              |
| 3:A5:68:LEU:HD12  | 3:A5:97:ALA:HB2   | 1.92                     | 0.52              |
| 3:B7:293:MET:HA   | 3:B7:298:ASN:HD21 | 1.74                     | 0.52              |
| 2:B8:262:TYR:HD2  | 2:B8:265:ILE:HD12 | 1.74                     | 0.52              |
| 2:C0:212:ILE:HD11 | 2:C0:275:ILE:HG21 | 1.92                     | 0.52              |
| 2:C6:27:GLU:HB3   | 2:C6:361:THR:HG21 | 1.91                     | 0.52              |
| 3:D7:282:ARG:HB2  | 3:E1:86:ARG:HH12  | 1.74                     | 0.52              |
| 2:D8:71:GLU:HB3   | 2:D8:98:ASP:HB3   | 1.92                     | 0.52              |
| 2:D8:211:ASP:HA   | 2:D8:214:ARG:HG2  | 1.91                     | 0.52              |
| 2:D8:250:VAL:HG12 | 2:D8:352:LYS:HE3  | 1.92                     | 0.52              |
| 2:E2:337:THR:HG22 | 2:E2:338:LYS:H    | 1.74                     | 0.52              |
| 3:E3:70:PRO:HD3   | 3:E3:94:GLN:HA    | 1.92                     | 0.52              |
| 3:E3:286:VAL:HB   | 3:E3:325:GLU:HG3  | 1.92                     | 0.52              |
| 7:b:67:HIS:HD2    | 7:d:19:GLU:HB3    | 1.75                     | 0.52              |
| 7:c:140:LEU:HA    | 7:c:143:ILE:HG22  | 1.92                     | 0.52              |
| 7:t:15:ARG:HG2    | 7:t:45:MET:HE1    | 1.91                     | 0.52              |
| 7:u:65:GLN:HE21   | 7:u:206:PHE:HZ    | 1.58                     | 0.52              |
| 7:u:97:ARG:HH22   | 7:w:149:ARG:HH12  | 1.57                     | 0.52              |
| 3:A1:46:ARG:HB2   | 3:A1:241:ARG:HA   | 1.91                     | 0.52              |
| 3:A1:190:HIS:HB2  | 3:A1:414:ASN:HD21 | 1.74                     | 0.52              |
| 2:A2:70:LEU:HD21  | 2:A2:149:LEU:HD13 | 1.92                     | 0.52              |
| 2:A4:274:PRO:HG3  | 2:A4:291:ILE:HD12 | 1.92                     | 0.52              |
| 3:B5:383:ASP:HA   | 3:B5:386:THR:HG22 | 1.92                     | 0.52              |
| 3:C5:191:GLN:HE21 | 3:C5:195:ASN:HD21 | 1.57                     | 0.52              |
| 2:C6:3:GLU:HA     | 2:C6:51:THR:HA    | 1.91                     | 0.52              |
| 3:F1:2:ARG:HB3    | 3:F1:131:GLN:HB2  | 1.92                     | 0.52              |
| 4:L:1399:TYR:HA   | 4:L:1402:GLN:HG2  | 1.92                     | 0.52              |
| 7:j:14:LYS:HG2    | 7:j:45:MET:HE2    | 1.91                     | 0.52              |
| 2:A0:265:ILE:HG22 | 2:A0:380:ASN:HD21 | 1.75                     | 0.51              |
| 2:A0:409:VAL:HA   | 2:A0:413:MET:HB2  | 1.92                     | 0.51              |
| 2:A4:104:ALA:HB2  | 2:A4:413:MET:HE2  | 1.91                     | 0.51              |
| 2:B4:84:ARG:HH21  | 7:f:197:LEU:HD21  | 1.75                     | 0.51              |
| 3:B7:372:THR:HG21 | 3:B7:426:GLN:HB2  | 1.92                     | 0.51              |
| 3:C1:333:VAL:HA   | 3:C1:336:LYS:HG2  | 1.91                     | 0.51              |
| 3:C7:32:PRO:HA    | 3:C7:84:LEU:HD11  | 1.92                     | 0.51              |
| 2:D6:32:PRO:HB3   | 2:D6:83:TYR:HE1   | 1.75                     | 0.51              |
| 3:F1:149:THR:HA   | 3:F1:152:ILE:HB   | 1.91                     | 0.51              |
| 7:g:158:THR:HB    | 7:g:161:TYR:HB2   | 1.92                     | 0.51              |
| 7:t:78:ALA:HB3    | 7:t:112:PHE:HE1   | 1.75                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A3:246:LEU:HB2  | 3:A3:353:VAL:H    | 1.75                     | 0.51              |
| 2:A4:311:LYS:HA   | 2:A4:342:GLN:HB2  | 1.92                     | 0.51              |
| 3:B3:207:LEU:HB3  | 3:B3:225:LEU:HD22 | 1.93                     | 0.51              |
| 3:C5:211:CYS:HB2  | 3:C5:217:LEU:HD12 | 1.92                     | 0.51              |
| 3:C9:281:TYR:HB3  | 3:D3:86:ARG:HG2   | 1.91                     | 0.51              |
| 2:E0:219:ILE:HD13 | 7:u:198:ARG:HH12  | 1.75                     | 0.51              |
| 3:E7:28:HIS:HA    | 3:E7:43:GLN:HG2   | 1.91                     | 0.51              |
| 7:p:71:LYS:HD3    | 7:p:106:GLN:HG2   | 1.93                     | 0.51              |
| 7:v:63:ILE:HG21   | 7:v:132:LEU:HD22  | 1.92                     | 0.51              |
| 2:A0:323:VAL:HG22 | 2:A0:373:ARG:HD3  | 1.91                     | 0.51              |
| 3:B1:323:THR:HG22 | 3:B1:353:VAL:HG21 | 1.92                     | 0.51              |
| 3:C1:49:VAL:HG11  | 3:C1:241:ARG:HB3  | 1.92                     | 0.51              |
| 3:C1:61:PRO:HD3   | 3:C1:84:LEU:HG    | 1.91                     | 0.51              |
| 2:C4:406:HIS:HD1  | 2:C4:407:TRP:CD1  | 2.28                     | 0.51              |
| 2:C6:167:LEU:HD21 | 2:C6:238:LEU:HD21 | 1.93                     | 0.51              |
| 3:D3:135:ILE:HB   | 3:D3:166:THR:HG22 | 1.93                     | 0.51              |
| 2:D4:294:SER:HA   | 2:D4:297:GLU:HG3  | 1.93                     | 0.51              |
| 3:D7:57:GLY:HA3   | 7:q:83:PRO:HB2    | 1.92                     | 0.51              |
| 2:E0:240:ALA:HB1  | 2:E0:356:ASN:HD22 | 1.75                     | 0.51              |
| 3:E3:132:GLY:HA3  | 3:E3:163:ILE:HG22 | 1.92                     | 0.51              |
| 3:F1:290:THR:HG21 | 3:F1:329:GLN:HB3  | 1.92                     | 0.51              |
| 5:P:239:ARG:HD2   | 6:R:86:ASP:HB3    | 1.92                     | 0.51              |
| 4:W:1214:LEU:HD22 | 4:W:1447:ALA:HB1  | 1.91                     | 0.51              |
| 2:A2:360:PRO:HD2  | 2:A2:372:MET:HA   | 1.91                     | 0.51              |
| 2:A4:248:LEU:HD23 | 2:A4:355:ILE:HD12 | 1.92                     | 0.51              |
| 3:A7:284:LEU:H    | 3:B1:55:THR:HB    | 1.75                     | 0.51              |
| 2:B2:156:ARG:HG2  | 4:W:1246:TYR:CZ   | 2.45                     | 0.51              |
| 3:C5:66:MET:HE3   | 3:C5:147:MET:HG3  | 1.92                     | 0.51              |
| 3:D7:77:ARG:HH22  | 3:D7:92:PHE:HZ    | 1.58                     | 0.51              |
| 2:F0:53:PHE:HB3   | 2:F0:61:HIS:HB3   | 1.91                     | 0.51              |
| 3:F1:229:VAL:HA   | 3:F1:300:MET:HE1  | 1.91                     | 0.51              |
| 1:J:262:THR:HA    | 5:O:455:TYR:HE1   | 1.74                     | 0.51              |
| 4:L:1406:LEU:HD22 | 4:Q:1298:PHE:HE1  | 1.75                     | 0.51              |
| 4:V:1382:GLU:HA   | 4:V:1385:LEU:HD12 | 1.93                     | 0.51              |
| 3:A3:358:PRO:HG2  | 3:A3:361:LEU:HD13 | 1.93                     | 0.51              |
| 3:B1:207:LEU:HB3  | 3:B1:225:LEU:HD22 | 1.93                     | 0.51              |
| 2:B6:133:GLN:HG2  | 2:B6:242:LEU:HD21 | 1.92                     | 0.51              |
| 2:C2:32:PRO:HG2   | 1:I:221:PRO:HG3   | 1.92                     | 0.51              |
| 2:C4:163:LYS:HG3  | 2:C4:164:LYS:HG3  | 1.92                     | 0.51              |
| 3:E1:2:ARG:HB2    | 3:E1:131:GLN:HB2  | 1.93                     | 0.51              |
| 2:E4:70:LEU:HD21  | 2:E4:114:ILE:HG21 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E4:388:PHE:HB3  | 2:E4:425:LEU:HD11 | 1.92                     | 0.51              |
| 2:E6:32:PRO:HA    | 2:E6:86:LEU:HD12  | 1.91                     | 0.51              |
| 2:A0:195:LEU:HD21 | 2:A0:264:ARG:HH21 | 1.74                     | 0.51              |
| 3:A1:294:PHE:HE2  | 3:A1:333:VAL:HG11 | 1.75                     | 0.51              |
| 2:B6:259:LEU:HD21 | 2:B6:316:CYS:HB2  | 1.92                     | 0.51              |
| 3:C1:164:MET:HB3  | 3:C1:197:ASP:H    | 1.75                     | 0.51              |
| 2:C2:204:LEU:HD21 | 2:C2:231:ILE:HD12 | 1.93                     | 0.51              |
| 3:C3:392:LYS:HE2  | 3:C3:395:LEU:HG   | 1.92                     | 0.51              |
| 2:C8:207:GLU:HB3  | 2:C8:304:LYS:NZ   | 2.26                     | 0.51              |
| 2:D2:398:MET:HE3  | 3:D3:345:ILE:HG23 | 1.91                     | 0.51              |
| 3:D7:124:ALA:HB1  | 3:D7:130:LEU:HD13 | 1.93                     | 0.51              |
| 3:E3:7:VAL:HG11   | 3:E3:151:LEU:HD23 | 1.93                     | 0.51              |
| 3:E7:139:LEU:HD12 | 3:E7:170:PHE:HE1  | 1.74                     | 0.51              |
| 3:F1:276:ARG:HA   | 3:F1:279:GLN:HB2  | 1.93                     | 0.51              |
| 5:P:519:LEU:HB2   | 5:P:521:PRO:HG3   | 1.91                     | 0.51              |
| 7:h:71:LYS:HZ1    | 7:h:109:GLU:HB2   | 1.76                     | 0.51              |
| 7:j:10:LEU:HD22   | 7:j:47:LEU:HD21   | 1.92                     | 0.51              |
| 7:t:65:GLN:HE21   | 7:t:206:PHE:HZ    | 1.59                     | 0.51              |
| 7:t:73:VAL:HA     | 7:t:109:GLU:O     | 2.11                     | 0.51              |
| 1:A:221:PRO:HG3   | 7:b:101:GLU:HG2   | 1.93                     | 0.51              |
| 3:A7:316:MET:HE2  | 3:A7:366:THR:HG23 | 1.93                     | 0.51              |
| 3:B3:68:LEU:HB3   | 3:B3:96:GLY:HA2   | 1.92                     | 0.51              |
| 2:C0:82:THR:HG21  | 1:I:252:VAL:HA    | 1.91                     | 0.51              |
| 2:C4:274:PRO:HG3  | 2:C4:374:ALA:HA   | 1.91                     | 0.51              |
| 3:C5:42:LEU:HD12  | 1:J:248:ARG:HH22  | 1.75                     | 0.51              |
| 3:D9:173:PRO:HD2  | 3:D9:205:GLU:OE2  | 2.11                     | 0.51              |
| 3:E9:138:SER:HA   | 3:E9:169:VAL:HG23 | 1.92                     | 0.51              |
| 7:a:127:ALA:HB1   | 7:c:157:PRO:HG3   | 1.93                     | 0.51              |
| 7:n:136:LEU:HA    | 7:n:141:THR:HG21  | 1.92                     | 0.51              |
| 3:A1:263:LEU:HD13 | 3:A1:422:TYR:CE2  | 2.46                     | 0.51              |
| 2:A8:292:THR:HG21 | 2:A8:331:ALA:HB1  | 1.92                     | 0.51              |
| 2:B2:292:THR:HG21 | 2:B2:331:ALA:HB1  | 1.93                     | 0.51              |
| 2:B6:53:PHE:HB3   | 2:B6:61:HIS:HB3   | 1.92                     | 0.51              |
| 3:D1:407:GLU:HA   | 3:D1:410:GLU:HB3  | 1.93                     | 0.51              |
| 2:E6:80:THR:HA    | 2:E6:84:ARG:HH11  | 1.76                     | 0.51              |
| 2:E6:317:LEU:HG   | 2:E6:377:MET:HB3  | 1.93                     | 0.51              |
| 7:m:96:TYR:HA     | 7:m:108:ILE:HD11  | 1.93                     | 0.51              |
| 3:B1:334:GLN:HE22 | 3:B1:347:ASN:HA   | 1.76                     | 0.51              |
| 2:C0:388:PHE:HB3  | 2:C0:425:LEU:HD21 | 1.92                     | 0.51              |
| 2:D4:280:LYS:HG2  | 2:D8:89:PRO:HD2   | 1.92                     | 0.51              |
| 2:D4:298:PRO:HB3  | 2:D4:307:PRO:HD2  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D5:39:ASP:HA    | 7:p:90:PRO:HG3    | 1.93                     | 0.51              |
| 3:D5:171:PRO:HG2  | 3:D5:185:ALA:HB2  | 1.91                     | 0.51              |
| 3:E5:163:ILE:HD11 | 3:E5:251:ARG:HB2  | 1.91                     | 0.51              |
| 2:F0:213:CYS:HA   | 2:F0:217:LEU:HB2  | 1.93                     | 0.51              |
| 7:m:75:LEU:HD21   | 7:m:144:LEU:HD13  | 1.92                     | 0.51              |
| 7:m:158:THR:HG23  | 7:m:160:GLY:H     | 1.75                     | 0.51              |
| 7:n:170:VAL:HG23  | 7:n:183:LEU:HB2   | 1.93                     | 0.51              |
| 7:r:82:ASP:HB3    | 7:r:85:CYS:HB2    | 1.93                     | 0.51              |
| 7:v:63:ILE:HD12   | 7:v:64:PRO:HD2    | 1.92                     | 0.51              |
| 7:v:96:TYR:HA     | 7:v:108:ILE:HD11  | 1.93                     | 0.51              |
| 3:A7:309:ARG:H    | 3:A7:372:THR:HG22 | 1.75                     | 0.51              |
| 3:C5:207:LEU:HD22 | 3:C5:225:LEU:HG   | 1.93                     | 0.51              |
| 3:C5:213:ARG:NH2  | 3:C5:297:LYS:HG3  | 2.26                     | 0.51              |
| 3:C5:244:GLY:HA2  | 3:C5:355:ASP:H    | 1.76                     | 0.51              |
| 2:E4:280:LYS:HD2  | 2:E8:88:HIS:HE2   | 1.76                     | 0.51              |
| 3:E9:42:LEU:HD13  | 3:E9:356:ILE:HD11 | 1.92                     | 0.51              |
| 3:F1:361:LEU:HD13 | 6:T:105:HIS:HB2   | 1.92                     | 0.51              |
| 4:M:1374:ARG:HD2  | 4:M:1376:ALA:H    | 1.76                     | 0.51              |
| 6:U:79:THR:HG23   | 6:U:82:ARG:H      | 1.76                     | 0.51              |
| 7:b:75:LEU:HD23   | 7:b:111:ILE:HB    | 1.93                     | 0.51              |
| 7:j:142:GLU:HA    | 7:j:145:LYS:HD3   | 1.93                     | 0.51              |
| 2:A0:284:GLU:HB2  | 2:A0:286:LEU:HD12 | 1.93                     | 0.50              |
| 2:A6:79:ARG:HG3   | 2:A6:92:LEU:HD22  | 1.93                     | 0.50              |
| 3:A7:117:LEU:HA   | 3:A7:120:VAL:HG12 | 1.92                     | 0.50              |
| 2:A8:214:ARG:HH22 | 3:A9:324:LYS:HD2  | 1.75                     | 0.50              |
| 2:C8:398:MET:HE1  | 3:C9:345:ILE:HA   | 1.91                     | 0.50              |
| 2:D6:265:ILE:HG22 | 2:D6:380:ASN:HD21 | 1.76                     | 0.50              |
| 3:E7:57:GLY:HA3   | 7:v:83:PRO:HB2    | 1.93                     | 0.50              |
| 2:F0:332:VAL:HA   | 2:F0:335:ILE:HG12 | 1.93                     | 0.50              |
| 3:A1:207:LEU:HD13 | 3:A1:225:LEU:HB3  | 1.93                     | 0.50              |
| 3:A3:227:HIS:HA   | 3:A3:230:SER:HB3  | 1.94                     | 0.50              |
| 3:C7:282:ARG:HB2  | 3:D1:86:ARG:HH12  | 1.76                     | 0.50              |
| 2:C8:310:GLY:HA3  | 2:C8:383:ALA:HB2  | 1.94                     | 0.50              |
| 3:C9:8:GLN:HE21   | 3:C9:65:LEU:HG    | 1.76                     | 0.50              |
| 2:E2:223:THR:HG22 | 3:E3:322:SER:HA   | 1.92                     | 0.50              |
| 2:E2:265:ILE:HG22 | 2:E2:380:ASN:HD21 | 1.75                     | 0.50              |
| 2:E2:296:PHE:CE2  | 2:E2:317:LEU:HD21 | 2.46                     | 0.50              |
| 3:E7:164:MET:H    | 3:E7:197:ASP:HB3  | 1.76                     | 0.50              |
| 2:B0:298:PRO:HB3  | 2:B0:307:PRO:HD2  | 1.93                     | 0.50              |
| 3:B5:66:MET:HE1   | 3:B5:151:LEU:HD22 | 1.92                     | 0.50              |
| 2:C0:286:LEU:HD22 | 2:C0:371:VAL:HG12 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E5:302:ALA:HB3  | 3:E5:377:MET:HE1  | 1.93                     | 0.50              |
| 4:N:1402:GLN:HA   | 4:N:1405:LEU:HG   | 1.93                     | 0.50              |
| 4:Q:1252:LEU:HD21 | 4:Q:1441:LEU:HB3  | 1.93                     | 0.50              |
| 7:r:154:TYR:HE1   | 7:r:158:THR:HG22  | 1.75                     | 0.50              |
| 2:A4:261:PRO:HG2  | 2:A4:265:ILE:HB   | 1.94                     | 0.50              |
| 2:B6:223:THR:HG22 | 3:B7:322:SER:HA   | 1.92                     | 0.50              |
| 3:C1:207:LEU:HB3  | 3:C1:225:LEU:HG   | 1.94                     | 0.50              |
| 2:C2:129:CYS:HB3  | 2:C2:132:LEU:HB3  | 1.94                     | 0.50              |
| 2:C8:195:LEU:HD21 | 2:C8:264:ARG:HH21 | 1.76                     | 0.50              |
| 3:E5:244:GLY:HA2  | 3:E5:355:ASP:HB2  | 1.94                     | 0.50              |
| 3:E7:87:PRO:HA    | 3:E7:90:PHE:HD2   | 1.77                     | 0.50              |
| 3:E9:287:PRO:HG3  | 3:E9:329:GLN:HE22 | 1.77                     | 0.50              |
| 7:o:88:LEU:HD11   | 7:o:185:ILE:HD13  | 1.92                     | 0.50              |
| 7:p:55:LEU:HD11   | 7:p:111:ILE:HD13  | 1.92                     | 0.50              |
| 7:x:184:PRO:HG3   | 7:x:189:LEU:HD12  | 1.94                     | 0.50              |
| 3:A1:37:CYS:HA    | 6:T:67:LEU:HD22   | 1.93                     | 0.50              |
| 3:A3:221:THR:HG21 | 5:P:219:LEU:HA    | 1.92                     | 0.50              |
| 2:C4:223:THR:HG22 | 3:C5:322:SER:HA   | 1.92                     | 0.50              |
| 3:E3:287:PRO:HG3  | 3:E3:329:GLN:HE21 | 1.76                     | 0.50              |
| 2:E4:203:MET:HE3  | 2:E4:267:PHE:HD2  | 1.77                     | 0.50              |
| 3:E7:286:VAL:HG22 | 3:E7:363:MET:HE1  | 1.93                     | 0.50              |
| 1:H:245:SER:O     | 1:H:249:SER:HB3   | 2.11                     | 0.50              |
| 7:a:78:ALA:HB3    | 7:a:112:PHE:HE1   | 1.76                     | 0.50              |
| 7:h:110:ILE:HB    | 7:h:131:TRP:CG    | 2.47                     | 0.50              |
| 8:l:38:PHE:HA     | 8:l:74:VAL:O      | 2.11                     | 0.50              |
| 7:m:119:ARG:HH21  | 7:m:137:GLU:HG2   | 1.76                     | 0.50              |
| 2:A2:7:ILE:HD13   | 2:A2:122:ILE:HD11 | 1.94                     | 0.50              |
| 2:A8:318:MET:HB2  | 2:A8:376:CYS:HB3  | 1.93                     | 0.50              |
| 3:B1:19:LYS:HE2   | 3:B1:223:GLY:HA2  | 1.93                     | 0.50              |
| 2:B2:174:SER:HB2  | 2:B2:207:GLU:HG2  | 1.94                     | 0.50              |
| 2:C2:134:GLY:HA3  | 2:C2:165:SER:HB3  | 1.92                     | 0.50              |
| 2:C2:313:MET:HE3  | 2:C2:380:ASN:HB3  | 1.94                     | 0.50              |
| 2:D6:273:ALA:HA   | 2:D6:275:ILE:HD12 | 1.94                     | 0.50              |
| 3:E3:392:LYS:HD2  | 3:E3:395:LEU:HD13 | 1.93                     | 0.50              |
| 2:E6:269:LEU:HD22 | 2:E6:303:ALA:HB3  | 1.94                     | 0.50              |
| 2:E6:276:ILE:HG23 | 2:E6:280:LYS:HB3  | 1.93                     | 0.50              |
| 2:E8:408:TYR:HB3  | 2:E8:413:MET:HG3  | 1.93                     | 0.50              |
| 3:F1:49:VAL:HG21  | 3:F1:240:LEU:HB3  | 1.94                     | 0.50              |
| 7:a:172:VAL:HG13  | 7:a:180:ALA:HB3   | 1.94                     | 0.50              |
| 7:d:5:VAL:HG11    | 7:d:149:ARG:HD3   | 1.94                     | 0.50              |
| 7:j:14:LYS:HD2    | 7:j:47:LEU:HD22   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:q:97:ARG:HH22   | 7:s:5:VAL:HG13    | 1.76                     | 0.50              |
| 7:s:9:PRO:HB2     | 7:s:143:ILE:HG13  | 1.92                     | 0.50              |
| 3:A1:86:ARG:HE    | 3:A1:87:PRO:HD2   | 1.76                     | 0.50              |
| 2:A2:227:LEU:HG   | 3:A3:324:LYS:HZ1  | 1.77                     | 0.50              |
| 3:B1:116:VAL:HA   | 3:B1:119:VAL:HG12 | 1.92                     | 0.50              |
| 2:B8:402:ARG:HD3  | 2:B8:405:VAL:HG11 | 1.93                     | 0.50              |
| 3:B9:267:LEU:HD21 | 3:B9:374:ILE:HG12 | 1.93                     | 0.50              |
| 3:C3:215:LEU:HB3  | 3:C3:217:LEU:HD23 | 1.94                     | 0.50              |
| 3:C3:323:THR:HG22 | 3:C3:353:VAL:HG21 | 1.93                     | 0.50              |
| 3:D7:68:LEU:HD22  | 3:D7:97:ALA:HB2   | 1.93                     | 0.50              |
| 2:D8:140:ALA:HA   | 2:D8:171:SER:HB3  | 1.94                     | 0.50              |
| 2:E0:238:LEU:HA   | 2:E0:318:MET:HE3  | 1.92                     | 0.50              |
| 4:V:1289:ARG:HH21 | 4:V:1294:VAL:HG22 | 1.77                     | 0.50              |
| 7:b:97:ARG:HH12   | 7:d:161:TYR:HA    | 1.77                     | 0.50              |
| 3:A3:249:ASP:H    | 3:A3:252:LYS:HB2  | 1.76                     | 0.50              |
| 2:A4:207:GLU:HA   | 2:A4:210:TYR:HD2  | 1.77                     | 0.50              |
| 1:B:247:TYR:O     | 1:B:251:TYR:HB2   | 2.12                     | 0.50              |
| 2:B0:29:GLY:HA2   | 1:C:224:LEU:HD12  | 1.92                     | 0.50              |
| 2:B0:339:ARG:HH11 | 4:Q:1235:ARG:HD2  | 1.77                     | 0.50              |
| 3:B1:169:VAL:HG12 | 3:B1:202:ILE:HB   | 1.94                     | 0.50              |
| 3:B1:238:CYS:HA   | 3:B1:241:ARG:HE   | 1.76                     | 0.50              |
| 3:B3:165:GLU:HG3  | 3:B3:198:GLU:HB2  | 1.94                     | 0.50              |
| 2:B8:247:ALA:HB3  | 2:B8:355:ILE:HD11 | 1.94                     | 0.50              |
| 3:B9:39:ASP:HA    | 7:h:90:PRO:HG3    | 1.93                     | 0.50              |
| 3:E1:278:SER:HA   | 3:E1:281:TYR:HB2  | 1.94                     | 0.50              |
| 3:E9:248:SER:HB2  | 3:E9:316:MET:HE1  | 1.93                     | 0.50              |
| 3:A1:178:THR:HB   | 3:A1:181:GLU:HG3  | 1.93                     | 0.50              |
| 2:A2:207:GLU:HG3  | 2:A2:304:LYS:NZ   | 2.27                     | 0.50              |
| 3:A9:11:GLN:HB2   | 3:A9:72:THR:HG21  | 1.94                     | 0.50              |
| 3:A9:213:ARG:HG3  | 3:A9:214:THR:HG23 | 1.93                     | 0.50              |
| 2:B0:175:PRO:HB3  | 2:B0:390:ARG:HD2  | 1.94                     | 0.50              |
| 3:B1:284:LEU:HG   | 3:B1:363:MET:HE2  | 1.93                     | 0.50              |
| 2:B4:387:VAL:HG23 | 2:B4:390:ARG:HH22 | 1.77                     | 0.50              |
| 3:B5:45:GLU:HG2   | 3:B5:46:ARG:HG2   | 1.93                     | 0.50              |
| 3:B9:57:GLY:HA3   | 7:h:83:PRO:HB2    | 1.93                     | 0.50              |
| 2:C6:323:VAL:HG22 | 2:C6:373:ARG:HG2  | 1.93                     | 0.50              |
| 3:C7:320:ARG:HH21 | 1:J:212:GLU:H     | 1.59                     | 0.50              |
| 3:C9:221:THR:HG23 | 3:C9:223:GLY:H    | 1.76                     | 0.50              |
| 2:D0:73:THR:HG22  | 3:D1:46:ARG:HH12  | 1.76                     | 0.50              |
| 2:D0:101:ASN:HA   | 2:D0:144:GLY:H    | 1.75                     | 0.50              |
| 3:D3:278:SER:HA   | 3:D3:281:TYR:HD2  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E2:286:LEU:HD11 | 2:E2:372:MET:H    | 1.77                     | 0.50              |
| 2:E8:267:PHE:HB3  | 2:E8:384:ILE:HD13 | 1.93                     | 0.50              |
| 3:F1:257:LEU:HD13 | 3:F1:312:THR:HG22 | 1.93                     | 0.50              |
| 7:b:64:PRO:HD2    | 7:b:67:HIS:HD1    | 1.76                     | 0.50              |
| 7:f:50:PHE:HD2    | 7:f:65:GLN:HG3    | 1.77                     | 0.50              |
| 7:n:55:LEU:HB3    | 7:n:132:LEU:HD23  | 1.93                     | 0.50              |
| 7:p:105:ASN:HD22  | 7:r:37:GLN:HE22   | 1.59                     | 0.50              |
| 7:t:9:PRO:HA      | 7:t:12:VAL:HG22   | 1.94                     | 0.50              |
| 2:A2:274:PRO:HB2  | 2:A2:371:VAL:HG21 | 1.92                     | 0.49              |
| 3:B1:284:LEU:HD23 | 3:B1:362:LYS:HE3  | 1.93                     | 0.49              |
| 2:B6:285:GLN:HB3  | 2:C0:56:THR:HA    | 1.93                     | 0.49              |
| 3:C9:66:MET:HE3   | 3:C9:147:MET:HG2  | 1.95                     | 0.49              |
| 3:D1:167:PHE:CG   | 3:D1:233:MET:HE3  | 2.47                     | 0.49              |
| 2:D8:226:ASN:HA   | 2:D8:229:ARG:HG2  | 1.94                     | 0.49              |
| 3:D9:95:THR:HG21  | 3:D9:108:GLU:HB3  | 1.94                     | 0.49              |
| 3:E1:11:GLN:HG3   | 3:E1:72:THR:HG21  | 1.93                     | 0.49              |
| 3:E9:149:THR:HA   | 3:E9:152:ILE:HD12 | 1.93                     | 0.49              |
| 3:E9:320:ARG:HH12 | 6:U:116:GLU:HA    | 1.76                     | 0.49              |
| 1:I:215:TYR:O     | 1:I:219:TYR:HB2   | 2.12                     | 0.49              |
| 7:f:15:ARG:O      | 7:f:19:GLU:HG2    | 2.11                     | 0.49              |
| 7:f:158:THR:HB    | 7:f:161:TYR:HB2   | 1.93                     | 0.49              |
| 7:j:78:ALA:HB3    | 7:j:112:PHE:HE1   | 1.77                     | 0.49              |
| 7:t:53:GLY:HA2    | 7:t:62:VAL:HG21   | 1.94                     | 0.49              |
| 2:A0:206:ASN:HB3  | 2:A0:210:TYR:CZ   | 2.47                     | 0.49              |
| 1:D:244:GLN:HE22  | 1:D:248:ARG:HB3   | 1.77                     | 0.49              |
| 3:D9:392:LYS:HG3  | 3:D9:395:LEU:HD23 | 1.94                     | 0.49              |
| 4:W:1251:ILE:HG23 | 4:W:1384:LYS:HB3  | 1.93                     | 0.49              |
| 7:s:94:ASN:HD22   | 7:s:94:ASN:C      | 2.20                     | 0.49              |
| 2:A0:107:HIS:C    | 2:A0:112:LYS:HZ1  | 2.20                     | 0.49              |
| 3:A5:173:PRO:HG3  | 3:A5:380:ARG:HG3  | 1.94                     | 0.49              |
| 2:A8:103:PHE:H    | 2:A8:408:TYR:HE1  | 1.58                     | 0.49              |
| 3:B7:215:LEU:HB3  | 3:B7:217:LEU:HG   | 1.94                     | 0.49              |
| 2:C0:115:VAL:HG21 | 2:C0:152:LEU:HD22 | 1.94                     | 0.49              |
| 3:C3:102:ALA:HB2  | 3:C3:403:MET:HE2  | 1.94                     | 0.49              |
| 2:D0:269:LEU:HD22 | 2:D0:303:ALA:HB2  | 1.94                     | 0.49              |
| 2:D2:272:TYR:HB3  | 2:D2:275:ILE:HD11 | 1.94                     | 0.49              |
| 3:D7:271:ALA:HA   | 3:D7:273:LEU:HG   | 1.95                     | 0.49              |
| 3:E3:259:PRO:HG2  | 3:E3:311:LEU:HD21 | 1.94                     | 0.49              |
| 3:E3:290:THR:HA   | 3:E3:293:MET:HE3  | 1.93                     | 0.49              |
| 7:a:130:PRO:HB3   | 7:c:159:TYR:CG    | 2.47                     | 0.49              |
| 7:s:50:PHE:HD1    | 7:s:140:LEU:HD21  | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:w:119:ARG:HH12  | 7:w:123:GLU:HB3   | 1.76                     | 0.49              |
| 3:A3:11:GLN:HA    | 3:A3:14:ASN:HB2   | 1.94                     | 0.49              |
| 3:A3:244:GLY:HA2  | 3:A3:355:ASP:HB2  | 1.94                     | 0.49              |
| 2:A6:344:VAL:HG13 | 2:A6:345:ASP:H    | 1.78                     | 0.49              |
| 3:A9:334:GLN:HE21 | 3:A9:349:MET:HG2  | 1.75                     | 0.49              |
| 2:B6:241:SER:HB2  | 2:B6:249:ASN:HB2  | 1.94                     | 0.49              |
| 3:B7:5:VAL:HB     | 3:B7:133:PHE:HD1  | 1.77                     | 0.49              |
| 2:C0:276:ILE:HD11 | 2:C0:280:LYS:HB2  | 1.92                     | 0.49              |
| 2:C4:180:ALA:HB3  | 2:C4:183:GLU:HB2  | 1.94                     | 0.49              |
| 2:C6:132:LEU:HD23 | 2:C6:164:LYS:HE3  | 1.94                     | 0.49              |
| 3:C9:289:LEU:HD23 | 3:C9:365:VAL:HG13 | 1.93                     | 0.49              |
| 3:D1:16:ILE:HA    | 3:D1:226:ASN:HB3  | 1.94                     | 0.49              |
| 2:D2:222:PRO:HG2  | 3:D3:324:LYS:NZ   | 2.27                     | 0.49              |
| 2:D8:93:ILE:HD11  | 2:D8:121:ARG:HG3  | 1.94                     | 0.49              |
| 2:D8:259:LEU:HD21 | 2:D8:316:CYS:HB2  | 1.94                     | 0.49              |
| 3:E1:64:ILE:HD12  | 3:E1:119:VAL:HG12 | 1.95                     | 0.49              |
| 2:E6:81:GLY:HA3   | 1:H:215:TYR:HE2   | 1.78                     | 0.49              |
| 2:E8:223:THR:HG21 | 3:E9:324:LYS:H    | 1.76                     | 0.49              |
| 6:R:76:LYS:HB3    | 7:b:162:GLY:HA3   | 1.93                     | 0.49              |
| 7:a:170:VAL:HG23  | 7:a:183:LEU:HB2   | 1.93                     | 0.49              |
| 7:c:71:LYS:HD2    | 7:c:109:GLU:HG2   | 1.94                     | 0.49              |
| 7:d:142:GLU:HA    | 7:d:145:LYS:HB2   | 1.95                     | 0.49              |
| 7:q:129:MET:HE3   | 7:q:131:TRP:HE1   | 1.77                     | 0.49              |
| 2:A4:101:ASN:HD22 | 2:A4:143:GLY:HA2  | 1.77                     | 0.49              |
| 2:A6:2:ARG:HH21   | 2:A6:242:LEU:HA   | 1.78                     | 0.49              |
| 2:B4:208:ALA:HB2  | 2:B4:304:LYS:HB2  | 1.95                     | 0.49              |
| 2:C0:244:PHE:HB2  | 2:C0:356:ASN:HD21 | 1.77                     | 0.49              |
| 4:M:1254:ARG:NH2  | 4:M:1266:ALA:HB1  | 2.27                     | 0.49              |
| 4:N:1285:ARG:HH22 | 4:N:1294:VAL:HA   | 1.76                     | 0.49              |
| 7:d:11:ASN:HB3    | 7:d:15:ARG:HH12   | 1.78                     | 0.49              |
| 7:e:185:ILE:HD13  | 7:e:195:ALA:HB3   | 1.94                     | 0.49              |
| 7:g:140:LEU:HA    | 7:g:143:ILE:HG22  | 1.93                     | 0.49              |
| 7:n:112:PHE:CG    | 7:n:129:MET:HE1   | 2.47                     | 0.49              |
| 7:t:172:VAL:HG11  | 7:t:204:THR:HG21  | 1.93                     | 0.49              |
| 2:A0:177:VAL:HG11 | 2:A0:210:TYR:CE1  | 2.48                     | 0.49              |
| 3:A5:113:ILE:HA   | 3:A5:147:MET:HE1  | 1.94                     | 0.49              |
| 3:A5:257:LEU:HB3  | 3:A5:266:PHE:HE2  | 1.77                     | 0.49              |
| 3:B1:24:ILE:HG23  | 3:B1:241:ARG:HH12 | 1.76                     | 0.49              |
| 3:B3:73:MET:HA    | 3:B3:76:VAL:HG12  | 1.93                     | 0.49              |
| 2:B4:311:LYS:H    | 2:B4:382:THR:HG22 | 1.76                     | 0.49              |
| 3:B5:117:LEU:HA   | 3:B5:120:VAL:HG12 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B6:137:MET:HE1  | 2:B6:154:LEU:HD11 | 1.95                     | 0.49              |
| 2:B6:262:TYR:HB2  | 2:B6:265:ILE:HG22 | 1.93                     | 0.49              |
| 2:C8:200:VAL:HG11 | 2:C8:255:PHE:HE2  | 1.77                     | 0.49              |
| 3:D3:271:ALA:HB2  | 3:D3:298:ASN:ND2  | 2.28                     | 0.49              |
| 2:D4:223:THR:HG22 | 3:D5:322:SER:HA   | 1.94                     | 0.49              |
| 2:D6:84:ARG:HH12  | 7:q:98:THR:HG21   | 1.76                     | 0.49              |
| 2:E2:184:PRO:HA   | 2:E2:391:MET:HE3  | 1.94                     | 0.49              |
| 2:E2:244:PHE:HB2  | 2:E2:356:ASN:HD21 | 1.77                     | 0.49              |
| 2:E6:53:PHE:HB3   | 2:E6:61:HIS:HB3   | 1.95                     | 0.49              |
| 3:A3:206:ALA:HB2  | 3:A3:302:ALA:HB2  | 1.95                     | 0.49              |
| 3:A9:200:GLN:HG2  | 3:A9:268:ILE:HD11 | 1.94                     | 0.49              |
| 3:B5:155:VAL:HA   | 3:B5:158:GLU:HG2  | 1.95                     | 0.49              |
| 3:B5:265:PHE:HB3  | 3:B5:374:ILE:HD13 | 1.95                     | 0.49              |
| 3:B7:17:GLY:HA2   | 3:B7:20:PHE:HB3   | 1.95                     | 0.49              |
| 3:C5:136:THR:HG22 | 3:C5:167:PHE:HB2  | 1.95                     | 0.49              |
| 2:C8:208:ALA:HB2  | 2:C8:304:LYS:H    | 1.78                     | 0.49              |
| 3:C9:189:VAL:HG11 | 3:C9:415:MET:HG3  | 1.95                     | 0.49              |
| 2:D2:189:LEU:HD21 | 2:D2:413:MET:HE3  | 1.95                     | 0.49              |
| 2:E2:195:LEU:HD13 | 2:E2:428:LEU:HD21 | 1.94                     | 0.49              |
| 2:E8:115:VAL:HG11 | 2:E8:152:LEU:HD22 | 1.93                     | 0.49              |
| 2:E8:310:GLY:HA3  | 2:E8:383:ALA:HB2  | 1.94                     | 0.49              |
| 8:k:50:VAL:O      | 8:k:54:ARG:HB2    | 2.13                     | 0.49              |
| 2:A6:3:GLU:HA     | 2:A6:51:THR:HA    | 1.95                     | 0.49              |
| 3:B5:4:ILE:HD11   | 3:B5:240:LEU:HD13 | 1.93                     | 0.49              |
| 3:B7:281:TYR:HD2  | 3:C1:87:PRO:HD3   | 1.77                     | 0.49              |
| 2:C2:259:LEU:HD21 | 2:C2:316:CYS:HB2  | 1.95                     | 0.49              |
| 3:D3:318:ARG:HG2  | 3:D3:354:CYS:HB2  | 1.93                     | 0.49              |
| 2:E6:18:ASN:HD21  | 1:H:215:TYR:HD1   | 1.59                     | 0.49              |
| 2:E6:195:LEU:HD12 | 2:E6:428:LEU:HD12 | 1.95                     | 0.49              |
| 7:n:106:GLN:HG3   | 7:p:6:PHE:HZ      | 1.77                     | 0.49              |
| 7:r:174:GLY:HA3   | 7:r:178:ARG:HD3   | 1.95                     | 0.49              |
| 2:A0:324:VAL:HG12 | 2:A0:326:LYS:H    | 1.78                     | 0.49              |
| 2:A2:210:TYR:HE1  | 2:A2:227:LEU:HD11 | 1.78                     | 0.49              |
| 3:A7:8:GLN:HG3    | 3:A7:65:LEU:HD13  | 1.94                     | 0.49              |
| 3:C7:32:PRO:HD3   | 3:C7:81:PHE:HE1   | 1.78                     | 0.49              |
| 2:D2:288:VAL:HG11 | 2:D2:323:VAL:HG13 | 1.94                     | 0.49              |
| 3:D9:207:LEU:HB3  | 3:D9:225:LEU:HG   | 1.94                     | 0.49              |
| 2:E0:2:ARG:HG2    | 2:E0:51:THR:HG22  | 1.95                     | 0.49              |
| 3:E3:320:ARG:HH12 | 1:F:214:ALA:HB2   | 1.78                     | 0.49              |
| 2:E8:325:PRO:HA   | 2:E8:328:VAL:HG22 | 1.95                     | 0.49              |
| 2:F0:26:LEU:HD21  | 2:F0:363:VAL:HG12 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F0:82:THR:HG21  | 6:T:123:PRO:HD3   | 1.93                     | 0.49              |
| 5:P:487:THR:HG22  | 5:P:489:LEU:H     | 1.77                     | 0.49              |
| 7:i:142:GLU:HA    | 7:i:145:LYS:HB2   | 1.95                     | 0.49              |
| 7:o:15:ARG:O      | 7:o:19:GLU:HG3    | 2.13                     | 0.49              |
| 7:u:4:PRO:HG3     | 7:u:179:GLU:HG2   | 1.94                     | 0.49              |
| 2:A2:191:THR:HG21 | 2:A2:425:LEU:HD13 | 1.95                     | 0.49              |
| 3:A5:289:LEU:HD23 | 3:A5:365:VAL:HG23 | 1.95                     | 0.49              |
| 3:A9:16:ILE:HG22  | 3:A9:226:ASN:CG   | 2.38                     | 0.49              |
| 3:B1:68:LEU:HD12  | 3:B1:143:THR:HG22 | 1.95                     | 0.49              |
| 3:B9:248:SER:HA   | 3:B9:252:LYS:HD2  | 1.94                     | 0.49              |
| 3:C1:298:ASN:ND2  | 3:C1:298:ASN:O    | 2.45                     | 0.49              |
| 3:C3:113:ILE:HA   | 3:C3:116:VAL:HG12 | 1.93                     | 0.49              |
| 2:D4:292:THR:HG21 | 2:D4:331:ALA:HB1  | 1.93                     | 0.49              |
| 3:E3:284:LEU:HD23 | 3:E3:362:LYS:HG2  | 1.94                     | 0.49              |
| 2:E4:207:GLU:HA   | 2:E4:210:TYR:HB2  | 1.95                     | 0.49              |
| 3:E5:252:LYS:HA   | 3:E5:255:VAL:HG12 | 1.95                     | 0.49              |
| 3:E9:311:LEU:HD12 | 3:E9:342:VAL:HG11 | 1.94                     | 0.49              |
| 3:E9:410:GLU:HA   | 3:E9:413:SER:HB3  | 1.94                     | 0.49              |
| 7:h:170:VAL:HG23  | 7:h:183:LEU:HB2   | 1.95                     | 0.49              |
| 7:s:146:ARG:HD2   | 7:s:156:VAL:HG21  | 1.94                     | 0.49              |
| 2:A2:244:PHE:HB2  | 2:A2:356:ASN:HD21 | 1.78                     | 0.48              |
| 2:B0:408:TYR:HB3  | 2:B0:413:MET:HE3  | 1.94                     | 0.48              |
| 3:C9:136:THR:HG22 | 3:C9:167:PHE:HB2  | 1.95                     | 0.48              |
| 2:D4:76:ASP:HA    | 2:D4:79:ARG:HG2   | 1.94                     | 0.48              |
| 3:D5:117:LEU:HA   | 3:D5:120:VAL:HG12 | 1.93                     | 0.48              |
| 2:E0:105:ARG:HA   | 2:E0:109:THR:HG22 | 1.95                     | 0.48              |
| 2:E2:180:ALA:HB3  | 2:E2:183:GLU:HB3  | 1.94                     | 0.48              |
| 2:E2:255:PHE:HZ   | 2:E2:378:ILE:HG21 | 1.78                     | 0.48              |
| 3:E5:229:VAL:HA   | 3:E5:300:MET:HE1  | 1.94                     | 0.48              |
| 3:E9:175:VAL:HG22 | 3:E9:205:GLU:HB3  | 1.95                     | 0.48              |
| 3:E9:308:GLY:HA3  | 3:E9:373:ALA:HB2  | 1.95                     | 0.48              |
| 1:J:244:GLN:HG2   | 7:m:162:GLY:HA3   | 1.95                     | 0.48              |
| 4:L:1440:ASP:HA   | 4:L:1443:GLU:OE1  | 2.13                     | 0.48              |
| 4:Q:1285:ARG:HH22 | 4:Q:1294:VAL:HG22 | 1.78                     | 0.48              |
| 7:g:67:HIS:HD2    | 7:i:23:LEU:HD12   | 1.78                     | 0.48              |
| 7:j:151:MET:HE2   | 7:j:154:TYR:HA    | 1.95                     | 0.48              |
| 3:A7:7:VAL:HB     | 3:A7:135:ILE:HG13 | 1.94                     | 0.48              |
| 2:A8:210:TYR:HE1  | 2:A8:227:LEU:HD21 | 1.77                     | 0.48              |
| 2:B2:398:MET:HG3  | 3:B3:346:PRO:HD2  | 1.95                     | 0.48              |
| 2:C4:292:THR:HG21 | 2:C4:331:ALA:HB1  | 1.94                     | 0.48              |
| 3:C5:272:PRO:HG3  | 3:C5:284:LEU:HD11 | 1.93                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C9:12:CYS:HB3   | 3:C9:138:SER:HB2  | 1.94                     | 0.48              |
| 3:D1:248:SER:HA   | 3:D1:252:LYS:HD3  | 1.95                     | 0.48              |
| 2:D4:323:VAL:HG22 | 2:D4:373:ARG:HG2  | 1.94                     | 0.48              |
| 2:D8:200:VAL:HG11 | 2:D8:255:PHE:HE1  | 1.77                     | 0.48              |
| 2:E6:434:GLU:HA   | 2:E6:437:ILE:HD12 | 1.95                     | 0.48              |
| 3:F1:135:ILE:HB   | 3:F1:166:THR:HG22 | 1.95                     | 0.48              |
| 7:g:146:ARG:HD2   | 7:g:156:VAL:HG11  | 1.95                     | 0.48              |
| 7:h:75:LEU:O      | 7:h:170:VAL:HA    | 2.13                     | 0.48              |
| 8:l:13:VAL:HG13   | 8:l:24:VAL:H      | 1.77                     | 0.48              |
| 8:l:51:PRO:HA     | 8:l:54:ARG:HE     | 1.79                     | 0.48              |
| 3:A1:248:SER:HA   | 3:A1:252:LYS:HG3  | 1.96                     | 0.48              |
| 3:A1:374:ILE:HD11 | 3:A1:377:MET:HE3  | 1.94                     | 0.48              |
| 3:A5:397:TRP:NE1  | 2:A6:257:THR:HA   | 2.28                     | 0.48              |
| 3:A9:39:ASP:HA    | 7:c:90:PRO:HG3    | 1.95                     | 0.48              |
| 3:B3:257:LEU:HD21 | 3:B3:314:SER:HB2  | 1.94                     | 0.48              |
| 2:B4:416:GLY:HA3  | 4:Q:1383:LEU:HD11 | 1.94                     | 0.48              |
| 3:C1:7:VAL:HB     | 3:C1:135:ILE:HG13 | 1.95                     | 0.48              |
| 3:C1:57:GLY:HA3   | 7:i:83:PRO:HB2    | 1.95                     | 0.48              |
| 3:C1:219:THR:HA   | 2:C2:326:LYS:HZ1  | 1.77                     | 0.48              |
| 3:C5:35:THR:HG22  | 8:k:44:SER:HB3    | 1.93                     | 0.48              |
| 2:C6:137:MET:HE1  | 2:C6:154:LEU:HB2  | 1.95                     | 0.48              |
| 3:C7:113:ILE:HA   | 3:C7:116:VAL:HG12 | 1.95                     | 0.48              |
| 3:C7:416:ASN:HA   | 3:C7:419:VAL:HG22 | 1.95                     | 0.48              |
| 3:C9:156:ARG:HH21 | 3:C9:164:MET:HG3  | 1.78                     | 0.48              |
| 3:C9:171:PRO:HG2  | 3:C9:185:ALA:HB2  | 1.95                     | 0.48              |
| 3:D3:156:ARG:HE   | 3:D3:164:MET:HG3  | 1.78                     | 0.48              |
| 2:D6:27:GLU:CD    | 2:D6:243:ARG:HH12 | 2.21                     | 0.48              |
| 3:D7:318:ARG:HA   | 3:D7:354:CYS:HB2  | 1.95                     | 0.48              |
| 3:E1:13:GLY:HA2   | 3:E1:136:THR:HG22 | 1.94                     | 0.48              |
| 3:E9:271:ALA:HB1  | 3:E9:292:GLN:HB3  | 1.95                     | 0.48              |
| 2:F0:177:VAL:HA   | 3:F1:331:LEU:HD21 | 1.95                     | 0.48              |
| 7:c:115:LEU:HD22  | 7:c:152:LYS:HZ2   | 1.78                     | 0.48              |
| 8:k:36:LEU:HD23   | 8:k:72:ILE:HB     | 1.95                     | 0.48              |
| 7:n:146:ARG:HH22  | 7:n:158:THR:HA    | 1.77                     | 0.48              |
| 3:A1:138:SER:HB3  | 11:A1:501:GDP:H5' | 1.96                     | 0.48              |
| 2:A6:387:VAL:HA   | 2:A6:390:ARG:NH1  | 2.28                     | 0.48              |
| 3:A9:290:THR:HG21 | 3:A9:329:GLN:HB3  | 1.94                     | 0.48              |
| 3:A9:326:VAL:O    | 3:A9:330:MET:HG2  | 2.13                     | 0.48              |
| 3:D3:91:VAL:HG11  | 3:D3:116:VAL:HG22 | 1.95                     | 0.48              |
| 2:E2:259:LEU:HD22 | 2:E2:316:CYS:HB2  | 1.96                     | 0.48              |
| 2:E4:70:LEU:HD12  | 2:E4:99:ALA:HB2   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:l:80:GLU:O      | 8:l:84:GLU:HG2    | 2.12                     | 0.48              |
| 8:l:99:SER:HB2    | 8:l:102:ARG:HB3   | 1.95                     | 0.48              |
| 7:n:14:LYS:HA     | 7:n:47:LEU:HD13   | 1.95                     | 0.48              |
| 7:v:114:SER:HB3   | 7:v:136:LEU:HD13  | 1.95                     | 0.48              |
| 2:A0:362:VAL:HB   | 2:A0:370:LYS:HB3  | 1.96                     | 0.48              |
| 3:B5:171:PRO:HG2  | 3:B5:185:ALA:HB2  | 1.95                     | 0.48              |
| 3:B5:293:MET:SD   | 3:B5:367:PHE:HB2  | 2.53                     | 0.48              |
| 3:B7:193:VAL:HG11 | 3:B7:418:LEU:HD22 | 1.95                     | 0.48              |
| 2:C2:210:TYR:CG   | 3:C3:324:LYS:HD3  | 2.48                     | 0.48              |
| 3:C9:215:LEU:HD21 | 3:C9:273:LEU:HD22 | 1.96                     | 0.48              |
| 3:E1:167:PHE:CE2  | 3:E1:233:MET:HG2  | 2.48                     | 0.48              |
| 3:E3:117:LEU:HA   | 3:E3:120:VAL:HG12 | 1.95                     | 0.48              |
| 1:K:244:GLN:HE22  | 7:o:162:GLY:HA3   | 1.79                     | 0.48              |
| 7:h:10:LEU:HG     | 7:h:47:LEU:HD11   | 1.95                     | 0.48              |
| 8:l:29:PHE:HB3    | 8:l:34:VAL:HG21   | 1.94                     | 0.48              |
| 7:v:84:LYS:HB2    | 7:v:168:PRO:HD3   | 1.94                     | 0.48              |
| 3:A5:207:LEU:HB3  | 3:A5:225:LEU:HD22 | 1.96                     | 0.48              |
| 3:B7:252:LYS:HG3  | 3:B7:350:LYS:NZ   | 2.28                     | 0.48              |
| 2:C2:212:ILE:HG23 | 2:C2:216:ASN:HD22 | 1.77                     | 0.48              |
| 2:C4:384:ILE:HD12 | 2:C4:387:VAL:HG21 | 1.95                     | 0.48              |
| 1:E:223:PRO:HG3   | 7:h:178:ARG:HD2   | 1.95                     | 0.48              |
| 4:L:1252:LEU:HD11 | 4:L:1442:TYR:HD1  | 1.79                     | 0.48              |
| 4:W:1276:LEU:C    | 4:W:1284:TRP:HE1  | 2.21                     | 0.48              |
| 7:f:97:ARG:HH12   | 7:h:161:TYR:HA    | 1.77                     | 0.48              |
| 7:p:50:PHE:HB2    | 7:p:65:GLN:HG3    | 1.95                     | 0.48              |
| 7:q:14:LYS:HB3    | 7:q:47:LEU:HD13   | 1.95                     | 0.48              |
| 2:A8:53:PHE:HB3   | 2:A8:61:HIS:HB3   | 1.96                     | 0.48              |
| 2:B0:310:GLY:HA3  | 2:B0:383:ALA:HB2  | 1.95                     | 0.48              |
| 2:B0:407:TRP:HE1  | 3:B1:258:ILE:HB   | 1.77                     | 0.48              |
| 2:B4:406:HIS:HA   | 2:B4:409:VAL:HG22 | 1.94                     | 0.48              |
| 3:B9:3:GLU:HA     | 3:B9:49:VAL:HA    | 1.96                     | 0.48              |
| 2:C4:181:VAL:HG12 | 3:C5:256:ASN:HB2  | 1.95                     | 0.48              |
| 2:D6:249:ASN:C    | 2:D6:249:ASN:HD22 | 2.19                     | 0.48              |
| 3:E1:290:THR:HG22 | 3:E1:293:MET:HE2  | 1.96                     | 0.48              |
| 3:E3:193:VAL:HG11 | 3:E3:418:LEU:HD11 | 1.96                     | 0.48              |
| 2:E4:265:ILE:HG22 | 2:E4:380:ASN:HD21 | 1.77                     | 0.48              |
| 2:E8:248:LEU:HB2  | 2:E8:355:ILE:H    | 1.79                     | 0.48              |
| 2:F0:286:LEU:HD13 | 2:F0:371:VAL:HG23 | 1.96                     | 0.48              |
| 7:d:55:LEU:HD11   | 7:d:111:ILE:HD12  | 1.96                     | 0.48              |
| 7:h:64:PRO:HD2    | 7:h:67:HIS:CE1    | 2.49                     | 0.48              |
| 7:q:37:GLN:HE22   | 7:q:40:PRO:HA     | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:q:185:ILE:HD13  | 7:q:195:ALA:HB3   | 1.95                     | 0.48              |
| 7:r:79:ASP:HB3    | 7:r:82:ASP:HB2    | 1.95                     | 0.48              |
| 2:A2:33:ASP:HB3   | 6:R:90:TRP:HZ3    | 1.78                     | 0.48              |
| 3:A3:117:LEU:HA   | 3:A3:120:VAL:HG12 | 1.95                     | 0.48              |
| 3:A5:117:LEU:HA   | 3:A5:120:VAL:HG12 | 1.96                     | 0.48              |
| 3:B1:156:ARG:HH22 | 3:B1:197:ASP:HB2  | 1.78                     | 0.48              |
| 3:B3:7:VAL:HB     | 3:B3:135:ILE:HG13 | 1.95                     | 0.48              |
| 3:B7:293:MET:HE1  | 3:B7:315:ALA:HB2  | 1.94                     | 0.48              |
| 3:B9:398:TYR:HB3  | 3:B9:403:MET:HE2  | 1.94                     | 0.48              |
| 2:C2:377:MET:HE3  | 2:C2:379:SER:HB3  | 1.95                     | 0.48              |
| 3:C5:36:TYR:HD2   | 8:k:47:ALA:HB1    | 1.79                     | 0.48              |
| 2:C6:404:PHE:HZ   | 3:C7:312:THR:HG21 | 1.78                     | 0.48              |
| 3:C7:7:VAL:HG11   | 3:C7:151:LEU:HD22 | 1.95                     | 0.48              |
| 3:C9:149:THR:HA   | 3:C9:152:ILE:HG12 | 1.95                     | 0.48              |
| 2:E8:126:ALA:HA   | 2:E8:132:LEU:HD21 | 1.96                     | 0.48              |
| 2:E8:286:LEU:HD21 | 2:E8:371:VAL:HG23 | 1.96                     | 0.48              |
| 7:v:95:TYR:HE1    | 7:v:197:LEU:HD23  | 1.79                     | 0.48              |
| 3:A9:330:MET:HE3  | 3:A9:351:SER:HB3  | 1.95                     | 0.48              |
| 2:B8:422:ARG:HH12 | 2:B8:425:LEU:HD22 | 1.78                     | 0.48              |
| 2:C4:178:SER:HB3  | 3:C5:347:ASN:ND2  | 2.29                     | 0.48              |
| 2:D6:11:GLN:HE22  | 3:D7:246:LEU:HD12 | 1.78                     | 0.48              |
| 2:E4:31:GLN:HE22  | 2:E4:37:PRO:HD3   | 1.79                     | 0.48              |
| 6:T:120:GLU:HA    | 6:T:127:ARG:HH22  | 1.79                     | 0.48              |
| 7:b:95:TYR:HE1    | 7:b:197:LEU:HD23  | 1.79                     | 0.48              |
| 7:d:183:LEU:HD23  | 7:d:196:LEU:HA    | 1.96                     | 0.48              |
| 7:g:183:LEU:HD13  | 7:g:196:LEU:HA    | 1.96                     | 0.48              |
| 7:o:97:ARG:HH12   | 7:q:5:VAL:HG12    | 1.79                     | 0.48              |
| 7:x:9:PRO:HA      | 7:x:12:VAL:HG22   | 1.96                     | 0.48              |
| 3:A1:235:GLY:HA3  | 3:A1:366:THR:HG21 | 1.95                     | 0.48              |
| 2:A2:181:VAL:HG12 | 3:A3:256:ASN:OD1  | 2.14                     | 0.48              |
| 3:A7:173:PRO:HB3  | 3:A7:380:ARG:HD2  | 1.95                     | 0.48              |
| 2:A8:398:MET:HE3  | 3:A9:346:PRO:HD2  | 1.96                     | 0.48              |
| 2:B0:80:THR:HA    | 2:B0:84:ARG:HE    | 1.78                     | 0.48              |
| 3:B3:8:GLN:OE1    | 3:B3:17:GLY:HA3   | 2.12                     | 0.48              |
| 3:B7:57:GLY:HA3   | 7:g:83:PRO:HB2    | 1.95                     | 0.48              |
| 2:B8:33:ASP:HB2   | 7:h:103:GLY:HA2   | 1.96                     | 0.48              |
| 3:C9:219:THR:HA   | 2:D0:326:LYS:NZ   | 2.29                     | 0.48              |
| 3:D1:237:THR:HG23 | 3:D1:240:LEU:HD12 | 1.96                     | 0.48              |
| 2:D4:320:ARG:HG2  | 2:D4:360:PRO:HD3  | 1.96                     | 0.48              |
| 2:D6:420:GLU:HA   | 2:D6:423:GLU:HB3  | 1.95                     | 0.48              |
| 3:D7:173:PRO:HD2  | 3:D7:380:ARG:HH21 | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E1:21:TRP:HA    | 3:E1:24:ILE:HG22  | 1.94                     | 0.48              |
| 3:E3:68:LEU:HD21  | 3:E3:109:GLY:HA2  | 1.95                     | 0.48              |
| 3:E5:170:PHE:HE1  | 3:E5:378:PHE:HE1  | 1.62                     | 0.48              |
| 3:E5:325:GLU:HA   | 3:E5:328:GLU:HG3  | 1.96                     | 0.48              |
| 2:F0:288:VAL:HG21 | 2:F0:323:VAL:HG23 | 1.95                     | 0.48              |
| 1:G:235:LEU:HD12  | 1:G:236:PRO:HD2   | 1.95                     | 0.48              |
| 1:H:215:TYR:O     | 1:H:219:TYR:HB2   | 2.14                     | 0.48              |
| 7:e:64:PRO:HD2    | 7:e:67:HIS:CE1    | 2.49                     | 0.48              |
| 7:i:10:LEU:HD13   | 7:i:147:HIS:HB2   | 1.95                     | 0.48              |
| 7:m:92:LEU:HA     | 7:m:196:LEU:HD21  | 1.94                     | 0.48              |
| 7:n:142:GLU:HA    | 7:n:145:LYS:HG2   | 1.94                     | 0.48              |
| 7:n:172:VAL:HG23  | 7:n:180:ALA:HB3   | 1.96                     | 0.48              |
| 7:s:75:LEU:HD23   | 7:s:111:ILE:HB    | 1.95                     | 0.48              |
| 7:v:50:PHE:HD2    | 7:v:65:GLN:HG3    | 1.78                     | 0.48              |
| 7:v:91:PHE:CD1    | 7:v:193:ASP:HB3   | 2.49                     | 0.48              |
| 3:A1:102:ALA:HB2  | 3:A1:403:MET:HE2  | 1.95                     | 0.47              |
| 3:A1:113:ILE:HA   | 3:A1:116:VAL:HG22 | 1.95                     | 0.47              |
| 2:A8:107:HIS:CE1  | 2:A8:151:CYS:HB3  | 2.49                     | 0.47              |
| 3:A9:171:PRO:HG2  | 3:A9:185:ALA:HB2  | 1.95                     | 0.47              |
| 2:D0:166:LYS:H    | 2:D0:199:ASP:HB2  | 1.79                     | 0.47              |
| 3:D1:316:MET:HE3  | 3:D1:316:MET:HB3  | 1.71                     | 0.47              |
| 2:D6:181:VAL:H    | 3:D7:256:ASN:HD22 | 1.61                     | 0.47              |
| 2:D8:203:MET:HE3  | 2:D8:267:PHE:HD2  | 1.79                     | 0.47              |
| 3:E1:57:GLY:HA3   | 7:s:83:PRO:HB2    | 1.95                     | 0.47              |
| 3:E1:268:ILE:HG12 | 3:E1:368:VAL:HG22 | 1.96                     | 0.47              |
| 3:E9:224:ASP:HA   | 3:E9:227:HIS:HB3  | 1.96                     | 0.47              |
| 7:d:134:ILE:HD13  | 7:d:140:LEU:HD22  | 1.96                     | 0.47              |
| 7:i:172:VAL:HG23  | 7:i:180:ALA:HB3   | 1.95                     | 0.47              |
| 7:j:149:ARG:HH11  | 7:j:161:TYR:HB3   | 1.77                     | 0.47              |
| 7:s:140:LEU:HA    | 7:s:143:ILE:HG22  | 1.96                     | 0.47              |
| 2:A2:136:LEU:HD22 | 2:A2:169:PHE:HE2  | 1.79                     | 0.47              |
| 2:A6:208:ALA:HA   | 2:A6:304:LYS:HE3  | 1.95                     | 0.47              |
| 2:A6:323:VAL:HG13 | 2:A6:355:ILE:HG23 | 1.96                     | 0.47              |
| 2:C4:262:TYR:HB2  | 2:C4:265:ILE:HD13 | 1.96                     | 0.47              |
| 2:C8:104:ALA:HB2  | 2:C8:413:MET:HE3  | 1.96                     | 0.47              |
| 3:D3:47:ILE:HG12  | 3:D3:51:TYR:HB2   | 1.95                     | 0.47              |
| 2:D8:310:GLY:HA3  | 2:D8:383:ALA:HB2  | 1.96                     | 0.47              |
| 3:E3:8:GLN:HE22   | 3:E3:63:ALA:HB1   | 1.78                     | 0.47              |
| 2:E6:328:VAL:HG21 | 2:E6:355:ILE:HG12 | 1.96                     | 0.47              |
| 3:F1:417:ASP:O    | 3:F1:421:GLU:HG3  | 2.14                     | 0.47              |
| 7:j:175:SER:HA    | 7:j:206:PHE:HE1   | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:m:73:VAL:HA     | 7:m:109:GLU:O     | 2.14                     | 0.47              |
| 7:r:170:VAL:HG23  | 7:r:183:LEU:HB2   | 1.95                     | 0.47              |
| 2:A2:9:VAL:HG13   | 2:A2:146:GLY:HA2  | 1.95                     | 0.47              |
| 2:A6:395:PHE:HD2  | 2:A6:422:ARG:HH21 | 1.61                     | 0.47              |
| 3:A9:42:LEU:HD21  | 1:C:245:SER:HB3   | 1.96                     | 0.47              |
| 2:B0:88:HIS:HB3   | 2:B0:91:GLN:HG2   | 1.95                     | 0.47              |
| 3:B1:28:HIS:HA    | 3:B1:43:GLN:HG2   | 1.96                     | 0.47              |
| 2:B4:364:PRO:HG2  | 1:E:222:LYS:HB3   | 1.96                     | 0.47              |
| 3:B5:375:GLN:HE21 | 3:B5:419:VAL:HG13 | 1.78                     | 0.47              |
| 2:C2:189:LEU:HD21 | 2:C2:418:PHE:HA   | 1.97                     | 0.47              |
| 3:C3:5:VAL:HG23   | 3:C3:130:LEU:HD11 | 1.95                     | 0.47              |
| 2:D4:88:HIS:CE1   | 2:D4:90:GLU:HG3   | 2.49                     | 0.47              |
| 2:E6:12:ALA:HB3   | 2:E6:140:ALA:HB2  | 1.96                     | 0.47              |
| 3:E7:49:VAL:HG11  | 3:E7:241:ARG:HG2  | 1.95                     | 0.47              |
| 1:J:207:LEU:HD12  | 1:J:208:PRO:HD2   | 1.95                     | 0.47              |
| 5:P:465:LEU:HD12  | 5:P:466:VAL:HG23  | 1.95                     | 0.47              |
| 7:h:79:ASP:HB3    | 7:h:82:ASP:HB2    | 1.96                     | 0.47              |
| 8:k:131:LEU:HB2   | 8:k:144:MET:HB3   | 1.96                     | 0.47              |
| 7:x:13:GLU:HA     | 7:x:16:ARG:HG2    | 1.96                     | 0.47              |
| 3:A5:361:LEU:HD12 | 5:P:285:GLN:HG2   | 1.97                     | 0.47              |
| 2:B0:276:ILE:HD12 | 2:B0:281:ALA:HA   | 1.96                     | 0.47              |
| 2:B4:5:ILE:HG23   | 2:B4:125:LEU:HD22 | 1.97                     | 0.47              |
| 3:C1:65:LEU:HB3   | 3:C1:73:MET:HE1   | 1.95                     | 0.47              |
| 2:C6:200:VAL:HG13 | 2:C6:268:MET:HE2  | 1.96                     | 0.47              |
| 2:D8:12:ALA:HB3   | 2:D8:140:ALA:HB2  | 1.96                     | 0.47              |
| 4:M:1401:ARG:HH21 | 4:V:1321:ILE:HD12 | 1.79                     | 0.47              |
| 7:e:90:PRO:HA     | 7:e:93:LEU:HD12   | 1.95                     | 0.47              |
| 7:f:78:ALA:HB3    | 7:f:112:PHE:HE1   | 1.79                     | 0.47              |
| 2:A0:67:PHE:HB2   | 2:A0:92:LEU:HG    | 1.97                     | 0.47              |
| 2:A4:88:HIS:HD2   | 2:A4:91:GLN:HB2   | 1.79                     | 0.47              |
| 3:A9:281:TYR:HD2  | 3:B3:87:PRO:HD3   | 1.80                     | 0.47              |
| 2:B2:53:PHE:HB3   | 2:B2:61:HIS:HB3   | 1.96                     | 0.47              |
| 3:B5:58:ARG:HH21  | 3:B5:84:LEU:HD12  | 1.80                     | 0.47              |
| 3:C3:68:LEU:HA    | 3:C3:93:GLY:HA3   | 1.95                     | 0.47              |
| 3:D1:377:MET:HA   | 3:D1:380:ARG:HD2  | 1.96                     | 0.47              |
| 2:E6:209:ILE:HG22 | 2:E6:227:LEU:HD22 | 1.95                     | 0.47              |
| 2:F0:414:GLU:HG3  | 2:F0:417:GLU:HG2  | 1.95                     | 0.47              |
| 4:L:1248:THR:HG23 | 4:L:1438:LEU:HD13 | 1.97                     | 0.47              |
| 6:U:116:GLU:O     | 6:U:120:GLU:HG2   | 2.14                     | 0.47              |
| 7:b:153:GLU:N     | 7:b:164:ARG:HH12  | 2.09                     | 0.47              |
| 7:d:15:ARG:HG2    | 7:d:45:MET:HE1    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:e:99:MET:HE1    | 7:e:201:TRP:CD1   | 2.48                     | 0.47              |
| 7:f:64:PRO:HD2    | 7:f:67:HIS:CE1    | 2.49                     | 0.47              |
| 7:g:134:ILE:HD13  | 7:g:140:LEU:HD23  | 1.95                     | 0.47              |
| 7:i:151:MET:HE3   | 7:i:152:LYS:HB2   | 1.96                     | 0.47              |
| 2:A0:34:GLY:HA3   | 2:A0:60:LYS:HZ3   | 1.80                     | 0.47              |
| 3:A1:198:GLU:HG2  | 3:A1:266:PHE:HE2  | 1.80                     | 0.47              |
| 3:A3:2:ARG:HG2    | 3:A3:131:GLN:HE22 | 1.79                     | 0.47              |
| 3:A5:32:PRO:HD3   | 3:A5:81:PHE:CE1   | 2.50                     | 0.47              |
| 3:B3:244:GLY:HA2  | 3:B3:355:ASP:HB2  | 1.97                     | 0.47              |
| 3:B5:97:ALA:HA    | 3:B5:103:LYS:HE2  | 1.95                     | 0.47              |
| 2:C0:183:GLU:HG2  | 2:C0:184:PRO:HD3  | 1.96                     | 0.47              |
| 4:W:1222:TRP:HZ2  | 4:W:1316:GLN:HG3  | 1.79                     | 0.47              |
| 8:l:40:LYS:HE3    | 8:l:43:HIS:HB2    | 1.97                     | 0.47              |
| 8:l:73:TYR:HB2    | 8:l:92:TRP:NE1    | 2.30                     | 0.47              |
| 7:p:10:LEU:O      | 7:p:14:LYS:HB2    | 2.14                     | 0.47              |
| 7:w:184:PRO:HB2   | 7:w:189:LEU:HB2   | 1.96                     | 0.47              |
| 2:A0:282:TYR:CE1  | 7:a:202:ARG:HD2   | 2.49                     | 0.47              |
| 2:A2:7:ILE:HG23   | 2:A2:137:MET:HG3  | 1.96                     | 0.47              |
| 3:A3:7:VAL:HB     | 3:A3:135:ILE:HG13 | 1.96                     | 0.47              |
| 3:A3:183:TYR:HB3  | 3:A3:398:TYR:HE2  | 1.80                     | 0.47              |
| 3:A3:313:ALA:HB3  | 3:A3:349:MET:HB3  | 1.97                     | 0.47              |
| 3:A5:32:PRO:HA    | 3:A5:84:LEU:HD13  | 1.96                     | 0.47              |
| 2:A8:402:ARG:HG3  | 2:A8:405:VAL:HG21 | 1.95                     | 0.47              |
| 2:B0:2:ARG:HG2    | 2:B0:51:THR:HG22  | 1.97                     | 0.47              |
| 2:B0:76:ASP:HA    | 2:B0:79:ARG:HG2   | 1.96                     | 0.47              |
| 3:B3:20:PHE:HA    | 3:B3:230:SER:OG   | 2.15                     | 0.47              |
| 2:B4:73:THR:HB    | 3:B5:2:ARG:HH22   | 1.78                     | 0.47              |
| 3:B5:113:ILE:HA   | 3:B5:116:VAL:HG12 | 1.96                     | 0.47              |
| 2:B6:265:ILE:HG13 | 2:B6:432:TYR:CZ   | 2.50                     | 0.47              |
| 3:C3:205:GLU:HA   | 3:C3:208:TYR:HB2  | 1.97                     | 0.47              |
| 2:C6:247:ALA:HB3  | 2:C6:355:ILE:HB   | 1.96                     | 0.47              |
| 2:C8:210:TYR:CE2  | 3:C9:324:LYS:HD2  | 2.50                     | 0.47              |
| 2:D0:217:LEU:HG   | 2:D0:275:ILE:HG22 | 1.96                     | 0.47              |
| 2:D0:287:SER:HA   | 2:D0:373:ARG:HH11 | 1.80                     | 0.47              |
| 3:D3:163:ILE:HD11 | 3:D3:251:ARG:HG3  | 1.95                     | 0.47              |
| 3:D5:60:VAL:HG21  | 3:D5:86:ARG:HG3   | 1.97                     | 0.47              |
| 2:D6:151:CYS:SG   | 2:D6:193:SER:HB3  | 2.54                     | 0.47              |
| 3:D7:20:PHE:HA    | 3:D7:230:SER:HB2  | 1.97                     | 0.47              |
| 2:D8:274:PRO:HG3  | 2:D8:374:ALA:HA   | 1.95                     | 0.47              |
| 2:E0:66:VAL:HG11  | 2:E0:122:ILE:HD11 | 1.97                     | 0.47              |
| 3:E7:276:ARG:NH1  | 3:E7:276:ARG:HA   | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E8:409:VAL:HA   | 2:E8:413:MET:HB2  | 1.97                     | 0.47              |
| 3:E9:206:ALA:O    | 3:E9:210:ILE:HG12 | 2.15                     | 0.47              |
| 2:F0:262:TYR:HB2  | 2:F0:265:ILE:HG12 | 1.97                     | 0.47              |
| 6:T:117:THR:O     | 6:T:121:TYR:HB2   | 2.14                     | 0.47              |
| 7:d:97:ARG:HD3    | 7:f:161:TYR:CE1   | 2.50                     | 0.47              |
| 7:g:8:SER:HB2     | 7:g:147:HIS:HA    | 1.97                     | 0.47              |
| 7:h:37:GLN:HE22   | 7:h:41:ASN:H      | 1.63                     | 0.47              |
| 7:h:141:THR:O     | 7:h:145:LYS:HG3   | 2.14                     | 0.47              |
| 8:k:15:ARG:HB3    | 8:k:22:VAL:HG13   | 1.96                     | 0.47              |
| 8:k:65:GLU:HB2    | 7:m:42:TYR:H      | 1.79                     | 0.47              |
| 7:m:184:PRO:HD2   | 7:m:195:ALA:HB1   | 1.96                     | 0.47              |
| 7:n:51:PRO:HG2    | 7:n:54:SER:HB3    | 1.96                     | 0.47              |
| 7:o:9:PRO:HA      | 7:o:12:VAL:HG22   | 1.96                     | 0.47              |
| 7:o:99:MET:HE1    | 7:o:201:TRP:CE2   | 2.50                     | 0.47              |
| 7:r:75:LEU:O      | 7:r:170:VAL:HA    | 2.13                     | 0.47              |
| 3:A1:279:GLN:HB3  | 5:O:231:PRO:HG3   | 1.96                     | 0.47              |
| 3:A7:198:GLU:HA   | 3:A7:264:HIS:HB2  | 1.96                     | 0.47              |
| 3:B7:164:MET:HB3  | 3:B7:197:ASP:H    | 1.80                     | 0.47              |
| 3:B9:12:CYS:HB3   | 3:B9:138:SER:HB2  | 1.96                     | 0.47              |
| 2:C4:325:PRO:HG3  | 5:O:458:ARG:HE    | 1.79                     | 0.47              |
| 2:C8:177:VAL:HG11 | 2:C8:210:TYR:HE1  | 1.80                     | 0.47              |
| 3:D7:32:PRO:HA    | 3:D7:84:LEU:HD11  | 1.97                     | 0.47              |
| 3:D9:117:LEU:HA   | 3:D9:120:VAL:HG12 | 1.96                     | 0.47              |
| 2:E8:394:LYS:HZ3  | 2:E8:397:LEU:HB3  | 1.78                     | 0.47              |
| 3:E9:65:LEU:HD22  | 3:E9:90:PHE:HE1   | 1.79                     | 0.47              |
| 3:F1:217:LEU:HD23 | 6:R:174:ARG:HH12  | 1.80                     | 0.47              |
| 7:h:115:LEU:HD21  | 7:h:145:LYS:HD3   | 1.97                     | 0.47              |
| 2:A4:214:ARG:NH1  | 2:A4:215:ARG:HG3  | 2.29                     | 0.47              |
| 3:A7:213:ARG:HD2  | 3:A7:297:LYS:HD2  | 1.96                     | 0.47              |
| 3:A9:259:PRO:HG2  | 3:A9:311:LEU:HD21 | 1.97                     | 0.47              |
| 2:B0:140:ALA:HA   | 2:B0:171:SER:HB3  | 1.96                     | 0.47              |
| 3:B1:280:GLN:HE22 | 3:B5:58:ARG:HD2   | 1.80                     | 0.47              |
| 3:B1:318:ARG:HE   | 3:B1:358:PRO:HD3  | 1.80                     | 0.47              |
| 2:B4:67:PHE:HB2   | 2:B4:92:LEU:HA    | 1.97                     | 0.47              |
| 2:B8:184:PRO:HG3  | 2:B8:394:LYS:HE3  | 1.97                     | 0.47              |
| 3:B9:263:LEU:HB2  | 3:B9:422:TYR:HE1  | 1.79                     | 0.47              |
| 2:C0:17:GLY:HA2   | 2:C0:20:CYS:HB3   | 1.97                     | 0.47              |
| 2:C0:53:PHE:HB3   | 2:C0:61:HIS:HB3   | 1.96                     | 0.47              |
| 3:C1:321:MET:HE2  | 3:C1:321:MET:HB3  | 1.75                     | 0.47              |
| 3:C7:281:TYR:CD2  | 3:D1:87:PRO:HD3   | 2.43                     | 0.47              |
| 3:C9:198:GLU:HG2  | 3:C9:266:PHE:HE2  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D3:293:MET:HA   | 3:D3:298:ASN:HD22 | 1.80                     | 0.47              |
| 2:D4:318:MET:HB2  | 2:D4:376:CYS:HB3  | 1.96                     | 0.47              |
| 2:D8:135:PHE:CE2  | 2:D8:164:LYS:HE2  | 2.49                     | 0.47              |
| 2:D8:429:GLU:HA   | 2:D8:432:TYR:HD2  | 1.80                     | 0.47              |
| 2:E8:16:ILE:HD11  | 2:E8:231:ILE:HG21 | 1.97                     | 0.47              |
| 3:F1:68:LEU:HD12  | 3:F1:143:THR:HG22 | 1.97                     | 0.47              |
| 7:a:140:LEU:HA    | 7:a:143:ILE:HG22  | 1.96                     | 0.47              |
| 7:e:63:ILE:HG23   | 7:e:67:HIS:ND1    | 2.29                     | 0.47              |
| 7:f:75:LEU:HD23   | 7:f:111:ILE:HB    | 1.96                     | 0.47              |
| 7:m:115:LEU:HD12  | 7:m:167:VAL:HB    | 1.97                     | 0.47              |
| 7:m:134:ILE:HG12  | 7:m:140:LEU:HD23  | 1.96                     | 0.47              |
| 7:u:112:PHE:HB3   | 7:u:133:SER:HB2   | 1.97                     | 0.47              |
| 7:v:55:LEU:HD23   | 7:v:132:LEU:HD13  | 1.96                     | 0.47              |
| 2:A0:395:PHE:CD1  | 2:A0:422:ARG:HD3  | 2.50                     | 0.47              |
| 3:B1:259:PRO:HG2  | 3:B1:311:LEU:HD21 | 1.97                     | 0.47              |
| 3:B5:318:ARG:HG2  | 3:B5:354:CYS:HB3  | 1.96                     | 0.47              |
| 2:B8:258:ASN:ND2  | 2:B8:352:LYS:HD2  | 2.30                     | 0.47              |
| 3:B9:131:GLN:HE22 | 3:B9:249:ASP:HB3  | 1.80                     | 0.47              |
| 3:B9:392:LYS:HG3  | 3:B9:395:LEU:HD12 | 1.96                     | 0.47              |
| 3:C5:10:GLY:HA2   | 3:C5:143:THR:HB   | 1.97                     | 0.47              |
| 2:D2:280:LYS:HE3  | 2:D6:90:GLU:OE1   | 2.15                     | 0.47              |
| 3:D9:213:ARG:HH12 | 3:D9:297:LYS:HE3  | 1.80                     | 0.47              |
| 2:E0:189:LEU:HD13 | 2:E0:413:MET:HE1  | 1.96                     | 0.47              |
| 2:E2:36:MET:HE2   | 2:E2:61:HIS:NE2   | 2.30                     | 0.47              |
| 2:E6:68:LEU:HD11  | 2:E6:118:SER:HB2  | 1.95                     | 0.47              |
| 2:E6:274:PRO:HG3  | 2:E6:374:ALA:HA   | 1.97                     | 0.47              |
| 3:E7:187:LEU:HD13 | 3:E7:403:MET:HE1  | 1.97                     | 0.47              |
| 3:E9:221:THR:HG22 | 2:F0:324:VAL:HG23 | 1.97                     | 0.47              |
| 7:d:64:PRO:HD2    | 7:d:67:HIS:CD2    | 2.51                     | 0.47              |
| 7:i:41:ASN:O      | 7:i:45:MET:HB2    | 2.15                     | 0.47              |
| 7:s:9:PRO:HG3     | 7:s:146:ARG:HH21  | 1.79                     | 0.47              |
| 7:t:8:SER:HB2     | 7:t:147:HIS:HA    | 1.97                     | 0.47              |
| 3:A1:252:LYS:HB3  | 3:A1:350:LYS:HZ1  | 1.80                     | 0.46              |
| 2:A2:272:TYR:HD2  | 2:A2:275:ILE:HG23 | 1.80                     | 0.46              |
| 3:A3:383:ASP:HA   | 3:A3:386:THR:HG22 | 1.97                     | 0.46              |
| 2:B2:310:GLY:HA3  | 2:B2:383:ALA:HB2  | 1.97                     | 0.46              |
| 3:B5:73:MET:HE1   | 3:B5:92:PHE:HA    | 1.97                     | 0.46              |
| 2:B6:387:VAL:HA   | 2:B6:390:ARG:NH1  | 2.31                     | 0.46              |
| 3:B7:179:VAL:HG12 | 2:B8:258:ASN:OD1  | 2.15                     | 0.46              |
| 3:B7:376:GLU:HA   | 3:B7:379:LYS:HG2  | 1.95                     | 0.46              |
| 2:B8:99:ALA:HA    | 2:B8:110:ILE:HD11 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B9:49:VAL:HG11  | 3:B9:241:ARG:HG2  | 1.97                     | 0.46              |
| 3:B9:349:MET:HE1  | 3:B9:367:PHE:HE1  | 1.80                     | 0.46              |
| 2:C0:298:PRO:HB3  | 2:C0:307:PRO:HD2  | 1.97                     | 0.46              |
| 2:C2:205:ASP:HB3  | 2:C2:303:ALA:HA   | 1.97                     | 0.46              |
| 3:C9:97:ALA:HA    | 3:C9:103:LYS:HE2  | 1.96                     | 0.46              |
| 3:E5:149:THR:HG21 | 3:E5:188:SER:HB2  | 1.96                     | 0.46              |
| 6:T:128:ARG:HG3   | 6:T:132:LYS:HE2   | 1.97                     | 0.46              |
| 7:f:115:LEU:HD21  | 7:f:145:LYS:HD3   | 1.97                     | 0.46              |
| 7:j:88:LEU:HD22   | 7:j:185:ILE:HG21  | 1.97                     | 0.46              |
| 7:m:136:LEU:HA    | 7:m:141:THR:HG21  | 1.96                     | 0.46              |
| 7:r:15:ARG:O      | 7:r:19:GLU:HB3    | 2.15                     | 0.46              |
| 3:A3:284:LEU:HD12 | 5:P:232:PHE:HZ    | 1.79                     | 0.46              |
| 3:A5:272:PRO:HG3  | 3:A5:364:SER:HA   | 1.97                     | 0.46              |
| 3:A9:42:LEU:HD22  | 3:A9:356:ILE:HD11 | 1.96                     | 0.46              |
| 2:C2:315:CYS:HB3  | 2:C2:377:MET:HE1  | 1.97                     | 0.46              |
| 3:C5:14:ASN:HB3   | 3:C5:76:VAL:HG21  | 1.97                     | 0.46              |
| 3:D3:377:MET:HG2  | 3:D3:380:ARG:HD3  | 1.97                     | 0.46              |
| 2:E0:11:GLN:HG3   | 2:E0:74:VAL:HG21  | 1.97                     | 0.46              |
| 3:E3:178:THR:HB   | 3:E3:181:GLU:HB3  | 1.96                     | 0.46              |
| 11:E5:501:GDP:C8  | 2:E6:248:LEU:HD21 | 2.50                     | 0.46              |
| 3:E7:28:HIS:HE2   | 3:E7:241:ARG:HH11 | 1.62                     | 0.46              |
| 2:E8:274:PRO:HG3  | 2:E8:374:ALA:HA   | 1.97                     | 0.46              |
| 3:E9:276:ARG:HA   | 3:E9:279:GLN:HG2  | 1.96                     | 0.46              |
| 2:F0:274:PRO:HB2  | 2:F0:276:ILE:HG12 | 1.97                     | 0.46              |
| 3:F1:198:GLU:HG3  | 3:F1:200:GLN:HE22 | 1.80                     | 0.46              |
| 4:Q:1438:LEU:HA   | 4:Q:1441:LEU:HD12 | 1.97                     | 0.46              |
| 6:R:132:LYS:HA    | 6:R:136:GLN:HB2   | 1.97                     | 0.46              |
| 4:V:1230:LYS:HG3  | 4:V:1277:THR:HG21 | 1.97                     | 0.46              |
| 7:c:9:PRO:HB2     | 7:c:143:ILE:HG13  | 1.97                     | 0.46              |
| 7:g:69:LYS:HA     | 7:g:206:PHE:HB3   | 1.96                     | 0.46              |
| 7:g:117:ARG:HH12  | 7:g:152:LYS:HE2   | 1.80                     | 0.46              |
| 7:m:23:LEU:HD23   | 7:m:23:LEU:HA     | 1.76                     | 0.46              |
| 2:A2:373:ARG:CZ   | 5:P:255:LYS:HD2   | 2.46                     | 0.46              |
| 2:A4:60:LYS:HD2   | 2:A4:60:LYS:HA    | 1.76                     | 0.46              |
| 2:C0:209:ILE:HD13 | 2:C0:231:ILE:HD11 | 1.97                     | 0.46              |
| 2:C4:200:VAL:HA   | 2:C4:266:HIS:HB2  | 1.96                     | 0.46              |
| 2:C4:209:ILE:HA   | 2:C4:212:ILE:HG12 | 1.96                     | 0.46              |
| 2:C4:272:TYR:HB3  | 2:C4:275:ILE:HD11 | 1.96                     | 0.46              |
| 3:D1:51:TYR:HE1   | 3:D1:61:PRO:HG3   | 1.81                     | 0.46              |
| 2:D8:53:PHE:HB3   | 2:D8:61:HIS:HB3   | 1.97                     | 0.46              |
| 2:D8:229:ARG:HH12 | 2:D8:366:GLY:HA2  | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E1:200:GLN:HG2  | 3:E1:268:ILE:HD11 | 1.98                     | 0.46              |
| 3:E1:385:PHE:HZ   | 3:E1:408:PHE:HB3  | 1.81                     | 0.46              |
| 7:v:75:LEU:HD23   | 7:v:111:ILE:HB    | 1.97                     | 0.46              |
| 2:A0:322:ASP:HB3  | 2:A0:373:ARG:NH2  | 2.30                     | 0.46              |
| 3:A5:57:GLY:HA3   | 7:a:83:PRO:HB2    | 1.97                     | 0.46              |
| 2:A8:88:HIS:HB3   | 2:A8:91:GLN:HG3   | 1.97                     | 0.46              |
| 2:B2:105:ARG:HG3  | 2:B2:110:ILE:HD13 | 1.96                     | 0.46              |
| 3:B3:156:ARG:HA   | 3:B3:156:ARG:HD2  | 1.63                     | 0.46              |
| 3:B3:190:HIS:CE1  | 3:B3:414:ASN:HD22 | 2.32                     | 0.46              |
| 3:C5:143:THR:HG23 | 3:C5:147:MET:HE2  | 1.97                     | 0.46              |
| 2:C8:154:LEU:HD23 | 2:C8:154:LEU:HA   | 1.80                     | 0.46              |
| 1:D:218:ASP:HB2   | 2:D8:363:VAL:HB   | 1.96                     | 0.46              |
| 1:D:239:LEU:HD21  | 3:D7:357:PRO:HG2  | 1.98                     | 0.46              |
| 3:D1:269:GLY:HA2  | 3:D1:300:MET:HE2  | 1.96                     | 0.46              |
| 2:D8:401:LYS:HB2  | 3:D9:344:TRP:CH2  | 2.51                     | 0.46              |
| 2:E0:328:VAL:HG21 | 2:E0:355:ILE:HD11 | 1.97                     | 0.46              |
| 3:E7:41:ASP:CG    | 7:v:94:ASN:HD22   | 2.23                     | 0.46              |
| 7:g:3:GLN:HE22    | 7:g:179:GLU:H     | 1.62                     | 0.46              |
| 8:k:15:ARG:HB2    | 8:k:24:VAL:HB     | 1.97                     | 0.46              |
| 7:q:111:ILE:HD13  | 7:q:132:LEU:HB2   | 1.97                     | 0.46              |
| 7:s:191:GLU:HG2   | 7:s:195:ALA:HB2   | 1.96                     | 0.46              |
| 2:A2:33:ASP:HB3   | 6:R:90:TRP:CZ3    | 2.51                     | 0.46              |
| 2:A2:307:PRO:HB2  | 2:A2:312:TYR:HE1  | 1.81                     | 0.46              |
| 3:A3:113:ILE:HA   | 3:A3:116:VAL:HG22 | 1.97                     | 0.46              |
| 2:A4:180:ALA:HB3  | 2:A4:183:GLU:HG3  | 1.98                     | 0.46              |
| 2:A4:318:MET:HB2  | 2:A4:376:CYS:HB3  | 1.96                     | 0.46              |
| 3:A5:19:LYS:HA    | 3:A5:22:GLU:HB2   | 1.97                     | 0.46              |
| 2:A8:208:ALA:HA   | 2:A8:304:LYS:HE2  | 1.97                     | 0.46              |
| 3:A9:97:ALA:HA    | 3:A9:103:LYS:HD2  | 1.97                     | 0.46              |
| 2:B0:70:LEU:HD12  | 2:B0:145:THR:HG22 | 1.96                     | 0.46              |
| 2:B0:397:LEU:HD11 | 3:B1:346:PRO:HD3  | 1.98                     | 0.46              |
| 3:B7:68:LEU:HA    | 3:B7:93:GLY:HA3   | 1.97                     | 0.46              |
| 3:C3:344:TRP:CD1  | 3:C3:344:TRP:H    | 2.33                     | 0.46              |
| 3:C5:113:ILE:HA   | 3:C5:116:VAL:HG12 | 1.97                     | 0.46              |
| 3:D7:276:ARG:HD2  | 5:P:551:GLU:HA    | 1.98                     | 0.46              |
| 3:E1:35:THR:HG22  | 7:s:83:PRO:HG3    | 1.97                     | 0.46              |
| 2:E4:407:TRP:CH2  | 3:E5:258:ILE:HB   | 2.50                     | 0.46              |
| 3:E7:273:LEU:HD23 | 3:E7:273:LEU:HA   | 1.79                     | 0.46              |
| 2:E8:135:PHE:HB2  | 2:E8:166:LYS:HG2  | 1.97                     | 0.46              |
| 6:R:110:ALA:HA    | 6:R:113:TRP:HD1   | 1.81                     | 0.46              |
| 6:T:58:LEU:HA     | 6:T:61:TRP:HD1    | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:V:1241:PHE:CD2  | 4:V:1242:PRO:HD3  | 2.51                     | 0.46              |
| 4:V:1285:ARG:NE   | 4:V:1289:ARG:HH12 | 2.11                     | 0.46              |
| 7:e:152:LYS:HD2   | 7:e:167:VAL:HG21  | 1.97                     | 0.46              |
| 7:g:18:ASN:HA     | 7:g:21:ARG:HG2    | 1.97                     | 0.46              |
| 7:g:96:TYR:HA     | 7:g:108:ILE:HD11  | 1.98                     | 0.46              |
| 7:g:173:ILE:HD11  | 7:g:177:GLY:HA2   | 1.96                     | 0.46              |
| 7:i:146:ARG:HD2   | 7:i:156:VAL:HG21  | 1.96                     | 0.46              |
| 7:o:96:TYR:HA     | 7:o:108:ILE:HD11  | 1.98                     | 0.46              |
| 2:A0:373:ARG:CZ   | 5:O:255:LYS:HZ2   | 2.28                     | 0.46              |
| 2:A2:271:SER:HB3  | 2:A2:301:MET:HE2  | 1.97                     | 0.46              |
| 3:A3:216:LYS:HB3  | 3:A3:275:SER:HB3  | 1.97                     | 0.46              |
| 3:A5:273:LEU:HB2  | 3:A5:292:GLN:HE22 | 1.79                     | 0.46              |
| 2:B2:269:LEU:HD22 | 2:B2:303:ALA:HB3  | 1.98                     | 0.46              |
| 3:B3:101:TRP:HE1  | 3:B3:188:SER:HB3  | 1.81                     | 0.46              |
| 2:B4:310:GLY:HA3  | 2:B4:383:ALA:HB2  | 1.98                     | 0.46              |
| 3:B5:257:LEU:HD21 | 3:B5:314:SER:HB2  | 1.97                     | 0.46              |
| 2:B6:76:ASP:HA    | 2:B6:79:ARG:HD2   | 1.98                     | 0.46              |
| 3:B7:217:LEU:HD21 | 5:P:370:LEU:HD11  | 1.97                     | 0.46              |
| 2:B8:79:ARG:HE    | 2:B8:92:LEU:HB3   | 1.81                     | 0.46              |
| 1:C:229:LYS:HE2   | 1:C:229:LYS:HB2   | 1.78                     | 0.46              |
| 3:C3:19:LYS:HZ3   | 3:C3:226:ASN:C    | 2.24                     | 0.46              |
| 3:D1:3:GLU:HA     | 3:D1:49:VAL:HA    | 1.98                     | 0.46              |
| 3:D1:272:PRO:HG3  | 3:D1:364:SER:HA   | 1.97                     | 0.46              |
| 2:D2:27:GLU:HB2   | 2:D2:361:THR:HG21 | 1.98                     | 0.46              |
| 2:D4:242:LEU:HD21 | 2:D4:251:ASP:HB2  | 1.97                     | 0.46              |
| 3:D5:296:ALA:HB2  | 3:D5:306:ARG:HH12 | 1.79                     | 0.46              |
| 2:D8:16:ILE:HD11  | 2:D8:138:PHE:HB3  | 1.98                     | 0.46              |
| 4:V:1214:LEU:HD21 | 4:V:1448:ALA:HA   | 1.97                     | 0.46              |
| 7:e:119:ARG:HH22  | 7:e:137:GLU:HG2   | 1.80                     | 0.46              |
| 7:h:51:PRO:HD2    | 7:h:54:SER:HB2    | 1.97                     | 0.46              |
| 3:A9:175:VAL:HG22 | 2:B0:333:ALA:HB2  | 1.97                     | 0.46              |
| 2:B0:238:LEU:HD23 | 2:B0:318:MET:HG3  | 1.96                     | 0.46              |
| 3:B3:182:PRO:HD2  | 3:B3:388:MET:HE1  | 1.98                     | 0.46              |
| 2:B4:154:LEU:HB3  | 2:B4:197:HIS:HB3  | 1.97                     | 0.46              |
| 2:B6:259:LEU:HD12 | 2:B6:268:MET:HE1  | 1.96                     | 0.46              |
| 2:C6:105:ARG:HA   | 2:C6:109:THR:OG1  | 2.15                     | 0.46              |
| 2:C6:154:LEU:HD11 | 2:C6:166:LYS:HD2  | 1.98                     | 0.46              |
| 3:C7:390:ARG:NH1  | 3:C7:391:ARG:HB3  | 2.30                     | 0.46              |
| 3:D1:2:ARG:HE     | 3:D1:2:ARG:HB2    | 1.62                     | 0.46              |
| 3:D1:403:MET:HB3  | 3:D1:407:GLU:OE2  | 2.15                     | 0.46              |
| 3:D3:57:GLY:HA3   | 7:o:83:PRO:HB2    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D5:316:MET:HG3  | 3:D5:352:SER:HB2  | 1.98                     | 0.46              |
| 2:D6:276:ILE:HD11 | 2:D6:280:LYS:HD2  | 1.97                     | 0.46              |
| 2:E0:105:ARG:HH22 | 3:E1:251:ARG:HD2  | 1.80                     | 0.46              |
| 2:E4:282:TYR:CZ   | 7:w:202:ARG:HD2   | 2.51                     | 0.46              |
| 3:E5:122:LYS:HB2  | 3:E5:122:LYS:HE2  | 1.72                     | 0.46              |
| 2:E8:184:PRO:HB3  | 2:E8:391:MET:HE1  | 1.97                     | 0.46              |
| 3:E9:49:VAL:HG11  | 3:E9:241:ARG:HG2  | 1.98                     | 0.46              |
| 4:Q:1395:GLU:HG2  | 4:Q:1435:ARG:HH21 | 1.81                     | 0.46              |
| 7:e:75:LEU:O      | 7:e:170:VAL:HA    | 2.16                     | 0.46              |
| 8:l:84:GLU:HA     | 8:l:87:ARG:HG3    | 1.98                     | 0.46              |
| 7:r:63:ILE:HD11   | 7:r:132:LEU:HD11  | 1.98                     | 0.46              |
| 7:x:170:VAL:HG23  | 7:x:183:LEU:HB2   | 1.97                     | 0.46              |
| 2:A0:109:THR:HG22 | 2:A0:110:ILE:H    | 1.81                     | 0.46              |
| 2:A2:242:LEU:HD11 | 2:A2:252:VAL:HG23 | 1.98                     | 0.46              |
| 3:A7:39:ASP:HA    | 7:b:90:PRO:HG3    | 1.97                     | 0.46              |
| 3:A7:66:MET:HE3   | 3:A7:66:MET:HB2   | 1.86                     | 0.46              |
| 3:B5:236:VAL:HA   | 3:B5:316:MET:HG3  | 1.96                     | 0.46              |
| 3:C5:311:LEU:HD23 | 3:C5:342:VAL:HG11 | 1.96                     | 0.46              |
| 3:C9:275:SER:HB3  | 3:C9:278:SER:HB2  | 1.97                     | 0.46              |
| 3:D3:253:LEU:HD13 | 3:D3:316:MET:HE3  | 1.96                     | 0.46              |
| 3:D3:392:LYS:HA   | 3:D3:392:LYS:HD3  | 1.73                     | 0.46              |
| 3:E5:246:LEU:HD23 | 3:E5:352:SER:HA   | 1.97                     | 0.46              |
| 3:E9:330:MET:HA   | 3:E9:333:VAL:HG22 | 1.97                     | 0.46              |
| 2:F0:318:MET:HB2  | 2:F0:376:CYS:SG   | 2.56                     | 0.46              |
| 3:F1:173:PRO:HG3  | 3:F1:380:ARG:HD3  | 1.98                     | 0.46              |
| 3:F1:284:LEU:HB3  | 3:F1:362:LYS:HE2  | 1.97                     | 0.46              |
| 4:Q:1285:ARG:HH12 | 4:Q:1294:VAL:HA   | 1.81                     | 0.46              |
| 4:W:1254:ARG:O    | 4:W:1258:GLN:HG2  | 2.15                     | 0.46              |
| 8:l:16:THR:HA     | 8:l:21:TYR:CE2    | 2.51                     | 0.46              |
| 7:t:95:TYR:O      | 7:t:99:MET:HB3    | 2.15                     | 0.46              |
| 7:u:42:TYR:HA     | 7:u:45:MET:HE2    | 1.98                     | 0.46              |
| 3:A3:361:LEU:HD11 | 5:P:228:LEU:HD23  | 1.97                     | 0.46              |
| 3:A5:51:TYR:HB3   | 3:A5:59:PHE:HB3   | 1.97                     | 0.46              |
| 3:A5:395:LEU:HD21 | 3:A5:408:PHE:CE2  | 2.43                     | 0.46              |
| 2:B0:407:TRP:CG   | 3:B1:255:VAL:HG23 | 2.51                     | 0.46              |
| 3:B3:103:LYS:HA   | 3:B3:107:THR:HG22 | 1.97                     | 0.46              |
| 3:C1:5:VAL:HB     | 3:C1:133:PHE:HD1  | 1.80                     | 0.46              |
| 2:C4:70:LEU:HB2   | 2:C4:145:THR:HG21 | 1.98                     | 0.46              |
| 2:C8:280:LYS:HZ2  | 2:D2:89:PRO:HD2   | 1.81                     | 0.46              |
| 1:D:214:ALA:HB2   | 2:D8:225:THR:HG23 | 1.98                     | 0.46              |
| 2:D2:141:VAL:HG12 | 2:D2:187:SER:HA   | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D3:303:SER:HB3  | 3:D3:377:MET:HE3  | 1.98                     | 0.46              |
| 2:D4:363:VAL:HG23 | 2:D4:366:GLY:HA3  | 1.98                     | 0.46              |
| 3:D7:107:THR:HG21 | 3:D7:401:GLU:HB2  | 1.97                     | 0.46              |
| 2:D8:2:ARG:CZ     | 5:P:532:ARG:HH21  | 2.29                     | 0.46              |
| 2:E0:258:ASN:HD22 | 2:E0:352:LYS:HD3  | 1.81                     | 0.46              |
| 3:E1:164:MET:HB3  | 3:E1:197:ASP:H    | 1.81                     | 0.46              |
| 3:E5:228:LEU:HD11 | 3:E5:273:LEU:HD21 | 1.98                     | 0.46              |
| 2:E6:401:LYS:HZ1  | 3:E7:344:TRP:CG   | 2.33                     | 0.46              |
| 2:F0:156:ARG:HA   | 2:F0:159:VAL:HG12 | 1.97                     | 0.46              |
| 7:w:9:PRO:O       | 7:w:13:GLU:HG2    | 2.16                     | 0.46              |
| 3:A1:200:GLN:HB3  | 3:A1:268:ILE:HG13 | 1.98                     | 0.46              |
| 3:A1:388:MET:HB3  | 3:A1:393:ALA:HB3  | 1.96                     | 0.46              |
| 2:A2:201:ALA:HB3  | 2:A2:267:PHE:HA   | 1.98                     | 0.46              |
| 2:A2:210:TYR:CE1  | 3:A3:324:LYS:HD2  | 2.51                     | 0.46              |
| 2:A2:407:TRP:CH2  | 3:A3:258:ILE:HG23 | 2.50                     | 0.46              |
| 3:A7:25:SER:HB2   | 3:A7:30:ILE:HB    | 1.98                     | 0.46              |
| 2:A8:180:ALA:HB3  | 2:A8:183:GLU:HG3  | 1.98                     | 0.46              |
| 2:B0:320:ARG:HD3  | 2:B0:360:PRO:HG3  | 1.98                     | 0.46              |
| 3:B5:272:PRO:HD3  | 3:B5:364:SER:HA   | 1.98                     | 0.46              |
| 2:B6:286:LEU:HD11 | 2:B6:372:MET:H    | 1.80                     | 0.46              |
| 3:B7:211:CYS:HA   | 3:B7:215:LEU:HB2  | 1.98                     | 0.46              |
| 2:C0:247:ALA:HB3  | 2:C0:355:ILE:HB   | 1.97                     | 0.46              |
| 3:C1:183:TYR:O    | 3:C1:187:LEU:HG   | 2.16                     | 0.46              |
| 3:C3:149:THR:HA   | 3:C3:152:ILE:HG12 | 1.97                     | 0.46              |
| 2:C8:198:THR:HG21 | 2:C8:201:ALA:HB2  | 1.98                     | 0.46              |
| 2:C8:207:GLU:HA   | 2:C8:210:TYR:CD1  | 2.51                     | 0.46              |
| 3:D3:30:ILE:HG23  | 3:D3:34:GLY:HA2   | 1.98                     | 0.46              |
| 3:D3:171:PRO:HG2  | 3:D3:185:ALA:HB2  | 1.97                     | 0.46              |
| 3:D3:272:PRO:HG2  | 3:D3:361:LEU:HD13 | 1.98                     | 0.46              |
| 2:D4:218:ASP:HB3  | 7:r:194:ARG:NH2   | 2.30                     | 0.46              |
| 2:D6:31:GLN:HG3   | 2:D6:37:PRO:HD3   | 1.98                     | 0.46              |
| 2:E6:123:ARG:HH12 | 2:E6:127:ASP:HB3  | 1.81                     | 0.46              |
| 3:F1:259:PRO:HG3  | 3:F1:311:LEU:HD22 | 1.97                     | 0.46              |
| 4:Q:1395:GLU:HA   | 4:Q:1398:LEU:HG   | 1.98                     | 0.46              |
| 6:R:127:ARG:HH11  | 6:R:128:ARG:NH1   | 2.13                     | 0.46              |
| 7:f:115:LEU:HA    | 7:f:115:LEU:HD23  | 1.78                     | 0.46              |
| 7:v:5:VAL:HG21    | 7:v:161:TYR:CE1   | 2.49                     | 0.46              |
| 7:x:78:ALA:HB3    | 7:x:112:PHE:HE1   | 1.81                     | 0.46              |
| 2:A0:175:PRO:HB3  | 2:A0:390:ARG:HD2  | 1.98                     | 0.45              |
| 2:A2:100:ALA:HA   | 3:A3:252:LYS:HD3  | 1.97                     | 0.45              |
| 2:A2:209:ILE:HD12 | 2:A2:227:LEU:HB3  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A5:131:GLN:HE22 | 3:A5:250:LEU:HB2  | 1.81                     | 0.45              |
| 3:B5:105:HIS:CD2  | 3:B5:150:LEU:HD12 | 2.51                     | 0.45              |
| 3:B9:8:GLN:HE22   | 3:B9:63:ALA:HB1   | 1.81                     | 0.45              |
| 3:C3:19:LYS:HE3   | 3:C3:19:LYS:HB3   | 1.71                     | 0.45              |
| 2:C8:209:ILE:HG23 | 2:C8:230:LEU:HD22 | 1.97                     | 0.45              |
| 3:D1:16:ILE:HD11  | 3:D1:229:VAL:HG21 | 1.97                     | 0.45              |
| 3:D1:253:LEU:HD11 | 3:D1:316:MET:SD   | 2.56                     | 0.45              |
| 3:D3:149:THR:HG21 | 3:D3:188:SER:HB2  | 1.99                     | 0.45              |
| 3:D3:177:ASP:HB2  | 2:D4:353:CYS:H    | 1.82                     | 0.45              |
| 2:D4:360:PRO:HG3  | 2:D4:374:ALA:HB2  | 1.97                     | 0.45              |
| 3:D5:70:PRO:HA    | 3:D5:73:MET:HE2   | 1.97                     | 0.45              |
| 2:D6:10:GLY:HA2   | 2:D6:145:THR:HG23 | 1.98                     | 0.45              |
| 2:D8:320:ARG:HH21 | 2:D8:360:PRO:HA   | 1.81                     | 0.45              |
| 3:E1:201:VAL:HG21 | 3:E1:374:ILE:HD11 | 1.98                     | 0.45              |
| 2:E2:230:LEU:HD23 | 2:E2:275:ILE:HD13 | 1.98                     | 0.45              |
| 3:E5:282:ARG:HD3  | 3:E5:283:ALA:H    | 1.81                     | 0.45              |
| 3:E9:34:GLY:HA3   | 3:E9:58:ARG:HG2   | 1.98                     | 0.45              |
| 2:F0:362:VAL:HG11 | 2:F0:370:LYS:HG2  | 1.98                     | 0.45              |
| 7:e:136:LEU:HA    | 7:e:141:THR:HG21  | 1.97                     | 0.45              |
| 2:A6:194:LEU:HG   | 2:A6:267:PHE:HE2  | 1.80                     | 0.45              |
| 3:A9:171:PRO:HB3  | 3:A9:181:GLU:HB3  | 1.97                     | 0.45              |
| 2:B0:210:TYR:CD2  | 3:B1:324:LYS:HD3  | 2.51                     | 0.45              |
| 2:B2:318:MET:HB2  | 2:B2:376:CYS:HB3  | 1.97                     | 0.45              |
| 2:B4:26:LEU:HD11  | 2:B4:364:PRO:HD2  | 1.98                     | 0.45              |
| 3:B5:192:LEU:HD21 | 3:B5:199:VAL:HG21 | 1.99                     | 0.45              |
| 3:B7:230:SER:HA   | 3:B7:233:MET:HB3  | 1.98                     | 0.45              |
| 2:C2:104:ALA:HA   | 2:C2:108:TYR:HD2  | 1.81                     | 0.45              |
| 3:C3:7:VAL:HG22   | 3:C3:64:ILE:HD13  | 1.98                     | 0.45              |
| 2:C6:101:ASN:HB3  | 2:C6:182:VAL:HG21 | 1.98                     | 0.45              |
| 2:D0:222:PRO:HD2  | 3:D1:324:LYS:HZ2  | 1.82                     | 0.45              |
| 3:D7:239:CYS:HB3  | 3:D7:248:SER:H    | 1.82                     | 0.45              |
| 3:D9:282:ARG:HH12 | 3:D9:284:LEU:HD22 | 1.80                     | 0.45              |
| 3:E7:312:THR:HA   | 3:E7:348:ASN:HB3  | 1.97                     | 0.45              |
| 3:F1:108:GLU:O    | 3:F1:111:GLU:HG3  | 2.15                     | 0.45              |
| 3:F1:353:VAL:HG12 | 3:F1:355:ASP:H    | 1.81                     | 0.45              |
| 7:m:9:PRO:HB2     | 7:m:143:ILE:HG23  | 1.98                     | 0.45              |
| 7:r:84:LYS:NZ     | 7:r:168:PRO:HD2   | 2.32                     | 0.45              |
| 7:w:141:THR:O     | 7:w:145:LYS:HG2   | 2.16                     | 0.45              |
| 2:A6:283:HIS:CE1  | 2:B0:85:HIS:O     | 2.69                     | 0.45              |
| 3:A9:391:ARG:HD3  | 2:B0:346:TRP:CD1  | 2.51                     | 0.45              |
| 2:B0:362:VAL:HG21 | 2:B0:370:LYS:HA   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C9:220:PRO:HD2  | 2:D0:326:LYS:HZ3  | 1.82                     | 0.45              |
| 2:D0:215:ARG:HH22 | 2:D0:300:SER:HB2  | 1.82                     | 0.45              |
| 2:D2:36:MET:HG3   | 2:D2:61:HIS:CE1   | 2.52                     | 0.45              |
| 2:D4:7:ILE:HG21   | 2:D4:153:LEU:HD21 | 1.98                     | 0.45              |
| 3:D9:242:PHE:HB3  | 3:D9:356:ILE:HD13 | 1.97                     | 0.45              |
| 3:E1:44:LEU:HA    | 3:E1:47:ILE:HG13  | 1.99                     | 0.45              |
| 2:E4:144:GLY:H    | 9:E4:501:GTP:PG   | 2.40                     | 0.45              |
| 3:E5:263:LEU:HB3  | 3:E5:370:ASN:HD21 | 1.82                     | 0.45              |
| 2:E6:80:THR:HA    | 2:E6:84:ARG:HD2   | 1.98                     | 0.45              |
| 3:E9:241:ARG:HH21 | 3:E9:242:PHE:HE1  | 1.64                     | 0.45              |
| 7:b:199:TRP:HE1   | 7:b:201:TRP:HB3   | 1.82                     | 0.45              |
| 7:c:142:GLU:HA    | 7:c:145:LYS:HB2   | 1.99                     | 0.45              |
| 7:h:4:PRO:HG3     | 7:h:179:GLU:HB2   | 1.99                     | 0.45              |
| 7:h:112:PHE:H     | 7:h:133:SER:HA    | 1.81                     | 0.45              |
| 3:A1:220:PRO:HB2  | 5:O:223:ARG:NH1   | 2.31                     | 0.45              |
| 3:A1:293:MET:HE1  | 3:A1:315:ALA:HA   | 1.99                     | 0.45              |
| 3:A1:294:PHE:HD2  | 3:A1:333:VAL:HG21 | 1.81                     | 0.45              |
| 2:B0:298:PRO:HA   | 2:B0:301:MET:HG2  | 1.96                     | 0.45              |
| 3:B1:49:VAL:HG23  | 3:B1:50:PHE:HD1   | 1.81                     | 0.45              |
| 1:C:245:SER:O     | 1:C:249:SER:HB3   | 2.17                     | 0.45              |
| 2:C8:141:VAL:HG12 | 2:C8:187:SER:HA   | 1.97                     | 0.45              |
| 3:D5:200:GLN:HB3  | 3:D5:268:ILE:HD11 | 1.98                     | 0.45              |
| 2:D6:406:HIS:HA   | 2:D6:409:VAL:HG12 | 1.98                     | 0.45              |
| 3:E1:192:LEU:HD21 | 3:E1:199:VAL:HG11 | 1.99                     | 0.45              |
| 2:E2:82:THR:HA    | 7:t:98:THR:HG23   | 1.98                     | 0.45              |
| 3:E5:12:CYS:HB2   | 3:E5:138:SER:HB2  | 1.99                     | 0.45              |
| 3:E7:296:ALA:HB2  | 3:E7:305:PRO:HD2  | 1.99                     | 0.45              |
| 3:E9:64:ILE:HA    | 3:E9:89:ASN:HB3   | 1.98                     | 0.45              |
| 2:F0:224:TYR:CE2  | 3:F1:323:THR:HG21 | 2.51                     | 0.45              |
| 7:f:41:ASN:O      | 7:f:45:MET:HG3    | 2.16                     | 0.45              |
| 7:h:12:VAL:HG12   | 7:h:15:ARG:NH2    | 2.24                     | 0.45              |
| 7:m:75:LEU:HA     | 7:m:111:ILE:O     | 2.17                     | 0.45              |
| 7:q:78:ALA:HB3    | 7:q:112:PHE:HE1   | 1.81                     | 0.45              |
| 7:r:194:ARG:HH12  | 7:r:198:ARG:HH21  | 1.65                     | 0.45              |
| 2:A0:182:VAL:HG11 | 3:A1:255:VAL:HG12 | 1.99                     | 0.45              |
| 2:A0:219:ILE:HG13 | 2:A0:222:PRO:HG3  | 1.98                     | 0.45              |
| 3:A5:233:MET:HE2  | 3:A5:233:MET:HB3  | 1.78                     | 0.45              |
| 3:B3:293:MET:HE1  | 3:B3:330:MET:HE1  | 1.98                     | 0.45              |
| 3:B3:420:SER:HA   | 3:B3:423:GLN:HG2  | 1.98                     | 0.45              |
| 3:B5:112:LEU:HD22 | 3:B5:147:MET:HE2  | 1.98                     | 0.45              |
| 3:B5:284:LEU:HD23 | 3:B5:362:LYS:HB3  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B7:276:ARG:NH1  | 3:B7:276:ARG:HA   | 2.32                     | 0.45              |
| 1:C:235:LEU:HD12  | 1:C:236:PRO:HD2   | 1.98                     | 0.45              |
| 2:C0:54:SER:HB2   | 2:C0:64:ARG:HD3   | 1.98                     | 0.45              |
| 2:C0:209:ILE:HA   | 2:C0:212:ILE:HG22 | 1.97                     | 0.45              |
| 3:C1:164:MET:H    | 3:C1:197:ASP:HB3  | 1.82                     | 0.45              |
| 2:C2:10:GLY:HA2   | 2:C2:145:THR:HG23 | 1.98                     | 0.45              |
| 2:C2:409:VAL:HA   | 2:C2:413:MET:HB3  | 1.99                     | 0.45              |
| 3:C3:259:PRO:HG2  | 3:C3:311:LEU:HD21 | 1.99                     | 0.45              |
| 3:C3:320:ARG:HD2  | 3:C3:320:ARG:HA   | 1.72                     | 0.45              |
| 2:C8:222:PRO:HG2  | 3:C9:324:LYS:HE3  | 1.99                     | 0.45              |
| 2:D0:115:VAL:HG21 | 2:D0:152:LEU:HD23 | 1.99                     | 0.45              |
| 2:D8:217:LEU:HD12 | 2:D8:277:SER:HB2  | 1.97                     | 0.45              |
| 3:E3:104:GLY:HA2  | 3:E3:109:GLY:HA3  | 1.99                     | 0.45              |
| 2:E8:323:VAL:HG23 | 2:E8:355:ILE:HG23 | 1.99                     | 0.45              |
| 3:E9:117:LEU:HA   | 3:E9:120:VAL:HG12 | 1.99                     | 0.45              |
| 4:M:1390:GLU:HG2  | 4:M:1393:ILE:HD11 | 1.98                     | 0.45              |
| 7:b:184:PRO:HB2   | 7:b:189:LEU:HB3   | 1.99                     | 0.45              |
| 7:d:4:PRO:HG3     | 7:d:179:GLU:HB2   | 1.99                     | 0.45              |
| 7:g:184:PRO:HB2   | 7:g:189:LEU:HB2   | 1.97                     | 0.45              |
| 8:l:79:ASP:HB3    | 8:l:82:ASP:HB2    | 1.98                     | 0.45              |
| 7:n:105:ASN:HD21  | 7:p:37:GLN:HE22   | 1.63                     | 0.45              |
| 7:p:10:LEU:HD12   | 7:p:147:HIS:CG    | 2.51                     | 0.45              |
| 7:p:47:LEU:HD21   | 7:p:176:ASP:HA    | 1.98                     | 0.45              |
| 7:p:170:VAL:HG23  | 7:p:183:LEU:HB2   | 1.98                     | 0.45              |
| 7:t:64:PRO:HD2    | 7:t:67:HIS:ND1    | 2.31                     | 0.45              |
| 7:x:171:ILE:HD11  | 7:x:179:GLU:HB2   | 1.99                     | 0.45              |
| 3:A1:37:CYS:HB3   | 6:T:67:LEU:HD13   | 1.98                     | 0.45              |
| 3:A1:271:ALA:HB1  | 3:A1:292:GLN:HB3  | 1.99                     | 0.45              |
| 3:A3:2:ARG:HG2    | 3:A3:131:GLN:NE2  | 2.32                     | 0.45              |
| 3:A3:276:ARG:HH11 | 5:P:227:LEU:HD12  | 1.80                     | 0.45              |
| 2:A6:283:HIS:HB3  | 2:B0:62:VAL:HG11  | 1.98                     | 0.45              |
| 3:A9:163:ILE:HD11 | 3:A9:251:ARG:HB2  | 1.98                     | 0.45              |
| 3:B1:49:VAL:HG21  | 3:B1:241:ARG:HG3  | 1.97                     | 0.45              |
| 2:B2:377:MET:HE3  | 2:B2:379:SER:HB3  | 1.99                     | 0.45              |
| 2:B4:283:HIS:HB3  | 2:B8:62:VAL:HG11  | 1.97                     | 0.45              |
| 2:C2:195:LEU:HD11 | 2:C2:428:LEU:HD22 | 1.98                     | 0.45              |
| 2:C4:306:ASP:HB3  | 2:C4:309:HIS:CE1  | 2.52                     | 0.45              |
| 3:C5:42:LEU:HD21  | 3:C5:356:ILE:HG13 | 1.99                     | 0.45              |
| 3:C5:397:TRP:HH2  | 2:C6:256:GLN:HE21 | 1.64                     | 0.45              |
| 2:C6:177:VAL:HG13 | 3:C7:327:ASP:HB3  | 1.98                     | 0.45              |
| 2:D2:104:ALA:HB2  | 2:D2:413:MET:HE2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:48:ALA:H     | 5:O:558:ARG:HD3   | 1.82                     | 0.45              |
| 2:E4:73:THR:HA    | 3:E5:46:ARG:HH21  | 1.80                     | 0.45              |
| 3:E5:309:ARG:HD3  | 3:E5:342:VAL:HA   | 1.98                     | 0.45              |
| 3:E5:316:MET:HE1  | 3:E5:368:VAL:HG22 | 1.98                     | 0.45              |
| 2:E6:271:SER:HB2  | 2:E6:377:MET:HG3  | 1.97                     | 0.45              |
| 3:F1:205:GLU:HB2  | 3:F1:302:ALA:HB2  | 1.98                     | 0.45              |
| 7:e:168:PRO:HG2   | 7:e:185:ILE:HG21  | 1.99                     | 0.45              |
| 7:i:15:ARG:HG2    | 7:i:45:MET:HE1    | 1.98                     | 0.45              |
| 8:k:8:PHE:HZ      | 8:k:26:PRO:HA     | 1.81                     | 0.45              |
| 7:q:10:LEU:HD12   | 7:q:147:HIS:CG    | 2.52                     | 0.45              |
| 7:q:77:PHE:HE2    | 7:q:171:ILE:HD12  | 1.81                     | 0.45              |
| 7:r:14:LYS:HD2    | 7:r:47:LEU:HD13   | 1.99                     | 0.45              |
| 2:A2:292:THR:HG21 | 2:A2:331:ALA:HB1  | 1.98                     | 0.45              |
| 2:A4:154:LEU:HD12 | 2:A4:193:SER:HB3  | 1.97                     | 0.45              |
| 3:A7:284:LEU:HD23 | 3:A7:362:LYS:HB3  | 1.99                     | 0.45              |
| 2:A8:250:VAL:HG13 | 2:A8:255:PHE:HE1  | 1.82                     | 0.45              |
| 3:B1:100:ASN:HB3  | 3:B1:103:LYS:HG2  | 1.98                     | 0.45              |
| 3:B1:235:GLY:HA3  | 3:B1:366:THR:HG21 | 1.98                     | 0.45              |
| 2:C0:311:LYS:HZ1  | 2:C0:342:GLN:HB2  | 1.81                     | 0.45              |
| 3:C5:309:ARG:HD3  | 3:C5:342:VAL:HA   | 1.98                     | 0.45              |
| 2:C6:388:PHE:HB3  | 2:C6:425:LEU:HD12 | 1.98                     | 0.45              |
| 2:C8:182:VAL:HG22 | 3:C9:256:ASN:HD21 | 1.81                     | 0.45              |
| 2:D0:88:HIS:HB3   | 2:D0:91:GLN:HG3   | 1.99                     | 0.45              |
| 2:D4:234:VAL:HG22 | 2:D4:272:TYR:HB2  | 1.98                     | 0.45              |
| 2:E6:285:GLN:HG3  | 2:E6:287:SER:HB3  | 1.99                     | 0.45              |
| 3:E9:211:CYS:HB3  | 3:E9:220:PRO:HG3  | 1.99                     | 0.45              |
| 3:E9:293:MET:HE3  | 3:E9:367:PHE:HB2  | 1.98                     | 0.45              |
| 2:F0:9:VAL:HG12   | 2:F0:68:LEU:HB2   | 1.98                     | 0.45              |
| 2:F0:11:GLN:HG2   | 2:F0:74:VAL:HG11  | 1.98                     | 0.45              |
| 7:a:134:ILE:HG12  | 7:a:140:LEU:HD22  | 1.98                     | 0.45              |
| 7:c:97:ARG:O      | 7:c:101:GLU:HG2   | 2.17                     | 0.45              |
| 8:k:74:VAL:HG13   | 8:k:102:ARG:HG3   | 1.99                     | 0.45              |
| 7:m:172:VAL:HG13  | 7:m:180:ALA:HB3   | 1.98                     | 0.45              |
| 7:o:95:TYR:O      | 7:o:99:MET:HB3    | 2.17                     | 0.45              |
| 2:A2:4:VAL:HG11   | 2:A2:136:LEU:HG   | 1.98                     | 0.45              |
| 2:A2:108:TYR:C    | 2:A2:112:LYS:HZ3  | 2.25                     | 0.45              |
| 2:A6:121:ARG:HA   | 2:A6:121:ARG:HD2  | 1.61                     | 0.45              |
| 3:A7:382:SER:HB2  | 3:A7:415:MET:HE1  | 1.98                     | 0.45              |
| 3:B1:215:LEU:HD11 | 3:B1:273:LEU:HD22 | 1.99                     | 0.45              |
| 2:B4:338:LYS:HE3  | 2:B4:340:THR:HG22 | 1.97                     | 0.45              |
| 3:B7:289:LEU:O    | 3:B7:293:MET:HG2  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B9:207:LEU:HD23 | 3:B9:225:LEU:HB3  | 1.97                     | 0.45              |
| 3:B9:282:ARG:HH22 | 3:B9:292:GLN:CD   | 2.25                     | 0.45              |
| 3:B9:334:GLN:HA   | 3:B9:341:PHE:CE2  | 2.52                     | 0.45              |
| 3:C1:260:PHE:HB2  | 3:C1:263:LEU:HD13 | 1.98                     | 0.45              |
| 3:C7:138:SER:HA   | 3:C7:169:VAL:HG22 | 1.98                     | 0.45              |
| 3:D7:198:GLU:HG2  | 3:D7:266:PHE:HE2  | 1.82                     | 0.45              |
| 3:D9:183:TYR:HE2  | 3:D9:395:LEU:HD13 | 1.82                     | 0.45              |
| 3:E1:229:VAL:HG12 | 3:E1:233:MET:HE2  | 1.99                     | 0.45              |
| 2:E6:288:VAL:HG22 | 2:E6:323:VAL:HG12 | 1.99                     | 0.45              |
| 3:E7:309:ARG:H    | 3:E7:372:THR:HG22 | 1.82                     | 0.45              |
| 3:E9:211:CYS:HA   | 3:E9:215:LEU:HB3  | 1.98                     | 0.45              |
| 2:F0:105:ARG:HH12 | 3:F1:251:ARG:HG2  | 1.81                     | 0.45              |
| 4:W:1284:TRP:HA   | 4:W:1287:MET:HE2  | 1.98                     | 0.45              |
| 7:a:153:GLU:N     | 7:a:164:ARG:HE    | 2.15                     | 0.45              |
| 7:c:37:GLN:NE2    | 7:c:37:GLN:C      | 2.75                     | 0.45              |
| 7:n:8:SER:HA      | 7:n:9:PRO:HD3     | 1.81                     | 0.45              |
| 7:r:72:SER:HB3    | 7:r:108:ILE:HG22  | 1.98                     | 0.45              |
| 7:v:140:LEU:HA    | 7:v:143:ILE:HG12  | 1.99                     | 0.45              |
| 3:A3:32:PRO:HB3   | 3:A3:81:PHE:HD1   | 1.81                     | 0.45              |
| 3:A3:290:THR:HA   | 3:A3:293:MET:HE3  | 1.98                     | 0.45              |
| 3:A7:68:LEU:HD12  | 3:A7:143:THR:HG22 | 1.98                     | 0.45              |
| 2:A8:207:GLU:HA   | 2:A8:210:TYR:CD2  | 2.52                     | 0.45              |
| 2:C0:296:PHE:CZ   | 2:C0:377:MET:HE1  | 2.52                     | 0.45              |
| 2:C2:82:THR:HG21  | 1:I:221:PRO:HD3   | 1.99                     | 0.45              |
| 3:C3:25:SER:HB2   | 3:C3:30:ILE:HB    | 1.97                     | 0.45              |
| 3:C3:57:GLY:HA3   | 7:j:83:PRO:HB2    | 1.99                     | 0.45              |
| 2:C4:406:HIS:CD2  | 3:C5:261:PRO:HD3  | 2.52                     | 0.45              |
| 3:C5:105:HIS:CD2  | 3:C5:150:LEU:HD13 | 2.51                     | 0.45              |
| 3:D1:131:GLN:HE22 | 3:D1:249:ASP:HB2  | 1.81                     | 0.45              |
| 3:D3:165:GLU:HG2  | 3:D3:198:GLU:HB2  | 1.99                     | 0.45              |
| 3:D3:384:GLN:HE21 | 2:D4:348:PRO:HB2  | 1.82                     | 0.45              |
| 3:D7:131:GLN:HE21 | 3:D7:250:LEU:HB2  | 1.82                     | 0.45              |
| 2:D8:167:LEU:HG   | 2:D8:200:VAL:HB   | 1.99                     | 0.45              |
| 2:E0:179:THR:HB   | 3:E1:351:SER:HB2  | 1.99                     | 0.45              |
| 3:F1:30:ILE:HG13  | 3:F1:51:TYR:CE1   | 2.47                     | 0.45              |
| 4:M:1251:ILE:HG23 | 4:M:1384:LYS:HB3  | 1.98                     | 0.45              |
| 6:U:58:LEU:HA     | 6:U:61:TRP:HD1    | 1.80                     | 0.45              |
| 7:d:75:LEU:O      | 7:d:170:VAL:HA    | 2.17                     | 0.45              |
| 8:l:54:ARG:CZ     | 7:n:160:GLY:HA3   | 2.47                     | 0.45              |
| 8:l:58:LYS:HA     | 8:l:62:PHE:HD2    | 1.82                     | 0.45              |
| 7:o:4:PRO:HG3     | 7:o:179:GLU:HB2   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A4:272:TYR:HD2  | 2:A4:275:ILE:HG12 | 1.81                     | 0.45              |
| 3:A5:32:PRO:HB3   | 3:A5:81:PHE:HA    | 1.98                     | 0.45              |
| 2:B4:183:GLU:HG2  | 2:B4:184:PRO:HD3  | 1.99                     | 0.45              |
| 2:B8:223:THR:HG22 | 3:B9:322:SER:HA   | 1.99                     | 0.45              |
| 3:C1:25:SER:HB2   | 3:C1:30:ILE:HB    | 1.98                     | 0.45              |
| 2:C6:198:THR:HG21 | 2:C6:201:ALA:HB2  | 1.99                     | 0.45              |
| 2:D0:71:GLU:HG2   | 2:D0:98:ASP:HB3   | 1.99                     | 0.45              |
| 3:D3:313:ALA:HB3  | 3:D3:349:MET:HE2  | 1.99                     | 0.45              |
| 3:D7:117:LEU:HA   | 3:D7:120:VAL:HG12 | 1.99                     | 0.45              |
| 2:D8:174:SER:HB2  | 2:D8:177:VAL:O    | 2.17                     | 0.45              |
| 3:E1:207:LEU:HB3  | 3:E1:225:LEU:HD22 | 1.98                     | 0.45              |
| 4:M:1279:ARG:HG3  | 4:M:1316:GLN:HE22 | 1.81                     | 0.45              |
| 7:f:56:LYS:HE3    | 7:f:60:ASN:HA     | 1.99                     | 0.45              |
| 7:u:146:ARG:HH12  | 7:u:156:VAL:HG21  | 1.82                     | 0.45              |
| 7:v:50:PHE:HD1    | 7:v:140:LEU:HD21  | 1.82                     | 0.45              |
| 7:x:88:LEU:HD11   | 7:x:185:ILE:HG12  | 1.98                     | 0.45              |
| 3:A1:198:GLU:HB3  | 3:A1:200:GLN:NE2  | 2.32                     | 0.44              |
| 3:A3:39:ASP:HA    | 6:R:74:GLY:H      | 1.82                     | 0.44              |
| 2:A4:112:LYS:HA   | 2:A4:115:VAL:HG12 | 1.98                     | 0.44              |
| 3:A5:98:GLY:H     | 3:A5:103:LYS:NZ   | 2.15                     | 0.44              |
| 3:A7:249:ASP:H    | 3:A7:252:LYS:HG3  | 1.82                     | 0.44              |
| 2:B0:75:VAL:HG13  | 2:B0:79:ARG:HH21  | 1.82                     | 0.44              |
| 2:D6:306:ASP:HB3  | 2:D6:309:HIS:CE1  | 2.52                     | 0.44              |
| 3:D9:341:PHE:HD2  | 3:D9:348:ASN:HD22 | 1.65                     | 0.44              |
| 3:E3:320:ARG:HA   | 3:E3:320:ARG:HD2  | 1.79                     | 0.44              |
| 3:E9:415:MET:HE2  | 3:E9:415:MET:HA   | 1.99                     | 0.44              |
| 3:F1:224:ASP:HA   | 3:F1:227:HIS:HB2  | 1.99                     | 0.44              |
| 4:L:1286:ARG:NE   | 4:L:1289:ARG:HH21 | 2.14                     | 0.44              |
| 5:O:231:PRO:HA    | 6:T:55:ASP:HA     | 1.97                     | 0.44              |
| 4:V:1395:GLU:HA   | 4:V:1398:LEU:HG   | 1.98                     | 0.44              |
| 7:h:97:ARG:NH2    | 7:j:160:GLY:HA3   | 2.31                     | 0.44              |
| 8:l:53:VAL:HA     | 8:l:154:LEU:HD21  | 1.99                     | 0.44              |
| 7:p:78:ALA:HB3    | 7:p:112:PHE:HE2   | 1.81                     | 0.44              |
| 2:A4:385:ALA:HB2  | 2:A4:432:TYR:HD2  | 1.81                     | 0.44              |
| 3:A9:19:LYS:HG3   | 3:A9:226:ASN:HB2  | 2.00                     | 0.44              |
| 3:B3:145:SER:HB2  | 3:B3:188:SER:HB3  | 2.00                     | 0.44              |
| 3:B3:150:LEU:HD11 | 3:B3:154:LYS:HE2  | 2.00                     | 0.44              |
| 3:B3:265:PHE:HB3  | 3:B3:374:ILE:HD13 | 1.98                     | 0.44              |
| 2:C6:213:CYS:HA   | 2:C6:217:LEU:HD23 | 1.99                     | 0.44              |
| 3:C9:284:LEU:HD23 | 3:C9:284:LEU:HA   | 1.91                     | 0.44              |
| 3:D1:230:SER:HA   | 3:D1:233:MET:HG3  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D7:5:VAL:HG21   | 3:D7:124:ALA:HB2  | 1.99                     | 0.44              |
| 3:E5:313:ALA:HB1  | 3:E5:367:PHE:HE1  | 1.82                     | 0.44              |
| 2:E8:136:LEU:HD22 | 2:E8:169:PHE:HE2  | 1.81                     | 0.44              |
| 4:M:1241:PHE:CD2  | 4:M:1242:PRO:HD3  | 2.51                     | 0.44              |
| 7:t:71:LYS:NZ     | 7:t:106:GLN:HG2   | 2.32                     | 0.44              |
| 7:u:63:ILE:HD11   | 7:u:67:HIS:CD2    | 2.51                     | 0.44              |
| 7:u:97:ARG:HH22   | 7:w:149:ARG:NH1   | 2.15                     | 0.44              |
| 7:w:169:SER:HA    | 7:w:185:ILE:HD11  | 1.99                     | 0.44              |
| 3:A3:286:VAL:HB   | 3:A3:325:GLU:HG2  | 1.99                     | 0.44              |
| 2:A8:26:LEU:HG    | 1:C:257:PRO:HD3   | 1.98                     | 0.44              |
| 2:B2:324:VAL:HG22 | 2:B2:326:LYS:H    | 1.83                     | 0.44              |
| 3:B3:42:LEU:HB3   | 1:E:241:PHE:HE2   | 1.82                     | 0.44              |
| 2:B8:254:GLU:HG2  | 2:B8:352:LYS:HE2  | 1.99                     | 0.44              |
| 3:C1:66:MET:HE2   | 3:C1:116:VAL:HG21 | 1.99                     | 0.44              |
| 3:C1:132:GLY:HA2  | 3:C1:162:ARG:HB3  | 1.98                     | 0.44              |
| 3:C1:133:PHE:HD2  | 3:C1:164:MET:HE1  | 1.83                     | 0.44              |
| 3:C3:164:MET:H    | 3:C3:197:ASP:HB2  | 1.81                     | 0.44              |
| 3:C7:135:ILE:HG21 | 3:C7:152:ILE:HD11 | 1.99                     | 0.44              |
| 2:C8:180:ALA:HB3  | 2:C8:183:GLU:HG3  | 2.00                     | 0.44              |
| 2:D0:363:VAL:HG23 | 2:D0:366:GLY:HA3  | 1.98                     | 0.44              |
| 3:D1:296:ALA:HB2  | 3:D1:305:PRO:HD2  | 2.00                     | 0.44              |
| 3:D3:234:SER:HB2  | 3:D3:241:ARG:HH12 | 1.81                     | 0.44              |
| 3:D3:282:ARG:HH22 | 3:D3:362:LYS:HZ1  | 1.65                     | 0.44              |
| 2:E2:198:THR:HG21 | 2:E2:201:ALA:HB2  | 1.99                     | 0.44              |
| 2:E2:311:LYS:HE3  | 2:E2:344:VAL:HA   | 1.99                     | 0.44              |
| 3:E5:158:GLU:HG2  | 3:E5:159:TYR:CD1  | 2.52                     | 0.44              |
| 3:E7:163:ILE:HD11 | 3:E7:251:ARG:HB2  | 1.99                     | 0.44              |
| 2:E8:88:HIS:CE1   | 2:E8:90:GLU:HB2   | 2.52                     | 0.44              |
| 3:E9:361:LEU:HD23 | 6:U:105:HIS:CE1   | 2.52                     | 0.44              |
| 4:M:1249:THR:HG22 | 4:M:1438:LEU:HD21 | 1.98                     | 0.44              |
| 4:V:1248:THR:HG22 | 4:V:1252:LEU:HD23 | 1.99                     | 0.44              |
| 7:q:129:MET:HE3   | 7:q:131:TRP:NE1   | 2.32                     | 0.44              |
| 3:A3:133:PHE:HD2  | 3:A3:164:MET:HE1  | 1.82                     | 0.44              |
| 3:A7:6:HIS:CE1    | 3:A7:8:GLN:HE22   | 2.35                     | 0.44              |
| 2:A8:107:HIS:HE1  | 2:A8:151:CYS:HB3  | 1.83                     | 0.44              |
| 3:A9:256:ASN:OD1  | 3:A9:350:LYS:HD3  | 2.18                     | 0.44              |
| 3:B3:201:VAL:HG21 | 3:B3:374:ILE:HD11 | 1.98                     | 0.44              |
| 3:B5:39:ASP:HA    | 7:f:90:PRO:HG3    | 1.98                     | 0.44              |
| 2:C8:306:ASP:HB3  | 2:C8:309:HIS:CE1  | 2.53                     | 0.44              |
| 3:C9:166:THR:HG22 | 3:C9:168:SER:HB3  | 1.98                     | 0.44              |
| 1:D:247:TYR:HA    | 2:D6:22:GLU:CD    | 2.42                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D2:194:LEU:HG   | 2:D2:267:PHE:HE1  | 1.82                     | 0.44              |
| 2:D2:423:GLU:HA   | 2:D2:426:ALA:HB3  | 2.00                     | 0.44              |
| 2:D6:82:THR:HB    | 2:D6:83:TYR:CZ    | 2.52                     | 0.44              |
| 2:D6:360:PRO:HG2  | 2:D6:371:VAL:HG13 | 1.99                     | 0.44              |
| 2:D6:407:TRP:HZ2  | 3:D7:258:ILE:HD12 | 1.83                     | 0.44              |
| 3:D9:39:ASP:HA    | 7:r:90:PRO:HG3    | 1.99                     | 0.44              |
| 2:E2:151:CYS:O    | 2:E2:155:GLU:HG2  | 2.18                     | 0.44              |
| 2:E2:320:ARG:HG3  | 2:E2:356:ASN:HB3  | 2.00                     | 0.44              |
| 3:E5:42:LEU:HD21  | 1:H:248:ARG:HH12  | 1.81                     | 0.44              |
| 4:N:1405:LEU:HA   | 4:N:1408:GLN:HB2  | 1.98                     | 0.44              |
| 6:R:48:ASP:HB2    | 7:b:154:TYR:CE1   | 2.52                     | 0.44              |
| 6:T:57:LYS:HD3    | 6:T:57:LYS:HA     | 1.76                     | 0.44              |
| 7:e:55:LEU:HD22   | 7:e:111:ILE:HD12  | 1.97                     | 0.44              |
| 7:m:65:GLN:HE21   | 7:m:65:GLN:C      | 2.23                     | 0.44              |
| 7:o:63:ILE:HD11   | 7:o:132:LEU:HD11  | 2.00                     | 0.44              |
| 7:o:82:ASP:HB2    | 7:o:85:CYS:HB2    | 2.00                     | 0.44              |
| 7:u:14:LYS:HG3    | 7:u:47:LEU:HB3    | 1.99                     | 0.44              |
| 2:A4:4:VAL:HB     | 2:A4:52:PHE:HE1   | 1.83                     | 0.44              |
| 2:B0:387:VAL:HG23 | 2:B0:390:ARG:HH12 | 1.82                     | 0.44              |
| 2:B2:180:ALA:HA   | 3:B3:350:LYS:HE2  | 2.00                     | 0.44              |
| 3:B9:86:ARG:HD2   | 3:B9:88:ASP:HB2   | 1.99                     | 0.44              |
| 2:C4:288:VAL:HA   | 2:C4:291:ILE:HG12 | 2.00                     | 0.44              |
| 3:C9:139:LEU:HD13 | 3:C9:168:SER:HB2  | 1.99                     | 0.44              |
| 3:E3:107:THR:HG22 | 3:E3:108:GLU:H    | 1.83                     | 0.44              |
| 2:E4:96:LYS:HD3   | 2:E4:96:LYS:HA    | 1.77                     | 0.44              |
| 2:E6:286:LEU:HD11 | 2:E6:371:VAL:HG23 | 1.99                     | 0.44              |
| 1:G:212:GLU:HG3   | 1:G:216:ARG:HG3   | 1.99                     | 0.44              |
| 1:K:255:PRO:HG3   | 7:o:178:ARG:HD2   | 1.99                     | 0.44              |
| 8:k:39:ALA:O      | 8:k:75:SER:HA     | 2.18                     | 0.44              |
| 7:m:63:ILE:HD11   | 7:m:132:LEU:HD13  | 2.00                     | 0.44              |
| 7:n:18:ASN:HD22   | 7:n:45:MET:HG3    | 1.82                     | 0.44              |
| 7:n:59:ASN:HD21   | 7:p:9:PRO:HA      | 1.83                     | 0.44              |
| 7:p:165:THR:HG21  | 7:p:182:PHE:HZ    | 1.83                     | 0.44              |
| 1:A:210:HIS:HB3   | 7:d:154:TYR:HH    | 1.83                     | 0.44              |
| 2:A2:137:MET:HE3  | 2:A2:154:LEU:HD13 | 1.99                     | 0.44              |
| 3:B1:187:LEU:HA   | 3:B1:190:HIS:CE1  | 2.52                     | 0.44              |
| 3:B1:190:HIS:HB2  | 3:B1:414:ASN:HD22 | 1.83                     | 0.44              |
| 3:B5:17:GLY:HA2   | 3:B5:20:PHE:HB3   | 2.00                     | 0.44              |
| 2:C0:21:TRP:CZ2   | 2:C0:65:CYS:HB3   | 2.53                     | 0.44              |
| 3:C5:191:GLN:NE2  | 3:C5:195:ASN:HD21 | 2.15                     | 0.44              |
| 2:C6:292:THR:HG21 | 2:C6:331:ALA:HB1  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C8:10:GLY:HA2   | 2:C8:145:THR:HG23 | 2.00                     | 0.44              |
| 3:C9:214:THR:HG22 | 3:C9:297:LYS:HZ3  | 1.81                     | 0.44              |
| 2:D6:28:HIS:CE1   | 2:D6:243:ARG:HD2  | 2.53                     | 0.44              |
| 2:D6:137:MET:HE1  | 2:D6:154:LEU:HD11 | 2.00                     | 0.44              |
| 3:D7:294:PHE:CZ   | 3:D7:333:VAL:HG11 | 2.52                     | 0.44              |
| 2:D8:204:LEU:HD21 | 2:D8:231:ILE:HG12 | 2.00                     | 0.44              |
| 3:E9:199:VAL:HG23 | 3:E9:264:HIS:HD2  | 1.83                     | 0.44              |
| 3:F1:199:VAL:HG23 | 3:F1:264:HIS:HD2  | 1.83                     | 0.44              |
| 1:J:223:PRO:HG3   | 7:n:178:ARG:HH21  | 1.82                     | 0.44              |
| 6:R:127:ARG:HG2   | 6:R:131:LEU:HD23  | 1.98                     | 0.44              |
| 7:f:111:ILE:HG12  | 7:f:132:LEU:HB2   | 2.00                     | 0.44              |
| 7:f:200:ASP:O     | 7:f:204:THR:HG22  | 2.18                     | 0.44              |
| 7:g:9:PRO:HA      | 7:g:12:VAL:HG22   | 1.99                     | 0.44              |
| 7:s:18:ASN:HA     | 7:s:21:ARG:HH12   | 1.81                     | 0.44              |
| 3:A1:294:PHE:CE2  | 3:A1:333:VAL:HG11 | 2.53                     | 0.44              |
| 2:A2:104:ALA:O    | 2:A2:108:TYR:HB2  | 2.17                     | 0.44              |
| 3:A7:206:ALA:HB2  | 3:A7:302:ALA:HB2  | 1.99                     | 0.44              |
| 3:A9:91:VAL:HG21  | 3:A9:116:VAL:HG22 | 2.00                     | 0.44              |
| 2:B8:75:VAL:HG11  | 2:B8:94:SER:HB2   | 1.98                     | 0.44              |
| 2:B8:258:ASN:HD22 | 2:B8:352:LYS:HD2  | 1.83                     | 0.44              |
| 2:C0:408:TYR:HB3  | 2:C0:413:MET:HG2  | 2.00                     | 0.44              |
| 2:C6:338:LYS:HB2  | 2:C6:338:LYS:HE2  | 1.84                     | 0.44              |
| 3:C7:318:ARG:HH12 | 3:C7:358:PRO:HB3  | 1.81                     | 0.44              |
| 2:C8:219:ILE:HG12 | 7:o:198:ARG:HH22  | 1.82                     | 0.44              |
| 2:D0:100:ALA:O    | 3:D1:255:VAL:HG11 | 2.18                     | 0.44              |
| 2:D2:202:VAL:HG22 | 2:D2:268:MET:HB2  | 1.99                     | 0.44              |
| 2:D4:68:LEU:HD11  | 2:D4:118:SER:HB3  | 1.99                     | 0.44              |
| 2:D6:259:LEU:HD11 | 2:D6:316:CYS:HB2  | 2.00                     | 0.44              |
| 3:E7:290:THR:HA   | 3:E7:293:MET:HE3  | 1.99                     | 0.44              |
| 7:a:53:GLY:HA2    | 7:a:62:VAL:HG21   | 1.99                     | 0.44              |
| 7:d:42:TYR:HA     | 7:d:45:MET:HG3    | 2.00                     | 0.44              |
| 7:g:55:LEU:HB3    | 7:g:63:ILE:HG23   | 1.99                     | 0.44              |
| 7:h:8:SER:HB2     | 7:h:147:HIS:HA    | 1.99                     | 0.44              |
| 7:j:9:PRO:HD3     | 7:j:146:ARG:HG2   | 1.98                     | 0.44              |
| 3:A3:8:GLN:HG3    | 3:A3:65:LEU:HD13  | 1.99                     | 0.44              |
| 3:A3:186:THR:HG22 | 3:A3:411:ALA:HB1  | 2.00                     | 0.44              |
| 3:A3:290:THR:HG21 | 3:A3:329:GLN:HG2  | 1.99                     | 0.44              |
| 3:A3:316:MET:HE2  | 3:A3:366:THR:HG23 | 2.00                     | 0.44              |
| 2:A4:102:ASN:HB3  | 2:A4:105:ARG:HG3  | 1.98                     | 0.44              |
| 2:A4:230:LEU:HD11 | 2:A4:275:ILE:HG23 | 1.99                     | 0.44              |
| 2:A8:84:ARG:HD3   | 7:c:197:LEU:HD11  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B1:11:GLN:HB3   | 3:B1:72:THR:HG21  | 1.99                     | 0.44              |
| 2:B6:311:LYS:HZ3  | 2:B6:344:VAL:HA   | 1.81                     | 0.44              |
| 2:B8:310:GLY:HA3  | 2:B8:383:ALA:HB2  | 2.00                     | 0.44              |
| 3:C5:64:ILE:HG12  | 3:C5:119:VAL:HG13 | 1.99                     | 0.44              |
| 3:C5:283:ALA:HA   | 3:C9:55:THR:H     | 1.82                     | 0.44              |
| 2:C6:210:TYR:HE1  | 2:C6:227:LEU:HD11 | 1.83                     | 0.44              |
| 3:C7:282:ARG:HA   | 3:D1:86:ARG:HH22  | 1.82                     | 0.44              |
| 3:D7:388:MET:HE2  | 2:D8:348:PRO:HD2  | 1.99                     | 0.44              |
| 2:D8:363:VAL:HB   | 2:D8:366:GLY:HA3  | 2.00                     | 0.44              |
| 2:E0:391:MET:HE3  | 2:E0:391:MET:HB3  | 1.77                     | 0.44              |
| 1:I:222:LYS:HE3   | 8:I:140:GLU:HG3   | 2.00                     | 0.44              |
| 6:U:127:ARG:HA    | 6:U:130:GLN:HE21  | 1.83                     | 0.44              |
| 7:b:171:ILE:HD11  | 7:b:179:GLU:HG2   | 1.98                     | 0.44              |
| 7:i:18:ASN:ND2    | 7:i:45:MET:HG3    | 2.32                     | 0.44              |
| 8:k:25:ARG:NH2    | 8:k:28:HIS:HA     | 2.33                     | 0.44              |
| 7:m:15:ARG:O      | 7:m:19:GLU:CB     | 2.65                     | 0.44              |
| 7:o:69:LYS:HB2    | 7:o:69:LYS:HE3    | 1.74                     | 0.44              |
| 7:r:75:LEU:HD23   | 7:r:173:ILE:HG21  | 2.00                     | 0.44              |
| 2:A2:74:VAL:HG13  | 2:A2:75:VAL:HG13  | 2.00                     | 0.44              |
| 2:A2:238:LEU:HD13 | 2:A2:318:MET:HE3  | 2.00                     | 0.44              |
| 2:A2:306:ASP:HB3  | 2:A2:309:HIS:CD2  | 2.53                     | 0.44              |
| 3:A3:309:ARG:H    | 3:A3:372:THR:HG22 | 1.82                     | 0.44              |
| 2:A6:119:LEU:HA   | 2:A6:122:ILE:HG12 | 1.99                     | 0.44              |
| 2:B4:82:THR:HG21  | 1:E:221:PRO:HD3   | 1.99                     | 0.44              |
| 2:B4:306:ASP:HB3  | 2:B4:309:HIS:CE1  | 2.53                     | 0.44              |
| 3:B5:65:LEU:HB2   | 3:B5:90:PHE:HA    | 1.99                     | 0.44              |
| 2:B6:311:LYS:NZ   | 2:B6:344:VAL:HA   | 2.33                     | 0.44              |
| 3:B7:281:TYR:CD2  | 3:C1:87:PRO:HD3   | 2.53                     | 0.44              |
| 2:B8:250:VAL:HG22 | 2:B8:352:LYS:HE3  | 2.00                     | 0.44              |
| 2:C0:71:GLU:HB3   | 2:C0:98:ASP:HB3   | 1.99                     | 0.44              |
| 3:C1:319:GLY:HA2  | 3:C1:357:PRO:HG3  | 1.99                     | 0.44              |
| 3:C3:294:PHE:HD1  | 3:C3:310:TYR:HE2  | 1.65                     | 0.44              |
| 2:C6:66:VAL:HG11  | 2:C6:122:ILE:HG12 | 2.00                     | 0.44              |
| 2:C8:434:GLU:HA   | 2:C8:437:ILE:HG12 | 2.00                     | 0.44              |
| 2:D0:123:ARG:HH21 | 2:D0:161:TYR:HE1  | 1.64                     | 0.44              |
| 2:D2:422:ARG:HD2  | 2:D2:422:ARG:HA   | 1.68                     | 0.44              |
| 2:D4:164:LYS:HD3  | 2:D4:164:LYS:HA   | 1.69                     | 0.44              |
| 3:D5:252:LYS:HG3  | 3:D5:350:LYS:HZ2  | 1.82                     | 0.44              |
| 2:D6:226:ASN:HA   | 2:D6:229:ARG:HG2  | 1.98                     | 0.44              |
| 3:D9:113:ILE:HD11 | 3:D9:151:LEU:HB2  | 1.99                     | 0.44              |
| 3:E9:265:PHE:HE2  | 3:E9:418:LEU:HD21 | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:b:194:ARG:HH11  | 7:b:197:LEU:HD12  | 1.83                     | 0.44              |
| 7:f:79:ASP:HB3    | 7:f:82:ASP:HB2    | 2.00                     | 0.44              |
| 7:h:84:LYS:HB3    | 7:h:168:PRO:HD3   | 2.00                     | 0.44              |
| 7:v:130:PRO:HD2   | 7:v:131:TRP:CE3   | 2.53                     | 0.44              |
| 7:w:93:LEU:O      | 7:w:97:ARG:HG2    | 2.18                     | 0.44              |
| 2:A2:408:TYR:HB3  | 2:A2:413:MET:HG3  | 1.99                     | 0.43              |
| 3:A3:131:GLN:HB3  | 3:A3:163:ILE:HD11 | 2.00                     | 0.43              |
| 3:A7:171:PRO:HB2  | 3:A7:380:ARG:HH22 | 1.83                     | 0.43              |
| 2:A8:68:LEU:HD23  | 2:A8:93:ILE:HB    | 2.00                     | 0.43              |
| 2:A8:262:TYR:HD2  | 2:A8:265:ILE:HD11 | 1.81                     | 0.43              |
| 2:A8:398:MET:HE2  | 3:A9:345:ILE:HG23 | 1.99                     | 0.43              |
| 2:B0:188:VAL:HG12 | 2:B0:421:ALA:HB1  | 1.99                     | 0.43              |
| 2:B0:294:SER:HA   | 2:B0:297:GLU:HG2  | 1.99                     | 0.43              |
| 3:B1:113:ILE:HA   | 3:B1:116:VAL:HG22 | 2.00                     | 0.43              |
| 3:B3:284:LEU:HD23 | 3:B3:362:LYS:HG2  | 1.99                     | 0.43              |
| 3:B3:293:MET:HG3  | 3:B3:294:PHE:CD2  | 2.53                     | 0.43              |
| 3:B5:175:VAL:HG12 | 3:B5:205:GLU:OE2  | 2.17                     | 0.43              |
| 2:B8:36:MET:HG2   | 2:B8:61:HIS:HE1   | 1.83                     | 0.43              |
| 2:B8:210:TYR:HB3  | 3:B9:324:LYS:NZ   | 2.33                     | 0.43              |
| 2:B8:221:ARG:HH12 | 3:B9:325:GLU:HB3  | 1.82                     | 0.43              |
| 2:C2:421:ALA:HA   | 2:C2:424:ASP:HB3  | 1.99                     | 0.43              |
| 2:C4:203:MET:HG3  | 2:C4:384:ILE:HD11 | 1.99                     | 0.43              |
| 3:C5:388:MET:HE2  | 3:C5:388:MET:HB3  | 1.91                     | 0.43              |
| 2:D8:77:GLU:HA    | 2:D8:80:THR:HG22  | 2.00                     | 0.43              |
| 3:E7:5:VAL:HG21   | 3:E7:124:ALA:HB2  | 2.00                     | 0.43              |
| 4:V:1248:THR:HG21 | 4:V:1438:LEU:HD21 | 2.00                     | 0.43              |
| 7:h:93:LEU:HB3    | 7:h:97:ARG:NH2    | 2.27                     | 0.43              |
| 7:o:142:GLU:HA    | 7:o:145:LYS:HB2   | 2.00                     | 0.43              |
| 7:t:64:PRO:HD2    | 7:t:67:HIS:CE1    | 2.52                     | 0.43              |
| 2:A0:352:LYS:HA   | 2:A0:352:LYS:HD3  | 1.87                     | 0.43              |
| 2:A2:370:LYS:HE3  | 2:A2:370:LYS:HB3  | 1.83                     | 0.43              |
| 3:A3:136:THR:HG21 | 3:A3:233:MET:HE1  | 1.98                     | 0.43              |
| 2:B2:154:LEU:HB3  | 2:B2:197:HIS:HB3  | 2.01                     | 0.43              |
| 2:B2:210:TYR:HB3  | 3:B3:324:LYS:NZ   | 2.33                     | 0.43              |
| 3:B3:68:LEU:HG    | 3:B3:147:MET:HE3  | 2.01                     | 0.43              |
| 2:B8:121:ARG:HH11 | 2:B8:124:LYS:HE2  | 1.84                     | 0.43              |
| 3:B9:215:LEU:HD11 | 3:B9:228:LEU:HD21 | 2.00                     | 0.43              |
| 3:C3:5:VAL:HB     | 3:C3:133:PHE:HD1  | 1.83                     | 0.43              |
| 2:C4:141:VAL:HG23 | 2:C4:173:PRO:HD3  | 1.99                     | 0.43              |
| 2:C4:184:PRO:HA   | 2:C4:391:MET:HE1  | 2.00                     | 0.43              |
| 2:C6:240:ALA:HB1  | 2:C6:356:ASN:HD22 | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C7:212:PHE:HB3  | 3:C7:213:ARG:HH11 | 1.83                     | 0.43              |
| 3:C7:290:THR:HA   | 3:C7:293:MET:HG2  | 2.01                     | 0.43              |
| 3:C7:359:LYS:HD2  | 3:C7:359:LYS:HA   | 1.72                     | 0.43              |
| 3:C9:150:LEU:O    | 3:C9:154:LYS:HG2  | 2.18                     | 0.43              |
| 3:C9:294:PHE:CZ   | 3:C9:349:MET:HE1  | 2.52                     | 0.43              |
| 2:D0:198:THR:HG21 | 2:D0:201:ALA:HB2  | 2.00                     | 0.43              |
| 3:D7:35:THR:HG22  | 7:q:83:PRO:HG3    | 1.99                     | 0.43              |
| 3:D7:174:LYS:HG3  | 3:D7:175:VAL:HG23 | 1.99                     | 0.43              |
| 2:E0:33:ASP:HB3   | 7:s:102:GLY:O     | 2.19                     | 0.43              |
| 2:E6:96:LYS:HE3   | 2:E6:96:LYS:HB3   | 1.82                     | 0.43              |
| 2:E8:296:PHE:CE1  | 2:E8:377:MET:HE1  | 2.54                     | 0.43              |
| 3:E9:356:ILE:HD12 | 6:U:113:TRP:HB3   | 2.01                     | 0.43              |
| 3:F1:60:VAL:HG21  | 3:F1:86:ARG:HH11  | 1.82                     | 0.43              |
| 7:x:79:ASP:HB3    | 7:x:82:ASP:HB2    | 2.00                     | 0.43              |
| 2:A0:292:THR:HG21 | 2:A0:331:ALA:HB1  | 2.00                     | 0.43              |
| 3:A1:361:LEU:HD11 | 5:O:228:LEU:HD23  | 1.98                     | 0.43              |
| 1:B:240:PRO:HB2   | 7:q:154:TYR:HD2   | 1.83                     | 0.43              |
| 2:B0:115:VAL:HG21 | 2:B0:152:LEU:HG   | 2.00                     | 0.43              |
| 3:B1:19:LYS:HA    | 3:B1:22:GLU:HG3   | 1.99                     | 0.43              |
| 2:B4:230:LEU:HD22 | 2:B4:275:ILE:HD12 | 1.99                     | 0.43              |
| 3:B5:67:ASP:HB3   | 3:B5:73:MET:HE2   | 2.01                     | 0.43              |
| 2:B6:288:VAL:HA   | 2:B6:291:ILE:HG12 | 2.01                     | 0.43              |
| 2:B8:66:VAL:HG21  | 2:B8:122:ILE:HD11 | 2.01                     | 0.43              |
| 2:B8:259:LEU:HD11 | 2:B8:316:CYS:HB2  | 2.01                     | 0.43              |
| 2:B8:268:MET:HE1  | 2:B8:380:ASN:HB2  | 2.01                     | 0.43              |
| 2:C4:9:VAL:HG23   | 2:C4:68:LEU:HD22  | 1.99                     | 0.43              |
| 2:C4:133:GLN:HE22 | 2:C4:251:ASP:HB3  | 1.84                     | 0.43              |
| 3:C7:47:ILE:HG22  | 3:C7:51:TYR:HB2   | 2.00                     | 0.43              |
| 3:C7:166:THR:HG23 | 3:C7:199:VAL:HA   | 2.00                     | 0.43              |
| 3:C9:68:LEU:HD22  | 3:C9:97:ALA:HB2   | 1.99                     | 0.43              |
| 3:C9:139:LEU:HA   | 3:C9:145:SER:HB3  | 1.99                     | 0.43              |
| 2:D0:240:ALA:HB1  | 2:D0:356:ASN:HD22 | 1.82                     | 0.43              |
| 3:D1:211:CYS:SG   | 3:D1:220:PRO:HB3  | 2.59                     | 0.43              |
| 2:D2:259:LEU:HD13 | 2:D2:316:CYS:HB2  | 2.01                     | 0.43              |
| 2:D4:251:ASP:OD2  | 2:D4:254:GLU:HG2  | 2.18                     | 0.43              |
| 2:D6:154:LEU:HD12 | 2:D6:193:SER:HB2  | 2.01                     | 0.43              |
| 3:D9:289:LEU:HD11 | 3:D9:363:MET:HG3  | 2.00                     | 0.43              |
| 3:E3:310:TYR:CD1  | 3:E3:371:SER:HB2  | 2.53                     | 0.43              |
| 3:E3:392:LYS:HD3  | 3:E3:392:LYS:HA   | 1.74                     | 0.43              |
| 3:E5:34:GLY:HA3   | 3:E5:58:ARG:NH1   | 2.33                     | 0.43              |
| 3:E7:116:VAL:HA   | 3:E7:119:VAL:HG12 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E7:173:PRO:HB3  | 3:E7:380:ARG:HE   | 1.82                     | 0.43              |
| 3:E7:257:LEU:HB3  | 3:E7:266:PHE:CZ   | 2.53                     | 0.43              |
| 2:F0:246:GLY:HA3  | 2:F0:356:ASN:HA   | 2.00                     | 0.43              |
| 3:F1:217:LEU:HD23 | 6:R:174:ARG:NH1   | 2.33                     | 0.43              |
| 6:T:163:HIS:HB2   | 6:T:167:THR:HG21  | 2.00                     | 0.43              |
| 7:e:96:TYR:HA     | 7:e:108:ILE:HD11  | 1.99                     | 0.43              |
| 7:e:173:ILE:HD11  | 7:e:177:GLY:HA2   | 2.01                     | 0.43              |
| 7:m:53:GLY:HA2    | 7:m:62:VAL:HG21   | 2.01                     | 0.43              |
| 7:n:15:ARG:O      | 7:n:19:GLU:HB2    | 2.18                     | 0.43              |
| 2:A8:363:VAL:HG23 | 2:A8:366:GLY:HA3  | 1.99                     | 0.43              |
| 2:B4:53:PHE:HB3   | 2:B4:61:HIS:HB3   | 2.00                     | 0.43              |
| 3:B7:330:MET:HE3  | 3:B7:351:SER:HB2  | 2.00                     | 0.43              |
| 2:B8:155:GLU:HA   | 2:B8:197:HIS:CE1  | 2.52                     | 0.43              |
| 2:C0:110:ILE:HG23 | 2:C0:111:GLY:H    | 1.84                     | 0.43              |
| 3:C1:198:GLU:HG3  | 3:C1:266:PHE:HE2  | 1.84                     | 0.43              |
| 2:C4:133:GLN:HE21 | 2:C4:252:VAL:HB   | 1.83                     | 0.43              |
| 3:C5:51:TYR:HE2   | 3:C5:61:PRO:HG3   | 1.82                     | 0.43              |
| 3:C7:3:GLU:H      | 3:C7:130:LEU:HA   | 1.84                     | 0.43              |
| 2:C8:407:TRP:CH2  | 3:C9:258:ILE:HB   | 2.53                     | 0.43              |
| 3:D1:274:THR:HG21 | 3:D1:279:GLN:HA   | 1.99                     | 0.43              |
| 2:D2:265:ILE:HG23 | 2:D2:432:TYR:CZ   | 2.52                     | 0.43              |
| 2:D2:274:PRO:HD3  | 2:D2:291:ILE:HD11 | 1.99                     | 0.43              |
| 3:D3:167:PHE:CE2  | 3:D3:233:MET:HG2  | 2.53                     | 0.43              |
| 2:D8:175:PRO:HB3  | 2:D8:390:ARG:HD2  | 2.00                     | 0.43              |
| 2:E2:210:TYR:CG   | 3:E3:324:LYS:HD3  | 2.53                     | 0.43              |
| 3:E9:244:GLY:HA2  | 3:E9:355:ASP:HB2  | 1.99                     | 0.43              |
| 4:L:1256:ILE:HG23 | 4:L:1287:MET:HE1  | 2.00                     | 0.43              |
| 7:c:14:LYS:HD2    | 7:c:47:LEU:HD12   | 2.01                     | 0.43              |
| 7:d:115:LEU:HD23  | 7:d:152:LYS:HZ2   | 1.84                     | 0.43              |
| 7:d:122:PHE:CD2   | 7:d:136:LEU:HB2   | 2.53                     | 0.43              |
| 7:f:71:LYS:HE2    | 7:f:106:GLN:HG2   | 2.00                     | 0.43              |
| 7:g:84:LYS:HB2    | 7:g:168:PRO:HD3   | 2.00                     | 0.43              |
| 7:m:130:PRO:HD2   | 7:m:131:TRP:CE3   | 2.53                     | 0.43              |
| 7:n:146:ARG:HD2   | 7:n:146:ARG:HA    | 1.75                     | 0.43              |
| 7:n:146:ARG:NH2   | 7:n:158:THR:HA    | 2.33                     | 0.43              |
| 7:v:165:THR:HB    | 7:v:182:PHE:HZ    | 1.83                     | 0.43              |
| 7:x:76:TYR:HA     | 7:x:169:SER:O     | 2.17                     | 0.43              |
| 1:A:246:CYS:O     | 1:A:250:GLU:HG2   | 2.19                     | 0.43              |
| 2:A0:104:ALA:HB2  | 2:A0:413:MET:HG2  | 2.00                     | 0.43              |
| 3:A3:169:VAL:HG12 | 3:A3:202:ILE:HB   | 2.01                     | 0.43              |
| 3:A5:152:ILE:HA   | 3:A5:164:MET:HE1  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A8:211:ASP:HA   | 2:A8:214:ARG:HE   | 1.84                     | 0.43              |
| 3:B1:73:MET:HE3   | 3:B1:90:PHE:HD1   | 1.83                     | 0.43              |
| 2:B6:401:LYS:HE3  | 3:B7:344:TRP:CD2  | 2.52                     | 0.43              |
| 3:C1:171:PRO:HB3  | 3:C1:181:GLU:CD   | 2.44                     | 0.43              |
| 3:C1:316:MET:HA   | 3:C1:352:SER:HB3  | 2.00                     | 0.43              |
| 3:C3:105:HIS:CD2  | 3:C3:150:LEU:HD13 | 2.53                     | 0.43              |
| 2:C6:274:PRO:HB2  | 2:C6:276:ILE:HG23 | 1.99                     | 0.43              |
| 3:C7:101:TRP:HB2  | 3:C7:184:ASN:HB3  | 2.00                     | 0.43              |
| 2:C8:28:HIS:HB2   | 2:C8:30:ILE:HG12  | 2.00                     | 0.43              |
| 1:D:253:ALA:HA    | 2:D6:26:LEU:HD13  | 2.00                     | 0.43              |
| 2:D0:326:LYS:HG3  | 2:D0:327:ASP:N    | 2.32                     | 0.43              |
| 3:E3:39:ASP:HA    | 7:t:90:PRO:HG3    | 2.00                     | 0.43              |
| 2:E4:26:LEU:HD12  | 2:E4:363:VAL:HG12 | 2.00                     | 0.43              |
| 2:E4:111:GLY:HA2  | 2:E4:114:ILE:HG22 | 1.99                     | 0.43              |
| 2:E4:274:PRO:HG2  | 2:E4:374:ALA:HA   | 2.00                     | 0.43              |
| 3:E7:202:ILE:HG21 | 3:E7:229:VAL:HG22 | 2.00                     | 0.43              |
| 2:F0:335:ILE:HB   | 2:F0:341:ILE:HD11 | 1.99                     | 0.43              |
| 2:F0:336:LYS:HD3  | 2:F0:343:PHE:HE2  | 1.84                     | 0.43              |
| 4:W:1317:ARG:HD3  | 4:W:1317:ARG:HA   | 1.85                     | 0.43              |
| 7:b:153:GLU:HA    | 7:b:164:ARG:NH2   | 2.32                     | 0.43              |
| 7:d:26:ALA:HA     | 7:d:36:ILE:HD12   | 1.99                     | 0.43              |
| 7:q:77:PHE:CG     | 7:q:150:VAL:HG11  | 2.53                     | 0.43              |
| 3:A1:273:LEU:HD23 | 3:A1:273:LEU:HA   | 1.86                     | 0.43              |
| 3:A1:362:LYS:HB2  | 5:O:234:TYR:HB2   | 2.00                     | 0.43              |
| 3:A3:309:ARG:HD3  | 3:A3:342:VAL:HA   | 2.01                     | 0.43              |
| 2:A4:313:MET:HG2  | 2:A4:344:VAL:HG11 | 2.00                     | 0.43              |
| 2:A6:264:ARG:HH12 | 2:A6:427:ALA:HB1  | 1.83                     | 0.43              |
| 3:A9:132:GLY:HA2  | 3:A9:162:ARG:HB3  | 2.00                     | 0.43              |
| 3:A9:215:LEU:HD11 | 3:A9:273:LEU:HB3  | 1.99                     | 0.43              |
| 3:B1:20:PHE:HA    | 3:B1:230:SER:HB2  | 2.00                     | 0.43              |
| 3:B5:131:GLN:HE22 | 3:B5:250:LEU:HB2  | 1.82                     | 0.43              |
| 2:B6:64:ARG:HH21  | 2:B6:128:ASN:HD21 | 1.67                     | 0.43              |
| 3:B7:68:LEU:HD23  | 3:B7:112:LEU:HD13 | 2.00                     | 0.43              |
| 3:B9:19:LYS:HD2   | 3:B9:22:GLU:HG3   | 1.99                     | 0.43              |
| 3:C7:66:MET:HG3   | 3:C7:116:VAL:HG21 | 2.00                     | 0.43              |
| 2:C8:388:PHE:HB3  | 2:C8:425:LEU:HD11 | 2.01                     | 0.43              |
| 3:D1:268:ILE:HG23 | 3:D1:300:MET:HE3  | 2.01                     | 0.43              |
| 2:D2:73:THR:HG23  | 3:D3:247:ASN:HD22 | 1.83                     | 0.43              |
| 2:D4:310:GLY:HA3  | 2:D4:383:ALA:HB2  | 1.99                     | 0.43              |
| 2:D6:154:LEU:HA   | 2:D6:154:LEU:HD23 | 1.78                     | 0.43              |
| 2:E0:48:ALA:N     | 5:O:558:ARG:HD3   | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E0:141:VAL:HG21 | 2:E0:172:TRP:CE3  | 2.53                     | 0.43              |
| 2:E8:70:LEU:HA    | 2:E8:95:GLY:HA3   | 2.00                     | 0.43              |
| 2:E8:297:GLU:HB3  | 2:E8:300:SER:HB2  | 2.00                     | 0.43              |
| 5:O:516:ASP:OD1   | 5:O:520:LEU:HA    | 2.19                     | 0.43              |
| 4:Q:1215:ARG:HD3  | 4:Q:1293:TYR:CE2  | 2.53                     | 0.43              |
| 7:c:75:LEU:HD11   | 7:c:144:LEU:HD13  | 2.01                     | 0.43              |
| 7:x:96:TYR:O      | 7:x:100:ASN:HB2   | 2.19                     | 0.43              |
| 1:A:235:LEU:HD23  | 1:A:236:PRO:HD2   | 2.00                     | 0.43              |
| 3:A1:233:MET:HE3  | 3:A1:233:MET:HB3  | 1.90                     | 0.43              |
| 2:A2:133:GLN:NE2  | 2:A2:252:VAL:HB   | 2.28                     | 0.43              |
| 2:A2:222:PRO:C    | 3:A3:324:LYS:HE2  | 2.44                     | 0.43              |
| 2:A2:320:ARG:O    | 2:A2:373:ARG:HA   | 2.19                     | 0.43              |
| 2:A4:63:PRO:HD2   | 2:A4:86:LEU:O     | 2.18                     | 0.43              |
| 3:A5:149:THR:HA   | 3:A5:152:ILE:HD12 | 2.01                     | 0.43              |
| 2:A6:283:HIS:HE1  | 2:B0:85:HIS:O     | 2.01                     | 0.43              |
| 1:B:231:VAL:H     | 5:P:507:ARG:HH22  | 1.66                     | 0.43              |
| 3:B3:28:HIS:HA    | 3:B3:43:GLN:HG2   | 2.01                     | 0.43              |
| 3:B7:207:LEU:HB3  | 3:B7:225:LEU:HG   | 1.99                     | 0.43              |
| 3:C3:318:ARG:NE   | 3:C3:358:PRO:HD3  | 2.32                     | 0.43              |
| 2:C6:401:LYS:HD2  | 3:C7:344:TRP:CD1  | 2.52                     | 0.43              |
| 3:C7:110:ALA:HB2  | 3:C7:150:LEU:HD21 | 2.01                     | 0.43              |
| 2:C8:4:VAL:HG21   | 2:C8:136:LEU:HD13 | 2.00                     | 0.43              |
| 2:C8:68:LEU:HG    | 2:C8:149:LEU:HD21 | 2.00                     | 0.43              |
| 2:C8:103:PHE:HB2  | 2:C8:186:ASN:HD22 | 1.84                     | 0.43              |
| 2:C8:259:LEU:HD13 | 2:C8:268:MET:HE2  | 2.00                     | 0.43              |
| 3:C9:152:ILE:HG22 | 3:C9:164:MET:HE1  | 2.01                     | 0.43              |
| 1:D:215:TYR:CD1   | 2:D8:22:GLU:HB3   | 2.52                     | 0.43              |
| 3:D1:50:PHE:HD2   | 3:D1:241:ARG:HD3  | 1.82                     | 0.43              |
| 2:D4:285:GLN:HB3  | 2:D8:56:THR:HA    | 2.01                     | 0.43              |
| 3:D5:7:VAL:HG22   | 3:D5:64:ILE:HB    | 2.01                     | 0.43              |
| 3:D5:382:SER:HB2  | 3:D5:415:MET:HG2  | 2.01                     | 0.43              |
| 3:D7:379:LYS:HD3  | 3:D7:379:LYS:HA   | 1.81                     | 0.43              |
| 2:F0:101:ASN:HB3  | 2:F0:182:VAL:HG21 | 2.01                     | 0.43              |
| 3:F1:238:CYS:SG   | 3:F1:316:MET:HE2  | 2.59                     | 0.43              |
| 4:W:1269:LEU:HA   | 4:W:1272:ILE:HD12 | 2.00                     | 0.43              |
| 7:a:174:GLY:HA3   | 7:a:178:ARG:HE    | 1.84                     | 0.43              |
| 7:c:12:VAL:HG12   | 7:c:15:ARG:NH2    | 2.33                     | 0.43              |
| 7:e:68:LEU:HD23   | 7:e:73:VAL:HG21   | 2.01                     | 0.43              |
| 7:f:72:SER:O      | 7:f:108:ILE:HA    | 2.17                     | 0.43              |
| 7:i:96:TYR:HA     | 7:i:108:ILE:HD11  | 2.00                     | 0.43              |
| 7:n:140:LEU:HG    | 7:n:144:LEU:HD23  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:q:183:LEU:HD13  | 7:q:196:LEU:HA    | 1.99                     | 0.43              |
| 7:u:55:LEU:HD23   | 7:u:132:LEU:HD23  | 2.01                     | 0.43              |
| 7:u:69:LYS:NZ     | 7:w:38:LEU:HB3    | 2.34                     | 0.43              |
| 7:v:4:PRO:HG3     | 7:v:179:GLU:HB2   | 2.01                     | 0.43              |
| 2:A0:188:VAL:HG12 | 2:A0:421:ALA:HB1  | 1.99                     | 0.43              |
| 3:A1:49:VAL:HG13  | 3:A1:50:PHE:CD2   | 2.54                     | 0.43              |
| 3:A1:221:THR:HG21 | 5:O:219:LEU:HA    | 2.00                     | 0.43              |
| 3:A1:309:ARG:HG3  | 3:A1:426:GLN:HA   | 2.00                     | 0.43              |
| 2:A4:167:LEU:HG   | 2:A4:200:VAL:HB   | 2.01                     | 0.43              |
| 2:B2:156:ARG:HA   | 2:B2:159:VAL:HG12 | 2.00                     | 0.43              |
| 3:B3:39:ASP:HA    | 7:e:90:PRO:HG3    | 2.00                     | 0.43              |
| 3:B3:330:MET:SD   | 3:B3:349:MET:HE2  | 2.58                     | 0.43              |
| 3:B5:21:TRP:HZ3   | 3:B5:50:PHE:HB3   | 1.83                     | 0.43              |
| 2:B6:31:GLN:HE22  | 2:B6:37:PRO:HD3   | 1.84                     | 0.43              |
| 3:B7:330:MET:HB2  | 3:B7:330:MET:HE2  | 1.78                     | 0.43              |
| 2:C0:181:VAL:HG22 | 3:C1:256:ASN:OD1  | 2.18                     | 0.43              |
| 3:C3:135:ILE:HG21 | 3:C3:152:ILE:HG21 | 2.01                     | 0.43              |
| 3:C5:47:ILE:HG22  | 3:C5:51:TYR:HB2   | 2.01                     | 0.43              |
| 2:C6:397:LEU:HD11 | 3:C7:346:PRO:HD3  | 2.00                     | 0.43              |
| 3:C7:165:GLU:HB2  | 3:C7:250:LEU:HD21 | 2.01                     | 0.43              |
| 2:C8:265:ILE:HG23 | 2:C8:432:TYR:HE2  | 1.84                     | 0.43              |
| 3:C9:282:ARG:HH12 | 3:C9:292:GLN:NE2  | 2.17                     | 0.43              |
| 2:D0:221:ARG:HG2  | 3:D1:325:GLU:OE2  | 2.18                     | 0.43              |
| 3:D3:16:ILE:HD11  | 3:D3:229:VAL:HG11 | 2.00                     | 0.43              |
| 3:D3:286:VAL:HB   | 3:D3:325:GLU:HG2  | 2.00                     | 0.43              |
| 2:D6:14:ILE:HD11  | 2:D6:69:ASP:HB2   | 2.00                     | 0.43              |
| 2:D6:82:THR:HB    | 2:D6:83:TYR:CE2   | 2.54                     | 0.43              |
| 2:D8:195:LEU:HD22 | 2:D8:428:LEU:HD12 | 2.01                     | 0.43              |
| 3:E7:239:CYS:HB3  | 3:E7:248:SER:H    | 1.83                     | 0.43              |
| 2:E8:209:ILE:HB   | 2:E8:227:LEU:HD22 | 2.01                     | 0.43              |
| 3:E9:237:THR:HG23 | 3:E9:241:ARG:HH11 | 1.84                     | 0.43              |
| 4:L:1405:LEU:HA   | 4:L:1408:GLN:HB2  | 2.01                     | 0.43              |
| 4:V:1439:MET:HE3  | 4:V:1439:MET:HB3  | 1.78                     | 0.43              |
| 7:b:149:ARG:HD2   | 7:b:149:ARG:HA    | 1.86                     | 0.43              |
| 2:A4:71:GLU:HG3   | 2:A4:73:THR:HG22  | 2.00                     | 0.43              |
| 2:A4:169:PHE:CD1  | 2:A4:202:VAL:HG12 | 2.54                     | 0.43              |
| 2:A4:338:LYS:HD2  | 2:A4:339:ARG:N    | 2.33                     | 0.43              |
| 3:A7:124:ALA:HB1  | 3:A7:130:LEU:HD22 | 2.01                     | 0.43              |
| 3:B1:200:GLN:HG3  | 3:B1:266:PHE:HB2  | 2.00                     | 0.43              |
| 2:B2:275:ILE:HG22 | 2:B2:368:LEU:HD21 | 2.00                     | 0.43              |
| 3:B5:73:MET:HA    | 3:B5:76:VAL:HG12  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B8:8:HIS:CE1    | 2:B8:17:GLY:HA3   | 2.53                     | 0.43              |
| 2:B8:36:MET:HG2   | 2:B8:61:HIS:CE1   | 2.53                     | 0.43              |
| 2:B8:80:THR:HA    | 2:B8:84:ARG:NH1   | 2.34                     | 0.43              |
| 2:B8:259:LEU:HD21 | 2:B8:316:CYS:HB2  | 1.99                     | 0.43              |
| 2:C2:221:ARG:HG3  | 3:C3:325:GLU:HB2  | 2.01                     | 0.43              |
| 3:C7:389:PHE:HE1  | 3:C7:408:PHE:HB3  | 1.84                     | 0.43              |
| 2:C8:222:PRO:C    | 3:C9:324:LYS:HE2  | 2.44                     | 0.43              |
| 3:D5:298:ASN:O    | 3:D5:299:MET:HE2  | 2.19                     | 0.43              |
| 2:D6:88:HIS:ND1   | 2:D6:89:PRO:HD2   | 2.34                     | 0.43              |
| 2:E2:132:LEU:HB3  | 2:E2:164:LYS:HD2  | 2.01                     | 0.43              |
| 3:E5:252:LYS:HB3  | 3:E5:350:LYS:HZ1  | 1.84                     | 0.43              |
| 2:E8:259:LEU:HD21 | 2:E8:316:CYS:HB2  | 2.00                     | 0.43              |
| 2:F0:121:ARG:HD2  | 2:F0:121:ARG:HA   | 1.77                     | 0.43              |
| 4:N:1256:ILE:HG12 | 4:N:1445:LEU:HB2  | 2.01                     | 0.43              |
| 7:h:115:LEU:HD23  | 7:h:115:LEU:HA    | 1.81                     | 0.43              |
| 7:j:75:LEU:HD23   | 7:j:111:ILE:HB    | 2.01                     | 0.43              |
| 8:l:37:PHE:CE1    | 8:l:53:VAL:HG11   | 2.53                     | 0.43              |
| 2:A0:22:GLU:HG2   | 5:O:241:ARG:HH12  | 1.84                     | 0.43              |
| 2:A0:88:HIS:HB3   | 2:A0:91:GLN:HB2   | 2.00                     | 0.43              |
| 3:A1:23:VAL:HG11  | 3:A1:230:SER:HB3  | 2.01                     | 0.43              |
| 3:A1:281:TYR:CD2  | 3:A5:87:PRO:HD3   | 2.53                     | 0.43              |
| 3:A3:337:ASN:HB3  | 3:A3:340:TYR:HB2  | 2.01                     | 0.43              |
| 2:A4:280:LYS:HB3  | 2:A8:89:PRO:HG3   | 2.01                     | 0.43              |
| 2:A8:395:PHE:HE2  | 2:A8:422:ARG:HB2  | 1.84                     | 0.43              |
| 3:B5:375:GLN:HG2  | 3:B5:379:LYS:HE3  | 1.99                     | 0.43              |
| 3:B7:295:ASP:HB3  | 3:B7:297:LYS:HG2  | 2.01                     | 0.43              |
| 3:B9:281:TYR:CD2  | 3:C3:87:PRO:HD3   | 2.53                     | 0.43              |
| 3:B9:304:ASP:HA   | 3:B9:305:PRO:HD3  | 1.91                     | 0.43              |
| 2:C0:3:GLU:HG3    | 2:C0:64:ARG:NH2   | 2.34                     | 0.43              |
| 2:C0:291:ILE:HD12 | 2:C0:375:VAL:HG13 | 2.00                     | 0.43              |
| 3:C7:162:ARG:HH22 | 3:C7:251:ARG:HH21 | 1.67                     | 0.43              |
| 3:C9:42:LEU:HD13  | 3:C9:356:ILE:HD11 | 2.00                     | 0.43              |
| 3:C9:107:THR:HG22 | 3:C9:108:GLU:H    | 1.84                     | 0.43              |
| 2:D6:360:PRO:HG3  | 2:D6:374:ALA:HB2  | 2.01                     | 0.43              |
| 3:D7:85:PHE:HB2   | 3:D7:90:PHE:HE1   | 1.84                     | 0.43              |
| 2:D8:76:ASP:HA    | 2:D8:79:ARG:HE    | 1.83                     | 0.43              |
| 2:E0:8:HIS:HD2    | 2:E0:138:PHE:HB2  | 1.83                     | 0.43              |
| 2:E2:70:LEU:HD12  | 2:E2:99:ALA:HB2   | 2.01                     | 0.43              |
| 3:E3:248:SER:HB2  | 3:E3:252:LYS:HG2  | 2.01                     | 0.43              |
| 3:E3:336:LYS:HE3  | 3:E3:336:LYS:HB3  | 1.71                     | 0.43              |
| 3:F1:337:ASN:HB3  | 3:F1:340:TYR:HB2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:231:PRO:HA    | 6:R:55:ASP:HA     | 2.01                     | 0.43              |
| 7:c:184:PRO:HG3   | 7:c:189:LEU:HD23  | 2.01                     | 0.43              |
| 8:l:25:ARG:HE     | 7:n:23:LEU:HD12   | 1.84                     | 0.43              |
| 7:o:113:VAL:HG12  | 7:o:134:ILE:HB    | 2.00                     | 0.43              |
| 7:o:189:LEU:HD23  | 7:o:189:LEU:HA    | 1.88                     | 0.43              |
| 2:A0:326:LYS:HD3  | 2:A0:326:LYS:HA   | 1.66                     | 0.42              |
| 2:A4:35:GLN:HA    | 2:A4:59:GLY:HA3   | 2.02                     | 0.42              |
| 2:A4:285:GLN:HB2  | 2:A8:56:THR:HA    | 2.01                     | 0.42              |
| 2:A4:385:ALA:HB2  | 2:A4:432:TYR:CD2  | 2.54                     | 0.42              |
| 3:A5:395:LEU:HA   | 3:A5:395:LEU:HD23 | 1.78                     | 0.42              |
| 3:A9:77:ARG:HH22  | 3:A9:92:PHE:HZ    | 1.67                     | 0.42              |
| 3:A9:391:ARG:HD3  | 2:B0:346:TRP:CG   | 2.54                     | 0.42              |
| 2:B0:64:ARG:HA    | 2:B0:125:LEU:HD11 | 2.01                     | 0.42              |
| 2:C0:161:TYR:HB3  | 2:C0:164:LYS:HG2  | 2.01                     | 0.42              |
| 2:C2:388:PHE:HB3  | 2:C2:425:LEU:HD11 | 2.01                     | 0.42              |
| 3:C5:67:ASP:HA    | 3:C5:143:THR:HG21 | 2.00                     | 0.42              |
| 2:C6:324:VAL:HG12 | 2:C6:326:LYS:HG2  | 2.00                     | 0.42              |
| 3:C7:9:GLY:HA3    | 3:C7:66:MET:HE2   | 2.00                     | 0.42              |
| 3:C9:20:PHE:HA    | 3:C9:230:SER:HB2  | 2.00                     | 0.42              |
| 3:C9:224:ASP:HB3  | 5:P:487:THR:HG23  | 2.00                     | 0.42              |
| 2:D6:219:ILE:HG13 | 7:s:198:ARG:HH21  | 1.84                     | 0.42              |
| 2:D6:255:PHE:O    | 2:D6:259:LEU:HB2  | 2.19                     | 0.42              |
| 3:D7:2:ARG:HB3    | 3:D7:131:GLN:HB2  | 2.01                     | 0.42              |
| 3:D7:112:LEU:HB3  | 3:D7:147:MET:HE1  | 2.01                     | 0.42              |
| 3:D7:204:ASN:HA   | 3:D7:207:LEU:HD12 | 2.01                     | 0.42              |
| 3:D7:367:PHE:HE1  | 3:D7:369:GLY:HA3  | 1.84                     | 0.42              |
| 2:D8:286:LEU:HD23 | 2:D8:286:LEU:HA   | 1.87                     | 0.42              |
| 2:D8:306:ASP:HA   | 2:D8:307:PRO:HD3  | 1.86                     | 0.42              |
| 3:D9:46:ARG:HG2   | 3:D9:240:LEU:O    | 2.19                     | 0.42              |
| 2:E0:109:THR:HG23 | 2:E0:110:ILE:HG23 | 2.01                     | 0.42              |
| 3:E3:265:PHE:HB2  | 3:E3:374:ILE:HD12 | 2.01                     | 0.42              |
| 3:E7:359:LYS:HD3  | 3:E7:359:LYS:HA   | 1.86                     | 0.42              |
| 8:l:37:PHE:CE2    | 8:l:39:ALA:HB2    | 2.54                     | 0.42              |
| 7:o:184:PRO:HG3   | 7:o:189:LEU:HD12  | 2.01                     | 0.42              |
| 7:s:15:ARG:O      | 7:s:19:GLU:HG3    | 2.19                     | 0.42              |
| 7:v:170:VAL:HG23  | 7:v:183:LEU:HB2   | 2.00                     | 0.42              |
| 7:w:93:LEU:HB3    | 7:w:97:ARG:HH12   | 1.83                     | 0.42              |
| 2:A8:237:SER:HA   | 2:A8:320:ARG:HD2  | 2.01                     | 0.42              |
| 2:B0:362:VAL:HG13 | 2:B0:368:LEU:HD12 | 2.01                     | 0.42              |
| 3:B3:256:ASN:ND2  | 3:B3:350:LYS:HE3  | 2.33                     | 0.42              |
| 2:B6:112:LYS:HA   | 2:B6:115:VAL:HG12 | 1.99                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B9:28:HIS:HA    | 3:B9:43:GLN:HG2   | 2.01                     | 0.42              |
| 3:C7:372:THR:HG21 | 3:C7:426:GLN:HB2  | 2.01                     | 0.42              |
| 3:C9:164:MET:HE2  | 3:C9:164:MET:HB2  | 1.81                     | 0.42              |
| 2:D0:12:ALA:HB3   | 2:D0:140:ALA:HB2  | 2.01                     | 0.42              |
| 3:D3:317:PHE:CD2  | 3:D3:321:MET:HE1  | 2.54                     | 0.42              |
| 2:D4:237:SER:HA   | 2:D4:320:ARG:HH11 | 1.83                     | 0.42              |
| 2:D6:304:LYS:HD2  | 2:D6:304:LYS:HA   | 1.83                     | 0.42              |
| 2:E6:388:PHE:HB3  | 2:E6:425:LEU:HD11 | 2.00                     | 0.42              |
| 3:E7:100:ASN:HB3  | 3:E7:103:LYS:HB2  | 2.00                     | 0.42              |
| 3:E9:267:LEU:HB3  | 3:E9:299:MET:SD   | 2.59                     | 0.42              |
| 2:F0:79:ARG:HE    | 2:F0:92:LEU:HB3   | 1.83                     | 0.42              |
| 4:W:1388:LEU:HD22 | 4:W:1392:PHE:HD2  | 1.83                     | 0.42              |
| 7:c:144:LEU:HD23  | 7:c:144:LEU:HA    | 1.91                     | 0.42              |
| 7:u:75:LEU:O      | 7:u:170:VAL:HA    | 2.19                     | 0.42              |
| 1:A:234:LYS:HA    | 1:A:234:LYS:HD2   | 1.82                     | 0.42              |
| 2:A0:2:ARG:HG3    | 2:A0:51:THR:HB    | 2.01                     | 0.42              |
| 2:A4:217:LEU:HD11 | 2:A4:275:ILE:HG22 | 2.00                     | 0.42              |
| 2:A6:7:ILE:HG21   | 2:A6:153:LEU:HD21 | 2.01                     | 0.42              |
| 2:A6:248:LEU:HD23 | 2:A6:355:ILE:HD13 | 2.00                     | 0.42              |
| 3:B3:293:MET:HA   | 3:B3:298:ASN:HD22 | 1.83                     | 0.42              |
| 3:B7:318:ARG:HD3  | 3:B7:358:PRO:HD3  | 1.99                     | 0.42              |
| 2:B8:265:ILE:HG22 | 2:B8:380:ASN:HD21 | 1.84                     | 0.42              |
| 2:B8:268:MET:HE2  | 2:B8:378:ILE:HG22 | 2.02                     | 0.42              |
| 3:C3:34:GLY:HA3   | 3:C3:58:ARG:HB2   | 2.00                     | 0.42              |
| 2:C4:76:ASP:HA    | 2:C4:79:ARG:HB2   | 2.01                     | 0.42              |
| 2:C6:217:LEU:HD21 | 2:C6:275:ILE:HG22 | 2.01                     | 0.42              |
| 2:C6:280:LYS:HA   | 2:C6:280:LYS:HD3  | 1.83                     | 0.42              |
| 3:C9:163:ILE:HD11 | 3:C9:251:ARG:HB2  | 2.01                     | 0.42              |
| 2:D0:282:TYR:HB3  | 7:p:202:ARG:CZ    | 2.50                     | 0.42              |
| 2:D0:335:ILE:HG23 | 2:D0:341:ILE:HD13 | 2.01                     | 0.42              |
| 3:D1:100:ASN:HB3  | 3:D1:103:LYS:HD3  | 2.02                     | 0.42              |
| 2:D2:73:THR:HG23  | 3:D3:247:ASN:ND2  | 2.34                     | 0.42              |
| 3:D7:286:VAL:HG22 | 3:D7:363:MET:HE1  | 2.02                     | 0.42              |
| 2:E0:181:VAL:O    | 2:E0:398:MET:HE1  | 2.19                     | 0.42              |
| 5:P:489:LEU:HG    | 5:P:494:LEU:HA    | 2.01                     | 0.42              |
| 6:R:65:HIS:CG     | 6:R:66:PRO:HD3    | 2.54                     | 0.42              |
| 7:f:72:SER:HB3    | 7:f:108:ILE:HG22  | 2.00                     | 0.42              |
| 7:j:110:ILE:O     | 7:j:131:TRP:HB2   | 2.20                     | 0.42              |
| 7:m:112:PHE:CD1   | 7:m:129:MET:HE1   | 2.55                     | 0.42              |
| 7:o:78:ALA:O      | 7:o:114:SER:HA    | 2.19                     | 0.42              |
| 7:o:104:ALA:HB1   | 7:q:41:ASN:HD22   | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:s:53:GLY:HA2    | 7:s:62:VAL:HG21   | 2.00                     | 0.42              |
| 1:A:211:GLY:O     | 3:A7:356:ILE:HG13 | 2.18                     | 0.42              |
| 3:A1:47:ILE:HG22  | 3:A1:51:TYR:HB2   | 2.02                     | 0.42              |
| 2:A2:282:TYR:CE2  | 5:P:252:ALA:HA    | 2.54                     | 0.42              |
| 2:A4:28:HIS:HE2   | 2:A4:243:ARG:HD2  | 1.84                     | 0.42              |
| 3:A9:228:LEU:HB3  | 3:A9:300:MET:HE2  | 2.02                     | 0.42              |
| 3:B5:171:PRO:HB3  | 3:B5:181:GLU:HB3  | 1.99                     | 0.42              |
| 2:B6:335:ILE:HD11 | 2:B6:341:ILE:HG13 | 2.01                     | 0.42              |
| 3:C5:19:LYS:HG3   | 3:C5:226:ASN:HB2  | 2.02                     | 0.42              |
| 3:C5:375:GLN:HB3  | 3:C5:419:VAL:HG23 | 2.02                     | 0.42              |
| 2:C6:104:ALA:HA   | 2:C6:108:TYR:HD2  | 1.85                     | 0.42              |
| 2:C6:219:ILE:HG22 | 2:C6:221:ARG:H    | 1.84                     | 0.42              |
| 3:C7:159:TYR:HB3  | 3:C7:162:ARG:HG2  | 2.01                     | 0.42              |
| 2:C8:430:LYS:HA   | 2:C8:430:LYS:HD3  | 1.82                     | 0.42              |
| 2:D2:282:TYR:HB3  | 7:q:202:ARG:CZ    | 2.49                     | 0.42              |
| 3:E5:403:MET:HE3  | 3:E5:403:MET:HB2  | 1.78                     | 0.42              |
| 3:E9:156:ARG:HH22 | 3:E9:197:ASP:HB2  | 1.83                     | 0.42              |
| 3:F1:289:LEU:HD22 | 3:F1:363:MET:HE2  | 2.01                     | 0.42              |
| 1:J:223:PRO:HG3   | 7:n:178:ARG:NH2   | 2.34                     | 0.42              |
| 4:M:1390:GLU:HA   | 4:M:1393:ILE:HG12 | 2.01                     | 0.42              |
| 4:V:1264:THR:H    | 4:V:1374:ARG:HH22 | 1.67                     | 0.42              |
| 7:c:37:GLN:C      | 7:c:37:GLN:HE21   | 2.28                     | 0.42              |
| 7:f:3:GLN:OE1     | 7:f:4:PRO:HA      | 2.20                     | 0.42              |
| 7:j:8:SER:HB3     | 7:j:11:ASN:HB2    | 2.01                     | 0.42              |
| 7:o:110:ILE:HB    | 7:o:131:TRP:CG    | 2.54                     | 0.42              |
| 7:s:99:MET:HE3    | 7:s:99:MET:HB3    | 1.65                     | 0.42              |
| 7:t:201:TRP:CD1   | 7:t:201:TRP:H     | 2.36                     | 0.42              |
| 2:A0:112:LYS:H    | 2:A0:112:LYS:HG2  | 1.70                     | 0.42              |
| 3:A1:282:ARG:HA   | 3:A5:86:ARG:HH12  | 1.84                     | 0.42              |
| 2:A2:225:THR:HG21 | 6:R:84:SER:HB3    | 2.01                     | 0.42              |
| 2:A4:70:LEU:HA    | 2:A4:95:GLY:HA3   | 2.02                     | 0.42              |
| 2:A4:133:GLN:HB3  | 2:A4:252:VAL:HG22 | 2.01                     | 0.42              |
| 3:A9:227:HIS:CD2  | 5:P:312:ILE:HG23  | 2.51                     | 0.42              |
| 2:B2:207:GLU:HA   | 2:B2:210:TYR:HB2  | 2.02                     | 0.42              |
| 2:B2:312:TYR:HE2  | 2:B2:341:ILE:HD11 | 1.84                     | 0.42              |
| 3:B3:4:ILE:HB     | 3:B3:50:PHE:HE1   | 1.84                     | 0.42              |
| 2:B4:248:LEU:HD23 | 2:B4:248:LEU:HA   | 1.90                     | 0.42              |
| 3:B7:383:ASP:HA   | 3:B7:386:THR:HG22 | 2.00                     | 0.42              |
| 2:B8:401:LYS:HE2  | 3:B9:344:TRP:CD2  | 2.54                     | 0.42              |
| 3:B9:171:PRO:HG2  | 3:B9:185:ALA:HB2  | 2.02                     | 0.42              |
| 3:C1:186:THR:HG22 | 3:C1:415:MET:HE2  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C2:168:ASN:HD22 | 2:C2:198:THR:HG21 | 1.83                     | 0.42              |
| 2:C2:215:ARG:HH21 | 2:C2:216:ASN:ND2  | 2.17                     | 0.42              |
| 2:C4:31:GLN:HA    | 1:J:256:LEU:HD21  | 2.02                     | 0.42              |
| 2:C4:405:VAL:HA   | 2:C4:408:TYR:HB2  | 2.00                     | 0.42              |
| 3:C5:8:GLN:HE21   | 3:C5:65:LEU:HG    | 1.84                     | 0.42              |
| 2:C6:102:ASN:HB3  | 2:C6:105:ARG:HB2  | 2.01                     | 0.42              |
| 2:C8:119:LEU:HD11 | 2:C8:156:ARG:HB3  | 2.01                     | 0.42              |
| 2:D0:181:VAL:HG22 | 2:D0:398:MET:HE1  | 2.00                     | 0.42              |
| 2:D4:173:PRO:HG2  | 2:D4:391:MET:HE2  | 2.02                     | 0.42              |
| 3:D5:253:LEU:HD11 | 3:D5:316:MET:HE1  | 2.01                     | 0.42              |
| 2:D6:99:ALA:HA    | 2:D6:110:ILE:HD11 | 2.01                     | 0.42              |
| 3:D7:276:ARG:HG2  | 5:P:548:PRO:HB2   | 2.01                     | 0.42              |
| 3:E5:237:THR:HG23 | 3:E5:241:ARG:HH21 | 1.84                     | 0.42              |
| 2:E8:320:ARG:HG3  | 2:E8:356:ASN:HD22 | 1.83                     | 0.42              |
| 4:M:1397:VAL:HG12 | 4:M:1401:ARG:NH1  | 2.35                     | 0.42              |
| 7:a:115:LEU:HD23  | 7:a:152:LYS:HG2   | 2.00                     | 0.42              |
| 7:d:97:ARG:HD3    | 7:f:161:TYR:HE1   | 1.84                     | 0.42              |
| 7:g:71:LYS:HE2    | 7:g:109:GLU:HB2   | 2.01                     | 0.42              |
| 7:q:175:SER:H     | 7:q:178:ARG:NH1   | 2.17                     | 0.42              |
| 3:A1:215:LEU:HD11 | 3:A1:273:LEU:HD22 | 2.01                     | 0.42              |
| 2:A4:318:MET:HE3  | 2:A4:318:MET:HB3  | 1.86                     | 0.42              |
| 3:A5:269:GLY:HA2  | 3:A5:300:MET:HE2  | 2.02                     | 0.42              |
| 3:A5:379:LYS:HA   | 3:A5:379:LYS:HD2  | 1.86                     | 0.42              |
| 3:A7:86:ARG:HA    | 3:A7:87:PRO:HD3   | 1.94                     | 0.42              |
| 3:B5:19:LYS:HD3   | 3:B5:19:LYS:HA    | 1.84                     | 0.42              |
| 3:B5:269:GLY:H    | 3:B5:367:PHE:HB3  | 1.85                     | 0.42              |
| 2:B6:271:SER:HB3  | 2:B6:377:MET:HB3  | 2.02                     | 0.42              |
| 3:B7:131:GLN:HE22 | 3:B7:249:ASP:HB2  | 1.84                     | 0.42              |
| 2:C0:119:LEU:HA   | 2:C0:122:ILE:HB   | 2.01                     | 0.42              |
| 3:C3:299:MET:HG3  | 3:C3:305:PRO:HG2  | 2.02                     | 0.42              |
| 3:C7:207:LEU:HB3  | 3:C7:225:LEU:HG   | 2.00                     | 0.42              |
| 2:C8:363:VAL:HG23 | 2:C8:366:GLY:HA3  | 2.00                     | 0.42              |
| 3:C9:390:ARG:HG3  | 3:C9:391:ARG:HG3  | 2.01                     | 0.42              |
| 3:D1:281:TYR:HE2  | 3:D5:58:ARG:NH1   | 2.18                     | 0.42              |
| 3:D3:97:ALA:HB3   | 3:D3:143:THR:HB   | 2.01                     | 0.42              |
| 3:D3:267:LEU:HD22 | 3:D3:301:CYS:HB3  | 2.01                     | 0.42              |
| 2:E0:276:ILE:HD12 | 2:E0:286:LEU:HD11 | 2.02                     | 0.42              |
| 3:E3:286:VAL:HG11 | 3:E3:326:VAL:HA   | 2.01                     | 0.42              |
| 3:E9:8:GLN:HG2    | 3:E9:17:GLY:HA3   | 2.01                     | 0.42              |
| 2:F0:172:TRP:CD2  | 2:F0:173:PRO:HD2  | 2.54                     | 0.42              |
| 3:F1:149:THR:HA   | 3:F1:152:ILE:HD12 | 2.00                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F1:165:GLU:HG3 | 3:F1:198:GLU:HG2  | 2.02                     | 0.42              |
| 1:K:215:TYR:O    | 1:K:219:TYR:HB2   | 2.20                     | 0.42              |
| 4:W:1260:CYS:SG  | 4:W:1286:ARG:HB2  | 2.59                     | 0.42              |
| 7:i:71:LYS:HG2   | 7:i:107:LYS:HA    | 2.00                     | 0.42              |
| 7:i:149:ARG:HH12 | 7:i:164:ARG:HD3   | 1.84                     | 0.42              |
| 8:k:14:LYS:HD3   | 8:k:96:GLU:OE2    | 2.20                     | 0.42              |
| 8:k:35:ALA:HB2   | 8:k:133:VAL:HG12  | 2.01                     | 0.42              |
| 7:v:89:LEU:HD11  | 7:v:129:MET:HG2   | 2.01                     | 0.42              |
| 2:A2:21:TRP:CZ3  | 2:A2:52:PHE:HB3   | 2.55                     | 0.42              |
| 2:A2:32:PRO:HG3  | 2:A2:83:TYR:HE1   | 1.85                     | 0.42              |
| 2:A6:207:GLU:HA  | 2:A6:210:TYR:HB2  | 2.01                     | 0.42              |
| 2:A8:403:ALA:HB2 | 3:A9:344:TRP:HZ3  | 1.85                     | 0.42              |
| 3:A9:159:TYR:HB3 | 3:A9:162:ARG:HG2  | 2.01                     | 0.42              |
| 2:B0:267:PHE:HE2 | 2:B0:428:LEU:HD21 | 1.84                     | 0.42              |
| 3:B7:105:HIS:CE1 | 3:B7:150:LEU:HD12 | 2.55                     | 0.42              |
| 2:C0:10:GLY:O    | 2:C0:14:ILE:HG12  | 2.20                     | 0.42              |
| 2:C2:133:GLN:HG3 | 2:C2:252:VAL:HB   | 2.02                     | 0.42              |
| 3:C3:20:PHE:CE2  | 3:C3:233:MET:HG2  | 2.54                     | 0.42              |
| 2:C8:108:TYR:HE2 | 2:C8:413:MET:HG2  | 1.85                     | 0.42              |
| 3:E1:135:ILE:HB  | 3:E1:166:THR:HG22 | 2.01                     | 0.42              |
| 3:E1:305:PRO:HB2 | 3:E1:310:TYR:CE1  | 2.55                     | 0.42              |
| 2:E4:381:SER:H   | 2:E4:384:ILE:HD12 | 1.84                     | 0.42              |
| 2:E6:338:LYS:HD3 | 2:E6:341:ILE:HD12 | 2.01                     | 0.42              |
| 3:E7:203:ASP:HB3 | 3:E7:377:MET:HE1  | 2.02                     | 0.42              |
| 2:E8:76:ASP:HA   | 2:E8:79:ARG:HB2   | 2.02                     | 0.42              |
| 3:E9:219:THR:HB  | 2:F0:324:VAL:HG21 | 2.01                     | 0.42              |
| 7:c:183:LEU:HD23 | 7:c:196:LEU:HA    | 2.02                     | 0.42              |
| 7:f:25:GLN:HE22  | 7:f:36:ILE:HD13   | 1.85                     | 0.42              |
| 7:i:14:LYS:HG3   | 7:i:47:LEU:HB2    | 2.01                     | 0.42              |
| 7:j:41:ASN:O     | 7:j:45:MET:HG3    | 2.20                     | 0.42              |
| 7:j:72:SER:HB3   | 7:j:108:ILE:HG22  | 2.02                     | 0.42              |
| 8:k:53:VAL:HA    | 8:k:154:LEU:HD21  | 2.01                     | 0.42              |
| 7:n:9:PRO:HB2    | 7:n:143:ILE:HG23  | 2.01                     | 0.42              |
| 7:n:112:PHE:HD2  | 7:n:133:SER:HB2   | 1.84                     | 0.42              |
| 7:p:139:PRO:O    | 7:p:143:ILE:HG12  | 2.20                     | 0.42              |
| 7:r:97:ARG:O     | 7:r:101:GLU:HB2   | 2.20                     | 0.42              |
| 7:t:7:ALA:HB3    | 7:t:161:TYR:HE2   | 1.85                     | 0.42              |
| 7:u:80:GLY:HA2   | 7:u:125:HIS:CD2   | 2.55                     | 0.42              |
| 1:A:254:LYS:HB3  | 2:A4:364:PRO:HG2  | 2.00                     | 0.42              |
| 3:A1:216:LYS:HE3 | 3:A1:216:LYS:HB3  | 1.87                     | 0.42              |
| 2:A2:28:HIS:CE1  | 2:A2:243:ARG:HD2  | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A3:279:GLN:HB3  | 5:P:231:PRO:HG3   | 2.01                     | 0.42              |
| 3:A5:268:ILE:N    | 3:A5:299:MET:HE1  | 2.32                     | 0.42              |
| 2:A6:2:ARG:NH2    | 2:A6:242:LEU:HA   | 2.35                     | 0.42              |
| 2:B2:107:HIS:HD2  | 2:B2:152:LEU:HB2  | 1.85                     | 0.42              |
| 3:B5:170:PHE:HD2  | 3:B5:201:VAL:HG13 | 1.85                     | 0.42              |
| 3:B5:405:GLU:HA   | 3:B5:408:PHE:CD1  | 2.55                     | 0.42              |
| 3:C1:265:PHE:HB3  | 3:C1:374:ILE:HD13 | 2.00                     | 0.42              |
| 3:C5:210:ILE:HG23 | 3:C5:214:THR:HB   | 2.01                     | 0.42              |
| 3:C5:326:VAL:HG13 | 3:C5:330:MET:HE3  | 2.02                     | 0.42              |
| 3:C5:380:ARG:NH1  | 3:C5:384:GLN:HE22 | 2.18                     | 0.42              |
| 3:C7:292:GLN:HG2  | 3:C7:298:ASN:ND2  | 2.34                     | 0.42              |
| 3:C7:406:MET:HE3  | 3:C7:406:MET:O    | 2.20                     | 0.42              |
| 2:C8:105:ARG:HA   | 2:C8:105:ARG:HD2  | 1.91                     | 0.42              |
| 3:D1:359:LYS:HG3  | 1:K:207:LEU:HD23  | 2.02                     | 0.42              |
| 3:D3:178:THR:H    | 2:D4:352:LYS:HA   | 1.84                     | 0.42              |
| 3:D3:279:GLN:HA   | 3:D3:282:ARG:HD2  | 2.02                     | 0.42              |
| 3:D7:171:PRO:HG2  | 3:D7:185:ALA:HB2  | 2.01                     | 0.42              |
| 3:D7:182:PRO:HG2  | 3:D7:388:MET:HE3  | 2.00                     | 0.42              |
| 2:D8:2:ARG:NH2    | 2:D8:48:ALA:HA    | 2.34                     | 0.42              |
| 2:D8:25:CYS:O     | 2:D8:30:ILE:HG22  | 2.20                     | 0.42              |
| 2:D8:28:HIS:CE1   | 2:D8:243:ARG:HH11 | 2.37                     | 0.42              |
| 2:D8:304:LYS:HD3  | 2:D8:304:LYS:HA   | 1.86                     | 0.42              |
| 3:E1:311:LEU:HD23 | 3:E1:342:VAL:HG21 | 2.01                     | 0.42              |
| 3:E3:291:GLN:NE2  | 3:E7:122:LYS:HB2  | 2.35                     | 0.42              |
| 2:E4:191:THR:HG21 | 2:E4:425:LEU:HD13 | 2.02                     | 0.42              |
| 3:E5:42:LEU:HD13  | 3:E5:356:ILE:HD11 | 2.02                     | 0.42              |
| 3:E5:132:GLY:HA2  | 3:E5:162:ARG:HB3  | 2.01                     | 0.42              |
| 3:E5:372:THR:O    | 3:E5:375:GLN:HG2  | 2.20                     | 0.42              |
| 2:F0:329:ASN:HA   | 2:F0:332:VAL:HG22 | 2.02                     | 0.42              |
| 3:F1:46:ARG:HD3   | 3:F1:46:ARG:HA    | 1.89                     | 0.42              |
| 1:I:247:TYR:O     | 1:I:251:TYR:HB2   | 2.19                     | 0.42              |
| 4:L:1286:ARG:HE   | 4:L:1289:ARG:HH21 | 1.67                     | 0.42              |
| 7:f:73:VAL:HA     | 7:f:109:GLU:O     | 2.20                     | 0.42              |
| 7:j:71:LYS:HD3    | 7:j:106:GLN:HE22  | 1.85                     | 0.42              |
| 7:p:56:LYS:HE2    | 7:p:56:LYS:HB2    | 1.91                     | 0.42              |
| 7:q:95:TYR:HA     | 7:q:98:THR:HG22   | 2.02                     | 0.42              |
| 7:u:97:ARG:NH1    | 7:w:149:ARG:HH22  | 2.17                     | 0.42              |
| 7:x:115:LEU:HD23  | 7:x:115:LEU:HA    | 1.68                     | 0.42              |
| 2:A4:340:THR:HG23 | 2:A4:341:ILE:HG23 | 2.02                     | 0.42              |
| 3:B3:7:VAL:O      | 3:B3:135:ILE:HA   | 2.20                     | 0.42              |
| 3:B3:112:LEU:HD23 | 3:B3:147:MET:HE2  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:244:GLN:HE22  | 1:C:249:SER:N     | 2.17                     | 0.42              |
| 3:C1:16:ILE:HD11  | 3:C1:229:VAL:HG11 | 2.02                     | 0.42              |
| 3:C1:207:LEU:HD21 | 3:C1:229:VAL:HG23 | 2.01                     | 0.42              |
| 3:C1:240:LEU:HD21 | 3:C1:249:ASP:HB2  | 2.00                     | 0.42              |
| 2:C2:76:ASP:HA    | 2:C2:79:ARG:HD2   | 2.01                     | 0.42              |
| 2:C2:96:LYS:HD2   | 2:C2:96:LYS:HA    | 1.76                     | 0.42              |
| 2:C2:184:PRO:HG2  | 2:C2:398:MET:HE1  | 2.01                     | 0.42              |
| 2:C2:227:LEU:O    | 2:C2:231:ILE:HG12 | 2.20                     | 0.42              |
| 3:C5:139:LEU:HD23 | 3:C5:145:SER:HA   | 2.02                     | 0.42              |
| 3:C9:237:THR:HG22 | 3:C9:250:LEU:HD11 | 2.02                     | 0.42              |
| 2:D0:310:GLY:HA3  | 2:D0:383:ALA:HB2  | 2.01                     | 0.42              |
| 2:D0:430:LYS:HA   | 2:D0:430:LYS:HD3  | 1.68                     | 0.42              |
| 3:D3:164:MET:HE3  | 3:D3:164:MET:HB3  | 1.85                     | 0.42              |
| 2:D6:269:LEU:HD22 | 2:D6:303:ALA:HB2  | 2.02                     | 0.42              |
| 2:D8:238:LEU:HA   | 2:D8:318:MET:SD   | 2.60                     | 0.42              |
| 2:D8:370:LYS:HB3  | 2:D8:370:LYS:HE3  | 1.80                     | 0.42              |
| 3:D9:97:ALA:HA    | 3:D9:103:LYS:HE3  | 2.02                     | 0.42              |
| 3:D9:278:SER:HB3  | 3:E3:87:PRO:HG2   | 2.02                     | 0.42              |
| 3:E3:215:LEU:HD11 | 3:E3:228:LEU:HD21 | 2.02                     | 0.42              |
| 3:E3:396:HIS:HA   | 3:E3:399:THR:HG22 | 2.01                     | 0.42              |
| 3:E5:36:TYR:HE1   | 7:u:90:PRO:HG2    | 1.84                     | 0.42              |
| 6:R:57:LYS:HA     | 6:R:57:LYS:HD3    | 1.82                     | 0.42              |
| 4:W:1441:LEU:HD23 | 4:W:1441:LEU:HA   | 1.90                     | 0.42              |
| 7:f:139:PRO:O     | 7:f:143:ILE:HG12  | 2.20                     | 0.42              |
| 3:A1:42:LEU:HB2   | 6:T:77:TYR:CD1    | 2.54                     | 0.42              |
| 3:A1:139:LEU:H    | 3:A1:139:LEU:HD12 | 1.84                     | 0.42              |
| 2:A2:268:MET:HG3  | 2:A2:380:ASN:HB2  | 2.01                     | 0.42              |
| 3:A3:22:GLU:HG2   | 3:A3:81:PHE:CD2   | 2.55                     | 0.42              |
| 3:A3:318:ARG:HD3  | 3:A3:358:PRO:HD3  | 2.02                     | 0.42              |
| 2:A8:77:GLU:HA    | 2:A8:80:THR:HG22  | 2.01                     | 0.42              |
| 2:B0:282:TYR:HD1  | 7:f:202:ARG:HD2   | 1.84                     | 0.42              |
| 2:B4:100:ALA:O    | 3:B5:255:VAL:HG11 | 2.19                     | 0.42              |
| 3:C1:240:LEU:HA   | 3:C1:240:LEU:HD23 | 1.90                     | 0.42              |
| 2:C2:81:GLY:HA3   | 1:I:215:TYR:HE2   | 1.84                     | 0.42              |
| 2:C8:395:PHE:HB3  | 2:C8:422:ARG:NH2  | 2.34                     | 0.42              |
| 3:C9:230:SER:HA   | 3:C9:233:MET:HE2  | 2.02                     | 0.42              |
| 3:D3:12:CYS:HB2   | 3:D3:138:SER:HB2  | 2.01                     | 0.42              |
| 2:D8:4:VAL:HB     | 2:D8:136:LEU:HD23 | 2.01                     | 0.42              |
| 2:E0:10:GLY:O     | 2:E0:14:ILE:HG12  | 2.20                     | 0.42              |
| 3:E1:7:VAL:HB     | 3:E1:135:ILE:HG13 | 2.02                     | 0.42              |
| 3:E1:289:LEU:HD11 | 3:E1:363:MET:HG3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E2:296:PHE:CE1  | 2:E2:335:ILE:HG21 | 2.55                     | 0.42              |
| 2:E2:297:GLU:HA   | 2:E2:298:PRO:HD3  | 1.93                     | 0.42              |
| 3:E3:271:ALA:HB1  | 3:E3:292:GLN:HB3  | 2.02                     | 0.42              |
| 2:F0:189:LEU:HD11 | 2:F0:418:PHE:HD1  | 1.84                     | 0.42              |
| 2:F0:209:ILE:HD13 | 2:F0:231:ILE:HD11 | 2.02                     | 0.42              |
| 7:a:66:SER:HA     | 7:a:69:LYS:NZ     | 2.35                     | 0.42              |
| 7:b:183:LEU:HD11  | 7:b:199:TRP:HE3   | 1.85                     | 0.42              |
| 7:g:55:LEU:HA     | 7:g:55:LEU:HD23   | 1.89                     | 0.42              |
| 7:q:9:PRO:HA      | 7:q:12:VAL:HG22   | 2.01                     | 0.42              |
| 7:v:14:LYS:HB2    | 7:v:47:LEU:HD23   | 2.01                     | 0.42              |
| 3:A1:229:VAL:O    | 3:A1:233:MET:HG2  | 2.20                     | 0.41              |
| 2:A2:70:LEU:HD22  | 2:A2:114:ILE:HD12 | 2.01                     | 0.41              |
| 3:A9:280:GLN:HG3  | 3:A9:281:TYR:CD1  | 2.54                     | 0.41              |
| 2:B0:107:HIS:CD2  | 2:B0:152:LEU:HB2  | 2.55                     | 0.41              |
| 3:B3:356:ILE:HD12 | 1:E:243:ALA:HB1   | 2.01                     | 0.41              |
| 3:B5:61:PRO:HD3   | 3:B5:84:LEU:HG    | 2.01                     | 0.41              |
| 3:B5:170:PHE:HE2  | 3:B5:201:VAL:HG22 | 1.84                     | 0.41              |
| 3:B7:395:LEU:HA   | 3:B7:395:LEU:HD12 | 1.82                     | 0.41              |
| 2:B8:132:LEU:HB3  | 2:B8:164:LYS:HE2  | 2.01                     | 0.41              |
| 2:B8:204:LEU:HD13 | 2:B8:231:ILE:HD12 | 2.01                     | 0.41              |
| 2:C0:402:ARG:HH22 | 2:C0:406:HIS:HB3  | 1.84                     | 0.41              |
| 2:C6:23:LEU:HD11  | 2:C6:233:GLN:NE2  | 2.35                     | 0.41              |
| 3:C9:274:THR:HG22 | 3:C9:282:ARG:HD3  | 2.00                     | 0.41              |
| 2:D0:200:VAL:HG13 | 2:D0:268:MET:HE2  | 2.02                     | 0.41              |
| 3:D1:7:VAL:HG11   | 3:D1:151:LEU:HD23 | 2.02                     | 0.41              |
| 3:D7:382:SER:HB3  | 3:D7:415:MET:HE1  | 2.02                     | 0.41              |
| 3:D9:84:LEU:HD12  | 3:D9:84:LEU:HA    | 1.90                     | 0.41              |
| 3:E1:19:LYS:HA    | 3:E1:19:LYS:HD3   | 1.90                     | 0.41              |
| 3:E3:103:LYS:HD3  | 3:E3:108:GLU:OE2  | 2.19                     | 0.41              |
| 3:E3:374:ILE:HD11 | 3:E3:422:TYR:CZ   | 2.55                     | 0.41              |
| 3:E5:271:ALA:HB1  | 3:E5:292:GLN:HB3  | 2.02                     | 0.41              |
| 3:E5:344:TRP:CD1  | 3:E5:345:ILE:HG13 | 2.55                     | 0.41              |
| 2:E6:10:GLY:O     | 2:E6:14:ILE:HG12  | 2.20                     | 0.41              |
| 3:E9:12:CYS:HB3   | 3:E9:138:SER:HB2  | 2.02                     | 0.41              |
| 3:E9:227:HIS:CD2  | 6:U:103:LEU:HD23  | 2.55                     | 0.41              |
| 2:F0:88:HIS:HA    | 2:F0:89:PRO:HD3   | 1.90                     | 0.41              |
| 5:O:223:ARG:H     | 5:O:223:ARG:HG2   | 1.65                     | 0.41              |
| 7:a:141:THR:O     | 7:a:145:LYS:HG2   | 2.20                     | 0.41              |
| 7:c:50:PHE:HB3    | 7:c:54:SER:HB2    | 2.02                     | 0.41              |
| 7:h:15:ARG:O      | 7:h:19:GLU:HG3    | 2.20                     | 0.41              |
| 7:s:64:PRO:HD2    | 7:s:67:HIS:CE1    | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A4:195:LEU:HD12 | 2:A4:428:LEU:HD13 | 2.02                     | 0.41              |
| 2:A6:174:SER:HB2  | 2:A6:177:VAL:HB   | 2.01                     | 0.41              |
| 2:A6:223:THR:OG1  | 2:A6:225:THR:HG22 | 2.20                     | 0.41              |
| 2:A8:52:PHE:HE2   | 2:A8:243:ARG:HH11 | 1.68                     | 0.41              |
| 2:A8:306:ASP:HB3  | 2:A8:309:HIS:CE1  | 2.56                     | 0.41              |
| 2:B0:242:LEU:HD11 | 2:B0:252:VAL:HG23 | 2.01                     | 0.41              |
| 3:B1:16:ILE:HG22  | 3:B1:226:ASN:CG   | 2.45                     | 0.41              |
| 3:B7:105:HIS:HD2  | 3:B7:106:TYR:CE1  | 2.38                     | 0.41              |
| 3:B7:187:LEU:HA   | 3:B7:190:HIS:CE1  | 2.54                     | 0.41              |
| 3:B7:213:ARG:H    | 3:B7:213:ARG:HD3  | 1.85                     | 0.41              |
| 2:B8:283:HIS:ND1  | 2:C2:60:LYS:HE3   | 2.35                     | 0.41              |
| 2:C0:273:ALA:H    | 2:C0:375:VAL:HG23 | 1.84                     | 0.41              |
| 2:C0:274:PRO:HD3  | 2:C0:375:VAL:HG22 | 2.03                     | 0.41              |
| 2:C4:209:ILE:HD11 | 2:C4:230:LEU:HB2  | 2.01                     | 0.41              |
| 2:C4:413:MET:HE3  | 2:C4:417:GLU:HG2  | 2.02                     | 0.41              |
| 2:C8:195:LEU:HD11 | 2:C8:264:ARG:HE   | 1.84                     | 0.41              |
| 1:D:251:TYR:HD2   | 2:D6:22:GLU:HG2   | 1.84                     | 0.41              |
| 3:D3:262:ARG:HG3  | 3:D3:263:LEU:H    | 1.85                     | 0.41              |
| 2:D4:181:VAL:HG22 | 3:D5:256:ASN:OD1  | 2.19                     | 0.41              |
| 2:D4:242:LEU:HD23 | 2:D4:242:LEU:HA   | 1.81                     | 0.41              |
| 3:D7:39:ASP:HA    | 7:q:90:PRO:HG3    | 2.02                     | 0.41              |
| 2:E0:11:GLN:O     | 2:E0:15:GLN:HG3   | 2.20                     | 0.41              |
| 2:E0:304:LYS:HD2  | 2:E0:304:LYS:HA   | 1.89                     | 0.41              |
| 3:E1:10:GLY:HA2   | 3:E1:143:THR:HG23 | 2.03                     | 0.41              |
| 3:E3:320:ARG:HH11 | 3:E3:355:ASP:HB2  | 1.85                     | 0.41              |
| 2:E4:204:LEU:HD12 | 2:E4:209:ILE:HD11 | 2.02                     | 0.41              |
| 3:E9:87:PRO:HA    | 3:E9:90:PHE:HD2   | 1.85                     | 0.41              |
| 3:F1:150:LEU:O    | 3:F1:154:LYS:HG3  | 2.19                     | 0.41              |
| 1:J:212:GLU:OE2   | 1:J:216:ARG:HB2   | 2.20                     | 0.41              |
| 7:b:74:ALA:HB2    | 7:b:199:TRP:CH2   | 2.55                     | 0.41              |
| 7:b:115:LEU:HB3   | 7:b:152:LYS:HD2   | 2.02                     | 0.41              |
| 7:b:170:VAL:HG13  | 7:b:183:LEU:HD12  | 2.00                     | 0.41              |
| 7:n:72:SER:HB3    | 7:n:199:TRP:HE1   | 1.85                     | 0.41              |
| 7:t:191:GLU:HG2   | 7:t:194:ARG:HH21  | 1.85                     | 0.41              |
| 2:A0:280:LYS:HZ3  | 2:A4:89:PRO:HG2   | 1.84                     | 0.41              |
| 3:A1:293:MET:HE2  | 3:A1:367:PHE:HD2  | 1.85                     | 0.41              |
| 2:A2:96:LYS:HD2   | 3:A3:2:ARG:HG3    | 2.01                     | 0.41              |
| 2:A4:188:VAL:HG21 | 2:A4:395:PHE:HB2  | 2.03                     | 0.41              |
| 3:C1:150:LEU:O    | 3:C1:154:LYS:HG2  | 2.20                     | 0.41              |
| 3:C1:313:ALA:HA   | 3:C1:369:GLY:HA2  | 2.02                     | 0.41              |
| 3:C3:61:PRO:HD3   | 3:C3:84:LEU:HG    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C8:407:TRP:HH2  | 3:C9:258:ILE:HB   | 1.85                     | 0.41              |
| 1:D:215:TYR:CE2   | 2:D8:83:TYR:HD2   | 2.38                     | 0.41              |
| 2:D0:167:LEU:HD13 | 2:D0:200:VAL:HB   | 2.01                     | 0.41              |
| 2:D0:383:ALA:O    | 2:D0:386:GLU:HG3  | 2.20                     | 0.41              |
| 3:D1:57:GLY:HA3   | 7:n:83:PRO:HB2    | 2.03                     | 0.41              |
| 2:D4:259:LEU:HD13 | 2:D4:316:CYS:HB2  | 2.01                     | 0.41              |
| 3:D5:377:MET:HE2  | 3:D5:377:MET:HB2  | 1.77                     | 0.41              |
| 2:D6:64:ARG:HA    | 2:D6:125:LEU:HD11 | 2.02                     | 0.41              |
| 2:D6:320:ARG:HE   | 2:D6:356:ASN:HD22 | 1.67                     | 0.41              |
| 3:E3:7:VAL:HB     | 3:E3:135:ILE:HG13 | 2.01                     | 0.41              |
| 3:E3:36:TYR:HE2   | 7:t:90:PRO:HG2    | 1.86                     | 0.41              |
| 2:E8:30:ILE:HG13  | 2:E8:34:GLY:HA2   | 2.01                     | 0.41              |
| 4:N:1287:MET:HG3  | 4:N:1444:TRP:CZ2  | 2.55                     | 0.41              |
| 5:O:523:ASP:OD1   | 5:O:525:VAL:HG13  | 2.20                     | 0.41              |
| 5:P:305:ARG:HA    | 5:P:308:TRP:CD1   | 2.56                     | 0.41              |
| 5:P:490:HIS:HB2   | 5:P:495:VAL:O     | 2.19                     | 0.41              |
| 6:T:65:HIS:CG     | 6:T:66:PRO:HD3    | 2.55                     | 0.41              |
| 7:a:84:LYS:HB3    | 7:a:168:PRO:HD3   | 2.02                     | 0.41              |
| 7:c:68:LEU:HD13   | 7:c:73:VAL:HG21   | 2.02                     | 0.41              |
| 7:d:10:LEU:HD23   | 7:d:147:HIS:HB2   | 2.02                     | 0.41              |
| 7:e:194:ARG:HH12  | 7:e:198:ARG:NH2   | 2.14                     | 0.41              |
| 7:m:139:PRO:O     | 7:m:143:ILE:HG12  | 2.20                     | 0.41              |
| 7:n:15:ARG:O      | 7:n:19:GLU:CB     | 2.69                     | 0.41              |
| 7:o:158:THR:OG1   | 7:o:161:TYR:HB2   | 2.20                     | 0.41              |
| 7:v:115:LEU:HD23  | 7:v:115:LEU:HA    | 1.78                     | 0.41              |
| 7:v:184:PRO:HG3   | 7:v:189:LEU:HD12  | 2.02                     | 0.41              |
| 7:w:114:SER:HB3   | 7:w:136:LEU:HD13  | 2.02                     | 0.41              |
| 7:x:149:ARG:HG2   | 7:x:161:TYR:CD2   | 2.56                     | 0.41              |
| 2:A2:274:PRO:HG3  | 2:A2:373:ARG:O    | 2.20                     | 0.41              |
| 3:A3:228:LEU:HD11 | 3:A3:273:LEU:HD11 | 2.01                     | 0.41              |
| 2:A4:221:ARG:HD3  | 3:A5:325:GLU:CD   | 2.46                     | 0.41              |
| 2:A4:422:ARG:HH12 | 2:A4:426:ALA:HB2  | 1.85                     | 0.41              |
| 3:A5:73:MET:HG3   | 3:A5:92:PHE:HD1   | 1.86                     | 0.41              |
| 2:B2:372:MET:HG2  | 2:B2:373:ARG:HG2  | 2.02                     | 0.41              |
| 3:B5:8:GLN:OE1    | 3:B5:17:GLY:HA3   | 2.20                     | 0.41              |
| 3:B9:332:ASN:O    | 3:B9:336:LYS:HG2  | 2.20                     | 0.41              |
| 2:C0:200:VAL:HG11 | 2:C0:255:PHE:HE1  | 1.86                     | 0.41              |
| 2:C0:319:TYR:CE1  | 2:C0:375:VAL:HG12 | 2.55                     | 0.41              |
| 2:C8:408:TYR:HB3  | 2:C8:413:MET:SD   | 2.61                     | 0.41              |
| 1:D:240:PRO:HB2   | 7:s:162:GLY:C     | 2.45                     | 0.41              |
| 1:D:241:PHE:N     | 7:s:162:GLY:HA2   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D1:64:ILE:HA    | 3:D1:89:ASN:HB3   | 2.03                     | 0.41              |
| 3:D3:20:PHE:CD1   | 3:D3:233:MET:HE2  | 2.56                     | 0.41              |
| 3:D5:68:LEU:H     | 3:D5:143:THR:HG21 | 1.84                     | 0.41              |
| 2:D6:141:VAL:HG12 | 2:D6:187:SER:HA   | 2.01                     | 0.41              |
| 2:D6:225:THR:HG22 | 2:D6:229:ARG:HH12 | 1.84                     | 0.41              |
| 2:D8:67:PHE:HB2   | 2:D8:92:LEU:HA    | 2.02                     | 0.41              |
| 2:E0:70:LEU:HD12  | 2:E0:145:THR:HG22 | 2.02                     | 0.41              |
| 2:E0:319:TYR:HB2  | 2:E0:355:ILE:HG12 | 2.03                     | 0.41              |
| 2:E2:413:MET:HE3  | 2:E2:417:GLU:HB3  | 2.02                     | 0.41              |
| 3:E7:113:ILE:HA   | 3:E7:116:VAL:HG12 | 2.01                     | 0.41              |
| 2:E8:71:GLU:HG3   | 2:E8:74:VAL:HG12  | 2.02                     | 0.41              |
| 7:g:9:PRO:HB2     | 7:g:143:ILE:HG13  | 2.02                     | 0.41              |
| 7:o:184:PRO:HG2   | 7:o:191:GLU:OE2   | 2.20                     | 0.41              |
| 7:t:56:LYS:HG2    | 7:t:60:ASN:HA     | 2.03                     | 0.41              |
| 7:w:9:PRO:HB2     | 7:w:143:ILE:HD12  | 2.03                     | 0.41              |
| 2:A0:22:GLU:CG    | 5:O:241:ARG:HH12  | 2.33                     | 0.41              |
| 3:A5:309:ARG:H    | 3:A5:372:THR:HG23 | 1.85                     | 0.41              |
| 3:A9:117:LEU:HB3  | 3:A9:121:ARG:NH1  | 2.36                     | 0.41              |
| 3:A9:293:MET:SD   | 3:A9:367:PHE:HB2  | 2.60                     | 0.41              |
| 3:B1:86:ARG:HD2   | 3:B1:88:ASP:HB3   | 2.03                     | 0.41              |
| 2:B2:76:ASP:HA    | 2:B2:79:ARG:HG2   | 2.03                     | 0.41              |
| 2:B6:154:LEU:HB3  | 2:B6:197:HIS:HB3  | 2.02                     | 0.41              |
| 2:B6:175:PRO:HB3  | 2:B6:390:ARG:NE   | 2.35                     | 0.41              |
| 2:C0:65:CYS:H     | 2:C0:91:GLN:NE2   | 2.19                     | 0.41              |
| 2:C0:103:PHE:HD2  | 2:C0:413:MET:HE1  | 1.86                     | 0.41              |
| 2:C0:315:CYS:HB3  | 2:C0:377:MET:HE2  | 2.02                     | 0.41              |
| 3:C1:346:PRO:HB2  | 3:C1:347:ASN:HD22 | 1.85                     | 0.41              |
| 2:C2:88:HIS:CD2   | 2:C2:121:ARG:HH21 | 2.38                     | 0.41              |
| 2:C4:273:ALA:HA   | 2:C4:275:ILE:HD12 | 2.03                     | 0.41              |
| 2:C4:377:MET:HE2  | 2:C4:379:SER:HB3  | 2.02                     | 0.41              |
| 3:C7:292:GLN:HG2  | 3:C7:298:ASN:HD22 | 1.85                     | 0.41              |
| 3:D3:362:LYS:HE2  | 3:D3:362:LYS:HB2  | 1.92                     | 0.41              |
| 3:D7:372:THR:O    | 3:D7:375:GLN:HG2  | 2.20                     | 0.41              |
| 3:D9:282:ARG:NH1  | 3:D9:284:LEU:HD13 | 2.36                     | 0.41              |
| 3:E3:153:SER:HB3  | 3:E3:191:GLN:HE21 | 1.85                     | 0.41              |
| 3:E3:253:LEU:HD21 | 3:E3:368:VAL:HG21 | 2.02                     | 0.41              |
| 2:E6:254:GLU:HA   | 2:E6:257:THR:HG22 | 2.02                     | 0.41              |
| 3:E7:112:LEU:HG   | 3:E7:147:MET:HE1  | 2.01                     | 0.41              |
| 2:F0:222:PRO:HD2  | 3:F1:324:LYS:NZ   | 2.36                     | 0.41              |
| 3:F1:293:MET:HE2  | 3:F1:367:PHE:CD1  | 2.56                     | 0.41              |
| 4:L:1254:ARG:O    | 4:L:1258:GLN:HG2  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:c:142:GLU:HA    | 7:c:145:LYS:HD2   | 2.02                     | 0.41              |
| 7:f:9:PRO:HA      | 7:f:12:VAL:HG22   | 2.02                     | 0.41              |
| 7:n:110:ILE:HB    | 7:n:131:TRP:CG    | 2.55                     | 0.41              |
| 7:w:21:ARG:HA     | 7:w:24:MET:SD     | 2.61                     | 0.41              |
| 2:A2:113:GLU:HG2  | 2:A2:114:ILE:HG13 | 2.03                     | 0.41              |
| 3:A3:113:ILE:HG23 | 3:A3:117:LEU:HD23 | 2.02                     | 0.41              |
| 3:A3:139:LEU:HA   | 3:A3:145:SER:HB3  | 2.01                     | 0.41              |
| 3:A3:296:ALA:HB2  | 3:A3:305:PRO:HD2  | 2.03                     | 0.41              |
| 3:A5:27:GLU:HG2   | 3:A5:359:LYS:HG2  | 2.01                     | 0.41              |
| 2:A6:231:ILE:O    | 2:A6:235:ILE:HG12 | 2.20                     | 0.41              |
| 2:A8:338:LYS:HG3  | 2:A8:340:THR:HG22 | 2.02                     | 0.41              |
| 3:A9:175:VAL:HG11 | 2:B0:329:ASN:HB3  | 2.02                     | 0.41              |
| 2:B0:12:ALA:HB3   | 2:B0:140:ALA:HB2  | 2.03                     | 0.41              |
| 2:B8:372:MET:HG2  | 2:B8:373:ARG:HG2  | 2.03                     | 0.41              |
| 3:C3:121:ARG:O    | 3:C3:125:GLU:HG2  | 2.20                     | 0.41              |
| 2:C4:71:GLU:HB3   | 3:C5:2:ARG:HH22   | 1.85                     | 0.41              |
| 3:C5:113:ILE:HG23 | 3:C5:117:LEU:HD23 | 2.03                     | 0.41              |
| 3:C5:166:THR:HG23 | 3:C5:199:VAL:HA   | 2.02                     | 0.41              |
| 3:C5:416:ASN:HA   | 3:C5:419:VAL:HG12 | 2.02                     | 0.41              |
| 2:C6:311:LYS:HD2  | 2:C6:342:GLN:NE2  | 2.33                     | 0.41              |
| 3:C7:207:LEU:HA   | 3:C7:210:ILE:HG22 | 2.03                     | 0.41              |
| 3:C9:151:LEU:HA   | 3:C9:151:LEU:HD12 | 1.81                     | 0.41              |
| 3:C9:322:SER:HB3  | 3:C9:325:GLU:HG2  | 2.03                     | 0.41              |
| 3:C9:376:GLU:HB3  | 3:C9:380:ARG:HH22 | 1.86                     | 0.41              |
| 1:D:251:TYR:CZ    | 2:D6:23:LEU:HD13  | 2.55                     | 0.41              |
| 2:D2:194:LEU:HD12 | 2:D2:198:THR:HG21 | 2.01                     | 0.41              |
| 3:D9:290:THR:HG21 | 3:D9:329:GLN:HB3  | 2.02                     | 0.41              |
| 2:E4:363:VAL:HG23 | 2:E4:366:GLY:HA3  | 2.01                     | 0.41              |
| 3:E5:315:ALA:HB3  | 3:E5:351:SER:HA   | 2.02                     | 0.41              |
| 3:E5:326:VAL:O    | 3:E5:330:MET:HG2  | 2.20                     | 0.41              |
| 3:E7:417:ASP:O    | 3:E7:421:GLU:HG2  | 2.21                     | 0.41              |
| 3:E9:122:LYS:HA   | 3:E9:122:LYS:HE3  | 2.03                     | 0.41              |
| 6:U:102:LEU:HG    | 6:U:103:LEU:HD22  | 2.03                     | 0.41              |
| 4:W:1241:PHE:CD2  | 4:W:1242:PRO:HD3  | 2.55                     | 0.41              |
| 7:m:79:ASP:HB3    | 7:m:82:ASP:HB2    | 2.03                     | 0.41              |
| 7:o:64:PRO:HD2    | 7:o:67:HIS:CE1    | 2.55                     | 0.41              |
| 7:r:171:ILE:HG12  | 7:r:182:PHE:HD1   | 1.85                     | 0.41              |
| 2:A2:272:TYR:CD2  | 2:A2:274:PRO:HD2  | 2.55                     | 0.41              |
| 2:A4:231:ILE:O    | 2:A4:235:ILE:HG12 | 2.20                     | 0.41              |
| 2:A8:288:VAL:HG13 | 2:A8:319:TYR:HE2  | 1.86                     | 0.41              |
| 2:B0:332:VAL:HA   | 2:B0:335:ILE:HG22 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:338:LYS:HZ2  | 2:B0:340:THR:N    | 2.16                     | 0.41              |
| 3:B1:383:ASP:HA   | 3:B1:386:THR:HG22 | 2.03                     | 0.41              |
| 3:B3:178:THR:HG22 | 2:B4:352:LYS:NZ   | 2.36                     | 0.41              |
| 3:B7:153:SER:HB3  | 3:B7:191:GLN:NE2  | 2.36                     | 0.41              |
| 2:C0:362:VAL:HG21 | 2:C0:370:LYS:HG3  | 2.03                     | 0.41              |
| 2:C0:370:LYS:NZ   | 8:k:161:PHE:HA    | 2.36                     | 0.41              |
| 3:C1:68:LEU:HB2   | 3:C1:97:ALA:HB2   | 2.02                     | 0.41              |
| 3:C1:313:ALA:HB1  | 3:C1:367:PHE:HE1  | 1.85                     | 0.41              |
| 2:C2:103:PHE:CE2  | 2:C2:189:LEU:HB2  | 2.56                     | 0.41              |
| 2:C2:401:LYS:HZ1  | 3:C3:344:TRP:CG   | 2.38                     | 0.41              |
| 3:C3:374:ILE:HD11 | 3:C3:422:TYR:CZ   | 2.55                     | 0.41              |
| 3:C5:60:VAL:HG21  | 3:C5:86:ARG:HH21  | 1.86                     | 0.41              |
| 2:C6:325:PRO:HA   | 2:C6:328:VAL:HB   | 2.02                     | 0.41              |
| 2:C8:301:MET:HE1  | 2:C8:377:MET:HE1  | 2.01                     | 0.41              |
| 3:C9:299:MET:HE1  | 3:C9:367:PHE:HD2  | 1.84                     | 0.41              |
| 2:D0:276:ILE:HD13 | 2:D0:286:LEU:HD11 | 2.01                     | 0.41              |
| 3:D5:267:LEU:HD21 | 3:D5:374:ILE:HG22 | 2.02                     | 0.41              |
| 2:D8:231:ILE:O    | 2:D8:235:ILE:HG12 | 2.21                     | 0.41              |
| 2:D8:357:TYR:HB3  | 5:P:535:ILE:HG21  | 2.03                     | 0.41              |
| 1:E:253:ALA:HB3   | 7:e:101:GLU:HG3   | 2.03                     | 0.41              |
| 2:E0:36:MET:HE2   | 2:E0:61:HIS:CE1   | 2.56                     | 0.41              |
| 3:E1:156:ARG:HH21 | 3:E1:164:MET:HB2  | 1.86                     | 0.41              |
| 3:E3:281:TYR:CD2  | 3:E7:87:PRO:HD3   | 2.55                     | 0.41              |
| 3:E3:398:TYR:HB3  | 3:E3:403:MET:HE1  | 2.02                     | 0.41              |
| 3:E5:139:LEU:HD22 | 3:E5:170:PHE:CE2  | 2.55                     | 0.41              |
| 2:E6:364:PRO:HG2  | 1:H:222:LYS:HB3   | 2.02                     | 0.41              |
| 3:E9:65:LEU:HD22  | 3:E9:90:PHE:CE1   | 2.56                     | 0.41              |
| 2:F0:260:VAL:HG11 | 2:F0:266:HIS:HA   | 2.01                     | 0.41              |
| 5:P:305:ARG:HG3   | 5:P:305:ARG:HH11  | 1.85                     | 0.41              |
| 4:Q:1285:ARG:HA   | 4:Q:1285:ARG:HD2  | 1.81                     | 0.41              |
| 6:T:57:LYS:NZ     | 7:a:153:GLU:HG2   | 2.35                     | 0.41              |
| 6:U:58:LEU:HD12   | 6:U:61:TRP:HD1    | 1.85                     | 0.41              |
| 4:V:1286:ARG:HH12 | 4:V:1290:LEU:HG   | 1.85                     | 0.41              |
| 7:a:152:LYS:HZ2   | 7:a:154:TYR:HD2   | 1.67                     | 0.41              |
| 7:b:95:TYR:CE1    | 7:b:197:LEU:HD23  | 2.56                     | 0.41              |
| 7:d:100:ASN:HD21  | 7:d:108:ILE:HG13  | 1.86                     | 0.41              |
| 7:e:78:ALA:HB3    | 7:e:112:PHE:HE1   | 1.84                     | 0.41              |
| 7:i:73:VAL:HG13   | 7:i:173:ILE:HB    | 2.03                     | 0.41              |
| 3:A1:411:ALA:O    | 3:A1:415:MET:HB2  | 2.21                     | 0.41              |
| 3:A3:256:ASN:HD22 | 3:A3:350:LYS:HD2  | 1.86                     | 0.41              |
| 2:A4:91:GLN:NE2   | 2:A4:125:LEU:HD11 | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A6:136:LEU:HD22 | 2:A6:169:PHE:HE2  | 1.85                     | 0.41              |
| 3:B1:230:SER:HA   | 3:B1:233:MET:HG2  | 2.03                     | 0.41              |
| 3:B3:178:THR:HG22 | 2:B4:352:LYS:HZ3  | 1.86                     | 0.41              |
| 2:B4:72:PRO:HD2   | 3:B5:2:ARG:HH21   | 1.85                     | 0.41              |
| 3:B5:106:TYR:HE1  | 3:B5:403:MET:HG2  | 1.84                     | 0.41              |
| 3:B9:281:TYR:HD1  | 3:C3:58:ARG:HD3   | 1.84                     | 0.41              |
| 2:C0:317:LEU:HB3  | 2:C0:319:TYR:CE1  | 2.55                     | 0.41              |
| 2:C4:15:GLN:HB3   | 2:C4:228:ASN:ND2  | 2.36                     | 0.41              |
| 2:C4:26:LEU:HD21  | 2:C4:363:VAL:HG12 | 2.03                     | 0.41              |
| 2:C6:258:ASN:HD22 | 2:C6:352:LYS:HD3  | 1.85                     | 0.41              |
| 3:C7:7:VAL:O      | 3:C7:135:ILE:HG13 | 2.21                     | 0.41              |
| 1:D:215:TYR:HA    | 2:D8:22:GLU:CD    | 2.46                     | 0.41              |
| 2:D0:387:VAL:HA   | 2:D0:390:ARG:NH1  | 2.36                     | 0.41              |
| 3:D1:20:PHE:HA    | 3:D1:230:SER:HB2  | 2.03                     | 0.41              |
| 2:D4:372:MET:HE2  | 2:D4:372:MET:HB3  | 1.96                     | 0.41              |
| 2:D8:15:GLN:HB3   | 2:D8:228:ASN:HD21 | 1.86                     | 0.41              |
| 3:D9:92:PHE:HB3   | 3:D9:93:GLY:H     | 1.75                     | 0.41              |
| 3:D9:379:LYS:HD3  | 3:D9:419:VAL:HG11 | 2.01                     | 0.41              |
| 3:E1:100:ASN:ND2  | 3:E1:103:LYS:HG3  | 2.36                     | 0.41              |
| 2:E2:205:ASP:OD1  | 2:E2:303:ALA:HA   | 2.21                     | 0.41              |
| 2:E4:247:ALA:HB3  | 2:E4:355:ILE:HB   | 2.02                     | 0.41              |
| 2:E4:387:VAL:HA   | 2:E4:390:ARG:NH1  | 2.36                     | 0.41              |
| 2:F0:213:CYS:HB3  | 2:F0:219:ILE:HD11 | 2.02                     | 0.41              |
| 2:F0:222:PRO:HD2  | 3:F1:324:LYS:HZ2  | 1.85                     | 0.41              |
| 3:F1:121:ARG:O    | 3:F1:125:GLU:HG3  | 2.21                     | 0.41              |
| 4:N:1287:MET:HG3  | 4:N:1444:TRP:CE2  | 2.55                     | 0.41              |
| 4:V:1286:ARG:HA   | 4:V:1286:ARG:HD2  | 1.82                     | 0.41              |
| 7:b:64:PRO:HD2    | 7:b:67:HIS:ND1    | 2.35                     | 0.41              |
| 7:e:14:LYS:HD3    | 7:e:47:LEU:HD13   | 2.02                     | 0.41              |
| 7:f:151:MET:HE1   | 7:f:154:TYR:HA    | 2.02                     | 0.41              |
| 7:j:139:PRO:O     | 7:j:143:ILE:HG12  | 2.21                     | 0.41              |
| 7:n:10:LEU:HB2    | 7:n:147:HIS:ND1   | 2.35                     | 0.41              |
| 7:p:200:ASP:O     | 7:p:204:THR:HG22  | 2.21                     | 0.41              |
| 7:s:74:ALA:HB2    | 7:s:172:VAL:HG12  | 2.02                     | 0.41              |
| 7:t:15:ARG:O      | 7:t:19:GLU:HG3    | 2.20                     | 0.41              |
| 7:t:110:ILE:O     | 7:t:131:TRP:HB2   | 2.20                     | 0.41              |
| 2:A0:137:MET:HE2  | 2:A0:154:LEU:HD13 | 2.03                     | 0.41              |
| 2:A0:391:MET:HA   | 2:A0:394:LYS:HB2  | 2.02                     | 0.41              |
| 3:A1:228:LEU:HA   | 3:A1:228:LEU:HD23 | 1.89                     | 0.41              |
| 3:A3:9:GLY:HA2    | 3:A3:66:MET:SD    | 2.61                     | 0.41              |
| 2:A4:214:ARG:HH11 | 2:A4:215:ARG:HG3  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A5:304:ASP:OD2  | 3:A5:306:ARG:HG2  | 2.21                     | 0.41              |
| 2:A6:238:LEU:HA   | 2:A6:318:MET:SD   | 2.61                     | 0.41              |
| 2:A6:403:ALA:HB2  | 3:A7:344:TRP:HZ3  | 1.86                     | 0.41              |
| 2:A8:78:VAL:HA    | 1:C:247:TYR:CE1   | 2.51                     | 0.41              |
| 2:A8:172:TRP:HZ2  | 2:A8:391:MET:HG2  | 1.86                     | 0.41              |
| 3:A9:20:PHE:HB2   | 3:A9:233:MET:HE3  | 2.02                     | 0.41              |
| 3:A9:281:TYR:HD2  | 3:B3:86:ARG:HA    | 1.86                     | 0.41              |
| 2:B0:189:LEU:HD11 | 2:B0:418:PHE:HE1  | 1.86                     | 0.41              |
| 3:B1:153:SER:HA   | 3:B1:195:ASN:HD22 | 1.85                     | 0.41              |
| 3:B1:192:LEU:HD21 | 3:B1:199:VAL:HG11 | 2.02                     | 0.41              |
| 2:B2:133:GLN:HG3  | 2:B2:252:VAL:HG12 | 2.02                     | 0.41              |
| 2:B2:185:TYR:HE2  | 2:B2:398:MET:HE3  | 1.86                     | 0.41              |
| 2:B2:259:LEU:HD21 | 2:B2:316:CYS:HB2  | 2.02                     | 0.41              |
| 3:B3:105:HIS:CD2  | 3:B3:150:LEU:HD13 | 2.56                     | 0.41              |
| 3:B3:325:GLU:O    | 3:B3:329:GLN:HB2  | 2.20                     | 0.41              |
| 2:B4:33:ASP:HB3   | 7:f:102:GLY:O     | 2.20                     | 0.41              |
| 2:B4:181:VAL:HG23 | 3:B5:256:ASN:HD22 | 1.85                     | 0.41              |
| 2:B4:207:GLU:HA   | 2:B4:210:TYR:HB2  | 2.02                     | 0.41              |
| 2:B6:332:VAL:O    | 2:B6:336:LYS:HG2  | 2.21                     | 0.41              |
| 2:B8:67:PHE:HB2   | 2:B8:92:LEU:HD13  | 2.03                     | 0.41              |
| 3:C3:21:TRP:CZ3   | 3:C3:50:PHE:HB3   | 2.56                     | 0.41              |
| 2:C4:28:HIS:CE1   | 2:C4:243:ARG:HD2  | 2.55                     | 0.41              |
| 2:C4:408:TYR:O    | 2:C4:413:MET:HB3  | 2.21                     | 0.41              |
| 2:C8:340:THR:HG23 | 2:C8:341:ILE:HD12 | 2.02                     | 0.41              |
| 3:C9:229:VAL:HG22 | 3:C9:300:MET:HE1  | 2.02                     | 0.41              |
| 2:D0:194:LEU:HD12 | 2:D0:194:LEU:HA   | 1.93                     | 0.41              |
| 2:D0:259:LEU:HD11 | 2:D0:316:CYS:HB2  | 2.02                     | 0.41              |
| 3:D1:321:MET:HE2  | 3:D1:321:MET:HB2  | 1.99                     | 0.41              |
| 2:D2:73:THR:HB    | 3:D3:2:ARG:HH22   | 1.86                     | 0.41              |
| 3:D3:113:ILE:HD12 | 3:D3:116:VAL:HB   | 2.02                     | 0.41              |
| 3:D3:148:GLY:O    | 3:D3:152:ILE:HG12 | 2.21                     | 0.41              |
| 2:D4:88:HIS:HB3   | 2:D4:91:GLN:HG3   | 2.02                     | 0.41              |
| 3:D5:7:VAL:HB     | 3:D5:135:ILE:HD13 | 2.03                     | 0.41              |
| 3:D5:268:ILE:HA   | 3:D5:367:PHE:O    | 2.20                     | 0.41              |
| 2:D6:8:HIS:HD1    | 2:D6:138:PHE:HB2  | 1.86                     | 0.41              |
| 2:D6:21:TRP:CE3   | 2:D6:63:PRO:HB3   | 2.56                     | 0.41              |
| 3:D7:17:GLY:HA2   | 3:D7:20:PHE:HB3   | 2.02                     | 0.41              |
| 3:D7:323:THR:HA   | 3:D7:326:VAL:HG12 | 2.02                     | 0.41              |
| 2:D8:30:ILE:HD12  | 2:D8:61:HIS:CD2   | 2.55                     | 0.41              |
| 2:D8:240:ALA:HB1  | 2:D8:356:ASN:ND2  | 2.36                     | 0.41              |
| 2:D8:265:ILE:HG12 | 2:D8:380:ASN:HD21 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D8:268:MET:HB3  | 2:D8:378:ILE:HG22 | 2.03                     | 0.41              |
| 2:E0:180:ALA:HB3  | 2:E0:183:GLU:HB3  | 2.02                     | 0.41              |
| 3:E1:305:PRO:HB2  | 3:E1:310:TYR:HE1  | 1.86                     | 0.41              |
| 2:E2:75:VAL:HG21  | 2:E2:94:SER:HB2   | 2.01                     | 0.41              |
| 2:E6:101:ASN:ND2  | 2:E6:143:GLY:HA2  | 2.35                     | 0.41              |
| 2:E6:234:VAL:HG22 | 2:E6:272:TYR:HB2  | 2.03                     | 0.41              |
| 2:E6:261:PRO:HB2  | 2:E6:262:TYR:HD1  | 1.85                     | 0.41              |
| 3:E7:153:SER:HB3  | 3:E7:191:GLN:HE21 | 1.86                     | 0.41              |
| 3:E7:290:THR:HA   | 3:E7:293:MET:HG2  | 2.03                     | 0.41              |
| 2:E8:231:ILE:HD13 | 2:E8:302:MET:HE3  | 2.02                     | 0.41              |
| 3:E9:265:PHE:CE2  | 3:E9:418:LEU:HD21 | 2.56                     | 0.41              |
| 2:F0:224:TYR:HB2  | 3:F1:245:GLN:HE21 | 1.84                     | 0.41              |
| 3:F1:256:ASN:HD22 | 3:F1:350:LYS:HG3  | 1.85                     | 0.41              |
| 4:M:1212:ARG:HA   | 4:M:1215:ARG:HG2  | 2.01                     | 0.41              |
| 5:O:528:GLU:HG3   | 5:O:530:ILE:HG23  | 2.03                     | 0.41              |
| 6:T:125:ARG:HH12  | 6:T:126:LEU:HD13  | 1.86                     | 0.41              |
| 4:W:1385:LEU:HD11 | 4:W:1445:LEU:HD21 | 2.03                     | 0.41              |
| 7:a:55:LEU:HG     | 7:a:132:LEU:HD12  | 2.02                     | 0.41              |
| 7:a:171:ILE:HD13  | 7:a:182:PHE:HD2   | 1.86                     | 0.41              |
| 7:c:78:ALA:HB1    | 7:c:85:CYS:SG     | 2.61                     | 0.41              |
| 7:e:55:LEU:HB2    | 7:e:63:ILE:HB     | 2.03                     | 0.41              |
| 7:h:69:LYS:HD2    | 7:h:69:LYS:HA     | 1.78                     | 0.41              |
| 7:j:19:GLU:HB3    | 7:j:40:PRO:HD3    | 2.02                     | 0.41              |
| 8:k:65:GLU:HA     | 7:m:42:TYR:CZ     | 2.55                     | 0.41              |
| 7:o:68:LEU:HD21   | 7:o:111:ILE:HD11  | 2.02                     | 0.41              |
| 7:o:172:VAL:HG12  | 7:o:180:ALA:HB3   | 2.02                     | 0.41              |
| 7:p:10:LEU:HG     | 7:p:143:ILE:HG22  | 2.03                     | 0.41              |
| 7:r:63:ILE:HA     | 7:r:64:PRO:HD3    | 1.93                     | 0.41              |
| 7:u:50:PHE:HB3    | 7:u:55:LEU:HD13   | 2.02                     | 0.41              |
| 2:A0:408:TYR:HB3  | 2:A0:413:MET:HG3  | 2.02                     | 0.41              |
| 2:A4:312:TYR:HA   | 2:A4:381:SER:HA   | 2.02                     | 0.41              |
| 2:A6:265:ILE:HG23 | 2:A6:432:TYR:CZ   | 2.56                     | 0.41              |
| 3:A9:276:ARG:HD3  | 3:A9:276:ARG:HA   | 1.85                     | 0.41              |
| 2:B0:8:HIS:HE1    | 2:B0:21:TRP:HE1   | 1.69                     | 0.41              |
| 2:B2:194:LEU:O    | 2:B2:198:THR:HG22 | 2.21                     | 0.41              |
| 3:B3:152:ILE:HA   | 3:B3:164:MET:HE1  | 2.02                     | 0.41              |
| 2:B4:406:HIS:CD2  | 3:B5:261:PRO:HB3  | 2.56                     | 0.41              |
| 3:B5:167:PHE:HD1  | 3:B5:202:ILE:HD11 | 1.85                     | 0.41              |
| 2:C0:167:LEU:HD23 | 2:C0:200:VAL:HB   | 2.03                     | 0.41              |
| 2:C0:227:LEU:O    | 2:C0:231:ILE:HG12 | 2.21                     | 0.41              |
| 2:C2:121:ARG:HA   | 2:C2:121:ARG:HD2  | 1.70                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C2:259:LEU:HD11 | 2:C2:316:CYS:HB2  | 2.02                     | 0.41              |
| 2:C4:250:VAL:HG13 | 2:C4:255:PHE:HE1  | 1.86                     | 0.41              |
| 3:C9:294:PHE:HZ   | 3:C9:349:MET:HE1  | 1.85                     | 0.41              |
| 3:D3:349:MET:HE3  | 3:D3:349:MET:HB2  | 1.73                     | 0.41              |
| 3:D5:101:TRP:H    | 3:D5:398:TYR:HE1  | 1.68                     | 0.41              |
| 3:D5:190:HIS:HA   | 3:D5:414:ASN:HD21 | 1.85                     | 0.41              |
| 3:D5:374:ILE:HD11 | 3:D5:422:TYR:CZ   | 2.56                     | 0.41              |
| 2:D8:93:ILE:H     | 2:D8:93:ILE:HD12  | 1.86                     | 0.41              |
| 2:E8:188:VAL:HG11 | 2:E8:395:PHE:CD1  | 2.56                     | 0.41              |
| 7:d:18:ASN:ND2    | 7:d:45:MET:HB3    | 2.36                     | 0.41              |
| 7:d:75:LEU:HD23   | 7:d:111:ILE:HB    | 2.01                     | 0.41              |
| 7:g:69:LYS:HD2    | 7:i:38:LEU:HD11   | 2.03                     | 0.41              |
| 7:m:183:LEU:HA    | 7:m:184:PRO:HD3   | 1.89                     | 0.41              |
| 7:o:149:ARG:HE    | 7:o:149:ARG:HB2   | 1.69                     | 0.41              |
| 7:x:42:TYR:HA     | 7:x:45:MET:HG3    | 2.02                     | 0.41              |
| 2:A0:54:SER:HB2   | 2:A0:64:ARG:HE    | 1.87                     | 0.40              |
| 3:A1:385:PHE:HE2  | 3:A1:408:PHE:HD2  | 1.67                     | 0.40              |
| 3:A3:17:GLY:HA2   | 3:A3:20:PHE:HB3   | 2.04                     | 0.40              |
| 3:A3:293:MET:HE3  | 3:A3:293:MET:HB3  | 1.95                     | 0.40              |
| 2:A4:213:CYS:SG   | 2:A4:219:ILE:HB   | 2.61                     | 0.40              |
| 2:A4:297:GLU:HG3  | 2:A4:300:SER:H    | 1.86                     | 0.40              |
| 2:A8:211:ASP:HA   | 2:A8:214:ARG:HG2  | 2.03                     | 0.40              |
| 3:B1:293:MET:SD   | 3:B1:367:PHE:HB2  | 2.60                     | 0.40              |
| 2:B2:336:LYS:HD3  | 2:B2:351:PHE:HE2  | 1.86                     | 0.40              |
| 2:B6:147:SER:HB2  | 2:B6:190:SER:HB3  | 2.02                     | 0.40              |
| 2:B8:103:PHE:HB2  | 2:B8:186:ASN:HD22 | 1.86                     | 0.40              |
| 3:C1:149:THR:HG21 | 3:C1:188:SER:HB3  | 2.02                     | 0.40              |
| 2:C2:280:LYS:HZ3  | 2:C6:90:GLU:HB2   | 1.86                     | 0.40              |
| 3:C3:252:LYS:HA   | 3:C3:255:VAL:HG12 | 2.03                     | 0.40              |
| 3:C5:216:LYS:HE2  | 3:C5:275:SER:HB2  | 2.03                     | 0.40              |
| 3:C7:215:LEU:HD21 | 3:C7:273:LEU:HD22 | 2.04                     | 0.40              |
| 2:D0:189:LEU:HD11 | 2:D0:418:PHE:CE1  | 2.57                     | 0.40              |
| 3:D1:201:VAL:HG21 | 3:D1:374:ILE:HD11 | 2.04                     | 0.40              |
| 3:D3:172:SER:HA   | 3:D3:173:PRO:HD3  | 1.88                     | 0.40              |
| 3:D9:24:ILE:HD13  | 3:D9:24:ILE:HA    | 1.96                     | 0.40              |
| 3:D9:403:MET:HE3  | 3:D9:403:MET:HB2  | 1.91                     | 0.40              |
| 2:E0:21:TRP:CZ2   | 2:E0:65:CYS:HB3   | 2.56                     | 0.40              |
| 3:E5:182:PRO:HB2  | 3:E5:388:MET:HE1  | 2.02                     | 0.40              |
| 3:E5:253:LEU:HD11 | 3:E5:316:MET:SD   | 2.61                     | 0.40              |
| 3:E5:281:TYR:CE1  | 3:E9:86:ARG:HA    | 2.56                     | 0.40              |
| 3:E7:86:ARG:HG3   | 3:E7:88:ASP:H     | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F0:267:PHE:HE2  | 2:F0:428:LEU:HD21 | 1.86                     | 0.40              |
| 3:F1:193:VAL:HG21 | 3:F1:418:LEU:HD21 | 2.03                     | 0.40              |
| 4:L:1293:TYR:HD1  | 4:L:1318:VAL:HG22 | 1.86                     | 0.40              |
| 6:R:59:THR:HA     | 6:R:62:ARG:NH1    | 2.36                     | 0.40              |
| 6:T:126:LEU:HD12  | 6:T:126:LEU:HA    | 1.89                     | 0.40              |
| 7:c:186:CYS:HA    | 7:c:190:GLU:HG2   | 2.03                     | 0.40              |
| 7:e:130:PRO:HD2   | 7:e:131:TRP:CE3   | 2.56                     | 0.40              |
| 7:g:95:TYR:HE1    | 7:g:197:LEU:HD23  | 1.86                     | 0.40              |
| 8:k:73:TYR:CZ     | 8:k:75:SER:HB2    | 2.56                     | 0.40              |
| 3:A1:42:LEU:HD21  | 3:A1:243:PRO:HD2  | 2.03                     | 0.40              |
| 3:A1:211:CYS:HB2  | 3:A1:217:LEU:HD11 | 2.02                     | 0.40              |
| 3:A1:217:LEU:HB2  | 3:A1:220:PRO:HG3  | 2.04                     | 0.40              |
| 3:A1:325:GLU:HA   | 3:A1:328:GLU:OE2  | 2.22                     | 0.40              |
| 3:A3:281:TYR:CD1  | 3:A7:87:PRO:HD3   | 2.53                     | 0.40              |
| 2:A4:402:ARG:HD3  | 2:A4:402:ARG:HA   | 1.83                     | 0.40              |
| 3:A5:179:VAL:HG22 | 2:A6:350:GLY:HA2  | 2.04                     | 0.40              |
| 2:A8:406:HIS:HA   | 2:A8:409:VAL:HG12 | 2.03                     | 0.40              |
| 3:B1:294:PHE:CD2  | 3:B1:333:VAL:HG21 | 2.56                     | 0.40              |
| 3:B5:237:THR:HG23 | 3:B5:241:ARG:NH1  | 2.36                     | 0.40              |
| 3:B7:73:MET:HG2   | 3:B7:92:PHE:HE1   | 1.87                     | 0.40              |
| 3:B7:228:LEU:HD11 | 5:P:371:ARG:HH21  | 1.86                     | 0.40              |
| 3:C3:111:GLU:HG2  | 3:C3:112:LEU:HD22 | 2.03                     | 0.40              |
| 2:C4:325:PRO:HA   | 2:C4:328:VAL:HG12 | 2.03                     | 0.40              |
| 3:C5:269:GLY:HA2  | 3:C5:300:MET:HG3  | 2.02                     | 0.40              |
| 3:C7:229:VAL:HG22 | 3:C7:233:MET:HE3  | 2.04                     | 0.40              |
| 2:C8:200:VAL:HG13 | 2:C8:268:MET:HG2  | 2.02                     | 0.40              |
| 2:D0:287:SER:O    | 2:D0:291:ILE:HG12 | 2.20                     | 0.40              |
| 2:D2:21:TRP:HZ3   | 2:D2:52:PHE:HB3   | 1.86                     | 0.40              |
| 3:D3:133:PHE:HB3  | 3:D3:135:ILE:HD11 | 2.02                     | 0.40              |
| 2:D8:88:HIS:CD2   | 2:D8:90:GLU:HB2   | 2.56                     | 0.40              |
| 3:D9:42:LEU:HD13  | 3:D9:356:ILE:HD11 | 2.03                     | 0.40              |
| 2:E0:124:LYS:HA   | 2:E0:124:LYS:HD2  | 1.79                     | 0.40              |
| 2:E2:11:GLN:HG2   | 2:E2:74:VAL:HG21  | 2.01                     | 0.40              |
| 3:E5:58:ARG:HH11  | 3:E5:58:ARG:HA    | 1.87                     | 0.40              |
| 3:E9:202:ILE:HG21 | 3:E9:229:VAL:HG22 | 2.04                     | 0.40              |
| 4:L:1255:CYS:HB3  | 4:L:1381:ILE:HG23 | 2.03                     | 0.40              |
| 4:L:1388:LEU:HD13 | 4:L:1392:PHE:CE2  | 2.57                     | 0.40              |
| 4:M:1405:LEU:HA   | 4:M:1408:GLN:HB2  | 2.02                     | 0.40              |
| 4:V:1289:ARG:NH2  | 4:V:1294:VAL:HG22 | 2.37                     | 0.40              |
| 4:W:1248:THR:HG23 | 4:W:1392:PHE:CE2  | 2.55                     | 0.40              |
| 7:c:63:ILE:HA     | 7:c:64:PRO:HD3    | 1.89                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:d:11:ASN:HB3    | 7:d:15:ARG:NH1    | 2.35                     | 0.40              |
| 7:h:84:LYS:CB     | 7:h:168:PRO:HD3   | 2.52                     | 0.40              |
| 8:k:35:ALA:HA     | 8:k:133:VAL:HA    | 2.04                     | 0.40              |
| 7:r:77:PHE:O      | 7:r:168:PRO:HA    | 2.22                     | 0.40              |
| 2:A0:372:MET:HG2  | 2:A0:373:ARG:HE   | 1.86                     | 0.40              |
| 3:A1:2:ARG:HB3    | 3:A1:131:GLN:HG2  | 2.03                     | 0.40              |
| 3:A3:257:LEU:HA   | 3:A3:312:THR:HG21 | 2.03                     | 0.40              |
| 2:A6:409:VAL:HA   | 2:A6:413:MET:O    | 2.21                     | 0.40              |
| 3:A7:67:ASP:OD1   | 3:A7:73:MET:HE1   | 2.22                     | 0.40              |
| 2:A8:68:LEU:HD23  | 2:A8:68:LEU:HA    | 1.90                     | 0.40              |
| 2:B0:35:GLN:NE2   | 2:B0:60:LYS:HG2   | 2.36                     | 0.40              |
| 3:B1:16:ILE:HD13  | 3:B1:16:ILE:HG21  | 1.88                     | 0.40              |
| 3:B1:103:LYS:HB3  | 3:B1:103:LYS:HE2  | 1.91                     | 0.40              |
| 3:B5:154:LYS:HB2  | 3:B5:154:LYS:HE2  | 1.80                     | 0.40              |
| 1:C:221:PRO:HG2   | 7:d:101:GLU:HG3   | 2.04                     | 0.40              |
| 3:C1:396:HIS:CG   | 2:C2:263:PRO:HD3  | 2.55                     | 0.40              |
| 3:C5:273:LEU:H    | 3:C5:292:GLN:NE2  | 2.19                     | 0.40              |
| 3:C7:21:TRP:HA    | 3:C7:24:ILE:HG22  | 2.02                     | 0.40              |
| 2:C8:181:VAL:HG13 | 2:C8:182:VAL:HG13 | 2.02                     | 0.40              |
| 3:C9:398:TYR:HB3  | 3:C9:403:MET:SD   | 2.62                     | 0.40              |
| 2:D0:191:THR:HG21 | 2:D0:425:LEU:HB2  | 2.02                     | 0.40              |
| 2:D0:216:ASN:HB3  | 2:D0:275:ILE:O    | 2.22                     | 0.40              |
| 2:D0:292:THR:HG21 | 2:D0:331:ALA:HB1  | 2.02                     | 0.40              |
| 3:D1:268:ILE:HA   | 3:D1:367:PHE:O    | 2.20                     | 0.40              |
| 2:D6:77:GLU:HA    | 2:D6:80:THR:HG22  | 2.03                     | 0.40              |
| 2:D6:109:THR:OG1  | 2:D6:411:GLU:HB3  | 2.21                     | 0.40              |
| 2:D6:140:ALA:HA   | 2:D6:171:SER:HB3  | 2.03                     | 0.40              |
| 3:D7:8:GLN:HE21   | 3:D7:65:LEU:HD22  | 1.87                     | 0.40              |
| 3:D9:388:MET:HB3  | 3:D9:393:ALA:HB3  | 2.03                     | 0.40              |
| 3:E1:30:ILE:HD11  | 3:E1:47:ILE:HD13  | 2.03                     | 0.40              |
| 3:E1:359:LYS:HE3  | 3:E1:359:LYS:HB3  | 1.99                     | 0.40              |
| 2:E2:18:ASN:HB3   | 1:F:219:TYR:HE1   | 1.87                     | 0.40              |
| 2:E4:9:VAL:HG22   | 2:E4:68:LEU:HD12  | 2.03                     | 0.40              |
| 3:E7:201:VAL:HG22 | 3:E7:266:PHE:O    | 2.22                     | 0.40              |
| 2:E8:191:THR:HA   | 2:E8:194:LEU:HG   | 2.04                     | 0.40              |
| 2:E8:221:ARG:HB3  | 2:E8:222:PRO:HD3  | 2.03                     | 0.40              |
| 3:E9:20:PHE:HA    | 3:E9:230:SER:HB2  | 2.04                     | 0.40              |
| 2:F0:82:THR:HA    | 7:x:98:THR:HB     | 2.04                     | 0.40              |
| 1:G:210:HIS:CE1   | 7:j:154:TYR:HB2   | 2.55                     | 0.40              |
| 1:H:247:TYR:HA    | 1:H:251:TYR:HD2   | 1.87                     | 0.40              |
| 1:I:240:PRO:HG2   | 1:I:242:ASN:HD21  | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:d:149:ARG:HD2   | 7:d:161:TYR:HB3   | 2.02                     | 0.40              |
| 8:k:54:ARG:HA     | 8:k:92:TRP:HZ3    | 1.86                     | 0.40              |
| 8:l:45:LYS:O      | 8:l:49:ILE:HG12   | 2.21                     | 0.40              |
| 7:m:151:MET:HE3   | 7:m:152:LYS:H     | 1.86                     | 0.40              |
| 7:o:53:GLY:HA2    | 7:o:62:VAL:HG21   | 2.03                     | 0.40              |
| 7:o:85:CYS:SG     | 7:o:168:PRO:HB3   | 2.61                     | 0.40              |
| 7:s:19:GLU:HB3    | 7:s:40:PRO:HD2    | 2.03                     | 0.40              |
| 2:A0:68:LEU:HD12  | 2:A0:68:LEU:HA    | 1.83                     | 0.40              |
| 3:A5:372:THR:HG21 | 3:A5:426:GLN:HB3  | 2.04                     | 0.40              |
| 3:A9:139:LEU:HA   | 3:A9:145:SER:HB2  | 2.03                     | 0.40              |
| 3:A9:302:ALA:C    | 3:A9:377:MET:HE1  | 2.47                     | 0.40              |
| 2:B0:28:HIS:CE1   | 2:B0:243:ARG:HD2  | 2.57                     | 0.40              |
| 2:B6:100:ALA:O    | 3:B7:255:VAL:HG11 | 2.22                     | 0.40              |
| 2:C0:195:LEU:HG   | 2:C0:264:ARG:HH12 | 1.87                     | 0.40              |
| 2:C4:15:GLN:HE22  | 3:C5:245:GLN:HA   | 1.87                     | 0.40              |
| 2:C4:404:PHE:HZ   | 3:C5:312:THR:HG21 | 1.85                     | 0.40              |
| 3:C5:281:TYR:CD2  | 3:C9:87:PRO:HD3   | 2.57                     | 0.40              |
| 3:C5:283:ALA:HB2  | 3:C9:54:ALA:HA    | 2.03                     | 0.40              |
| 3:C9:214:THR:HG22 | 3:C9:297:LYS:NZ   | 2.37                     | 0.40              |
| 3:C9:281:TYR:HD1  | 3:D3:87:PRO:HD3   | 1.87                     | 0.40              |
| 1:D:250:GLU:HG2   | 2:D6:22:GLU:OE2   | 2.21                     | 0.40              |
| 2:D2:390:ARG:O    | 2:D2:394:LYS:HG2  | 2.22                     | 0.40              |
| 2:E0:407:TRP:CG   | 3:E1:255:VAL:HG23 | 2.57                     | 0.40              |
| 2:E4:398:MET:HE2  | 3:E5:345:ILE:HG23 | 2.02                     | 0.40              |
| 2:E6:200:VAL:HG13 | 2:E6:268:MET:HE1  | 2.03                     | 0.40              |
| 2:E8:316:CYS:SG   | 2:E8:318:MET:HE3  | 2.61                     | 0.40              |
| 3:E9:209:ASP:HB2  | 3:E9:213:ARG:NH2  | 2.36                     | 0.40              |
| 5:O:521:PRO:HB2   | 5:O:522:VAL:H     | 1.68                     | 0.40              |
| 7:j:194:ARG:HH12  | 7:j:197:LEU:HB2   | 1.86                     | 0.40              |
| 7:o:201:TRP:CD1   | 7:o:201:TRP:H     | 2.38                     | 0.40              |
| 7:s:42:TYR:HA     | 7:s:45:MET:HB2    | 2.03                     | 0.40              |
| 7:v:75:LEU:O      | 7:v:170:VAL:HA    | 2.21                     | 0.40              |
| 2:A2:167:LEU:HD11 | 2:A2:252:VAL:HG13 | 2.02                     | 0.40              |
| 3:A5:306:ARG:HB2  | 3:A5:340:TYR:CZ   | 2.56                     | 0.40              |
| 3:A5:318:ARG:HG2  | 3:A5:358:PRO:HD3  | 2.02                     | 0.40              |
| 2:A8:308:ARG:CZ   | 4:W:1241:PHE:HB3  | 2.52                     | 0.40              |
| 2:B2:250:VAL:HG11 | 2:B2:352:LYS:HE3  | 2.02                     | 0.40              |
| 2:B4:100:ALA:HA   | 3:B5:252:LYS:HD3  | 2.03                     | 0.40              |
| 2:C0:3:GLU:HA     | 2:C0:51:THR:HG23  | 2.03                     | 0.40              |
| 3:C1:70:PRO:HD3   | 3:C1:93:GLY:O     | 2.22                     | 0.40              |
| 3:C1:304:ASP:HB3  | 3:C1:307:HIS:CD2  | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C3:68:LEU:HB3   | 3:C3:96:GLY:HA2   | 2.04                     | 0.40              |
| 3:C3:164:MET:HB3  | 3:C3:197:ASP:H    | 1.86                     | 0.40              |
| 2:C6:265:ILE:HG22 | 2:C6:380:ASN:HD21 | 1.85                     | 0.40              |
| 2:C6:326:LYS:HE2  | 5:P:458:ARG:NH1   | 2.33                     | 0.40              |
| 2:C6:384:ILE:HD12 | 2:C6:384:ILE:HA   | 1.98                     | 0.40              |
| 3:C7:246:LEU:HD12 | 3:C7:246:LEU:HA   | 1.95                     | 0.40              |
| 2:C8:207:GLU:HB3  | 2:C8:304:LYS:HZ2  | 1.87                     | 0.40              |
| 3:C9:321:MET:HE2  | 3:C9:321:MET:HB3  | 1.70                     | 0.40              |
| 2:D6:4:VAL:HG22   | 2:D6:51:THR:HB    | 2.03                     | 0.40              |
| 2:D6:244:PHE:HD2  | 2:D6:356:ASN:HD21 | 1.69                     | 0.40              |
| 3:D7:172:SER:HB3  | 3:D7:203:ASP:HB3  | 2.03                     | 0.40              |
| 2:D8:6:SER:HB3    | 2:D8:8:HIS:NE2    | 2.37                     | 0.40              |
| 3:D9:28:HIS:NE2   | 3:D9:241:ARG:HD2  | 2.36                     | 0.40              |
| 3:D9:372:THR:HG21 | 3:D9:426:GLN:HB2  | 2.03                     | 0.40              |
| 3:E1:131:GLN:HE22 | 3:E1:250:LEU:HB2  | 1.86                     | 0.40              |
| 3:E3:281:TYR:HD2  | 3:E7:87:PRO:HD3   | 1.86                     | 0.40              |
| 2:F0:88:HIS:HB3   | 2:F0:91:GLN:HE22  | 1.85                     | 0.40              |
| 4:Q:1244:TYR:O    | 4:Q:1248:THR:HG23 | 2.22                     | 0.40              |
| 6:T:88:GLU:HG2    | 6:T:89:ASP:H      | 1.86                     | 0.40              |
| 7:a:142:GLU:HG3   | 7:a:146:ARG:NH1   | 2.37                     | 0.40              |
| 7:s:73:VAL:HA     | 7:s:109:GLU:O     | 2.20                     | 0.40              |
| 7:t:172:VAL:HG12  | 7:t:180:ALA:HB3   | 2.02                     | 0.40              |
| 7:u:71:LYS:HE2    | 7:u:106:GLN:HB3   | 2.03                     | 0.40              |
| 7:v:82:ASP:HA     | 7:v:83:PRO:HD3    | 1.97                     | 0.40              |
| 7:v:110:ILE:HB    | 7:v:131:TRP:CG    | 2.57                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | A     | 57/351 (16%) | 45 (79%) | 12 (21%) | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | B     | 58/351 (16%)  | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 1   | C     | 58/351 (16%)  | 53 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 1   | D     | 58/351 (16%)  | 50 (86%)  | 8 (14%)  | 0        | 100         | 100 |
| 1   | E     | 58/351 (16%)  | 53 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 1   | F     | 58/351 (16%)  | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 1   | G     | 58/351 (16%)  | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 1   | H     | 58/351 (16%)  | 53 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 1   | I     | 58/351 (16%)  | 54 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 1   | J     | 58/351 (16%)  | 49 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 1   | K     | 58/351 (16%)  | 54 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 2   | A0    | 424/453 (94%) | 391 (92%) | 33 (8%)  | 0        | 100         | 100 |
| 2   | A2    | 424/453 (94%) | 391 (92%) | 32 (8%)  | 1 (0%)   | 43          | 71  |
| 2   | A4    | 424/453 (94%) | 387 (91%) | 35 (8%)  | 2 (0%)   | 24          | 55  |
| 2   | A6    | 424/453 (94%) | 379 (89%) | 45 (11%) | 0        | 100         | 100 |
| 2   | A8    | 424/453 (94%) | 413 (97%) | 11 (3%)  | 0        | 100         | 100 |
| 2   | B0    | 424/453 (94%) | 413 (97%) | 11 (3%)  | 0        | 100         | 100 |
| 2   | B2    | 424/453 (94%) | 415 (98%) | 9 (2%)   | 0        | 100         | 100 |
| 2   | B4    | 424/453 (94%) | 410 (97%) | 14 (3%)  | 0        | 100         | 100 |
| 2   | B6    | 424/453 (94%) | 406 (96%) | 18 (4%)  | 0        | 100         | 100 |
| 2   | B8    | 424/453 (94%) | 409 (96%) | 15 (4%)  | 0        | 100         | 100 |
| 2   | C0    | 424/453 (94%) | 391 (92%) | 32 (8%)  | 1 (0%)   | 43          | 71  |
| 2   | C2    | 424/453 (94%) | 381 (90%) | 42 (10%) | 1 (0%)   | 43          | 71  |
| 2   | C4    | 424/453 (94%) | 383 (90%) | 38 (9%)  | 3 (1%)   | 18          | 49  |
| 2   | C6    | 424/453 (94%) | 384 (91%) | 39 (9%)  | 1 (0%)   | 43          | 71  |
| 2   | C8    | 424/453 (94%) | 392 (92%) | 32 (8%)  | 0        | 100         | 100 |
| 2   | D0    | 424/453 (94%) | 393 (93%) | 31 (7%)  | 0        | 100         | 100 |
| 2   | D2    | 424/453 (94%) | 379 (89%) | 44 (10%) | 1 (0%)   | 43          | 71  |
| 2   | D4    | 424/453 (94%) | 390 (92%) | 33 (8%)  | 1 (0%)   | 43          | 71  |
| 2   | D6    | 424/453 (94%) | 395 (93%) | 28 (7%)  | 1 (0%)   | 43          | 71  |
| 2   | D8    | 424/453 (94%) | 383 (90%) | 40 (9%)  | 1 (0%)   | 43          | 71  |
| 2   | E0    | 424/453 (94%) | 398 (94%) | 26 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | E2    | 424/453 (94%) | 390 (92%) | 33 (8%)  | 1 (0%)   | 43          | 71  |
| 2   | E4    | 424/453 (94%) | 385 (91%) | 39 (9%)  | 0        | 100         | 100 |
| 2   | E6    | 424/453 (94%) | 381 (90%) | 41 (10%) | 2 (0%)   | 24          | 55  |
| 2   | E8    | 424/453 (94%) | 384 (91%) | 39 (9%)  | 1 (0%)   | 43          | 71  |
| 2   | F0    | 424/453 (94%) | 410 (97%) | 14 (3%)  | 0        | 100         | 100 |
| 3   | A1    | 424/449 (94%) | 384 (91%) | 39 (9%)  | 1 (0%)   | 43          | 71  |
| 3   | A3    | 424/449 (94%) | 402 (95%) | 22 (5%)  | 0        | 100         | 100 |
| 3   | A5    | 424/449 (94%) | 386 (91%) | 38 (9%)  | 0        | 100         | 100 |
| 3   | A7    | 424/449 (94%) | 405 (96%) | 19 (4%)  | 0        | 100         | 100 |
| 3   | A9    | 424/449 (94%) | 403 (95%) | 21 (5%)  | 0        | 100         | 100 |
| 3   | B1    | 424/449 (94%) | 401 (95%) | 23 (5%)  | 0        | 100         | 100 |
| 3   | B3    | 424/449 (94%) | 405 (96%) | 19 (4%)  | 0        | 100         | 100 |
| 3   | B5    | 424/449 (94%) | 404 (95%) | 20 (5%)  | 0        | 100         | 100 |
| 3   | B7    | 424/449 (94%) | 405 (96%) | 19 (4%)  | 0        | 100         | 100 |
| 3   | B9    | 424/449 (94%) | 404 (95%) | 20 (5%)  | 0        | 100         | 100 |
| 3   | C1    | 424/449 (94%) | 391 (92%) | 32 (8%)  | 1 (0%)   | 43          | 71  |
| 3   | C3    | 424/449 (94%) | 402 (95%) | 22 (5%)  | 0        | 100         | 100 |
| 3   | C5    | 424/449 (94%) | 384 (91%) | 40 (9%)  | 0        | 100         | 100 |
| 3   | C7    | 424/449 (94%) | 383 (90%) | 40 (9%)  | 1 (0%)   | 43          | 71  |
| 3   | C9    | 424/449 (94%) | 382 (90%) | 42 (10%) | 0        | 100         | 100 |
| 3   | D1    | 424/449 (94%) | 381 (90%) | 42 (10%) | 1 (0%)   | 43          | 71  |
| 3   | D3    | 424/449 (94%) | 380 (90%) | 43 (10%) | 1 (0%)   | 43          | 71  |
| 3   | D5    | 424/449 (94%) | 382 (90%) | 40 (9%)  | 2 (0%)   | 24          | 55  |
| 3   | D7    | 424/449 (94%) | 386 (91%) | 36 (8%)  | 2 (0%)   | 24          | 55  |
| 3   | D9    | 424/449 (94%) | 383 (90%) | 40 (9%)  | 1 (0%)   | 43          | 71  |
| 3   | E1    | 424/449 (94%) | 382 (90%) | 40 (9%)  | 2 (0%)   | 24          | 55  |
| 3   | E3    | 424/449 (94%) | 396 (93%) | 28 (7%)  | 0        | 100         | 100 |
| 3   | E5    | 424/449 (94%) | 376 (89%) | 48 (11%) | 0        | 100         | 100 |
| 3   | E7    | 424/449 (94%) | 384 (91%) | 39 (9%)  | 1 (0%)   | 43          | 71  |
| 3   | E9    | 424/449 (94%) | 388 (92%) | 33 (8%)  | 3 (1%)   | 18          | 49  |
| 3   | F1    | 424/449 (94%) | 380 (90%) | 41 (10%) | 3 (1%)   | 18          | 49  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | L     | 154/1678 (9%) | 150 (97%) | 3 (2%)   | 1 (1%)   | 21          | 51  |
| 4   | M     | 154/1678 (9%) | 152 (99%) | 1 (1%)   | 1 (1%)   | 21          | 51  |
| 4   | N     | 154/1678 (9%) | 151 (98%) | 2 (1%)   | 1 (1%)   | 21          | 51  |
| 4   | Q     | 154/1678 (9%) | 148 (96%) | 5 (3%)   | 1 (1%)   | 21          | 51  |
| 4   | V     | 154/1678 (9%) | 150 (97%) | 3 (2%)   | 1 (1%)   | 21          | 51  |
| 4   | W     | 154/1678 (9%) | 148 (96%) | 5 (3%)   | 1 (1%)   | 21          | 51  |
| 5   | O     | 209/583 (36%) | 174 (83%) | 32 (15%) | 3 (1%)   | 9           | 34  |
| 5   | P     | 209/583 (36%) | 160 (77%) | 42 (20%) | 7 (3%)   | 3           | 19  |
| 6   | R     | 109/336 (32%) | 85 (78%)  | 24 (22%) | 0        | 100         | 100 |
| 6   | S     | 20/336 (6%)   | 17 (85%)  | 3 (15%)  | 0        | 100         | 100 |
| 6   | T     | 109/336 (32%) | 85 (78%)  | 24 (22%) | 0        | 100         | 100 |
| 6   | U     | 89/336 (26%)  | 73 (82%)  | 16 (18%) | 0        | 100         | 100 |
| 7   | a     | 159/220 (72%) | 138 (87%) | 21 (13%) | 0        | 100         | 100 |
| 7   | b     | 159/220 (72%) | 137 (86%) | 22 (14%) | 0        | 100         | 100 |
| 7   | c     | 197/220 (90%) | 185 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 7   | d     | 197/220 (90%) | 182 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 7   | e     | 197/220 (90%) | 184 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 7   | f     | 197/220 (90%) | 184 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 7   | g     | 197/220 (90%) | 187 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 7   | h     | 197/220 (90%) | 189 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 7   | i     | 197/220 (90%) | 183 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 7   | j     | 197/220 (90%) | 187 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 7   | m     | 197/220 (90%) | 181 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 7   | n     | 197/220 (90%) | 181 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 7   | o     | 197/220 (90%) | 187 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 7   | p     | 197/220 (90%) | 186 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 7   | q     | 197/220 (90%) | 186 (94%) | 11 (6%)  | 0        | 100         | 100 |
| 7   | r     | 197/220 (90%) | 185 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 7   | s     | 197/220 (90%) | 185 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 7   | t     | 197/220 (90%) | 188 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 7   | u     | 197/220 (90%) | 188 (95%) | 9 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 7   | v     | 197/220 (90%)     | 186 (94%)   | 11 (6%)   | 0        | 100         | 100 |
| 7   | w     | 197/220 (90%)     | 179 (91%)   | 18 (9%)   | 0        | 100         | 100 |
| 7   | x     | 197/220 (90%)     | 181 (92%)   | 16 (8%)   | 0        | 100         | 100 |
| 8   | k     | 139/189 (74%)     | 133 (96%)   | 6 (4%)    | 0        | 100         | 100 |
| 8   | l     | 139/189 (74%)     | 122 (88%)   | 17 (12%)  | 0        | 100         | 100 |
| All | All   | 28890/45109 (64%) | 26676 (92%) | 2162 (8%) | 52 (0%)  | 44          | 71  |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C4    | 219 | ILE  |
| 3   | C7    | 125 | GLU  |
| 3   | D3    | 178 | THR  |
| 3   | D7    | 178 | THR  |
| 3   | E1    | 95  | THR  |
| 2   | E2    | 163 | LYS  |
| 3   | F1    | 55  | THR  |
| 5   | O     | 511 | ASP  |
| 5   | O     | 521 | PRO  |
| 5   | P     | 511 | ASP  |
| 5   | P     | 521 | PRO  |
| 3   | A1    | 338 | SER  |
| 2   | C0    | 110 | ILE  |
| 2   | C2    | 110 | ILE  |
| 3   | D5    | 55  | THR  |
| 3   | D9    | 178 | THR  |
| 2   | E6    | 163 | LYS  |
| 3   | F1    | 296 | ALA  |
| 5   | O     | 278 | GLN  |
| 5   | P     | 278 | GLN  |
| 2   | A2    | 273 | ALA  |
| 2   | C4    | 274 | PRO  |
| 3   | D7    | 393 | ALA  |
| 3   | E1    | 178 | THR  |
| 2   | E6    | 403 | ALA  |
| 3   | E7    | 355 | ASP  |
| 3   | E9    | 178 | THR  |
| 5   | P     | 253 | ALA  |
| 2   | C4    | 218 | ASP  |
| 2   | D8    | 278 | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L     | 1242 | PRO  |
| 2   | A4    | 261  | PRO  |
| 2   | C6    | 261  | PRO  |
| 3   | E9    | 351  | SER  |
| 3   | F1    | 259  | PRO  |
| 5   | P     | 500  | LEU  |
| 4   | W     | 1242 | PRO  |
| 2   | A4    | 403  | ALA  |
| 3   | D5    | 108  | GLU  |
| 3   | E9    | 393  | ALA  |
| 5   | P     | 514  | SER  |
| 3   | C1    | 272  | PRO  |
| 4   | M     | 1242 | PRO  |
| 2   | D6    | 274  | PRO  |
| 2   | E8    | 261  | PRO  |
| 3   | D1    | 272  | PRO  |
| 2   | D2    | 261  | PRO  |
| 5   | P     | 530  | ILE  |
| 4   | Q     | 1242 | PRO  |
| 4   | V     | 1242 | PRO  |
| 2   | D4    | 274  | PRO  |
| 4   | N     | 1242 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | A     | 54/305 (18%) | 54 (100%) | 0        | 100         | 100 |
| 1   | B     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |
| 1   | C     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |
| 1   | D     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |
| 1   | E     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |
| 1   | F     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |
| 1   | G     | 55/305 (18%) | 55 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | H     | 55/305 (18%)  | 55 (100%)  | 0        | 100         | 100 |
| 1   | I     | 55/305 (18%)  | 55 (100%)  | 0        | 100         | 100 |
| 1   | J     | 55/305 (18%)  | 55 (100%)  | 0        | 100         | 100 |
| 1   | K     | 55/305 (18%)  | 55 (100%)  | 0        | 100         | 100 |
| 2   | A0    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | A2    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | A4    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | A6    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | A8    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | B0    | 359/379 (95%) | 358 (100%) | 1 (0%)   | 86          | 85  |
| 2   | B2    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | B4    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | B6    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | B8    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | C0    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | C2    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | C4    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | C6    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | C8    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | D0    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | D2    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | D4    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | D6    | 359/379 (95%) | 358 (100%) | 1 (0%)   | 86          | 85  |
| 2   | D8    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | E0    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | E2    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | E4    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | E6    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | E8    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 2   | F0    | 359/379 (95%) | 359 (100%) | 0        | 100         | 100 |
| 3   | A1    | 364/381 (96%) | 364 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | A3    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | A5    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | A7    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | A9    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | B1    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | B3    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | B5    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | B7    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | B9    | 364/381 (96%)  | 363 (100%) | 1 (0%)   | 86          | 85  |
| 3   | C1    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | C3    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | C5    | 364/381 (96%)  | 363 (100%) | 1 (0%)   | 86          | 85  |
| 3   | C7    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | C9    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | D1    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | D3    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | D5    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | D7    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | D9    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | E1    | 364/381 (96%)  | 363 (100%) | 1 (0%)   | 86          | 85  |
| 3   | E3    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | E5    | 364/381 (96%)  | 363 (100%) | 1 (0%)   | 86          | 85  |
| 3   | E7    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | E9    | 364/381 (96%)  | 364 (100%) | 0        | 100         | 100 |
| 3   | F1    | 364/381 (96%)  | 363 (100%) | 1 (0%)   | 86          | 85  |
| 4   | L     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |
| 4   | M     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |
| 4   | N     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |
| 4   | Q     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |
| 4   | V     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |
| 4   | W     | 143/1401 (10%) | 143 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 5   | O     | 193/502 (38%)     | 193 (100%)   | 0        | 100         | 100 |
| 5   | P     | 193/502 (38%)     | 193 (100%)   | 0        | 100         | 100 |
| 6   | R     | 101/280 (36%)     | 101 (100%)   | 0        | 100         | 100 |
| 6   | S     | 20/280 (7%)       | 20 (100%)    | 0        | 100         | 100 |
| 6   | T     | 101/280 (36%)     | 101 (100%)   | 0        | 100         | 100 |
| 6   | U     | 81/280 (29%)      | 81 (100%)    | 0        | 100         | 100 |
| 7   | a     | 139/190 (73%)     | 139 (100%)   | 0        | 100         | 100 |
| 7   | b     | 139/190 (73%)     | 139 (100%)   | 0        | 100         | 100 |
| 7   | c     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | d     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | e     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | f     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | g     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | h     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | i     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | j     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | m     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | n     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | o     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | p     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | q     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | r     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | s     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | t     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | u     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | v     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 7   | w     | 174/190 (92%)     | 173 (99%)    | 1 (1%)   | 78          | 81  |
| 7   | x     | 174/190 (92%)     | 174 (100%)   | 0        | 100         | 100 |
| 8   | k     | 127/164 (77%)     | 127 (100%)   | 0        | 100         | 100 |
| 8   | l     | 127/164 (77%)     | 127 (100%)   | 0        | 100         | 100 |
| All | All   | 24961/38153 (65%) | 24946 (100%) | 15 (0%)  | 87          | 89  |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B0    | 309 | HIS  |
| 3   | B9    | 347 | ASN  |
| 3   | C5    | 416 | ASN  |
| 2   | D6    | 249 | ASN  |
| 3   | E1    | 191 | GLN  |
| 3   | E5    | 424 | GLN  |
| 3   | F1    | 332 | ASN  |
| 7   | c     | 37  | GLN  |
| 7   | e     | 25  | GLN  |
| 7   | f     | 37  | GLN  |
| 7   | j     | 37  | GLN  |
| 7   | m     | 65  | GLN  |
| 7   | s     | 94  | ASN  |
| 7   | u     | 37  | GLN  |
| 7   | w     | 106 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (336) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 210 | HIS  |
| 2   | A0    | 101 | ASN  |
| 2   | A0    | 216 | ASN  |
| 2   | A0    | 266 | HIS  |
| 2   | A0    | 329 | ASN  |
| 3   | A1    | 14  | ASN  |
| 3   | A1    | 184 | ASN  |
| 3   | A1    | 190 | HIS  |
| 3   | A1    | 191 | GLN  |
| 3   | A1    | 226 | ASN  |
| 3   | A1    | 256 | ASN  |
| 3   | A1    | 298 | ASN  |
| 3   | A1    | 334 | GLN  |
| 2   | A2    | 133 | GLN  |
| 2   | A2    | 216 | ASN  |
| 2   | A2    | 309 | HIS  |
| 2   | A2    | 329 | ASN  |
| 2   | A2    | 356 | ASN  |
| 3   | A3    | 200 | GLN  |
| 3   | A3    | 227 | HIS  |
| 3   | A3    | 245 | GLN  |
| 3   | A3    | 298 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A3    | 334 | GLN  |
| 3   | A3    | 375 | GLN  |
| 3   | A3    | 414 | ASN  |
| 2   | A4    | 15  | GLN  |
| 2   | A4    | 50  | ASN  |
| 2   | A4    | 88  | HIS  |
| 2   | A4    | 101 | ASN  |
| 2   | A4    | 102 | ASN  |
| 3   | A5    | 14  | ASN  |
| 3   | A5    | 15  | GLN  |
| 3   | A5    | 256 | ASN  |
| 3   | A5    | 292 | GLN  |
| 3   | A5    | 396 | HIS  |
| 2   | A6    | 88  | HIS  |
| 2   | A6    | 186 | ASN  |
| 2   | A6    | 283 | HIS  |
| 2   | A6    | 329 | ASN  |
| 3   | A7    | 6   | HIS  |
| 3   | A7    | 8   | GLN  |
| 3   | A7    | 14  | ASN  |
| 3   | A7    | 200 | GLN  |
| 3   | A7    | 204 | ASN  |
| 3   | A7    | 279 | GLN  |
| 3   | A7    | 335 | ASN  |
| 3   | A7    | 416 | ASN  |
| 3   | A7    | 426 | GLN  |
| 3   | A9    | 8   | GLN  |
| 3   | A9    | 191 | GLN  |
| 3   | A9    | 227 | HIS  |
| 2   | B0    | 35  | GLN  |
| 2   | B0    | 50  | ASN  |
| 2   | B0    | 206 | ASN  |
| 3   | B1    | 14  | ASN  |
| 3   | B1    | 131 | GLN  |
| 3   | B1    | 137 | HIS  |
| 3   | B1    | 280 | GLN  |
| 3   | B1    | 334 | GLN  |
| 3   | B1    | 348 | ASN  |
| 2   | B2    | 11  | GLN  |
| 2   | B2    | 15  | GLN  |
| 2   | B2    | 356 | ASN  |
| 3   | B3    | 6   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B3    | 100 | ASN  |
| 3   | B3    | 191 | GLN  |
| 3   | B3    | 329 | GLN  |
| 3   | B3    | 348 | ASN  |
| 3   | B3    | 414 | ASN  |
| 2   | B4    | 18  | ASN  |
| 2   | B4    | 35  | GLN  |
| 2   | B4    | 139 | ASN  |
| 2   | B4    | 356 | ASN  |
| 3   | B5    | 131 | GLN  |
| 3   | B5    | 291 | GLN  |
| 3   | B5    | 337 | ASN  |
| 3   | B5    | 414 | ASN  |
| 2   | B6    | 91  | GLN  |
| 2   | B6    | 309 | HIS  |
| 3   | B7    | 15  | GLN  |
| 3   | B7    | 195 | ASN  |
| 3   | B7    | 247 | ASN  |
| 2   | B8    | 31  | GLN  |
| 2   | B8    | 101 | ASN  |
| 2   | B8    | 139 | ASN  |
| 2   | B8    | 216 | ASN  |
| 2   | B8    | 358 | GLN  |
| 3   | B9    | 8   | GLN  |
| 3   | B9    | 83  | GLN  |
| 3   | B9    | 94  | GLN  |
| 3   | B9    | 131 | GLN  |
| 3   | B9    | 227 | HIS  |
| 3   | B9    | 256 | ASN  |
| 3   | B9    | 335 | ASN  |
| 3   | B9    | 416 | ASN  |
| 3   | B9    | 423 | GLN  |
| 1   | C     | 261 | GLN  |
| 2   | C0    | 11  | GLN  |
| 2   | C0    | 50  | ASN  |
| 2   | C0    | 91  | GLN  |
| 2   | C0    | 101 | ASN  |
| 2   | C0    | 107 | HIS  |
| 2   | C0    | 233 | GLN  |
| 2   | C0    | 249 | ASN  |
| 2   | C0    | 285 | GLN  |
| 2   | C0    | 309 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C1    | 6   | HIS  |
| 3   | C1    | 52  | ASN  |
| 3   | C1    | 94  | GLN  |
| 3   | C1    | 247 | ASN  |
| 3   | C1    | 298 | ASN  |
| 3   | C1    | 334 | GLN  |
| 3   | C1    | 416 | ASN  |
| 2   | C2    | 31  | GLN  |
| 2   | C2    | 329 | ASN  |
| 2   | C2    | 358 | GLN  |
| 3   | C3    | 8   | GLN  |
| 3   | C3    | 11  | GLN  |
| 3   | C3    | 15  | GLN  |
| 3   | C3    | 134 | GLN  |
| 3   | C3    | 204 | ASN  |
| 3   | C3    | 292 | GLN  |
| 3   | C3    | 298 | ASN  |
| 3   | C3    | 348 | ASN  |
| 3   | C3    | 414 | ASN  |
| 3   | C3    | 423 | GLN  |
| 2   | C4    | 15  | GLN  |
| 2   | C4    | 31  | GLN  |
| 2   | C4    | 102 | ASN  |
| 2   | C4    | 133 | GLN  |
| 2   | C4    | 216 | ASN  |
| 2   | C4    | 329 | ASN  |
| 3   | C5    | 52  | ASN  |
| 3   | C5    | 195 | ASN  |
| 3   | C5    | 348 | ASN  |
| 3   | C5    | 384 | GLN  |
| 3   | C5    | 416 | ASN  |
| 2   | C6    | 233 | GLN  |
| 2   | C6    | 256 | GLN  |
| 2   | C6    | 329 | ASN  |
| 2   | C6    | 342 | GLN  |
| 3   | C7    | 334 | GLN  |
| 3   | C7    | 347 | ASN  |
| 3   | C7    | 370 | ASN  |
| 3   | C7    | 396 | HIS  |
| 3   | C7    | 423 | GLN  |
| 3   | C7    | 426 | GLN  |
| 2   | C8    | 15  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C8    | 35  | GLN  |
| 2   | C8    | 216 | ASN  |
| 3   | C9    | 8   | GLN  |
| 3   | C9    | 14  | ASN  |
| 3   | C9    | 94  | GLN  |
| 3   | C9    | 100 | ASN  |
| 3   | C9    | 329 | GLN  |
| 1   | D     | 244 | GLN  |
| 2   | D0    | 50  | ASN  |
| 2   | D0    | 91  | GLN  |
| 2   | D0    | 192 | HIS  |
| 2   | D0    | 283 | HIS  |
| 2   | D0    | 329 | ASN  |
| 3   | D1    | 8   | GLN  |
| 3   | D1    | 89  | ASN  |
| 3   | D1    | 190 | HIS  |
| 3   | D1    | 375 | GLN  |
| 3   | D1    | 396 | HIS  |
| 3   | D1    | 424 | GLN  |
| 2   | D2    | 11  | GLN  |
| 2   | D2    | 15  | GLN  |
| 2   | D2    | 50  | ASN  |
| 2   | D2    | 85  | HIS  |
| 2   | D2    | 91  | GLN  |
| 2   | D2    | 107 | HIS  |
| 2   | D2    | 128 | ASN  |
| 2   | D2    | 176 | GLN  |
| 2   | D2    | 258 | ASN  |
| 2   | D2    | 293 | ASN  |
| 3   | D3    | 28  | HIS  |
| 3   | D3    | 100 | ASN  |
| 3   | D3    | 105 | HIS  |
| 3   | D3    | 134 | GLN  |
| 3   | D3    | 184 | ASN  |
| 3   | D3    | 298 | ASN  |
| 3   | D3    | 384 | GLN  |
| 2   | D4    | 35  | GLN  |
| 2   | D4    | 85  | HIS  |
| 2   | D4    | 91  | GLN  |
| 3   | D5    | 15  | GLN  |
| 3   | D5    | 48  | ASN  |
| 3   | D5    | 100 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D5    | 137 | HIS  |
| 3   | D5    | 256 | ASN  |
| 3   | D5    | 292 | GLN  |
| 3   | D5    | 298 | ASN  |
| 3   | D5    | 335 | ASN  |
| 3   | D5    | 414 | ASN  |
| 2   | D6    | 11  | GLN  |
| 2   | D6    | 15  | GLN  |
| 2   | D6    | 85  | HIS  |
| 2   | D6    | 216 | ASN  |
| 2   | D6    | 249 | ASN  |
| 2   | D6    | 258 | ASN  |
| 2   | D6    | 356 | ASN  |
| 3   | D7    | 245 | GLN  |
| 3   | D7    | 256 | ASN  |
| 3   | D7    | 298 | ASN  |
| 3   | D7    | 414 | ASN  |
| 3   | D7    | 426 | GLN  |
| 2   | D8    | 50  | ASN  |
| 2   | D8    | 192 | HIS  |
| 2   | D8    | 216 | ASN  |
| 3   | D9    | 99  | ASN  |
| 3   | D9    | 298 | ASN  |
| 3   | D9    | 348 | ASN  |
| 3   | D9    | 375 | GLN  |
| 2   | E0    | 18  | ASN  |
| 2   | E0    | 61  | HIS  |
| 2   | E0    | 168 | ASN  |
| 2   | E0    | 258 | ASN  |
| 2   | E0    | 356 | ASN  |
| 2   | E0    | 393 | HIS  |
| 3   | E1    | 14  | ASN  |
| 3   | E1    | 334 | GLN  |
| 3   | E1    | 347 | ASN  |
| 3   | E1    | 375 | GLN  |
| 2   | E2    | 101 | ASN  |
| 2   | E2    | 233 | GLN  |
| 2   | E2    | 283 | HIS  |
| 2   | E2    | 356 | ASN  |
| 3   | E3    | 8   | GLN  |
| 3   | E3    | 28  | HIS  |
| 3   | E3    | 245 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | E3    | 264 | HIS  |
| 3   | E3    | 307 | HIS  |
| 3   | E3    | 335 | ASN  |
| 3   | E3    | 426 | GLN  |
| 2   | E4    | 18  | ASN  |
| 2   | E4    | 35  | GLN  |
| 2   | E4    | 216 | ASN  |
| 2   | E4    | 256 | GLN  |
| 2   | E4    | 258 | ASN  |
| 2   | E4    | 358 | GLN  |
| 3   | E5    | 6   | HIS  |
| 3   | E5    | 15  | GLN  |
| 3   | E5    | 134 | GLN  |
| 3   | E5    | 195 | ASN  |
| 3   | E5    | 292 | GLN  |
| 3   | E5    | 424 | GLN  |
| 2   | E6    | 107 | HIS  |
| 3   | E7    | 14  | ASN  |
| 3   | E7    | 48  | ASN  |
| 3   | E7    | 191 | GLN  |
| 3   | E7    | 204 | ASN  |
| 3   | E7    | 280 | GLN  |
| 3   | E7    | 334 | GLN  |
| 3   | E7    | 335 | ASN  |
| 2   | E8    | 102 | ASN  |
| 2   | E8    | 133 | GLN  |
| 2   | E8    | 139 | ASN  |
| 2   | E8    | 216 | ASN  |
| 2   | E8    | 356 | ASN  |
| 3   | E9    | 48  | ASN  |
| 3   | E9    | 99  | ASN  |
| 3   | E9    | 195 | ASN  |
| 3   | E9    | 264 | HIS  |
| 3   | E9    | 279 | GLN  |
| 2   | F0    | 28  | HIS  |
| 2   | F0    | 31  | GLN  |
| 2   | F0    | 258 | ASN  |
| 2   | F0    | 393 | HIS  |
| 3   | F1    | 15  | GLN  |
| 3   | F1    | 264 | HIS  |
| 3   | F1    | 292 | GLN  |
| 3   | F1    | 332 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | L     | 1228 | GLN  |
| 4   | L     | 1245 | ASN  |
| 4   | M     | 1316 | GLN  |
| 4   | M     | 1403 | GLN  |
| 4   | N     | 1245 | ASN  |
| 4   | N     | 1280 | GLN  |
| 5   | O     | 556  | HIS  |
| 5   | P     | 216  | GLN  |
| 5   | P     | 481  | HIS  |
| 4   | Q     | 1245 | ASN  |
| 6   | R     | 54   | ASN  |
| 6   | U     | 130  | GLN  |
| 4   | V     | 1280 | GLN  |
| 4   | V     | 1402 | GLN  |
| 7   | a     | 94   | ASN  |
| 7   | a     | 105  | ASN  |
| 7   | b     | 67   | HIS  |
| 7   | b     | 94   | ASN  |
| 7   | c     | 37   | GLN  |
| 7   | d     | 67   | HIS  |
| 7   | d     | 100  | ASN  |
| 7   | e     | 25   | GLN  |
| 7   | e     | 41   | ASN  |
| 7   | f     | 25   | GLN  |
| 7   | f     | 37   | GLN  |
| 7   | f     | 41   | ASN  |
| 7   | f     | 125  | HIS  |
| 7   | g     | 11   | ASN  |
| 7   | g     | 41   | ASN  |
| 7   | h     | 37   | GLN  |
| 7   | h     | 128  | HIS  |
| 7   | i     | 65   | GLN  |
| 7   | i     | 125  | HIS  |
| 8   | k     | 113  | ASN  |
| 8   | l     | 17   | GLN  |
| 8   | l     | 18   | GLN  |
| 8   | l     | 147  | GLN  |
| 7   | m     | 125  | HIS  |
| 7   | n     | 37   | GLN  |
| 7   | n     | 59   | ASN  |
| 7   | n     | 100  | ASN  |
| 7   | n     | 203  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | o     | 27  | GLN  |
| 7   | o     | 203 | ASN  |
| 7   | p     | 11  | ASN  |
| 7   | p     | 18  | ASN  |
| 7   | p     | 37  | GLN  |
| 7   | p     | 203 | ASN  |
| 7   | q     | 11  | ASN  |
| 7   | r     | 37  | GLN  |
| 7   | r     | 59  | ASN  |
| 7   | s     | 94  | ASN  |
| 7   | t     | 11  | ASN  |
| 7   | t     | 18  | ASN  |
| 7   | u     | 27  | GLN  |
| 7   | u     | 65  | GLN  |
| 7   | v     | 181 | GLN  |
| 7   | w     | 3   | GLN  |
| 7   | w     | 25  | GLN  |
| 7   | x     | 94  | ASN  |
| 7   | x     | 106 | GLN  |
| 7   | x     | 128 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 26 are monoatomic - leaving 52 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 |
| 9   | GTP  | A2    | 501 | -    | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.58 | 8 (16%)  |
| 9   | GTP  | B0    | 501 | 10   | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.59 | 10 (20%) |
| 9   | GTP  | C3    | 501 | 10   | 33,34,34     | 0.91 | 2 (6%)   | 50,54,54    | 1.59 | 9 (18%)  |
| 9   | GTP  | D8    | 501 | 10   | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.58 | 9 (18%)  |
| 11  | GDP  | C9    | 501 | -    | 29,30,30     | 1.16 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 9   | GTP  | E8    | 501 | -    | 33,34,34     | 0.97 | 2 (6%)   | 50,54,54    | 1.62 | 10 (20%) |
| 11  | GDP  | C3    | 502 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.77 | 7 (15%)  |
| 11  | GDP  | A5    | 502 | -    | 29,30,30     | 1.16 | 4 (13%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 9   | GTP  | D0    | 501 | 10   | 33,34,34     | 0.90 | 2 (6%)   | 50,54,54    | 1.59 | 9 (18%)  |
| 11  | GDP  | E5    | 501 | -    | 29,30,30     | 1.18 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 11  | GDP  | D7    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 11  | GDP  | F1    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.78 | 6 (13%)  |
| 9   | GTP  | B4    | 501 | -    | 33,34,34     | 0.88 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 11  | GDP  | E1    | 502 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.74 | 7 (15%)  |
| 11  | GDP  | B5    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 11  | GDP  | D9    | 501 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.78 | 7 (15%)  |
| 11  | GDP  | D3    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.76 | 8 (17%)  |
| 11  | GDP  | E3    | 501 | -    | 29,30,30     | 1.18 | 3 (10%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 11  | GDP  | E7    | 501 | -    | 29,30,30     | 1.19 | 3 (10%)  | 45,47,47    | 1.81 | 7 (15%)  |
| 11  | GDP  | A1    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.76 | 7 (15%)  |
| 9   | GTP  | C4    | 501 | 10   | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.63 | 9 (18%)  |
| 11  | GDP  | D5    | 501 | -    | 29,30,30     | 1.18 | 3 (10%)  | 45,47,47    | 1.81 | 7 (15%)  |
| 9   | GTP  | D2    | 501 | 10   | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.63 | 9 (18%)  |
| 9   | GTP  | E2    | 501 | 10   | 33,34,34     | 0.92 | 2 (6%)   | 50,54,54    | 1.68 | 9 (18%)  |
| 9   | GTP  | E4    | 501 | 10   | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.63 | 10 (20%) |
| 11  | GDP  | D1    | 501 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.77 | 7 (15%)  |
| 11  | GDP  | C5    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.77 | 7 (15%)  |
| 9   | GTP  | B8    | 501 | 10   | 33,34,34     | 0.92 | 1 (3%)   | 50,54,54    | 1.64 | 8 (16%)  |
| 11  | GDP  | B3    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.79 | 7 (15%)  |
| 9   | GTP  | D4    | 501 | 10   | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.52 | 10 (20%) |
| 9   | GTP  | F0    | 501 | 10   | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.68 | 11 (22%) |
| 11  | GDP  | A9    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.80 | 8 (17%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | GTP  | A0    | 501 | 10   | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.62 | 9 (18%)  |
| 9   | GTP  | D6    | 501 | 10   | 33,34,34     | 0.95 | 0        | 50,54,54    | 1.57 | 8 (16%)  |
| 9   | GTP  | A4    | 501 | 10   | 33,34,34     | 0.88 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 9   | GTP  | C6    | 501 | 10   | 33,34,34     | 0.93 | 1 (3%)   | 50,54,54    | 1.59 | 9 (18%)  |
| 9   | GTP  | C0    | 501 | 10   | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.55 | 9 (18%)  |
| 11  | GDP  | C1    | 501 | -    | 29,30,30     | 1.19 | 3 (10%)  | 45,47,47    | 1.74 | 7 (15%)  |
| 9   | GTP  | B6    | 501 | 10   | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.55 | 8 (16%)  |
| 9   | GTP  | E6    | 501 | 10   | 33,34,34     | 0.98 | 2 (6%)   | 50,54,54    | 1.64 | 11 (22%) |
| 11  | GDP  | C7    | 501 | -    | 29,30,30     | 1.18 | 3 (10%)  | 45,47,47    | 1.73 | 7 (15%)  |
| 11  | GDP  | A7    | 502 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.79 | 7 (15%)  |
| 9   | GTP  | B2    | 501 | -    | 33,34,34     | 0.88 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 11  | GDP  | E9    | 502 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.74 | 7 (15%)  |
| 9   | GTP  | A6    | 501 | 10   | 33,34,34     | 0.94 | 1 (3%)   | 50,54,54    | 1.64 | 9 (18%)  |
| 11  | GDP  | B9    | 501 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.83 | 7 (15%)  |
| 11  | GDP  | B1    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.88 | 7 (15%)  |
| 9   | GTP  | C8    | 501 | 10   | 33,34,34     | 0.91 | 1 (3%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 11  | GDP  | B7    | 501 | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 9   | GTP  | A8    | 501 | -    | 33,34,34     | 0.94 | 1 (3%)   | 50,54,54    | 1.62 | 11 (22%) |
| 11  | GDP  | A3    | 501 | -    | 29,30,30     | 1.24 | 4 (13%)  | 45,47,47    | 1.81 | 9 (20%)  |
| 9   | GTP  | E0    | 501 | 10   | 33,34,34     | 0.93 | 1 (3%)   | 50,54,54    | 1.64 | 11 (22%) |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 9   | GTP  | A2    | 501 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 9   | GTP  | B0    | 501 | 10   | -       | 7/22/38/38 | 0/3/3/3 |
| 9   | GTP  | C3    | 501 | 10   | -       | 7/22/38/38 | 0/3/3/3 |
| 9   | GTP  | D8    | 501 | 10   | -       | 4/22/38/38 | 0/3/3/3 |
| 11  | GDP  | C9    | 501 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 9   | GTP  | E8    | 501 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 11  | GDP  | C3    | 502 | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 11  | GDP  | A5    | 502 | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 9   | GTP  | D0    | 501 | 10   | -       | 6/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 11  | GDP  | E5    | 501 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 11  | GDP  | D7    | 501 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 11  | GDP  | F1    | 501 | -    | -       | 2/16/32/32  | 0/3/3/3 |
| 9   | GTP  | B4    | 501 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 11  | GDP  | E1    | 502 | -    | -       | 2/16/32/32  | 0/3/3/3 |
| 11  | GDP  | B5    | 501 | -    | -       | 2/16/32/32  | 0/3/3/3 |
| 11  | GDP  | D9    | 501 | -    | -       | 6/16/32/32  | 0/3/3/3 |
| 11  | GDP  | D3    | 501 | -    | -       | 5/16/32/32  | 0/3/3/3 |
| 11  | GDP  | E3    | 501 | -    | -       | 0/16/32/32  | 0/3/3/3 |
| 11  | GDP  | E7    | 501 | -    | -       | 8/16/32/32  | 0/3/3/3 |
| 11  | GDP  | A1    | 501 | -    | -       | 2/16/32/32  | 0/3/3/3 |
| 9   | GTP  | C4    | 501 | 10   | -       | 7/22/38/38  | 0/3/3/3 |
| 11  | GDP  | D5    | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 9   | GTP  | D2    | 501 | 10   | -       | 1/22/38/38  | 0/3/3/3 |
| 9   | GTP  | E2    | 501 | 10   | -       | 7/22/38/38  | 0/3/3/3 |
| 9   | GTP  | E4    | 501 | 10   | -       | 8/22/38/38  | 0/3/3/3 |
| 11  | GDP  | D1    | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 11  | GDP  | C5    | 501 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 9   | GTP  | B8    | 501 | 10   | -       | 9/22/38/38  | 0/3/3/3 |
| 11  | GDP  | B3    | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 9   | GTP  | D4    | 501 | 10   | -       | 7/22/38/38  | 0/3/3/3 |
| 9   | GTP  | F0    | 501 | 10   | -       | 10/22/38/38 | 0/3/3/3 |
| 11  | GDP  | A9    | 501 | -    | -       | 5/16/32/32  | 0/3/3/3 |
| 9   | GTP  | A0    | 501 | 10   | -       | 9/22/38/38  | 0/3/3/3 |
| 9   | GTP  | D6    | 501 | 10   | -       | 4/22/38/38  | 0/3/3/3 |
| 9   | GTP  | A4    | 501 | 10   | -       | 6/22/38/38  | 0/3/3/3 |
| 9   | GTP  | C6    | 501 | 10   | -       | 3/22/38/38  | 0/3/3/3 |
| 9   | GTP  | C0    | 501 | 10   | -       | 2/22/38/38  | 0/3/3/3 |
| 11  | GDP  | C1    | 501 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 9   | GTP  | B6    | 501 | 10   | -       | 6/22/38/38  | 0/3/3/3 |
| 9   | GTP  | E6    | 501 | 10   | -       | 6/22/38/38  | 0/3/3/3 |
| 11  | GDP  | C7    | 501 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 11  | GDP  | A7    | 502 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 9   | GTP  | B2    | 501 | -    | -       | 8/22/38/38  | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 11  | GDP  | E9    | 502 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 9   | GTP  | A6    | 501 | 10   | -       | 5/22/38/38  | 0/3/3/3 |
| 11  | GDP  | B9    | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 11  | GDP  | B1    | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 9   | GTP  | C8    | 501 | 10   | -       | 6/22/38/38  | 0/3/3/3 |
| 11  | GDP  | B7    | 501 | -    | -       | 2/16/32/32  | 0/3/3/3 |
| 9   | GTP  | A8    | 501 | -    | -       | 5/22/38/38  | 0/3/3/3 |
| 11  | GDP  | A3    | 501 | -    | -       | 11/16/32/32 | 0/3/3/3 |
| 9   | GTP  | E0    | 501 | 10   | -       | 9/22/38/38  | 0/3/3/3 |

All (108) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | A3    | 501 | GDP  | C5-C4 | 3.14  | 1.47        | 1.38     |
| 11  | C5    | 501 | GDP  | C5-C4 | 3.10  | 1.47        | 1.38     |
| 11  | E7    | 501 | GDP  | C5-C4 | 3.08  | 1.47        | 1.38     |
| 11  | C1    | 501 | GDP  | C5-C4 | 3.05  | 1.47        | 1.38     |
| 11  | F1    | 501 | GDP  | C5-C4 | 3.04  | 1.47        | 1.38     |
| 11  | D5    | 501 | GDP  | C5-C4 | 3.03  | 1.47        | 1.38     |
| 11  | A1    | 501 | GDP  | C5-C4 | 3.02  | 1.47        | 1.38     |
| 11  | C3    | 502 | GDP  | C5-C4 | 3.02  | 1.47        | 1.38     |
| 11  | E5    | 501 | GDP  | C5-C4 | 3.01  | 1.47        | 1.38     |
| 11  | B1    | 501 | GDP  | C5-C4 | 3.00  | 1.47        | 1.38     |
| 11  | D7    | 501 | GDP  | C5-C4 | 3.00  | 1.47        | 1.38     |
| 11  | A7    | 502 | GDP  | C5-C4 | 3.00  | 1.47        | 1.38     |
| 11  | B5    | 501 | GDP  | C5-C4 | 2.99  | 1.46        | 1.38     |
| 11  | D3    | 501 | GDP  | C5-C4 | 2.99  | 1.46        | 1.38     |
| 11  | B3    | 501 | GDP  | C5-C4 | 2.99  | 1.46        | 1.38     |
| 11  | E3    | 501 | GDP  | C5-C4 | 2.98  | 1.46        | 1.38     |
| 11  | A9    | 501 | GDP  | C5-C4 | 2.98  | 1.46        | 1.38     |
| 11  | E1    | 502 | GDP  | C5-C4 | 2.97  | 1.46        | 1.38     |
| 11  | B7    | 501 | GDP  | C5-C4 | 2.96  | 1.46        | 1.38     |
| 11  | B9    | 501 | GDP  | C5-C4 | 2.95  | 1.46        | 1.38     |
| 11  | E9    | 502 | GDP  | C5-C4 | 2.95  | 1.46        | 1.38     |
| 11  | C9    | 501 | GDP  | C5-C4 | 2.93  | 1.46        | 1.38     |
| 11  | C7    | 501 | GDP  | C5-C4 | 2.92  | 1.46        | 1.38     |
| 11  | D1    | 501 | GDP  | C5-C4 | 2.90  | 1.46        | 1.38     |
| 11  | D9    | 501 | GDP  | C5-C4 | 2.89  | 1.46        | 1.38     |
| 11  | A9    | 501 | GDP  | C6-N1 | -2.79 | 1.33        | 1.38     |
| 11  | A5    | 502 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 11  | E7    | 501 | GDP  | C6-N1  | -2.77 | 1.33        | 1.38     |
| 11  | F1    | 501 | GDP  | C6-N1  | -2.74 | 1.33        | 1.38     |
| 11  | B5    | 501 | GDP  | C6-N1  | -2.73 | 1.33        | 1.38     |
| 11  | C9    | 501 | GDP  | C6-N1  | -2.72 | 1.33        | 1.38     |
| 11  | E1    | 502 | GDP  | C6-N1  | -2.71 | 1.33        | 1.38     |
| 11  | C7    | 501 | GDP  | C6-N1  | -2.70 | 1.33        | 1.38     |
| 11  | D5    | 501 | GDP  | C6-N1  | -2.69 | 1.33        | 1.38     |
| 11  | D7    | 501 | GDP  | C6-N1  | -2.69 | 1.33        | 1.38     |
| 11  | A3    | 501 | GDP  | PA-O3A | 2.68  | 1.62        | 1.59     |
| 11  | D9    | 501 | GDP  | C6-N1  | -2.66 | 1.33        | 1.38     |
| 11  | E3    | 501 | GDP  | C6-N1  | -2.65 | 1.33        | 1.38     |
| 11  | B3    | 501 | GDP  | C6-N1  | -2.64 | 1.33        | 1.38     |
| 11  | B1    | 501 | GDP  | C6-N1  | -2.64 | 1.33        | 1.38     |
| 11  | D3    | 501 | GDP  | C6-N1  | -2.64 | 1.33        | 1.38     |
| 11  | E5    | 501 | GDP  | C6-N1  | -2.64 | 1.33        | 1.38     |
| 11  | B7    | 501 | GDP  | C6-N1  | -2.62 | 1.33        | 1.38     |
| 11  | B9    | 501 | GDP  | C6-N1  | -2.61 | 1.34        | 1.38     |
| 11  | C5    | 501 | GDP  | C6-N1  | -2.61 | 1.34        | 1.38     |
| 11  | E9    | 502 | GDP  | C6-N1  | -2.60 | 1.34        | 1.38     |
| 11  | C3    | 502 | GDP  | C6-N1  | -2.59 | 1.34        | 1.38     |
| 11  | D1    | 501 | GDP  | C6-N1  | -2.57 | 1.34        | 1.38     |
| 11  | A1    | 501 | GDP  | C6-N1  | -2.57 | 1.34        | 1.38     |
| 11  | A3    | 501 | GDP  | C6-N1  | -2.54 | 1.34        | 1.38     |
| 11  | A5    | 502 | GDP  | C6-N1  | -2.53 | 1.34        | 1.38     |
| 11  | A7    | 502 | GDP  | C6-N1  | -2.53 | 1.34        | 1.38     |
| 11  | C1    | 501 | GDP  | C6-N1  | -2.51 | 1.34        | 1.38     |
| 9   | E2    | 501 | GTP  | C2-N3  | 2.29  | 1.38        | 1.33     |
| 9   | C4    | 501 | GTP  | C2-N3  | 2.24  | 1.38        | 1.33     |
| 11  | B7    | 501 | GDP  | C5-N7  | -2.23 | 1.34        | 1.39     |
| 11  | E3    | 501 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 11  | C5    | 501 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 9   | E6    | 501 | GTP  | C2-N3  | 2.20  | 1.38        | 1.33     |
| 11  | E7    | 501 | GDP  | C5-N7  | -2.20 | 1.34        | 1.39     |
| 9   | C3    | 501 | GTP  | C2-N3  | 2.19  | 1.38        | 1.33     |
| 11  | F1    | 501 | GDP  | C5-N7  | -2.19 | 1.34        | 1.39     |
| 9   | F0    | 501 | GTP  | C2-N3  | 2.18  | 1.38        | 1.33     |
| 11  | A9    | 501 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 11  | A1    | 501 | GDP  | C5-N7  | -2.18 | 1.34        | 1.39     |
| 11  | E5    | 501 | GDP  | C5-N7  | -2.17 | 1.34        | 1.39     |
| 11  | A5    | 502 | GDP  | C4-N9  | -2.16 | 1.32        | 1.38     |
| 9   | E8    | 501 | GTP  | C2-N3  | 2.16  | 1.38        | 1.33     |
| 9   | E4    | 501 | GTP  | C2-N3  | 2.16  | 1.38        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 11  | A7    | 502 | GDP  | C5-N7  | -2.16 | 1.34        | 1.39     |
| 11  | E1    | 502 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 11  | A3    | 501 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 11  | C3    | 502 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 11  | B3    | 501 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 11  | E9    | 502 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 11  | C1    | 501 | GDP  | C5-N7  | -2.15 | 1.34        | 1.39     |
| 9   | C6    | 501 | GTP  | C2-N3  | 2.14  | 1.38        | 1.33     |
| 9   | B8    | 501 | GTP  | C2-N3  | 2.13  | 1.38        | 1.33     |
| 9   | D2    | 501 | GTP  | C2-N3  | 2.13  | 1.38        | 1.33     |
| 11  | B5    | 501 | GDP  | C5-N7  | -2.13 | 1.34        | 1.39     |
| 9   | A2    | 501 | GTP  | C2-N3  | 2.12  | 1.38        | 1.33     |
| 9   | B0    | 501 | GTP  | C2-N3  | 2.12  | 1.38        | 1.33     |
| 11  | B9    | 501 | GDP  | C5-N7  | -2.12 | 1.34        | 1.39     |
| 11  | C9    | 501 | GDP  | C5-N7  | -2.11 | 1.34        | 1.39     |
| 9   | A8    | 501 | GTP  | C2-N3  | 2.11  | 1.38        | 1.33     |
| 11  | D7    | 501 | GDP  | C5-N7  | -2.11 | 1.34        | 1.39     |
| 9   | E0    | 501 | GTP  | C2-N3  | 2.10  | 1.38        | 1.33     |
| 11  | B1    | 501 | GDP  | C5-N7  | -2.10 | 1.34        | 1.39     |
| 9   | A0    | 501 | GTP  | C2-N3  | 2.09  | 1.38        | 1.33     |
| 11  | A5    | 502 | GDP  | C5-N7  | -2.09 | 1.34        | 1.39     |
| 9   | C3    | 501 | GTP  | C5-N7  | -2.09 | 1.34        | 1.39     |
| 9   | A6    | 501 | GTP  | C2-N3  | 2.08  | 1.38        | 1.33     |
| 11  | D1    | 501 | GDP  | C5-N7  | -2.08 | 1.34        | 1.39     |
| 9   | D0    | 501 | GTP  | C2-N3  | 2.08  | 1.38        | 1.33     |
| 9   | C8    | 501 | GTP  | C2-N3  | 2.08  | 1.38        | 1.33     |
| 9   | C0    | 501 | GTP  | C2-N3  | 2.08  | 1.38        | 1.33     |
| 11  | C7    | 501 | GDP  | C5-N7  | -2.06 | 1.34        | 1.39     |
| 11  | D5    | 501 | GDP  | C5-N7  | -2.06 | 1.34        | 1.39     |
| 11  | D9    | 501 | GDP  | C5-N7  | -2.05 | 1.35        | 1.39     |
| 9   | B6    | 501 | GTP  | C2-N3  | 2.04  | 1.38        | 1.33     |
| 9   | D4    | 501 | GTP  | C2-N3  | 2.04  | 1.38        | 1.33     |
| 9   | E6    | 501 | GTP  | PA-O3A | 2.04  | 1.61        | 1.59     |
| 11  | D3    | 501 | GDP  | C5-N7  | -2.04 | 1.35        | 1.39     |
| 9   | E2    | 501 | GTP  | C5-N7  | -2.03 | 1.35        | 1.39     |
| 9   | D0    | 501 | GTP  | C5-N7  | -2.01 | 1.35        | 1.39     |
| 11  | C9    | 501 | GDP  | C4-N9  | -2.01 | 1.32        | 1.38     |
| 9   | D8    | 501 | GTP  | C2-N3  | 2.01  | 1.38        | 1.33     |
| 9   | E8    | 501 | GTP  | PA-O3A | 2.00  | 1.61        | 1.59     |

All (416) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | B1    | 501 | GDP  | C5-C4-N3 | -6.45 | 118.12      | 128.39   |
| 11  | E7    | 501 | GDP  | C5-C4-N3 | -6.43 | 118.15      | 128.39   |
| 11  | B9    | 501 | GDP  | C5-C4-N3 | -6.42 | 118.17      | 128.39   |
| 11  | D5    | 501 | GDP  | C5-C4-N3 | -6.32 | 118.32      | 128.39   |
| 11  | C5    | 501 | GDP  | C5-C4-N3 | -6.25 | 118.44      | 128.39   |
| 11  | B7    | 501 | GDP  | C5-C4-N3 | -6.18 | 118.56      | 128.39   |
| 11  | B3    | 501 | GDP  | C5-C4-N3 | -6.17 | 118.57      | 128.39   |
| 11  | A9    | 501 | GDP  | C5-C4-N3 | -6.16 | 118.58      | 128.39   |
| 11  | E5    | 501 | GDP  | C5-C4-N3 | -6.16 | 118.59      | 128.39   |
| 11  | F1    | 501 | GDP  | C5-C4-N3 | -6.13 | 118.64      | 128.39   |
| 11  | C3    | 502 | GDP  | C5-C4-N3 | -6.10 | 118.67      | 128.39   |
| 11  | A7    | 502 | GDP  | C5-C4-N3 | -6.09 | 118.70      | 128.39   |
| 11  | A1    | 501 | GDP  | C5-C4-N3 | -6.04 | 118.77      | 128.39   |
| 11  | E3    | 501 | GDP  | C5-C4-N3 | -5.99 | 118.86      | 128.39   |
| 11  | C1    | 501 | GDP  | C5-C4-N3 | -5.98 | 118.87      | 128.39   |
| 11  | D7    | 501 | GDP  | C5-C4-N3 | -5.95 | 118.92      | 128.39   |
| 11  | D3    | 501 | GDP  | C5-C4-N3 | -5.94 | 118.93      | 128.39   |
| 11  | D1    | 501 | GDP  | C5-C4-N3 | -5.94 | 118.94      | 128.39   |
| 11  | E1    | 502 | GDP  | C5-C4-N3 | -5.91 | 118.98      | 128.39   |
| 11  | A3    | 501 | GDP  | C5-C4-N3 | -5.91 | 118.98      | 128.39   |
| 11  | B5    | 501 | GDP  | C5-C4-N3 | -5.83 | 119.11      | 128.39   |
| 11  | D9    | 501 | GDP  | C5-C4-N3 | -5.83 | 119.11      | 128.39   |
| 11  | C7    | 501 | GDP  | C5-C4-N3 | -5.78 | 119.20      | 128.39   |
| 11  | C9    | 501 | GDP  | C5-C4-N3 | -5.77 | 119.20      | 128.39   |
| 11  | E9    | 502 | GDP  | C5-C4-N3 | -5.69 | 119.33      | 128.39   |
| 9   | E2    | 501 | GTP  | C5-C4-N3 | -5.59 | 119.49      | 128.39   |
| 9   | F0    | 501 | GTP  | C5-C4-N3 | -5.42 | 119.76      | 128.39   |
| 11  | A5    | 502 | GDP  | C5-C4-N3 | -5.39 | 119.82      | 128.39   |
| 11  | B1    | 501 | GDP  | C2-N3-C4 | 5.38  | 121.58      | 112.30   |
| 9   | C4    | 501 | GTP  | C5-C4-N3 | -5.37 | 119.84      | 128.39   |
| 9   | E6    | 501 | GTP  | C5-C4-N3 | -5.33 | 119.91      | 128.39   |
| 9   | B8    | 501 | GTP  | C5-C4-N3 | -5.28 | 119.98      | 128.39   |
| 9   | E8    | 501 | GTP  | C5-C4-N3 | -5.25 | 120.03      | 128.39   |
| 11  | B9    | 501 | GDP  | C2-N3-C4 | 5.25  | 121.34      | 112.30   |
| 9   | C3    | 501 | GTP  | C5-C4-N3 | -5.21 | 120.10      | 128.39   |
| 9   | A6    | 501 | GTP  | C5-C4-N3 | -5.14 | 120.22      | 128.39   |
| 11  | B7    | 501 | GDP  | C2-N3-C4 | 5.13  | 121.14      | 112.30   |
| 11  | D5    | 501 | GDP  | C2-N3-C4 | 5.13  | 121.14      | 112.30   |
| 9   | B0    | 501 | GTP  | C5-C4-N3 | -5.12 | 120.24      | 128.39   |
| 9   | D2    | 501 | GTP  | C5-C4-N3 | -5.10 | 120.27      | 128.39   |
| 9   | E4    | 501 | GTP  | C5-C4-N3 | -5.10 | 120.27      | 128.39   |
| 11  | A7    | 502 | GDP  | C2-N3-C4 | 5.08  | 121.05      | 112.30   |
| 11  | E5    | 501 | GDP  | C2-N3-C4 | 5.07  | 121.03      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | C5    | 501 | GDP  | C2-N3-C4 | 5.05  | 121.00      | 112.30   |
| 9   | B2    | 501 | GTP  | C5-C4-N3 | -5.05 | 120.36      | 128.39   |
| 11  | A1    | 501 | GDP  | C2-N3-C4 | 5.05  | 120.99      | 112.30   |
| 9   | D8    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.38      | 128.39   |
| 11  | A9    | 501 | GDP  | C2-N3-C4 | 5.03  | 120.97      | 112.30   |
| 9   | A0    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.39      | 128.39   |
| 9   | C8    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 11  | D1    | 501 | GDP  | C2-N3-C4 | 5.00  | 120.91      | 112.30   |
| 11  | C3    | 502 | GDP  | C2-N3-C4 | 4.99  | 120.90      | 112.30   |
| 9   | C6    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 11  | F1    | 501 | GDP  | C2-N3-C4 | 4.98  | 120.89      | 112.30   |
| 11  | B3    | 501 | GDP  | C2-N3-C4 | 4.98  | 120.88      | 112.30   |
| 11  | D9    | 501 | GDP  | C2-N3-C4 | 4.97  | 120.85      | 112.30   |
| 11  | E7    | 501 | GDP  | C2-N3-C4 | 4.96  | 120.85      | 112.30   |
| 9   | D0    | 501 | GTP  | C5-C4-N3 | -4.95 | 120.52      | 128.39   |
| 11  | C1    | 501 | GDP  | C2-N3-C4 | 4.93  | 120.79      | 112.30   |
| 11  | E7    | 501 | GDP  | N9-C4-N3 | 4.93  | 135.80      | 125.95   |
| 9   | A2    | 501 | GTP  | C5-C4-N3 | -4.92 | 120.55      | 128.39   |
| 11  | E1    | 502 | GDP  | C2-N3-C4 | 4.92  | 120.77      | 112.30   |
| 9   | C0    | 501 | GTP  | C5-C4-N3 | -4.92 | 120.56      | 128.39   |
| 11  | D3    | 501 | GDP  | C2-N3-C4 | 4.91  | 120.76      | 112.30   |
| 9   | A8    | 501 | GTP  | C5-C4-N3 | -4.91 | 120.57      | 128.39   |
| 11  | D7    | 501 | GDP  | C2-N3-C4 | 4.91  | 120.75      | 112.30   |
| 9   | B4    | 501 | GTP  | C5-C4-N3 | -4.90 | 120.58      | 128.39   |
| 11  | A5    | 502 | GDP  | C2-N3-C4 | 4.89  | 120.72      | 112.30   |
| 9   | E0    | 501 | GTP  | C5-C4-N3 | -4.89 | 120.61      | 128.39   |
| 11  | C9    | 501 | GDP  | C2-N3-C4 | 4.89  | 120.71      | 112.30   |
| 11  | E9    | 502 | GDP  | C2-N3-C4 | 4.88  | 120.71      | 112.30   |
| 9   | B6    | 501 | GTP  | C5-C4-N3 | -4.87 | 120.63      | 128.39   |
| 11  | C7    | 501 | GDP  | C2-N3-C4 | 4.85  | 120.65      | 112.30   |
| 11  | B5    | 501 | GDP  | C2-N3-C4 | 4.83  | 120.62      | 112.30   |
| 11  | E3    | 501 | GDP  | C2-N3-C4 | 4.82  | 120.59      | 112.30   |
| 9   | E2    | 501 | GTP  | C2-N3-C4 | 4.78  | 120.53      | 112.30   |
| 9   | D6    | 501 | GTP  | C5-C4-N3 | -4.77 | 120.80      | 128.39   |
| 9   | D4    | 501 | GTP  | C5-C4-N3 | -4.76 | 120.81      | 128.39   |
| 9   | A4    | 501 | GTP  | C5-C4-N3 | -4.76 | 120.81      | 128.39   |
| 9   | F0    | 501 | GTP  | C2-N3-C4 | 4.75  | 120.48      | 112.30   |
| 9   | A6    | 501 | GTP  | C2-N3-C4 | 4.74  | 120.47      | 112.30   |
| 9   | E8    | 501 | GTP  | C2-N3-C4 | 4.74  | 120.47      | 112.30   |
| 11  | A3    | 501 | GDP  | C2-N3-C4 | 4.71  | 120.42      | 112.30   |
| 9   | C4    | 501 | GTP  | C2-N3-C4 | 4.71  | 120.41      | 112.30   |
| 9   | E6    | 501 | GTP  | C2-N3-C4 | 4.70  | 120.39      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11  | D5    | 501 | GDP  | N9-C4-N3 | 4.70 | 135.35      | 125.95   |
| 9   | B2    | 501 | GTP  | C2-N3-C4 | 4.69 | 120.37      | 112.30   |
| 9   | D8    | 501 | GTP  | C2-N3-C4 | 4.69 | 120.37      | 112.30   |
| 9   | B8    | 501 | GTP  | C2-N3-C4 | 4.68 | 120.35      | 112.30   |
| 11  | C5    | 501 | GDP  | N9-C4-N3 | 4.66 | 135.27      | 125.95   |
| 9   | B0    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.33      | 112.30   |
| 9   | D2    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.32      | 112.30   |
| 9   | A4    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.31      | 112.30   |
| 9   | A0    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.31      | 112.30   |
| 9   | B4    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.30      | 112.30   |
| 9   | E4    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 9   | C8    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.25      | 112.30   |
| 11  | B3    | 501 | GDP  | N9-C4-N3 | 4.61 | 135.18      | 125.95   |
| 11  | A7    | 502 | GDP  | N9-C4-N3 | 4.61 | 135.17      | 125.95   |
| 9   | C0    | 501 | GTP  | C2-N3-C4 | 4.60 | 120.23      | 112.30   |
| 11  | E3    | 501 | GDP  | N9-C4-N3 | 4.60 | 135.16      | 125.95   |
| 9   | D0    | 501 | GTP  | C2-N3-C4 | 4.60 | 120.22      | 112.30   |
| 11  | B9    | 501 | GDP  | N9-C4-N3 | 4.59 | 135.14      | 125.95   |
| 9   | A2    | 501 | GTP  | C2-N3-C4 | 4.59 | 120.21      | 112.30   |
| 11  | A9    | 501 | GDP  | N9-C4-N3 | 4.59 | 135.12      | 125.95   |
| 9   | C3    | 501 | GTP  | C2-N3-C4 | 4.57 | 120.18      | 112.30   |
| 9   | D6    | 501 | GTP  | C2-N3-C4 | 4.56 | 120.16      | 112.30   |
| 11  | B1    | 501 | GDP  | N9-C4-N3 | 4.56 | 135.06      | 125.95   |
| 11  | C3    | 502 | GDP  | N9-C4-N3 | 4.55 | 135.05      | 125.95   |
| 11  | F1    | 501 | GDP  | N9-C4-N3 | 4.55 | 135.05      | 125.95   |
| 9   | A8    | 501 | GTP  | C2-N3-C4 | 4.54 | 120.11      | 112.30   |
| 9   | B6    | 501 | GTP  | C2-N3-C4 | 4.53 | 120.11      | 112.30   |
| 11  | B7    | 501 | GDP  | N9-C4-N3 | 4.53 | 135.01      | 125.95   |
| 9   | D4    | 501 | GTP  | C2-N3-C4 | 4.52 | 120.08      | 112.30   |
| 9   | C6    | 501 | GTP  | C2-N3-C4 | 4.51 | 120.07      | 112.30   |
| 11  | E5    | 501 | GDP  | N9-C4-N3 | 4.50 | 134.95      | 125.95   |
| 11  | E1    | 502 | GDP  | N9-C4-N3 | 4.47 | 134.90      | 125.95   |
| 9   | E0    | 501 | GTP  | C2-N3-C4 | 4.46 | 119.97      | 112.30   |
| 11  | A1    | 501 | GDP  | N9-C4-N3 | 4.44 | 134.83      | 125.95   |
| 11  | D7    | 501 | GDP  | N9-C4-N3 | 4.40 | 134.75      | 125.95   |
| 11  | D3    | 501 | GDP  | N9-C4-N3 | 4.38 | 134.71      | 125.95   |
| 11  | A3    | 501 | GDP  | N9-C4-N3 | 4.37 | 134.69      | 125.95   |
| 11  | D9    | 501 | GDP  | N9-C4-N3 | 4.36 | 134.68      | 125.95   |
| 11  | E9    | 502 | GDP  | N9-C4-N3 | 4.34 | 134.64      | 125.95   |
| 11  | B5    | 501 | GDP  | N9-C4-N3 | 4.29 | 134.53      | 125.95   |
| 11  | C1    | 501 | GDP  | N9-C4-N3 | 4.29 | 134.53      | 125.95   |
| 11  | D1    | 501 | GDP  | N9-C4-N3 | 4.28 | 134.51      | 125.95   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | C7    | 501 | GDP  | N9-C4-N3 | 4.26  | 134.48      | 125.95   |
| 11  | C9    | 501 | GDP  | N9-C4-N3 | 4.13  | 134.22      | 125.95   |
| 11  | A5    | 502 | GDP  | N9-C4-N3 | 3.98  | 133.91      | 125.95   |
| 9   | E2    | 501 | GTP  | N9-C4-N3 | 3.82  | 133.58      | 125.95   |
| 11  | A5    | 502 | GDP  | C6-C5-N7 | 3.66  | 136.95      | 130.29   |
| 9   | E6    | 501 | GTP  | N9-C4-N3 | 3.56  | 133.08      | 125.95   |
| 9   | C3    | 501 | GTP  | N9-C4-N3 | 3.52  | 133.00      | 125.95   |
| 9   | E8    | 501 | GTP  | N9-C4-N3 | 3.47  | 132.90      | 125.95   |
| 9   | F0    | 501 | GTP  | N9-C4-N3 | 3.47  | 132.89      | 125.95   |
| 9   | B8    | 501 | GTP  | N9-C4-N3 | 3.46  | 132.88      | 125.95   |
| 11  | D9    | 501 | GDP  | C6-C5-N7 | 3.46  | 136.58      | 130.29   |
| 9   | C4    | 501 | GTP  | N9-C4-N3 | 3.46  | 132.86      | 125.95   |
| 11  | C9    | 501 | GDP  | C6-C5-N7 | 3.41  | 136.50      | 130.29   |
| 11  | C7    | 501 | GDP  | C6-C5-N7 | 3.40  | 136.49      | 130.29   |
| 11  | E9    | 502 | GDP  | C6-C5-N7 | 3.39  | 136.47      | 130.29   |
| 11  | C1    | 501 | GDP  | C6-C5-N7 | 3.37  | 136.41      | 130.29   |
| 9   | C6    | 501 | GTP  | N9-C4-N3 | 3.36  | 132.68      | 125.95   |
| 9   | A6    | 501 | GTP  | N9-C4-N3 | 3.36  | 132.68      | 125.95   |
| 9   | E4    | 501 | GTP  | N9-C4-N3 | 3.36  | 132.67      | 125.95   |
| 11  | B1    | 501 | GDP  | C6-C5-N7 | 3.35  | 136.39      | 130.29   |
| 11  | D1    | 501 | GDP  | C6-C5-N7 | 3.34  | 136.37      | 130.29   |
| 11  | D3    | 501 | GDP  | C6-C5-N7 | 3.33  | 136.35      | 130.29   |
| 9   | B0    | 501 | GTP  | N9-C4-N3 | 3.32  | 132.60      | 125.95   |
| 11  | A1    | 501 | GDP  | C6-C5-N7 | 3.30  | 136.29      | 130.29   |
| 11  | F1    | 501 | GDP  | C6-C5-N7 | 3.28  | 136.27      | 130.29   |
| 9   | E0    | 501 | GTP  | N9-C4-N3 | 3.27  | 132.49      | 125.95   |
| 11  | D7    | 501 | GDP  | C6-C5-N7 | 3.27  | 136.23      | 130.29   |
| 11  | B9    | 501 | GDP  | C6-C5-N7 | 3.26  | 136.22      | 130.29   |
| 11  | B5    | 501 | GDP  | C6-C5-N7 | 3.25  | 136.21      | 130.29   |
| 9   | A8    | 501 | GTP  | N9-C4-N3 | 3.24  | 132.44      | 125.95   |
| 9   | E2    | 501 | GTP  | C2-N1-C6 | -3.23 | 119.25      | 125.11   |
| 9   | C0    | 501 | GTP  | N9-C4-N3 | 3.23  | 132.41      | 125.95   |
| 11  | E1    | 502 | GDP  | C6-C5-N7 | 3.21  | 136.14      | 130.29   |
| 9   | D2    | 501 | GTP  | N9-C4-N3 | 3.21  | 132.37      | 125.95   |
| 11  | C3    | 502 | GDP  | C6-C5-N7 | 3.21  | 136.12      | 130.29   |
| 11  | A9    | 501 | GDP  | C6-C5-N7 | 3.20  | 136.11      | 130.29   |
| 9   | D8    | 501 | GTP  | N9-C4-N3 | 3.19  | 132.34      | 125.95   |
| 11  | E5    | 501 | GDP  | C6-C5-N7 | 3.19  | 136.10      | 130.29   |
| 11  | A7    | 502 | GDP  | C6-C5-N7 | 3.17  | 136.06      | 130.29   |
| 9   | B6    | 501 | GTP  | N9-C4-N3 | 3.17  | 132.29      | 125.95   |
| 9   | C8    | 501 | GTP  | N9-C4-N3 | 3.16  | 132.28      | 125.95   |
| 11  | B7    | 501 | GDP  | C6-C5-N7 | 3.16  | 136.04      | 130.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | D5    | 501 | GDP  | C6-C5-N7 | 3.15  | 136.03      | 130.29   |
| 9   | D0    | 501 | GTP  | N9-C4-N3 | 3.14  | 132.24      | 125.95   |
| 9   | A2    | 501 | GTP  | N9-C4-N3 | 3.14  | 132.23      | 125.95   |
| 9   | A0    | 501 | GTP  | N9-C4-N3 | 3.14  | 132.23      | 125.95   |
| 11  | A3    | 501 | GDP  | C6-C5-N7 | 3.13  | 135.99      | 130.29   |
| 11  | C5    | 501 | GDP  | C6-C5-N7 | 3.12  | 135.97      | 130.29   |
| 9   | B8    | 501 | GTP  | C2-N1-C6 | -3.11 | 119.47      | 125.11   |
| 11  | E3    | 501 | GDP  | C6-C5-N7 | 3.11  | 135.94      | 130.29   |
| 9   | F0    | 501 | GTP  | C2-N1-C6 | -3.09 | 119.50      | 125.11   |
| 9   | E8    | 501 | GTP  | C2-N1-C6 | -3.08 | 119.52      | 125.11   |
| 11  | B3    | 501 | GDP  | C6-C5-N7 | 3.07  | 135.88      | 130.29   |
| 9   | E4    | 501 | GTP  | C2-N1-C6 | -3.07 | 119.55      | 125.11   |
| 9   | E6    | 501 | GTP  | C2-N1-C6 | -3.06 | 119.57      | 125.11   |
| 9   | A2    | 501 | GTP  | C2-N1-C6 | -3.05 | 119.59      | 125.11   |
| 9   | B0    | 501 | GTP  | C2-N1-C6 | -3.03 | 119.62      | 125.11   |
| 9   | A8    | 501 | GTP  | C2-N1-C6 | -3.02 | 119.62      | 125.11   |
| 9   | C4    | 501 | GTP  | C2-N1-C6 | -3.02 | 119.64      | 125.11   |
| 9   | B2    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.98      | 125.95   |
| 9   | B4    | 501 | GTP  | N9-C4-N3 | 3.00  | 131.96      | 125.95   |
| 9   | C8    | 501 | GTP  | C2-N1-C6 | -3.00 | 119.67      | 125.11   |
| 9   | A6    | 501 | GTP  | C2-N1-C6 | -2.99 | 119.70      | 125.11   |
| 9   | D6    | 501 | GTP  | N9-C4-N3 | 2.97  | 131.90      | 125.95   |
| 9   | B2    | 501 | GTP  | C2-N1-C6 | -2.97 | 119.72      | 125.11   |
| 9   | D2    | 501 | GTP  | C2-N1-C6 | -2.97 | 119.72      | 125.11   |
| 9   | D8    | 501 | GTP  | C2-N1-C6 | -2.97 | 119.72      | 125.11   |
| 9   | A4    | 501 | GTP  | N9-C4-N3 | 2.97  | 131.89      | 125.95   |
| 9   | A0    | 501 | GTP  | C2-N1-C6 | -2.94 | 119.77      | 125.11   |
| 9   | D4    | 501 | GTP  | N9-C4-N3 | 2.94  | 131.83      | 125.95   |
| 9   | E0    | 501 | GTP  | C2-N1-C6 | -2.89 | 119.88      | 125.11   |
| 9   | D0    | 501 | GTP  | C2-N1-C6 | -2.88 | 119.89      | 125.11   |
| 9   | D6    | 501 | GTP  | N9-C8-N7 | -2.87 | 108.07      | 113.40   |
| 9   | C8    | 501 | GTP  | N9-C8-N7 | -2.85 | 108.11      | 113.40   |
| 9   | C3    | 501 | GTP  | C2-N1-C6 | -2.85 | 119.94      | 125.11   |
| 9   | D6    | 501 | GTP  | C2-N1-C6 | -2.84 | 119.95      | 125.11   |
| 11  | E7    | 501 | GDP  | C6-C5-N7 | 2.82  | 135.43      | 130.29   |
| 9   | B4    | 501 | GTP  | C2-N1-C6 | -2.82 | 120.00      | 125.11   |
| 9   | A8    | 501 | GTP  | N9-C8-N7 | -2.79 | 108.22      | 113.40   |
| 9   | E0    | 501 | GTP  | N9-C8-N7 | -2.79 | 108.22      | 113.40   |
| 9   | A4    | 501 | GTP  | C2-N1-C6 | -2.79 | 120.04      | 125.11   |
| 9   | A4    | 501 | GTP  | N9-C8-N7 | -2.79 | 108.22      | 113.40   |
| 9   | C6    | 501 | GTP  | C2-N1-C6 | -2.79 | 120.05      | 125.11   |
| 9   | B4    | 501 | GTP  | N9-C8-N7 | -2.78 | 108.24      | 113.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | E2    | 501 | GTP  | C5-C6-N1    | 2.77  | 120.31      | 113.25   |
| 9   | A2    | 501 | GTP  | N9-C8-N7    | -2.77 | 108.26      | 113.40   |
| 9   | D8    | 501 | GTP  | N9-C8-N7    | -2.76 | 108.28      | 113.40   |
| 9   | B6    | 501 | GTP  | C2-N1-C6    | -2.75 | 120.11      | 125.11   |
| 9   | A6    | 501 | GTP  | N9-C8-N7    | -2.75 | 108.29      | 113.40   |
| 9   | B8    | 501 | GTP  | N9-C8-N7    | -2.75 | 108.30      | 113.40   |
| 9   | B6    | 501 | GTP  | N9-C8-N7    | -2.74 | 108.33      | 113.40   |
| 9   | F0    | 501 | GTP  | C8-N7-C5    | 2.72  | 109.11      | 104.26   |
| 9   | C0    | 501 | GTP  | C2-N1-C6    | -2.72 | 120.18      | 125.11   |
| 9   | F0    | 501 | GTP  | N9-C8-N7    | -2.71 | 108.38      | 113.40   |
| 11  | B1    | 501 | GDP  | C4-C5-N7    | -2.70 | 106.39      | 110.67   |
| 9   | E4    | 501 | GTP  | N9-C8-N7    | -2.70 | 108.39      | 113.40   |
| 9   | A2    | 501 | GTP  | O6-C6-C5    | -2.70 | 119.41      | 126.53   |
| 9   | B2    | 501 | GTP  | N9-C8-N7    | -2.70 | 108.40      | 113.40   |
| 9   | A0    | 501 | GTP  | O2B-PB-O3A  | 2.69  | 114.54      | 107.27   |
| 9   | A8    | 501 | GTP  | O6-C6-C5    | -2.69 | 119.44      | 126.53   |
| 9   | E6    | 501 | GTP  | N9-C8-N7    | -2.68 | 108.43      | 113.40   |
| 11  | B9    | 501 | GDP  | C4-C5-N7    | -2.68 | 106.43      | 110.67   |
| 9   | D2    | 501 | GTP  | N9-C8-N7    | -2.67 | 108.46      | 113.40   |
| 11  | C1    | 501 | GDP  | C4-C5-N7    | -2.66 | 106.45      | 110.67   |
| 9   | B0    | 501 | GTP  | N9-C8-N7    | -2.66 | 108.47      | 113.40   |
| 9   | C0    | 501 | GTP  | N9-C8-N7    | -2.65 | 108.48      | 113.40   |
| 9   | C6    | 501 | GTP  | N9-C8-N7    | -2.65 | 108.48      | 113.40   |
| 9   | E8    | 501 | GTP  | N9-C8-N7    | -2.64 | 108.50      | 113.40   |
| 11  | B1    | 501 | GDP  | C3'-C2'-C1' | 2.64  | 106.46      | 101.46   |
| 9   | E6    | 501 | GTP  | C5-C6-N1    | 2.64  | 119.97      | 113.25   |
| 9   | B0    | 501 | GTP  | C5-C6-N1    | 2.64  | 119.96      | 113.25   |
| 9   | A2    | 501 | GTP  | C5-C6-N1    | 2.63  | 119.95      | 113.25   |
| 9   | D4    | 501 | GTP  | N9-C8-N7    | -2.63 | 108.53      | 113.40   |
| 9   | E4    | 501 | GTP  | C5-C6-N1    | 2.63  | 119.94      | 113.25   |
| 9   | A6    | 501 | GTP  | C5-C6-N1    | 2.62  | 119.93      | 113.25   |
| 9   | E8    | 501 | GTP  | C5-C6-N1    | 2.62  | 119.93      | 113.25   |
| 9   | C4    | 501 | GTP  | N9-C8-N7    | -2.62 | 108.55      | 113.40   |
| 9   | D4    | 501 | GTP  | C2-N1-C6    | -2.61 | 120.37      | 125.11   |
| 11  | C9    | 501 | GDP  | C4-C5-N7    | -2.61 | 106.54      | 110.67   |
| 9   | C4    | 501 | GTP  | C8-N7-C5    | 2.60  | 108.90      | 104.26   |
| 11  | D3    | 501 | GDP  | C4-C5-N7    | -2.59 | 106.56      | 110.67   |
| 9   | B2    | 501 | GTP  | C5-C6-N1    | 2.59  | 119.85      | 113.25   |
| 9   | B8    | 501 | GTP  | C8-N7-C5    | 2.59  | 108.87      | 104.26   |
| 9   | C8    | 501 | GTP  | C5-C6-N1    | 2.59  | 119.84      | 113.25   |
| 9   | B2    | 501 | GTP  | C8-N7-C5    | 2.59  | 108.87      | 104.26   |
| 9   | F0    | 501 | GTP  | C5-C6-N1    | 2.59  | 119.84      | 113.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | A3    | 501 | GDP  | O2A-PA-O3A  | 2.58  | 114.26      | 107.27   |
| 9   | B8    | 501 | GTP  | C5-C6-N1    | 2.58  | 119.83      | 113.25   |
| 9   | D8    | 501 | GTP  | C5-C6-N1    | 2.58  | 119.81      | 113.25   |
| 11  | A1    | 501 | GDP  | C4-C5-N7    | -2.58 | 106.59      | 110.67   |
| 9   | A8    | 501 | GTP  | C5-C6-N1    | 2.57  | 119.80      | 113.25   |
| 9   | D0    | 501 | GTP  | N9-C8-N7    | -2.57 | 108.64      | 113.40   |
| 11  | E5    | 501 | GDP  | C4-C5-N7    | -2.57 | 106.61      | 110.67   |
| 9   | A4    | 501 | GTP  | C5-C6-N1    | 2.56  | 119.77      | 113.25   |
| 9   | C8    | 501 | GTP  | C8-N7-C5    | 2.56  | 108.82      | 104.26   |
| 9   | C4    | 501 | GTP  | C5-C6-N1    | 2.56  | 119.76      | 113.25   |
| 9   | B4    | 501 | GTP  | C8-N7-C5    | 2.56  | 108.81      | 104.26   |
| 11  | D1    | 501 | GDP  | C4-C5-N7    | -2.56 | 106.62      | 110.67   |
| 11  | F1    | 501 | GDP  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 11  | C3    | 502 | GDP  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 11  | C7    | 501 | GDP  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 11  | C5    | 501 | GDP  | C4-C5-N7    | -2.55 | 106.63      | 110.67   |
| 9   | A6    | 501 | GTP  | O6-C6-C5    | -2.55 | 119.81      | 126.53   |
| 9   | D2    | 501 | GTP  | C8-N7-C5    | 2.55  | 108.80      | 104.26   |
| 9   | D6    | 501 | GTP  | C5-C6-N1    | 2.54  | 119.72      | 113.25   |
| 9   | C6    | 501 | GTP  | C5-C6-N1    | 2.54  | 119.72      | 113.25   |
| 9   | D0    | 501 | GTP  | C5-C6-N1    | 2.54  | 119.72      | 113.25   |
| 11  | D5    | 501 | GDP  | C4-C5-N7    | -2.54 | 106.64      | 110.67   |
| 9   | A6    | 501 | GTP  | O2B-PB-O3A  | 2.54  | 114.13      | 107.27   |
| 9   | D2    | 501 | GTP  | C5-C6-N1    | 2.54  | 119.71      | 113.25   |
| 9   | A0    | 501 | GTP  | N9-C8-N7    | -2.53 | 108.70      | 113.40   |
| 9   | E6    | 501 | GTP  | C8-N7-C5    | 2.53  | 108.77      | 104.26   |
| 9   | D6    | 501 | GTP  | C8-N7-C5    | 2.53  | 108.77      | 104.26   |
| 11  | A3    | 501 | GDP  | C3'-C2'-C1' | 2.53  | 106.25      | 101.46   |
| 9   | A6    | 501 | GTP  | C8-N7-C5    | 2.53  | 108.76      | 104.26   |
| 9   | E0    | 501 | GTP  | C5-C6-N1    | 2.53  | 119.68      | 113.25   |
| 9   | A0    | 501 | GTP  | C5-C6-N1    | 2.52  | 119.68      | 113.25   |
| 9   | B4    | 501 | GTP  | C5-C6-N1    | 2.52  | 119.67      | 113.25   |
| 11  | B7    | 501 | GDP  | C4-C5-N7    | -2.51 | 106.69      | 110.67   |
| 9   | D8    | 501 | GTP  | C8-N7-C5    | 2.51  | 108.73      | 104.26   |
| 9   | C0    | 501 | GTP  | C5-C6-N1    | 2.51  | 119.64      | 113.25   |
| 9   | E0    | 501 | GTP  | O6-C6-C5    | -2.51 | 119.91      | 126.53   |
| 9   | E4    | 501 | GTP  | O6-C6-C5    | -2.51 | 119.91      | 126.53   |
| 9   | C3    | 501 | GTP  | C5-C6-N1    | 2.50  | 119.62      | 113.25   |
| 9   | D4    | 501 | GTP  | C5-C6-N1    | 2.50  | 119.62      | 113.25   |
| 11  | A9    | 501 | GDP  | C4-C5-N7    | -2.50 | 106.71      | 110.67   |
| 9   | D0    | 501 | GTP  | O6-C6-C5    | -2.50 | 119.94      | 126.53   |
| 9   | E0    | 501 | GTP  | C8-N7-C5    | 2.50  | 108.71      | 104.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | B5    | 501 | GDP  | C4-C5-N7    | -2.49 | 106.72      | 110.67   |
| 9   | B6    | 501 | GTP  | C8-N7-C5    | 2.49  | 108.70      | 104.26   |
| 9   | E4    | 501 | GTP  | C8-N7-C5    | 2.49  | 108.70      | 104.26   |
| 9   | B0    | 501 | GTP  | O6-C6-C5    | -2.49 | 119.97      | 126.53   |
| 9   | E2    | 501 | GTP  | N9-C8-N7    | -2.49 | 108.79      | 113.40   |
| 9   | E8    | 501 | GTP  | C8-N7-C5    | 2.48  | 108.68      | 104.26   |
| 9   | B8    | 501 | GTP  | O6-C6-C5    | -2.48 | 119.98      | 126.53   |
| 9   | B0    | 501 | GTP  | C8-N7-C5    | 2.48  | 108.68      | 104.26   |
| 9   | C8    | 501 | GTP  | O6-C6-C5    | -2.48 | 119.99      | 126.53   |
| 9   | A2    | 501 | GTP  | C8-N7-C5    | 2.48  | 108.67      | 104.26   |
| 11  | B3    | 501 | GDP  | C3'-C2'-C1' | 2.47  | 106.14      | 101.46   |
| 9   | E6    | 501 | GTP  | O6-C6-C5    | -2.47 | 120.01      | 126.53   |
| 11  | A5    | 502 | GDP  | C4-C5-N7    | -2.47 | 106.75      | 110.67   |
| 11  | B3    | 501 | GDP  | C4-C5-N7    | -2.47 | 106.75      | 110.67   |
| 9   | C3    | 501 | GTP  | O6-C6-C5    | -2.46 | 120.03      | 126.53   |
| 9   | A0    | 501 | GTP  | C8-N7-C5    | 2.46  | 108.64      | 104.26   |
| 9   | E2    | 501 | GTP  | O6-C6-C5    | -2.46 | 120.05      | 126.53   |
| 11  | D9    | 501 | GDP  | C4-C5-N7    | -2.46 | 106.78      | 110.67   |
| 11  | A7    | 502 | GDP  | C3'-C2'-C1' | 2.45  | 106.10      | 101.46   |
| 11  | D7    | 501 | GDP  | C4-C5-N7    | -2.45 | 106.79      | 110.67   |
| 9   | A8    | 501 | GTP  | C8-N7-C5    | 2.44  | 108.61      | 104.26   |
| 11  | E7    | 501 | GDP  | C4-C5-N7    | -2.44 | 106.81      | 110.67   |
| 11  | A3    | 501 | GDP  | C4-C5-N7    | -2.44 | 106.81      | 110.67   |
| 11  | E9    | 502 | GDP  | C4-C5-N7    | -2.44 | 106.81      | 110.67   |
| 9   | E8    | 501 | GTP  | O6-C6-C5    | -2.44 | 120.10      | 126.53   |
| 9   | B6    | 501 | GTP  | C5-C6-N1    | 2.43  | 119.44      | 113.25   |
| 9   | B6    | 501 | GTP  | O6-C6-C5    | -2.43 | 120.12      | 126.53   |
| 11  | A7    | 502 | GDP  | C4-C5-N7    | -2.42 | 106.83      | 110.67   |
| 9   | E2    | 501 | GTP  | C8-N7-C5    | 2.42  | 108.57      | 104.26   |
| 9   | A0    | 501 | GTP  | O6-C6-C5    | -2.42 | 120.16      | 126.53   |
| 11  | E3    | 501 | GDP  | C4-C5-N7    | -2.42 | 106.84      | 110.67   |
| 9   | C0    | 501 | GTP  | C8-N7-C5    | 2.42  | 108.56      | 104.26   |
| 9   | C4    | 501 | GTP  | O6-C6-C5    | -2.41 | 120.18      | 126.53   |
| 9   | C6    | 501 | GTP  | O6-C6-C5    | -2.41 | 120.18      | 126.53   |
| 9   | D0    | 501 | GTP  | C8-N7-C5    | 2.41  | 108.55      | 104.26   |
| 9   | A4    | 501 | GTP  | C8-N7-C5    | 2.41  | 108.55      | 104.26   |
| 11  | A1    | 501 | GDP  | C3'-C2'-C1' | 2.40  | 106.00      | 101.46   |
| 9   | D4    | 501 | GTP  | C8-N7-C5    | 2.40  | 108.53      | 104.26   |
| 11  | D5    | 501 | GDP  | C3'-C2'-C1' | 2.40  | 106.00      | 101.46   |
| 9   | F0    | 501 | GTP  | O2B-PB-O3A  | 2.39  | 113.74      | 107.27   |
| 9   | D8    | 501 | GTP  | O6-C6-C5    | -2.39 | 120.21      | 126.53   |
| 9   | E6    | 501 | GTP  | O2A-PA-O3A  | 2.39  | 113.74      | 107.27   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 9   | D2    | 501 | GTP  | O6-C6-C5    | -2.39 | 120.22      | 126.53   |
| 11  | E1    | 502 | GDP  | C4-C5-N7    | -2.39 | 106.88      | 110.67   |
| 9   | D6    | 501 | GTP  | O6-C6-C5    | -2.38 | 120.24      | 126.53   |
| 9   | F0    | 501 | GTP  | C3'-C2'-C1' | 2.38  | 105.96      | 101.46   |
| 11  | C9    | 501 | GDP  | C3'-C2'-C1' | 2.37  | 105.95      | 101.46   |
| 9   | C6    | 501 | GTP  | C8-N7-C5    | 2.37  | 108.47      | 104.26   |
| 9   | A4    | 501 | GTP  | O6-C6-C5    | -2.36 | 120.30      | 126.53   |
| 11  | F1    | 501 | GDP  | C3'-C2'-C1' | 2.36  | 105.93      | 101.46   |
| 9   | C6    | 501 | GTP  | O3G-PG-O3B  | 2.36  | 112.55      | 104.64   |
| 9   | C3    | 501 | GTP  | N9-C8-N7    | -2.35 | 109.03      | 113.40   |
| 9   | A8    | 501 | GTP  | O2B-PB-O3A  | 2.35  | 113.61      | 107.27   |
| 9   | E0    | 501 | GTP  | O2B-PB-O3A  | 2.32  | 113.55      | 107.27   |
| 11  | D1    | 501 | GDP  | C3'-C2'-C1' | 2.32  | 105.84      | 101.46   |
| 9   | B4    | 501 | GTP  | O6-C6-C5    | -2.29 | 120.49      | 126.53   |
| 9   | E2    | 501 | GTP  | C3'-C2'-C1' | 2.29  | 105.79      | 101.46   |
| 9   | F0    | 501 | GTP  | O6-C6-C5    | -2.28 | 120.51      | 126.53   |
| 9   | C3    | 501 | GTP  | C8-N7-C5    | 2.27  | 108.31      | 104.26   |
| 11  | E7    | 501 | GDP  | C3'-C2'-C1' | 2.27  | 105.75      | 101.46   |
| 11  | A7    | 502 | GDP  | O6-C6-C5    | -2.25 | 120.59      | 126.53   |
| 9   | E0    | 501 | GTP  | O2A-PA-O3A  | 2.24  | 113.33      | 107.27   |
| 11  | D3    | 501 | GDP  | C3'-C2'-C1' | 2.23  | 105.68      | 101.46   |
| 9   | D4    | 501 | GTP  | O2B-PB-O3A  | 2.23  | 113.29      | 107.27   |
| 9   | C0    | 501 | GTP  | O6-C6-C5    | -2.22 | 120.69      | 126.53   |
| 9   | E6    | 501 | GTP  | C3'-C2'-C1' | 2.21  | 105.64      | 101.46   |
| 11  | B5    | 501 | GDP  | C3'-C2'-C1' | 2.20  | 105.62      | 101.46   |
| 9   | E6    | 501 | GTP  | O2B-PB-O3A  | 2.20  | 113.21      | 107.27   |
| 9   | C4    | 501 | GTP  | C3'-C2'-C1' | 2.19  | 105.61      | 101.46   |
| 11  | C5    | 501 | GDP  | C3'-C2'-C1' | 2.18  | 105.59      | 101.46   |
| 11  | D1    | 501 | GDP  | O6-C6-C5    | -2.18 | 120.78      | 126.53   |
| 11  | D7    | 501 | GDP  | O6-C6-C5    | -2.17 | 120.80      | 126.53   |
| 9   | E4    | 501 | GTP  | C3'-C2'-C1' | 2.16  | 105.55      | 101.46   |
| 11  | A3    | 501 | GDP  | O3B-PB-O3A  | 2.16  | 111.87      | 104.64   |
| 11  | A3    | 501 | GDP  | O6-C6-C5    | -2.15 | 120.86      | 126.53   |
| 11  | D9    | 501 | GDP  | O6-C6-C5    | -2.15 | 120.86      | 126.53   |
| 9   | C3    | 501 | GTP  | O3G-PG-O3B  | 2.14  | 111.83      | 104.64   |
| 9   | D4    | 501 | GTP  | O6-C6-C5    | -2.14 | 120.87      | 126.53   |
| 9   | B2    | 501 | GTP  | O6-C6-C5    | -2.14 | 120.89      | 126.53   |
| 11  | C5    | 501 | GDP  | O6-C6-C5    | -2.13 | 120.90      | 126.53   |
| 11  | C1    | 501 | GDP  | C2'-C3'-C4' | 2.13  | 106.72      | 102.61   |
| 9   | B0    | 501 | GTP  | O2A-PA-O3A  | 2.13  | 113.02      | 107.27   |
| 11  | E9    | 502 | GDP  | C2'-C1'-N9  | -2.12 | 107.34      | 113.25   |
| 11  | E9    | 502 | GDP  | O6-C6-C5    | -2.12 | 120.93      | 126.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 11  | E3    | 501 | GDP  | O6-C6-C5    | -2.12 | 120.94      | 126.53   |
| 11  | A9    | 501 | GDP  | O3B-PB-O3A  | 2.11  | 111.72      | 104.64   |
| 11  | B7    | 501 | GDP  | O6-C6-C5    | -2.11 | 120.96      | 126.53   |
| 11  | A1    | 501 | GDP  | O6-C6-C5    | -2.10 | 120.98      | 126.53   |
| 11  | A5    | 502 | GDP  | O6-C6-C5    | -2.10 | 120.98      | 126.53   |
| 9   | E4    | 501 | GTP  | O2A-PA-O3A  | 2.10  | 112.95      | 107.27   |
| 11  | C1    | 501 | GDP  | O6-C6-C5    | -2.09 | 121.01      | 126.53   |
| 11  | B3    | 501 | GDP  | O6-C6-C5    | -2.09 | 121.01      | 126.53   |
| 11  | B9    | 501 | GDP  | O6-C6-C5    | -2.09 | 121.01      | 126.53   |
| 11  | E1    | 502 | GDP  | O6-C6-C5    | -2.09 | 121.02      | 126.53   |
| 11  | B1    | 501 | GDP  | O6-C6-C5    | -2.08 | 121.05      | 126.53   |
| 11  | E5    | 501 | GDP  | O6-C6-C5    | -2.07 | 121.06      | 126.53   |
| 9   | D4    | 501 | GTP  | C3'-C2'-C1' | 2.07  | 105.38      | 101.46   |
| 9   | E0    | 501 | GTP  | C3'-C2'-C1' | 2.07  | 105.37      | 101.46   |
| 9   | D0    | 501 | GTP  | C3'-C2'-C1' | 2.06  | 105.36      | 101.46   |
| 9   | F0    | 501 | GTP  | O2A-PA-O3A  | 2.06  | 112.84      | 107.27   |
| 11  | D5    | 501 | GDP  | O6-C6-C5    | -2.05 | 121.13      | 126.53   |
| 11  | E7    | 501 | GDP  | O6-C6-C5    | -2.05 | 121.13      | 126.53   |
| 11  | C7    | 501 | GDP  | O6-C6-C5    | -2.04 | 121.14      | 126.53   |
| 11  | A9    | 501 | GDP  | C3'-C2'-C1' | 2.04  | 105.31      | 101.46   |
| 9   | D2    | 501 | GTP  | C3'-C2'-C1' | 2.03  | 105.30      | 101.46   |
| 9   | E8    | 501 | GTP  | O2A-PA-O3A  | 2.03  | 112.75      | 107.27   |
| 11  | C3    | 502 | GDP  | O6-C6-C5    | -2.02 | 121.19      | 126.53   |
| 9   | D8    | 501 | GTP  | C3'-C2'-C1' | 2.02  | 105.29      | 101.46   |
| 9   | C0    | 501 | GTP  | C3'-C2'-C1' | 2.02  | 105.29      | 101.46   |
| 11  | D3    | 501 | GDP  | C2'-C3'-C4' | 2.02  | 106.51      | 102.61   |
| 11  | C3    | 502 | GDP  | C3'-C2'-C1' | 2.02  | 105.28      | 101.46   |
| 11  | A9    | 501 | GDP  | O6-C6-C5    | -2.02 | 121.21      | 126.53   |
| 11  | C7    | 501 | GDP  | O2A-PA-O3A  | 2.02  | 112.72      | 107.27   |
| 11  | E1    | 502 | GDP  | C3'-C2'-C1' | 2.02  | 105.28      | 101.46   |
| 11  | B9    | 501 | GDP  | C3'-C2'-C1' | 2.01  | 105.27      | 101.46   |
| 11  | D9    | 501 | GDP  | C5-C6-N1    | 2.01  | 118.38      | 113.25   |
| 11  | D3    | 501 | GDP  | O6-C6-C5    | -2.01 | 121.23      | 126.53   |
| 9   | B0    | 501 | GTP  | C3'-C2'-C1' | 2.01  | 105.26      | 101.46   |
| 9   | A8    | 501 | GTP  | O2A-PA-O3A  | 2.01  | 112.70      | 107.27   |
| 9   | A8    | 501 | GTP  | C3'-C2'-C1' | 2.00  | 105.25      | 101.46   |
| 9   | E8    | 501 | GTP  | C3'-C2'-C1' | 2.00  | 105.25      | 101.46   |

There are no chirality outliers.

All (253) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | A0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | A0    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | A0    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | A2    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | A2    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | A4    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | A4    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | A4    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | A6    | 501 | GTP  | PB-O3A-PA-O5'   |
| 9   | A6    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | A6    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | A6    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | A8    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | A8    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | B0    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | B0    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B2    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | B2    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | B2    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B4    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | B4    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | B4    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B6    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | B6    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | B6    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B8    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | B8    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | B8    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | B8    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | C3    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | C3    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | C3    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | C4    | 501 | GTP  | PB-O3B-PG-O2G   |
| 9   | C4    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | C4    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | C4    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | C8    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | C8    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | C8    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | D0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | D0    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | D0    | 501 | GTP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | D4    | 501 | GTP  | PB-O3A-PA-O5'   |
| 9   | D6    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | D8    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | D8    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | E0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | E0    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E0    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | E2    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | E2    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E4    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | E4    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E4    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | E6    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | E6    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E6    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | E8    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | E8    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E8    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | F0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | F0    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | F0    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 11  | A3    | 501 | GDP  | PA-O3A-PB-O3B   |
| 11  | A3    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | A3    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | A3    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | A7    | 502 | GDP  | C5'-O5'-PA-O3A  |
| 11  | A7    | 502 | GDP  | C5'-O5'-PA-O1A  |
| 11  | A7    | 502 | GDP  | C5'-O5'-PA-O2A  |
| 11  | A9    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | A9    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | A9    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | B1    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | B1    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | B1    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | B3    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | B3    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | B5    | 501 | GDP  | PA-O3A-PB-O2B   |
| 11  | B7    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | B7    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | B9    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | B9    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | B9    | 501 | GDP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | C1    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | C1    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | C3    | 502 | GDP  | C5'-O5'-PA-O3A  |
| 11  | C3    | 502 | GDP  | C5'-O5'-PA-O1A  |
| 11  | C3    | 502 | GDP  | C5'-O5'-PA-O2A  |
| 11  | C5    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 11  | C7    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | C7    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | C9    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | D1    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | D1    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | D5    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | D5    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | D7    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | D7    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | D9    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | D9    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | E1    | 502 | GDP  | C5'-O5'-PA-O3A  |
| 11  | E1    | 502 | GDP  | C5'-O5'-PA-O2A  |
| 11  | E7    | 501 | GDP  | PA-O3A-PB-O3B   |
| 11  | E7    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | E7    | 501 | GDP  | C5'-O5'-PA-O1A  |
| 11  | E7    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | E9    | 502 | GDP  | PA-O3A-PB-O2B   |
| 11  | E9    | 502 | GDP  | C5'-O5'-PA-O3A  |
| 11  | E9    | 502 | GDP  | C5'-O5'-PA-O2A  |
| 11  | F1    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | F1    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 9   | A2    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | A2    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | B2    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | B2    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | B6    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | B6    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | B8    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | C3    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | C3    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | C4    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | C6    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | D6    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | E2    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 11  | A3    | 501 | GDP  | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | E7    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | A0    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | A0    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | C4    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | C8    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | D4    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | D4    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | E2    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | E4    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | E4    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 11  | A1    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 11  | A1    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 11  | E7    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 9   | C8    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 11  | C5    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | C6    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 11  | A3    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 11  | D9    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | C0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | F0    | 501 | GTP  | PB-O3A-PA-O1A   |
| 11  | C5    | 501 | GDP  | PB-O3A-PA-O1A   |
| 9   | D0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | A0    | 501 | GTP  | PB-O3A-PA-O5'   |
| 9   | B8    | 501 | GTP  | PB-O3A-PA-O5'   |
| 9   | A4    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 11  | D3    | 501 | GDP  | PA-O3A-PB-O1B   |
| 11  | E5    | 501 | GDP  | PA-O3A-PB-O1B   |
| 11  | E7    | 501 | GDP  | PA-O3A-PB-O1B   |
| 9   | E0    | 501 | GTP  | PB-O3B-PG-O3G   |
| 9   | D0    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | E8    | 501 | GTP  | PB-O3A-PA-O2A   |
| 9   | F0    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 11  | C1    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 11  | D3    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | A4    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | A8    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | B0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | E2    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | E6    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | E8    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | F0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 11  | C9    | 501 | GDP  | C4'-C5'-O5'-PA  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | D9    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 9   | A2    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 9   | C0    | 501 | GTP  | C5'-O5'-PA-O3A  |
| 9   | D8    | 501 | GTP  | C5'-O5'-PA-O1A  |
| 9   | E2    | 501 | GTP  | C5'-O5'-PA-O2A  |
| 11  | C7    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | C9    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | D1    | 501 | GDP  | C5'-O5'-PA-O3A  |
| 11  | D7    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 11  | D9    | 501 | GDP  | C5'-O5'-PA-O2A  |
| 9   | A0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | A6    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | B2    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | B4    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | B6    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | B8    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | C3    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | C4    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | C8    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | D8    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | E0    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | C6    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | A0    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | A8    | 501 | GTP  | PB-O3A-PA-O1A   |
| 9   | B2    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | E0    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | E0    | 501 | GTP  | PB-O3A-PA-O1A   |
| 9   | E6    | 501 | GTP  | PB-O3A-PA-O2A   |
| 11  | A3    | 501 | GDP  | PB-O3A-PA-O2A   |
| 11  | A9    | 501 | GDP  | PB-O3A-PA-O2A   |
| 9   | B0    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | E4    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 11  | C1    | 501 | GDP  | C4'-C5'-O5'-PA  |
| 9   | A2    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 9   | D6    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 11  | E7    | 501 | GDP  | C4'-C5'-O5'-PA  |
| 9   | A4    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | B4    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 9   | A0    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | A8    | 501 | GTP  | PB-O3A-PA-O2A   |
| 11  | C5    | 501 | GDP  | PB-O3A-PA-O2A   |
| 11  | C7    | 501 | GDP  | PB-O3A-PA-O2A   |

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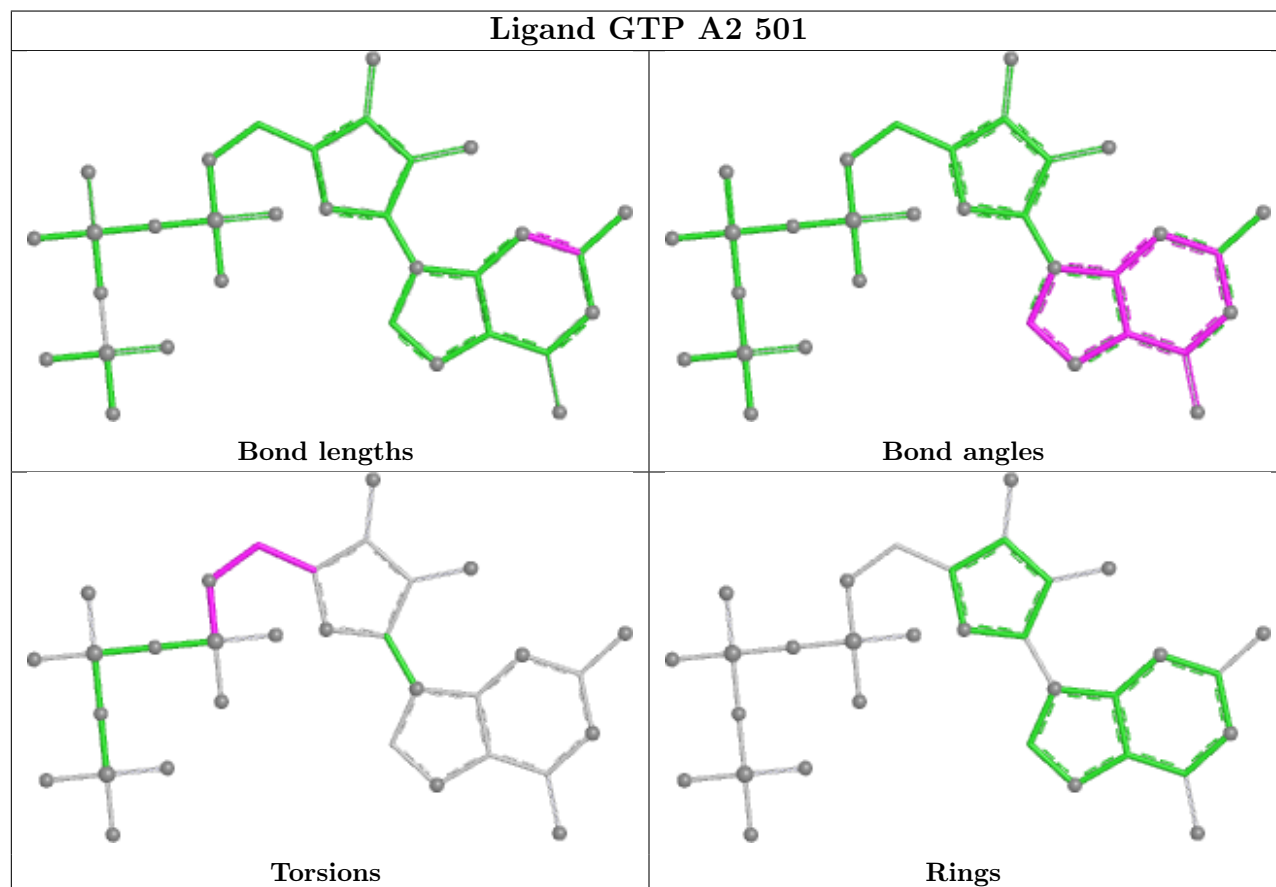
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 9   | D4    | 501 | GTP  | C4'-C5'-O5'-PA  |
| 11  | A3    | 501 | GDP  | C4'-C5'-O5'-PA  |
| 11  | D5    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | D4    | 501 | GTP  | PB-O3B-PG-O1G   |
| 11  | A3    | 501 | GDP  | PA-O3A-PB-O1B   |
| 9   | D4    | 501 | GTP  | PB-O3B-PG-O2G   |
| 9   | D4    | 501 | GTP  | PB-O3B-PG-O3G   |
| 9   | E0    | 501 | GTP  | PB-O3B-PG-O2G   |
| 9   | E2    | 501 | GTP  | PB-O3B-PG-O2G   |
| 11  | A3    | 501 | GDP  | PA-O3A-PB-O2B   |
| 11  | A5    | 502 | GDP  | PA-O3A-PB-O2B   |
| 11  | D3    | 501 | GDP  | PA-O3A-PB-O2B   |
| 11  | D3    | 501 | GDP  | PA-O3A-PB-O3B   |
| 11  | E5    | 501 | GDP  | PA-O3A-PB-O2B   |
| 11  | E5    | 501 | GDP  | PA-O3A-PB-O3B   |
| 11  | E9    | 502 | GDP  | PA-O3A-PB-O3B   |
| 11  | B3    | 501 | GDP  | C4'-C5'-O5'-PA  |
| 9   | F0    | 501 | GTP  | O4'-C4'-C5'-O5' |
| 9   | D0    | 501 | GTP  | C3'-C4'-C5'-O5' |
| 11  | D3    | 501 | GDP  | O4'-C4'-C5'-O5' |
| 9   | B0    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | B0    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | B2    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | B8    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | E0    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | E4    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | E4    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | E6    | 501 | GTP  | PB-O3A-PA-O1A   |
| 9   | E8    | 501 | GTP  | PB-O3A-PA-O1A   |
| 9   | F0    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | F0    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | F0    | 501 | GTP  | PB-O3A-PA-O2A   |
| 11  | A9    | 501 | GDP  | PB-O3A-PA-O1A   |
| 11  | D7    | 501 | GDP  | PB-O3A-PA-O2A   |
| 11  | B5    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 11  | E5    | 501 | GDP  | C3'-C4'-C5'-O5' |
| 9   | B8    | 501 | GTP  | PA-O3A-PB-O1B   |
| 9   | C3    | 501 | GTP  | PA-O3A-PB-O2B   |
| 9   | D2    | 501 | GTP  | PG-O3B-PB-O2B   |
| 9   | D6    | 501 | GTP  | PG-O3B-PB-O2B   |
| 11  | A3    | 501 | GDP  | PB-O3A-PA-O1A   |
| 11  | D9    | 501 | GDP  | PB-O3A-PA-O2A   |

There are no ring outliers.

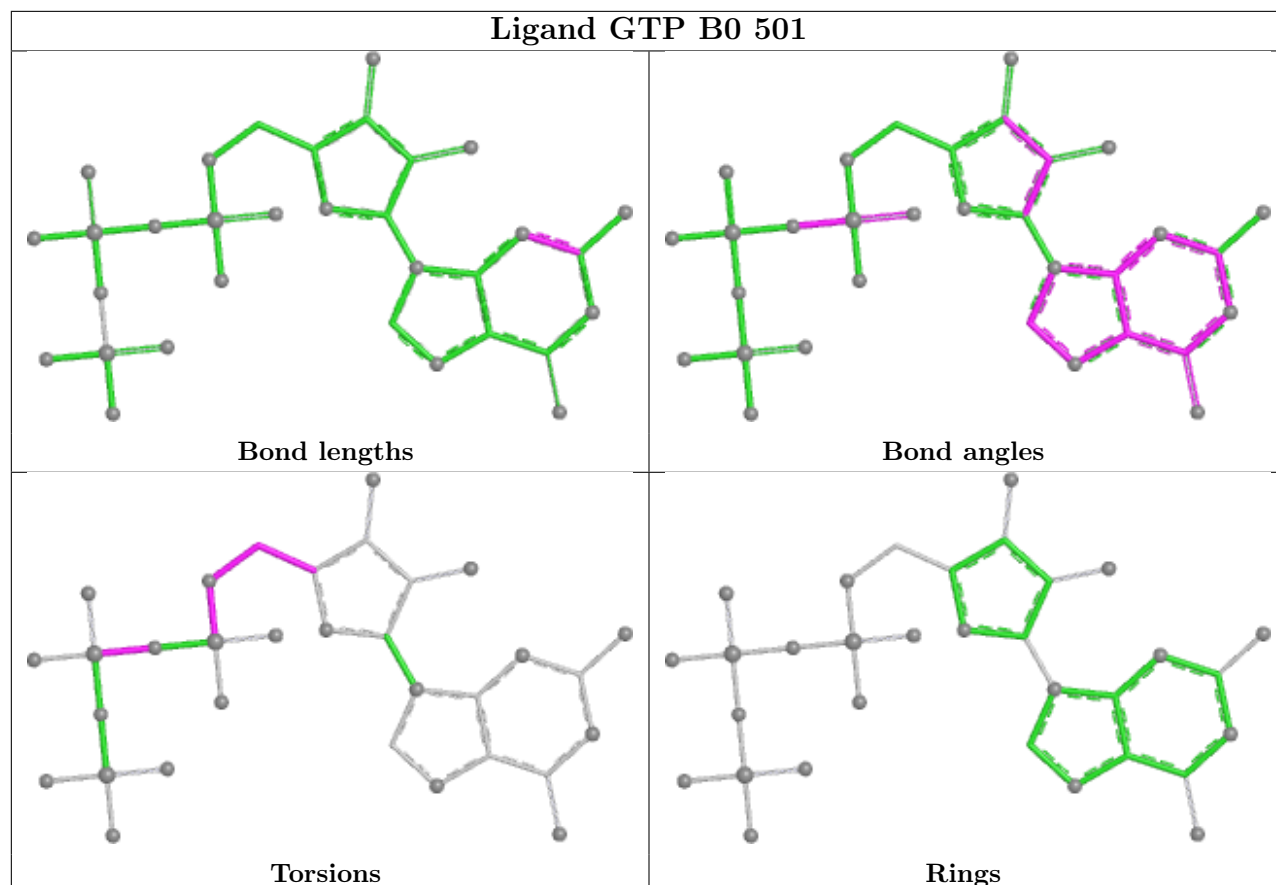
5 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | E5    | 501 | GDP  | 2       | 0            |
| 11  | E7    | 501 | GDP  | 1       | 0            |
| 11  | A1    | 501 | GDP  | 1       | 0            |
| 9   | E4    | 501 | GTP  | 1       | 0            |
| 11  | B3    | 501 | GDP  | 1       | 0            |

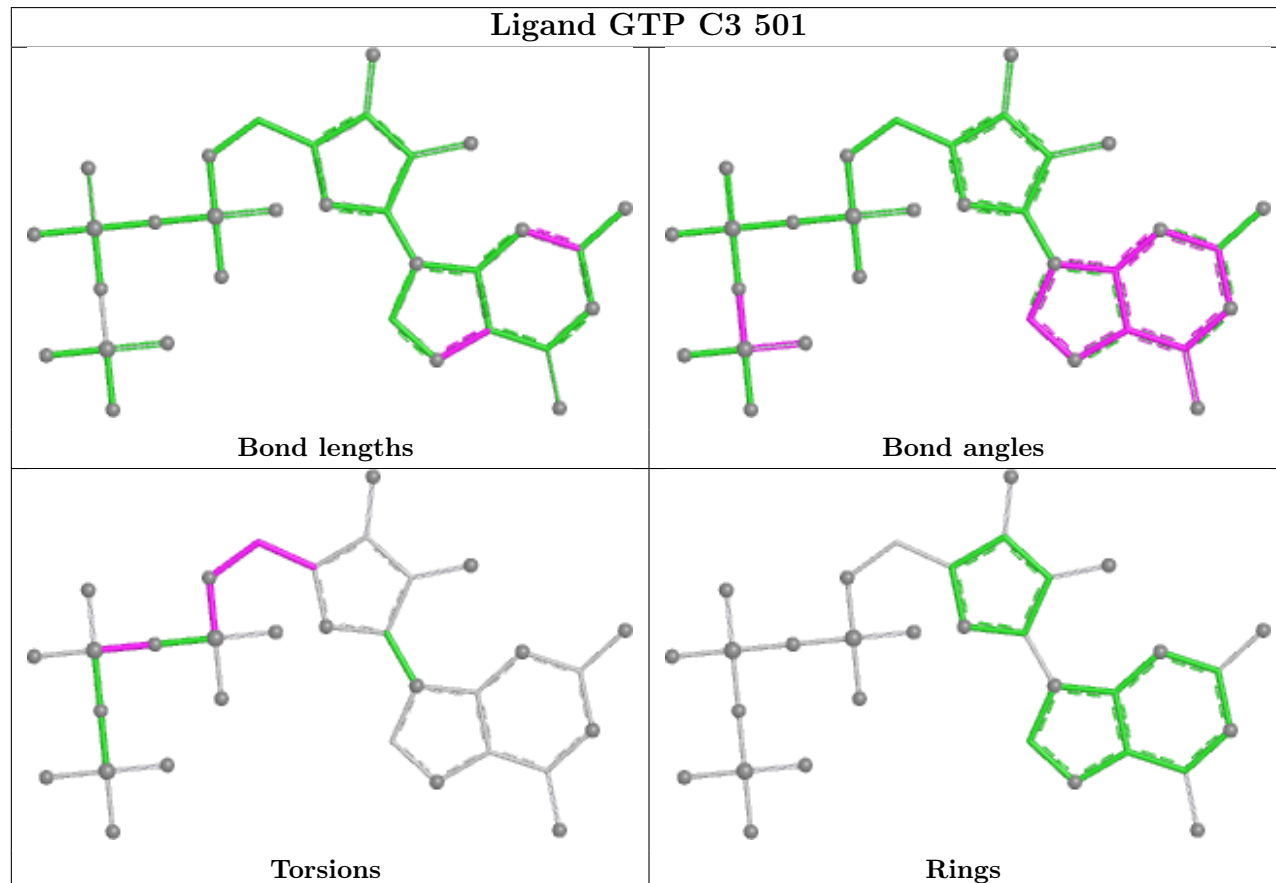
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



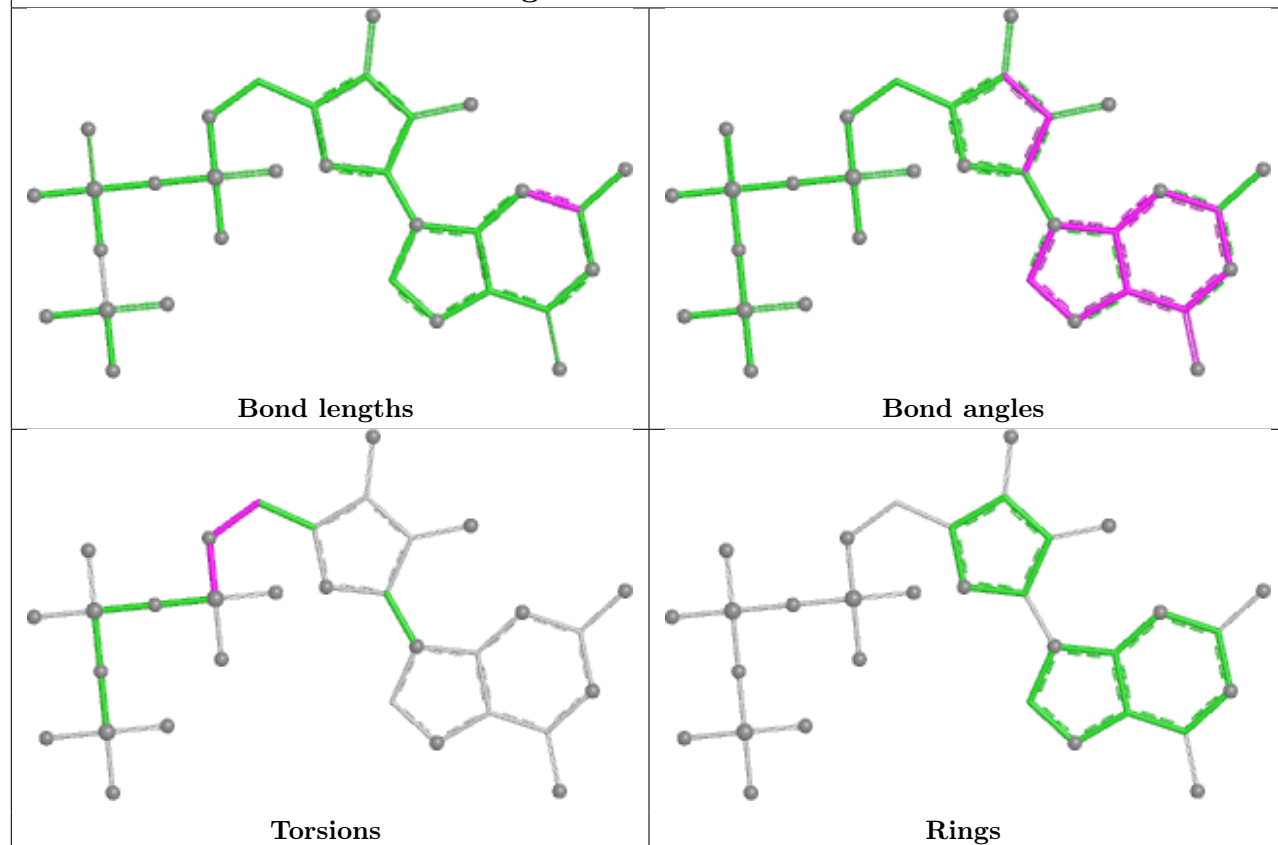
## Ligand GTP B0 501



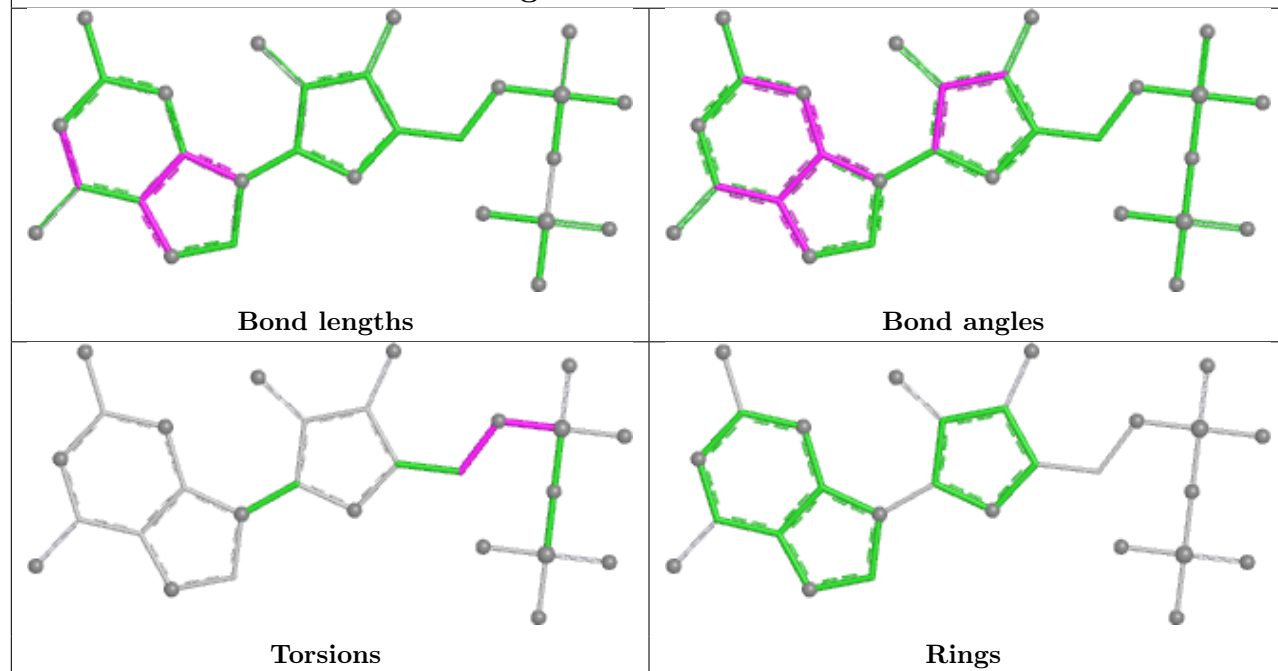
## Ligand GTP C3 501

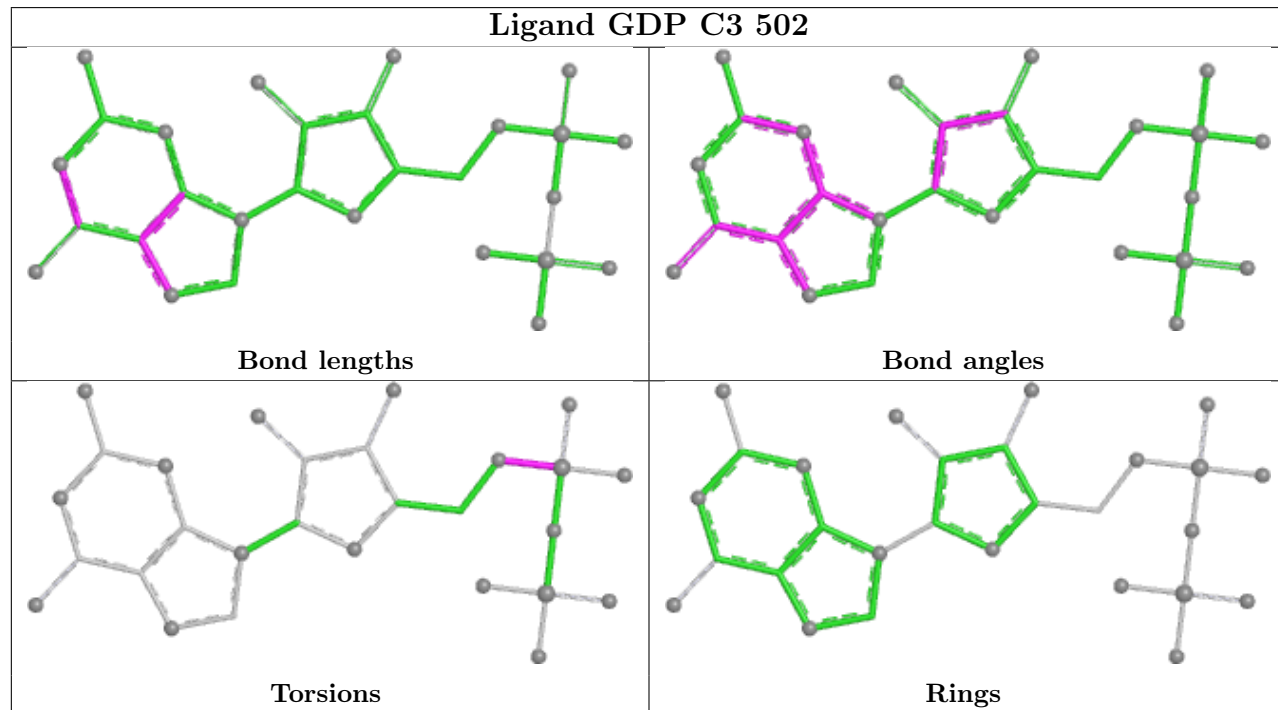
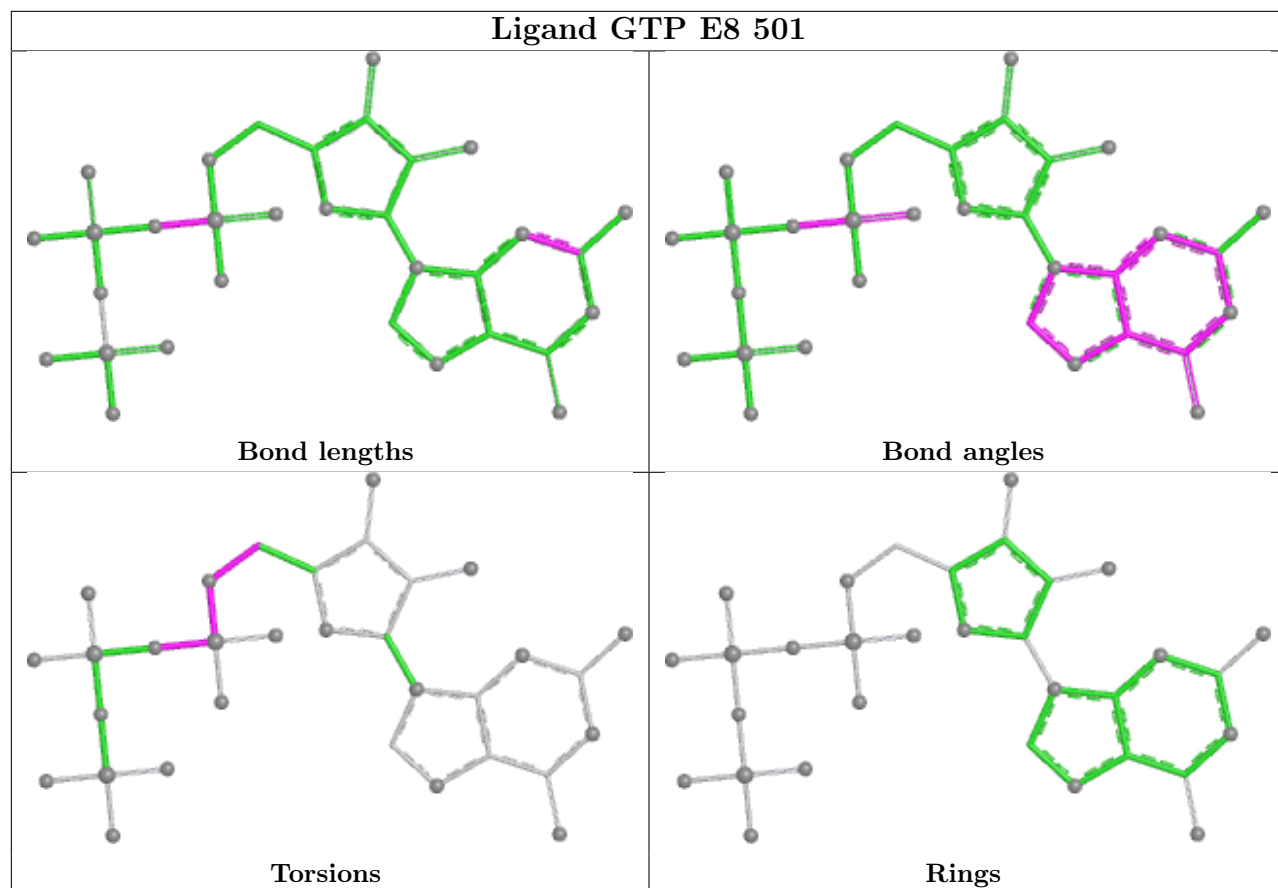


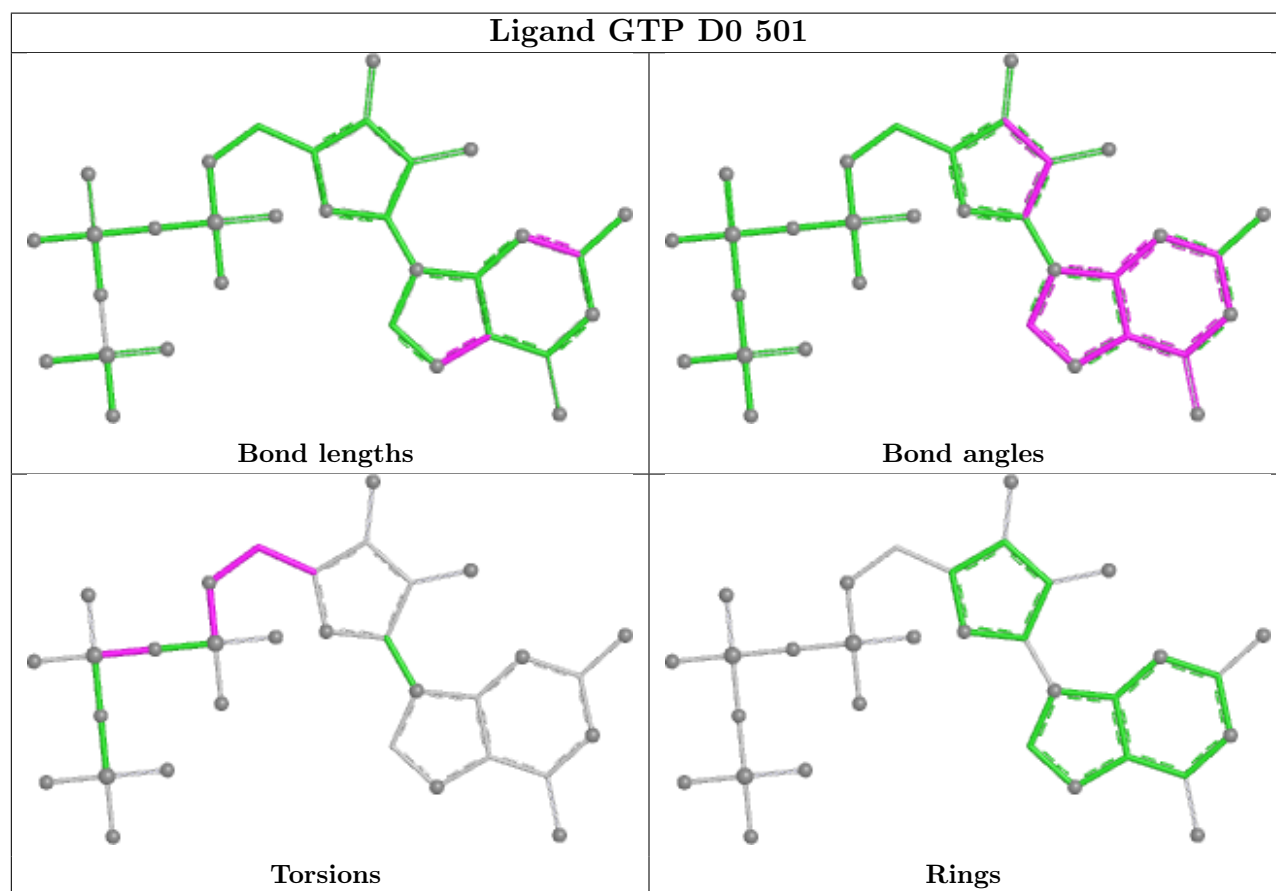
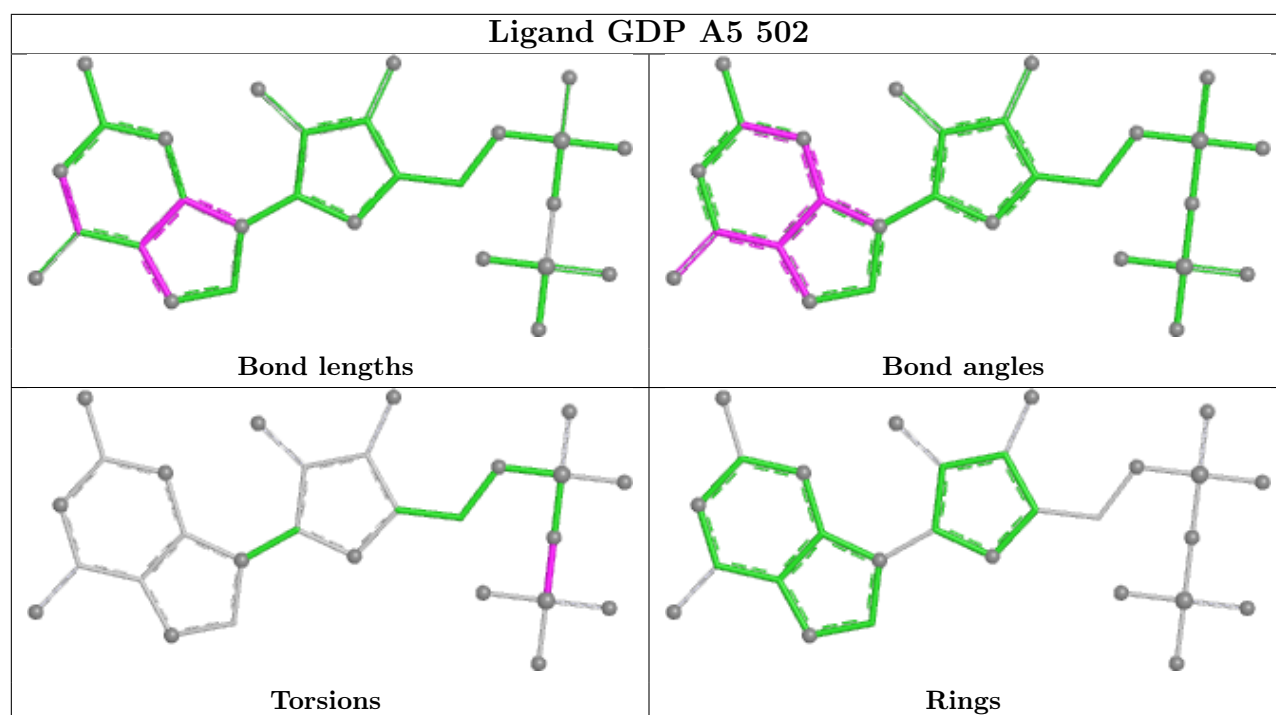
## Ligand GTP D8 501

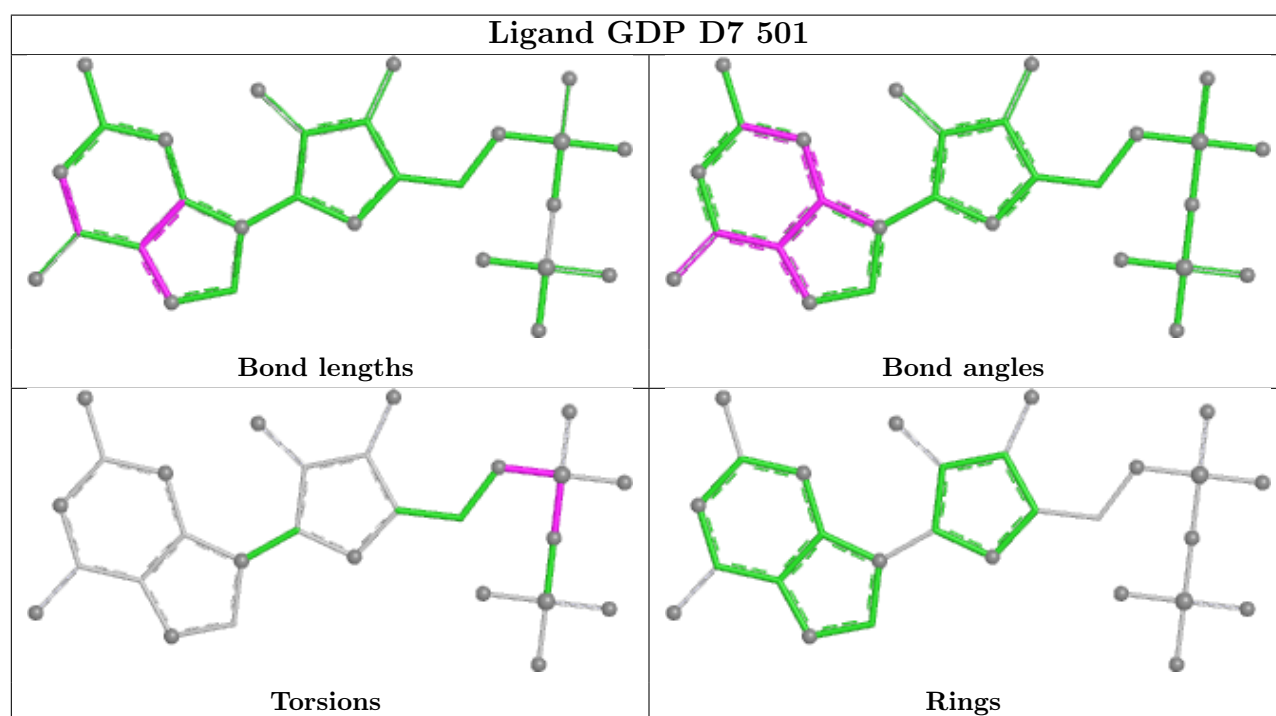
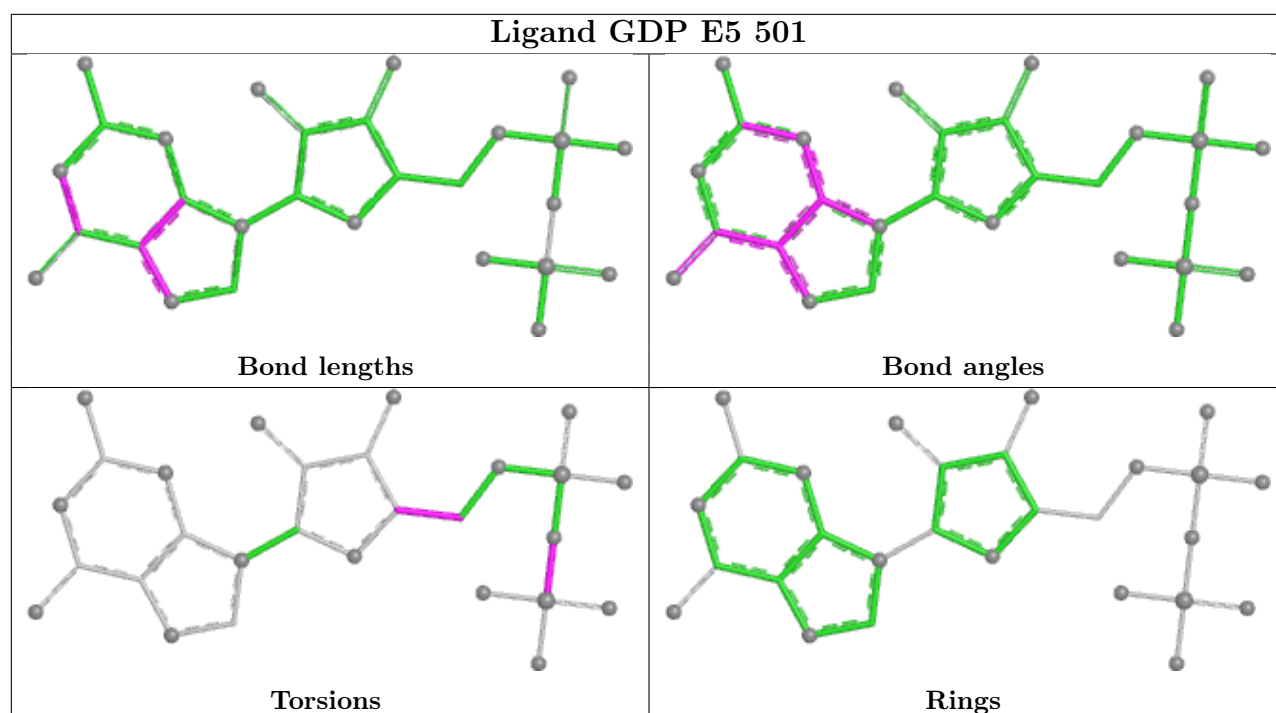


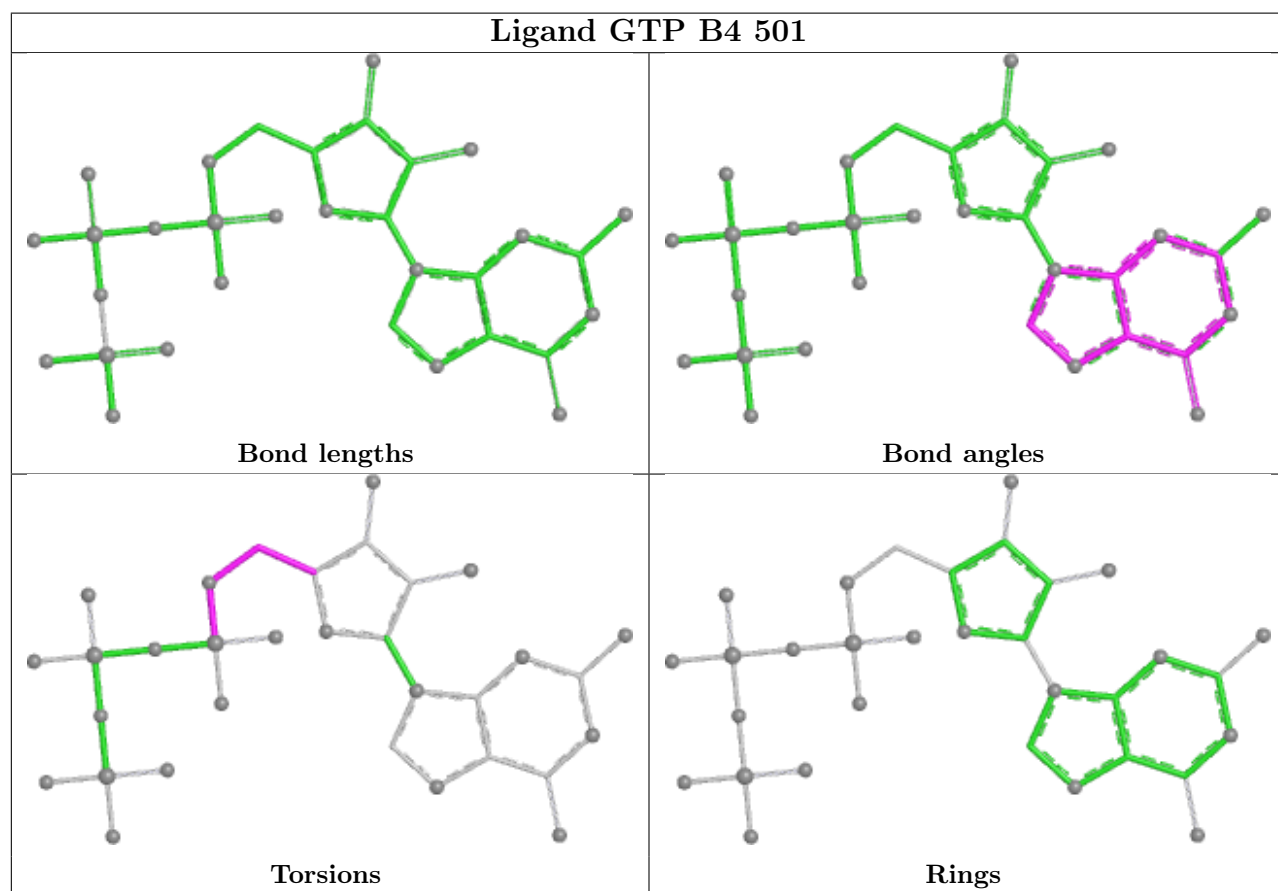
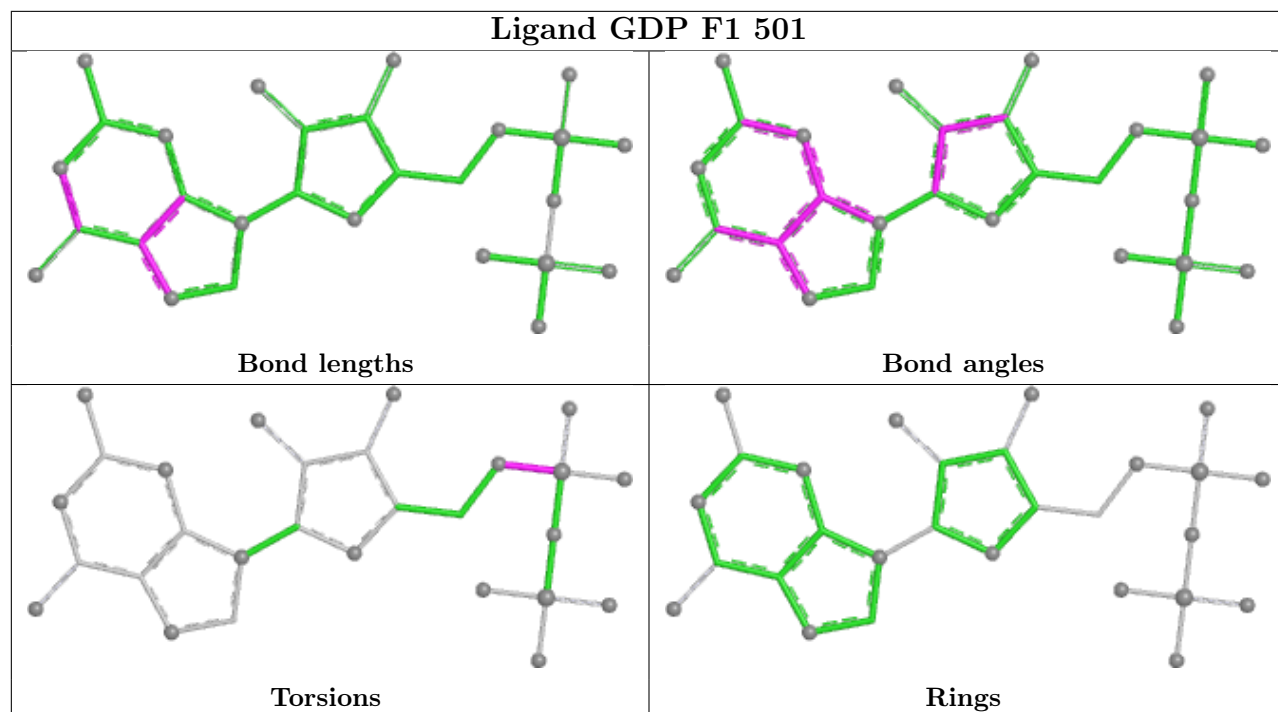
## Ligand GDP C9 501

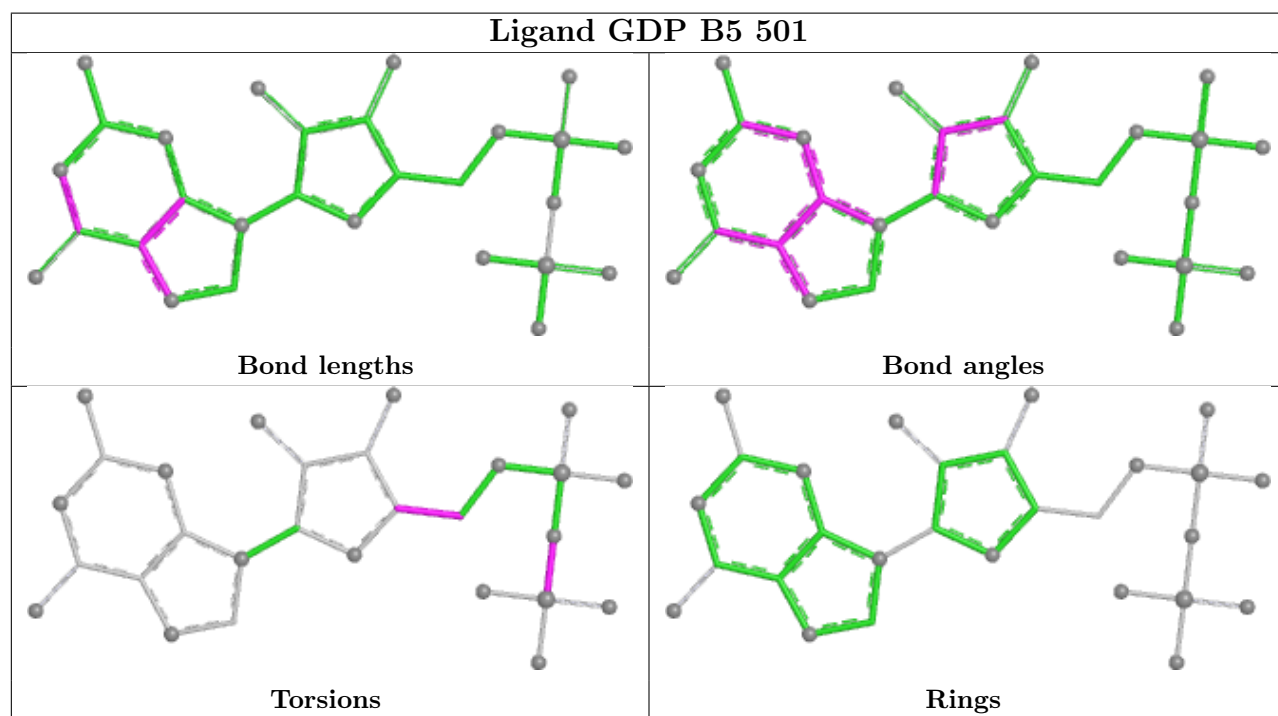
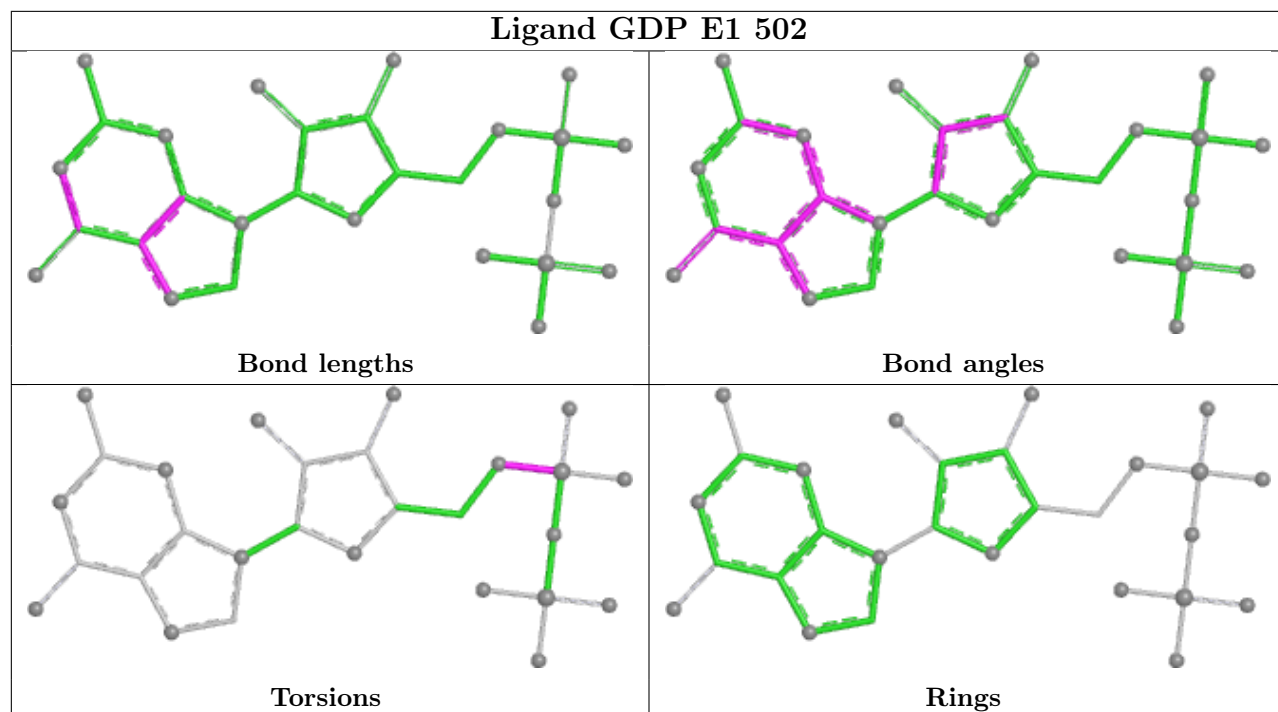


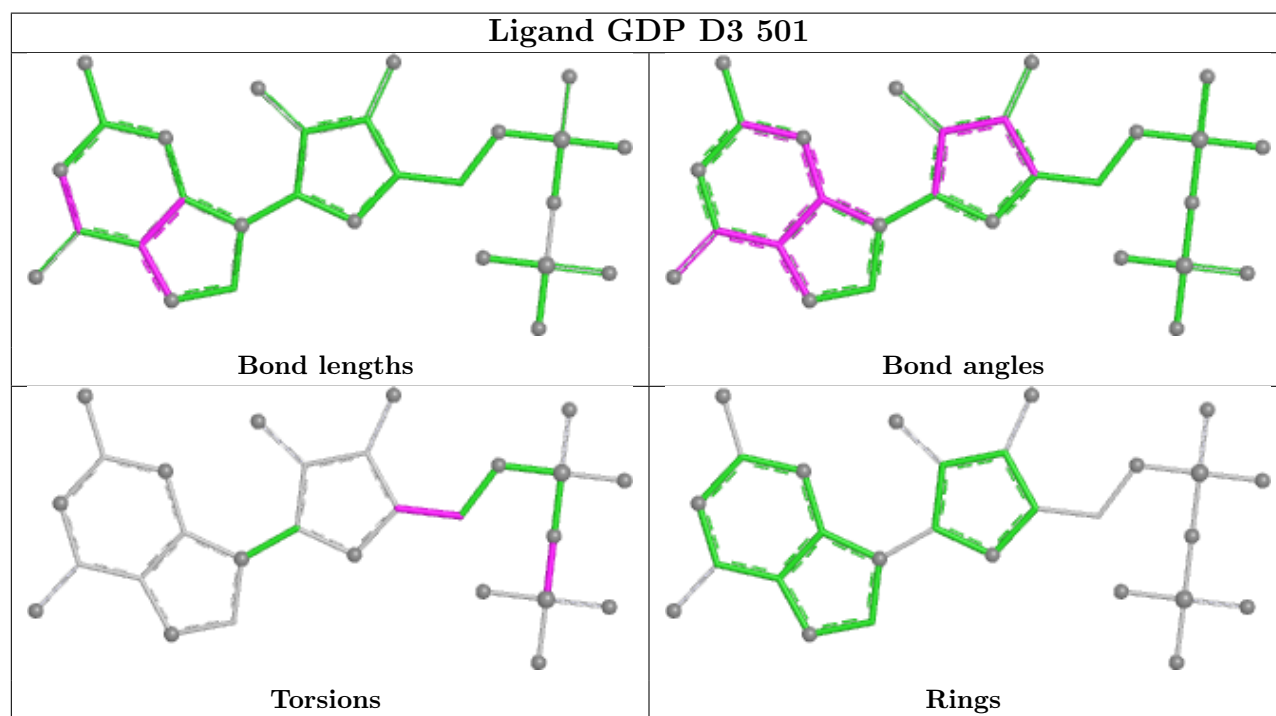
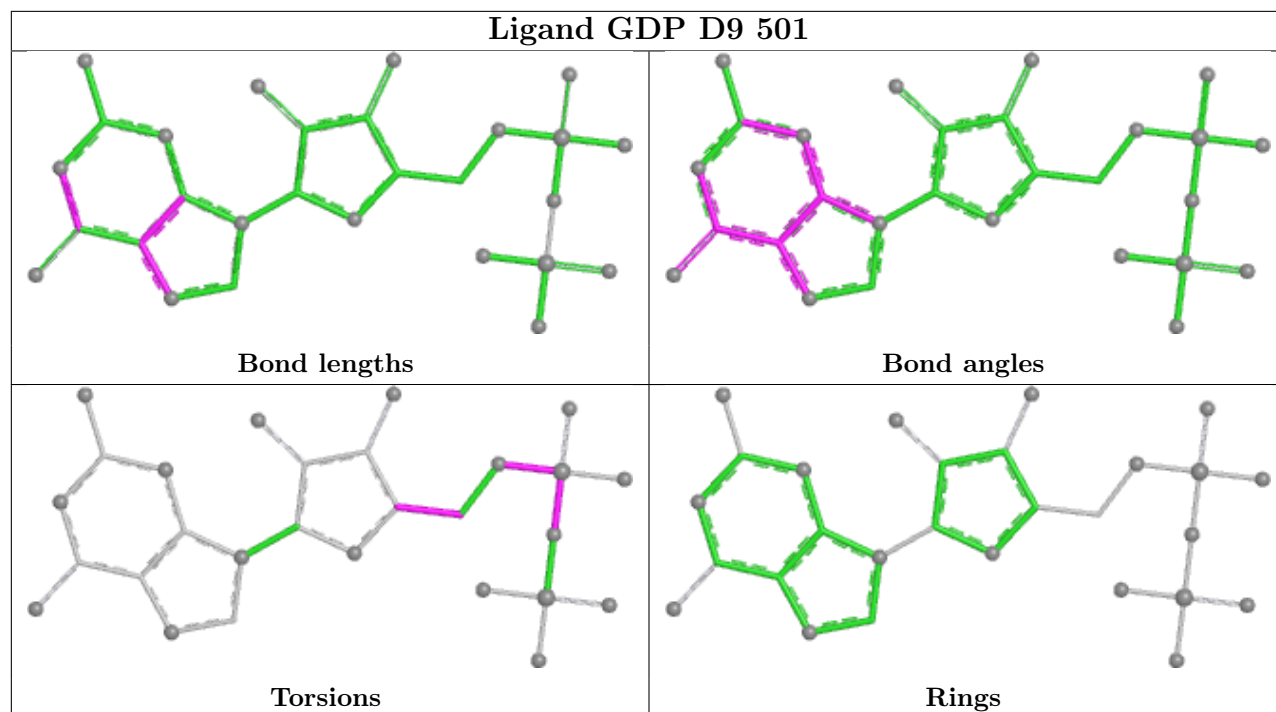


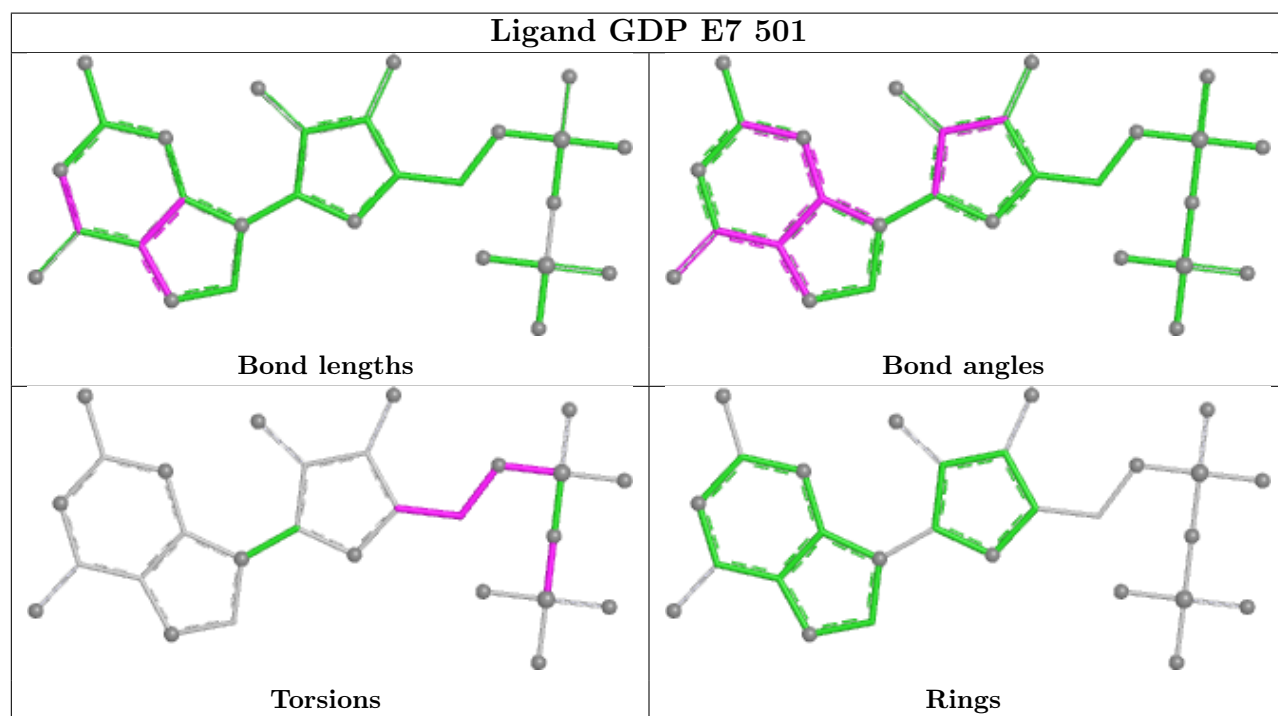
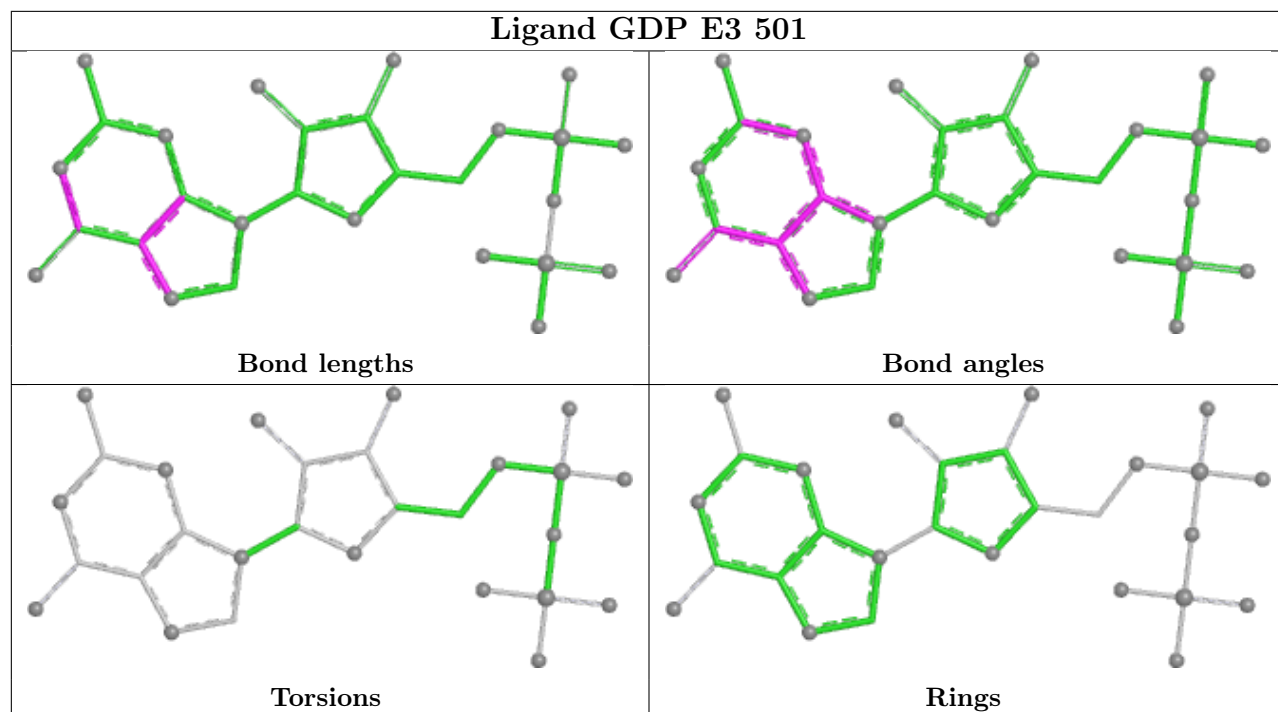


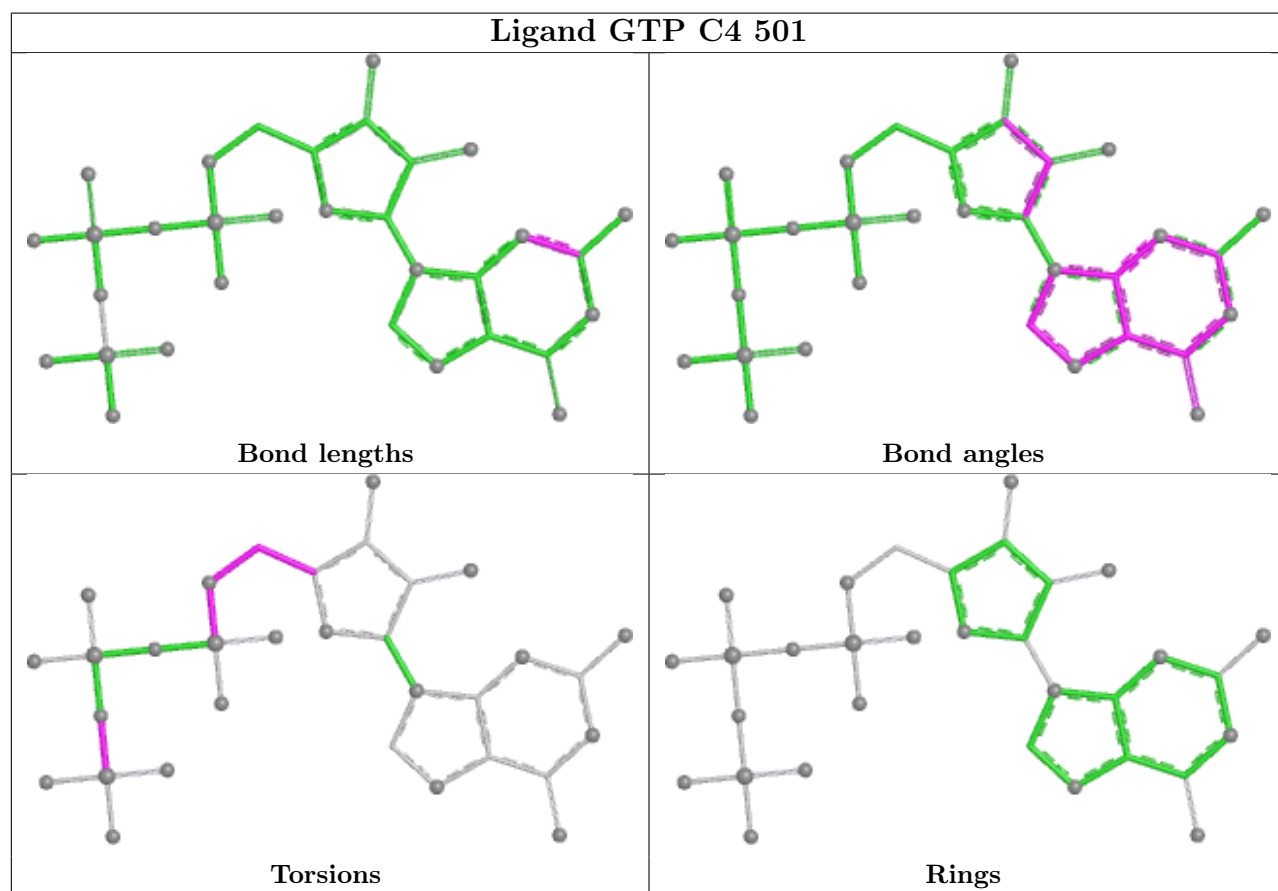
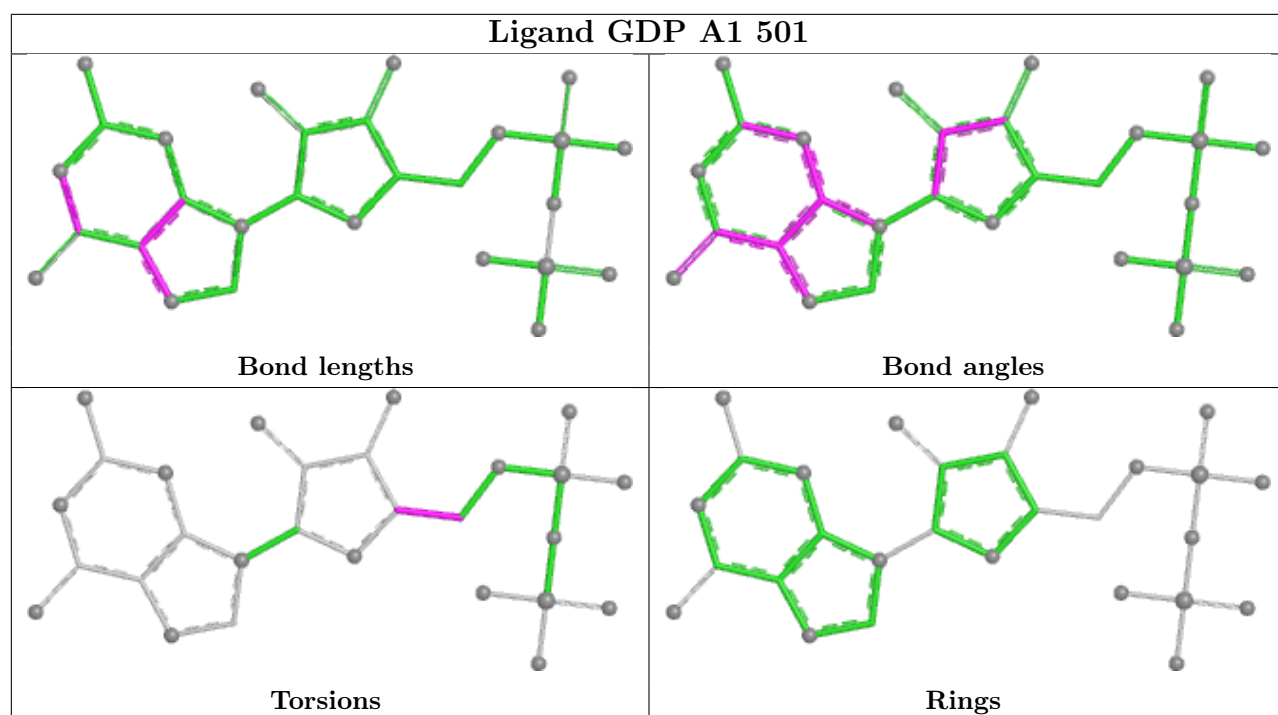


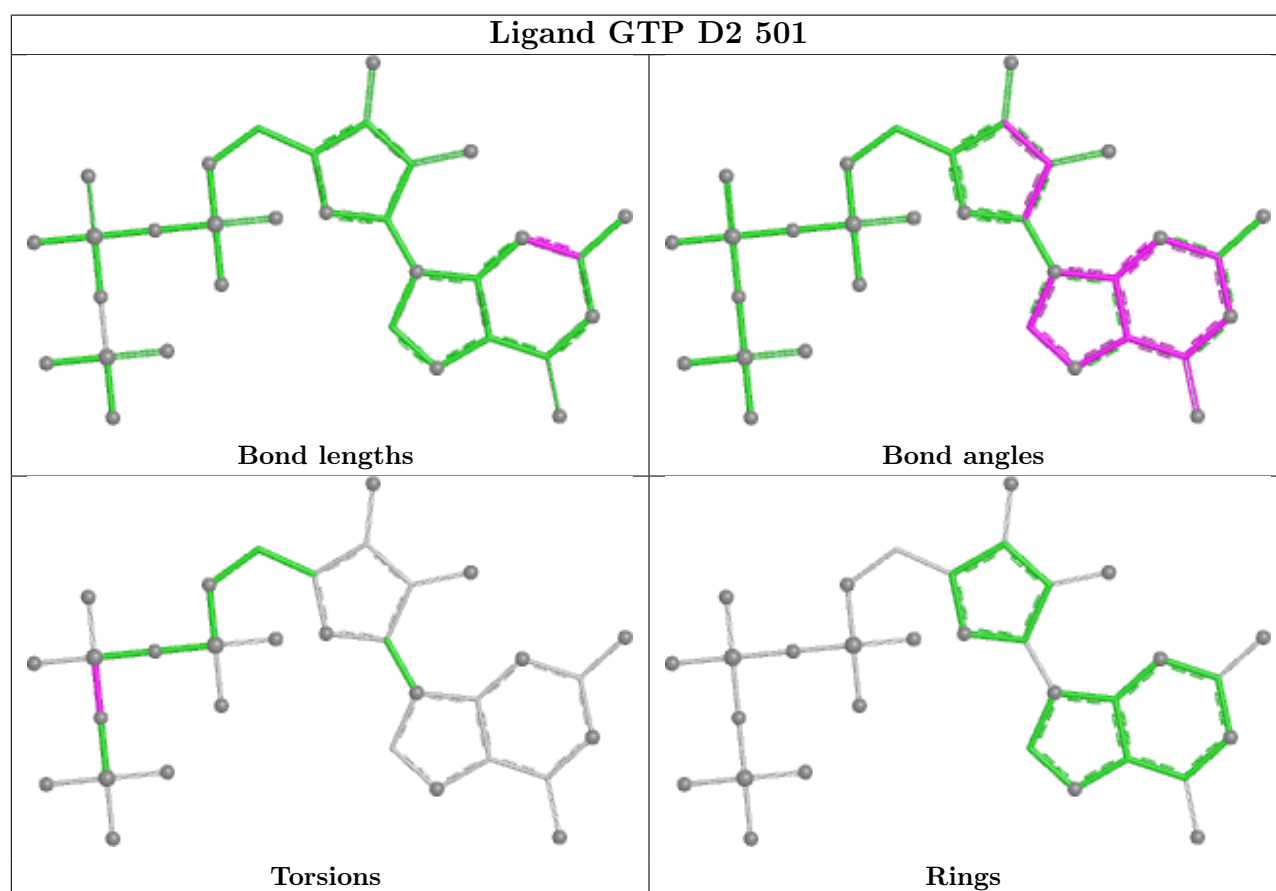
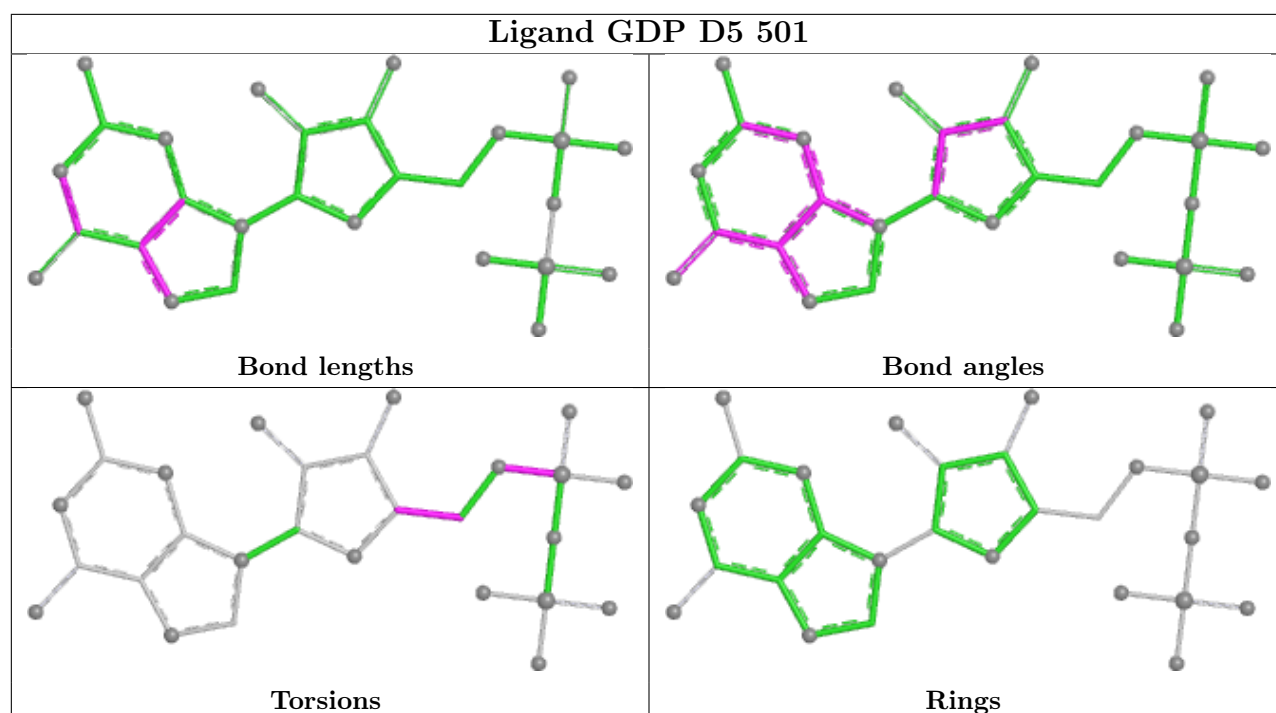




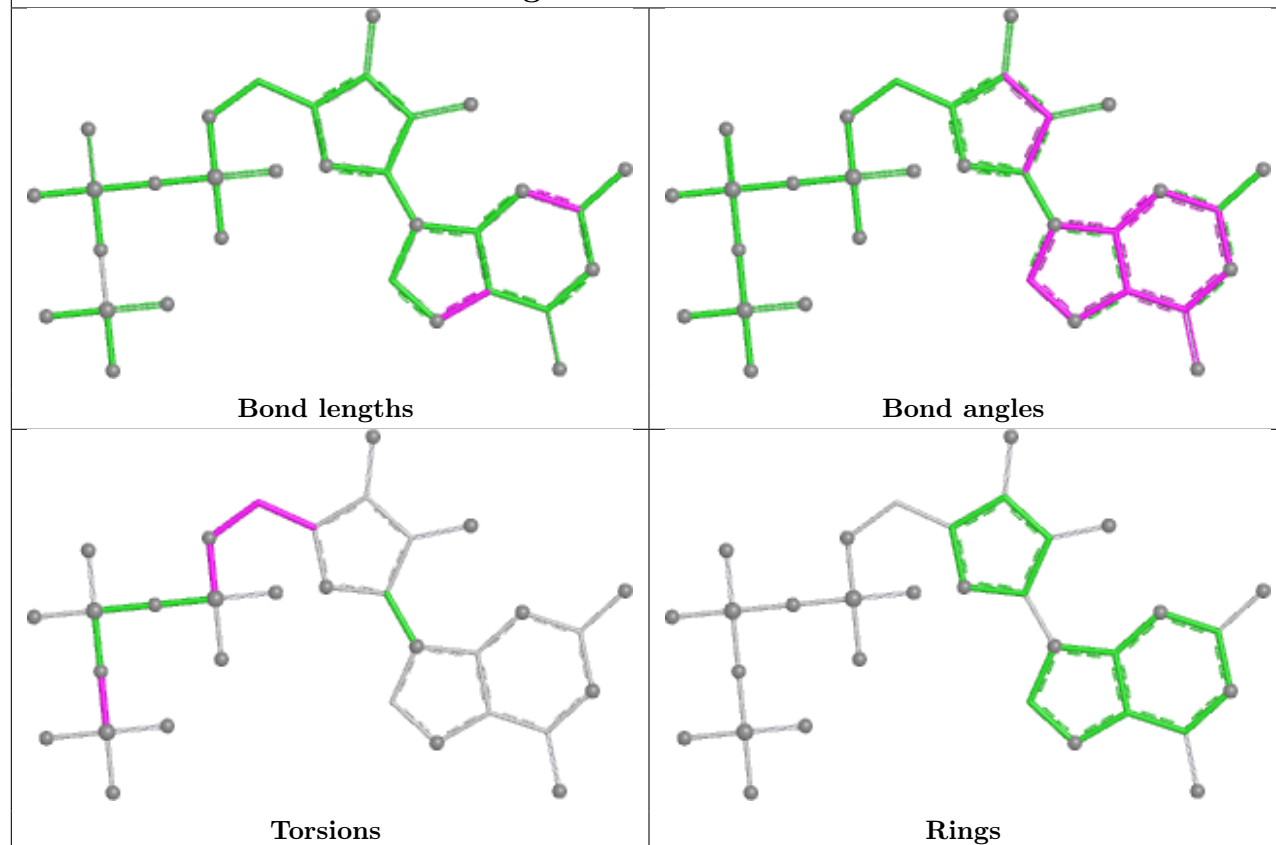




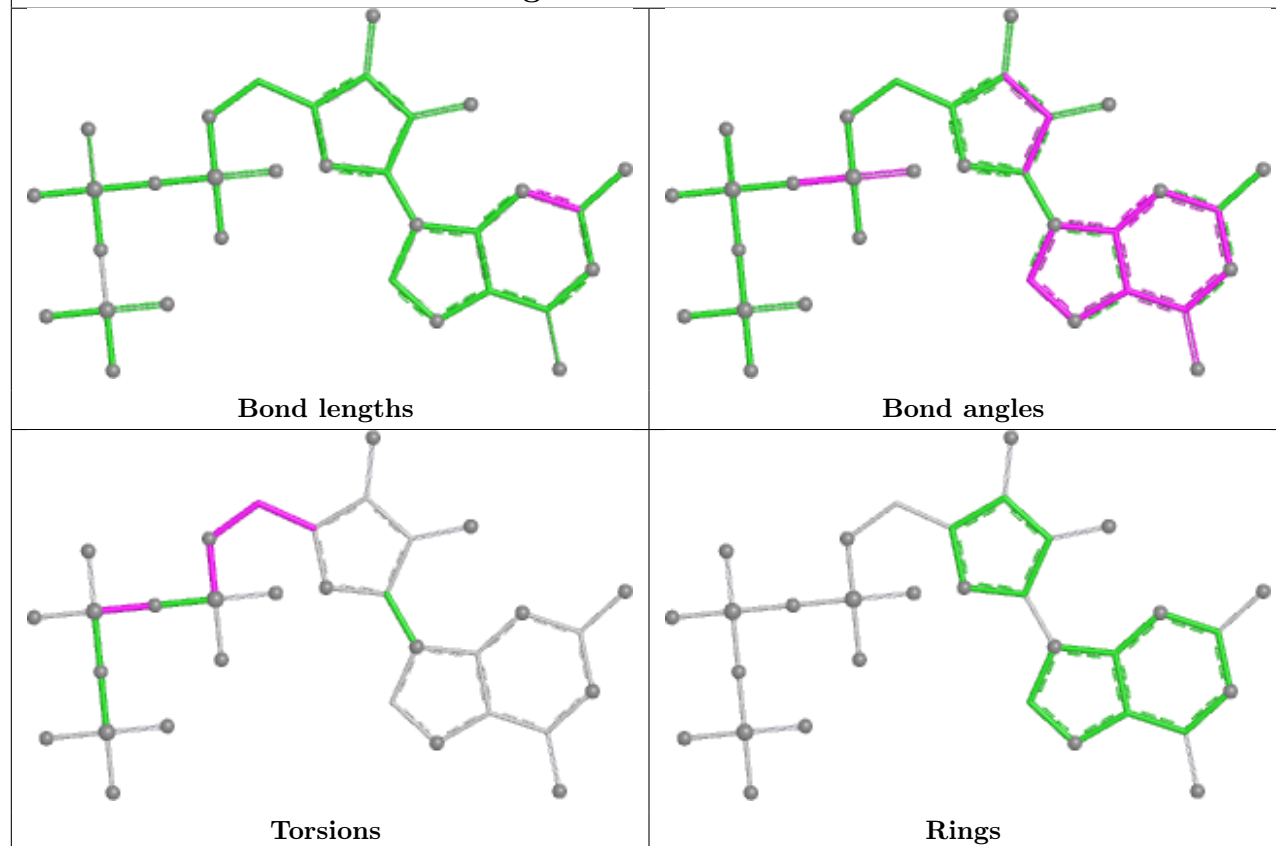


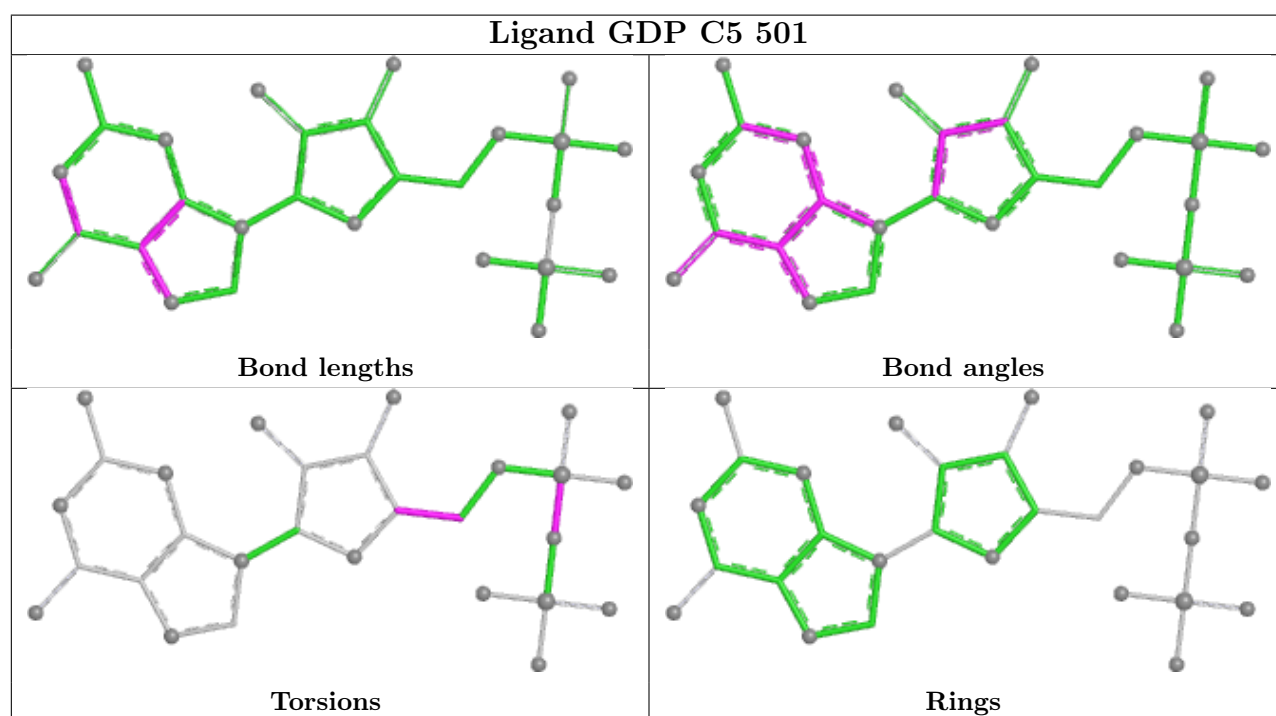
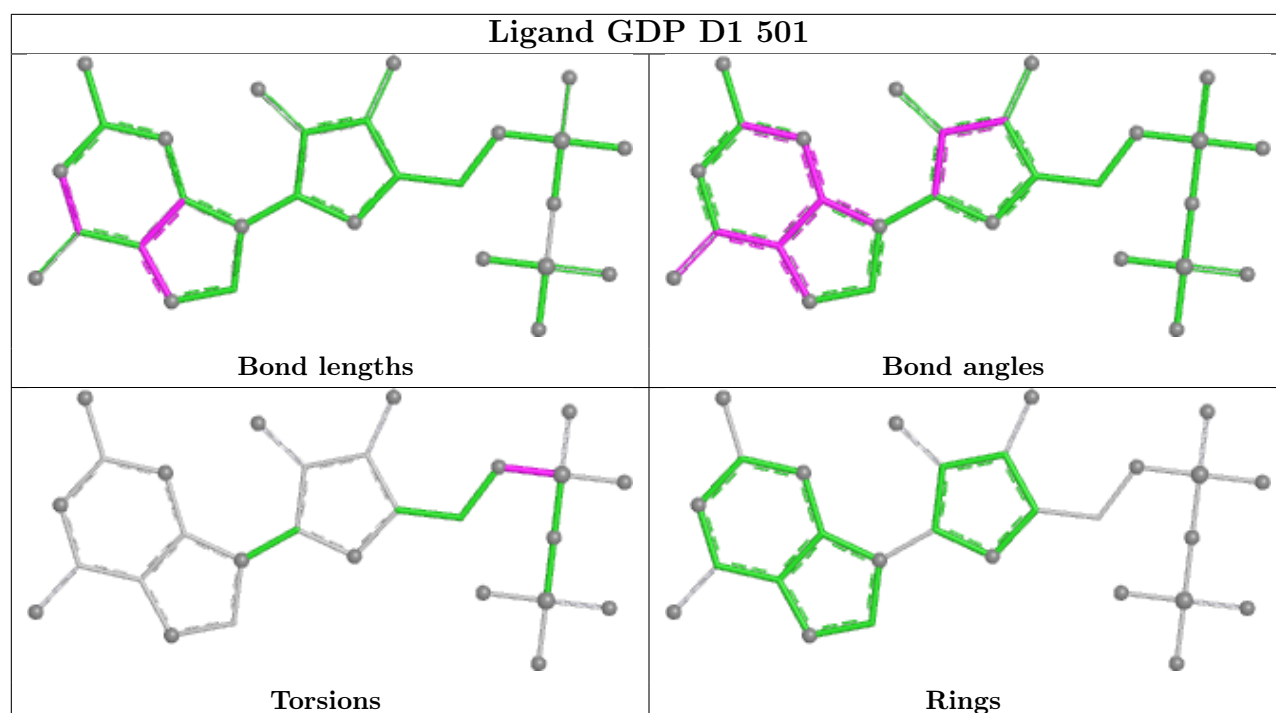


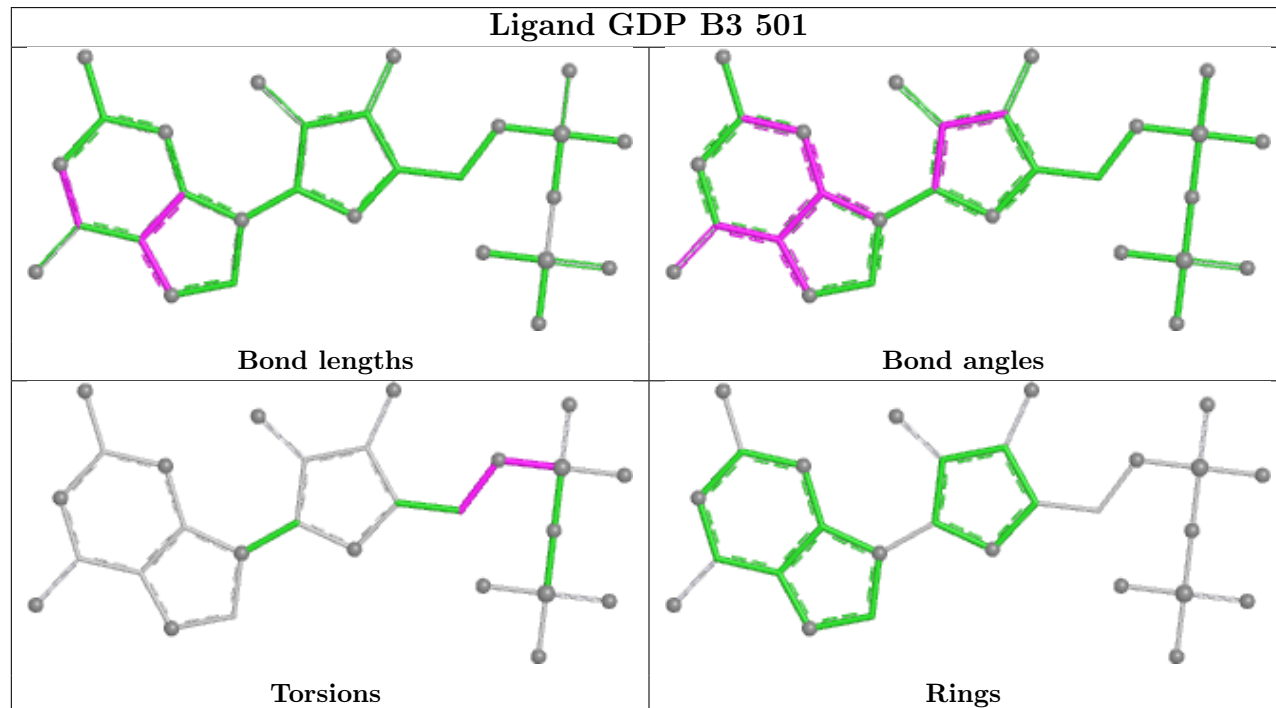
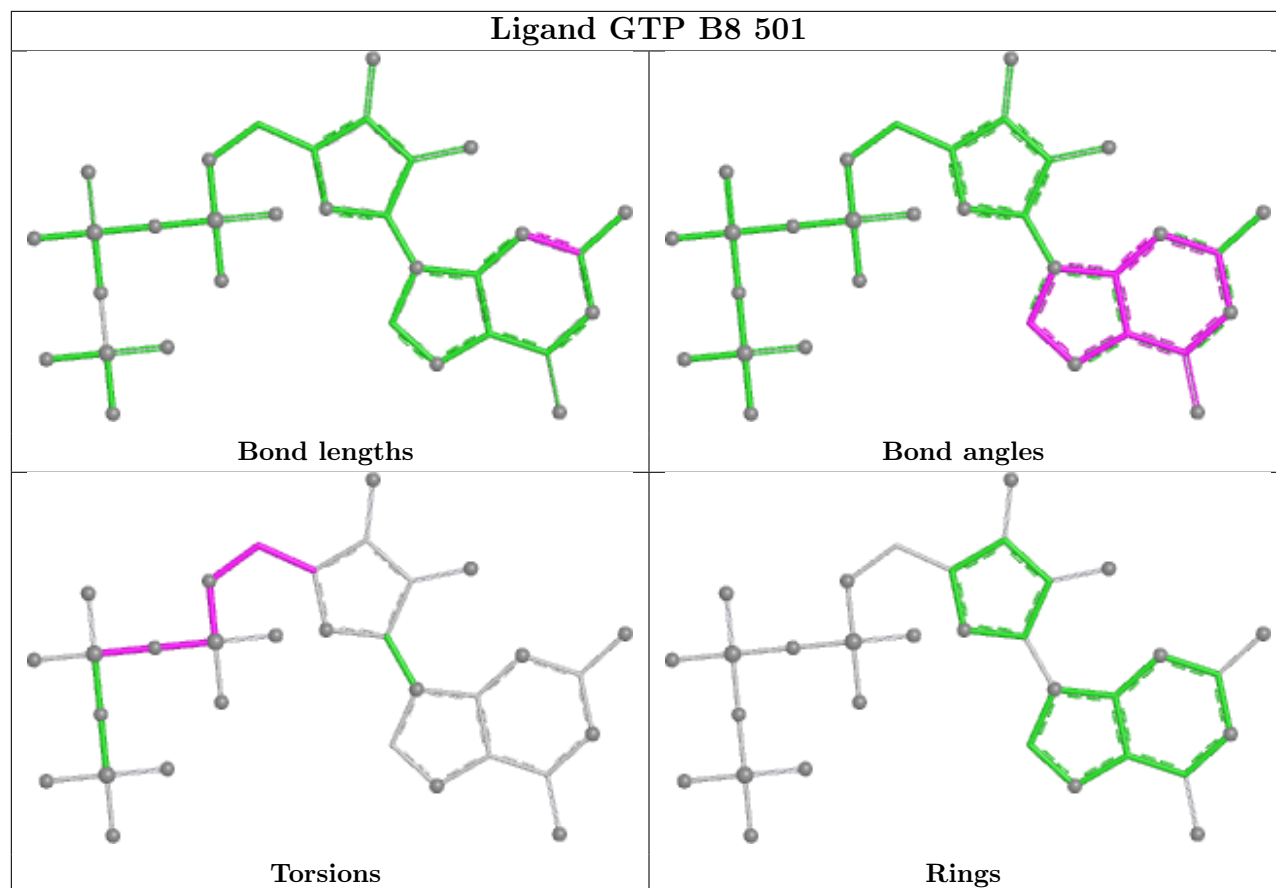
## Ligand GTP E2 501



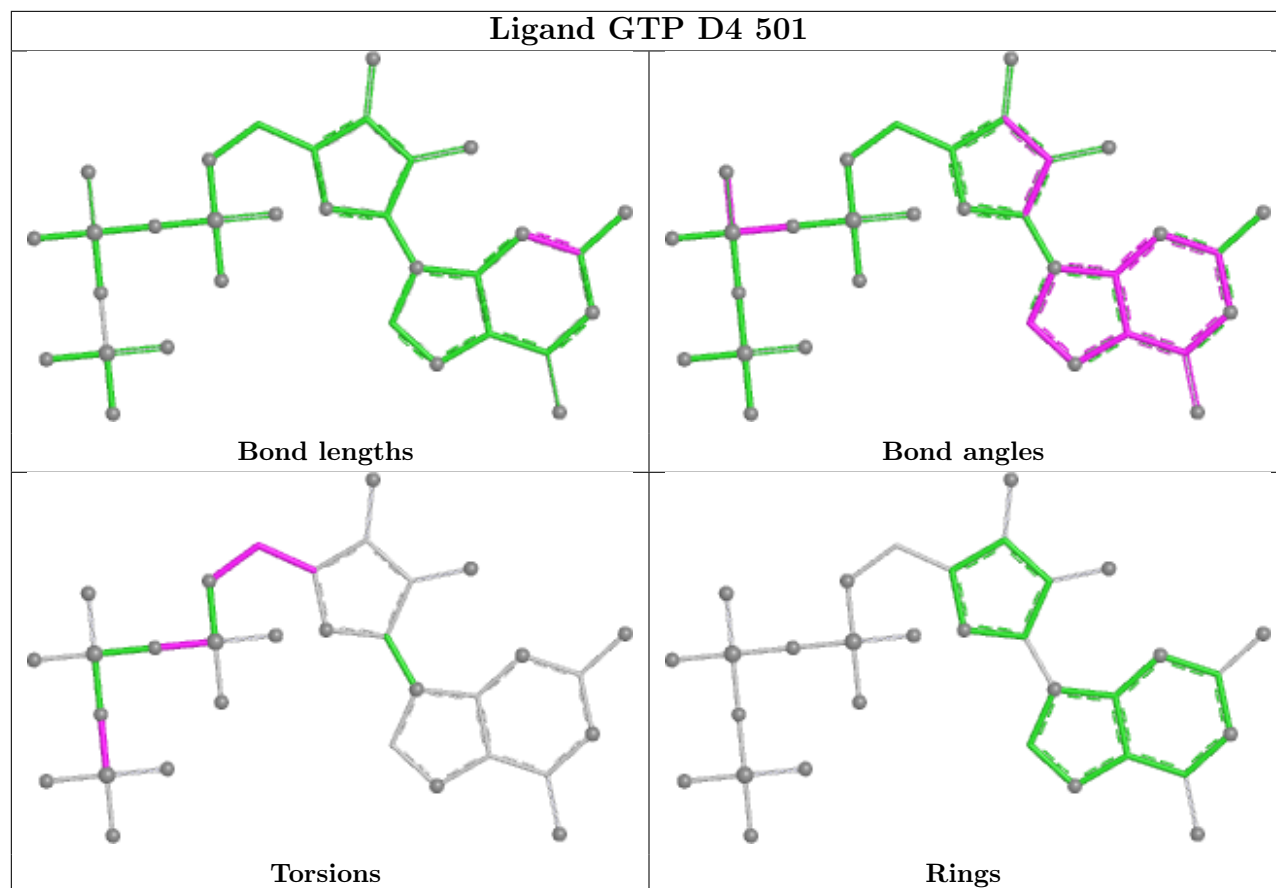
## Ligand GTP E4 501



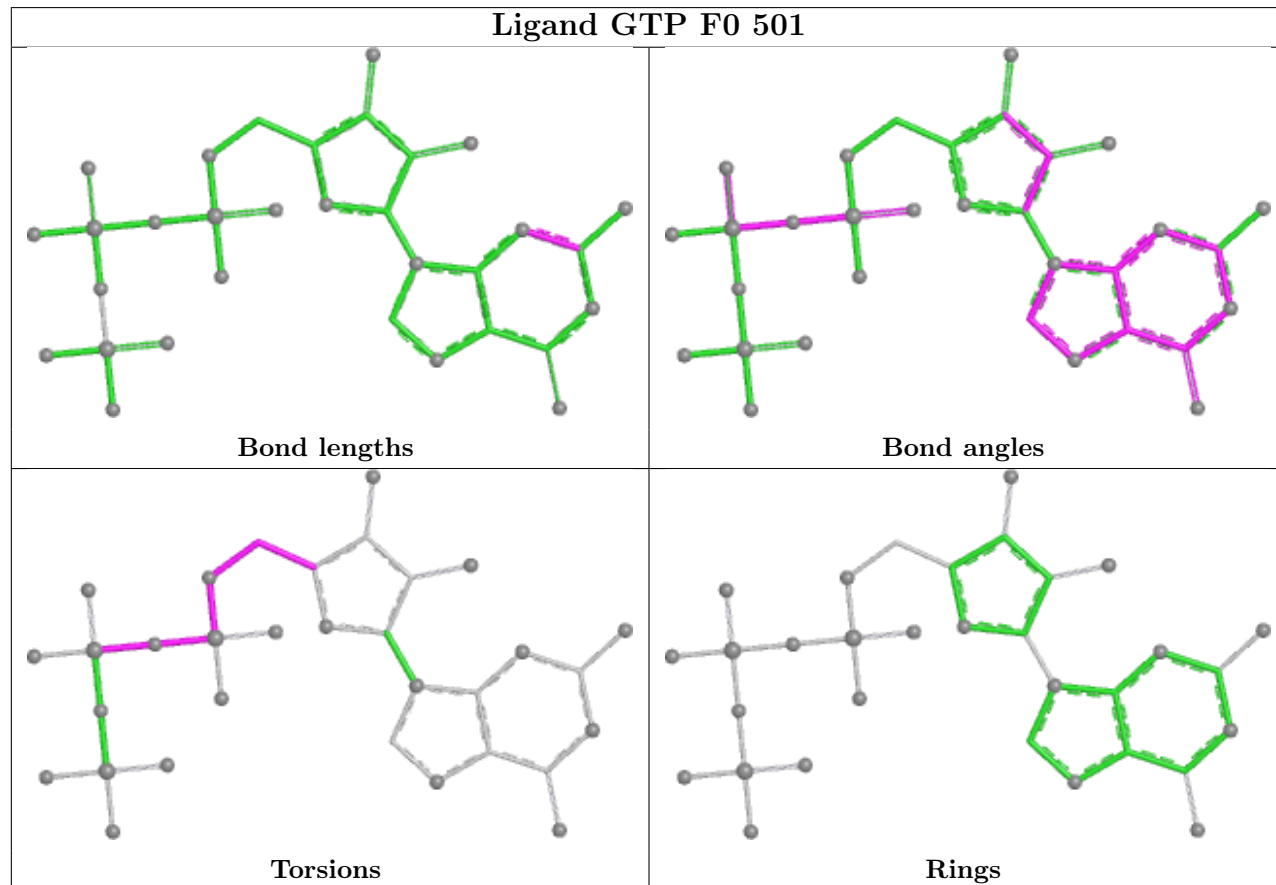


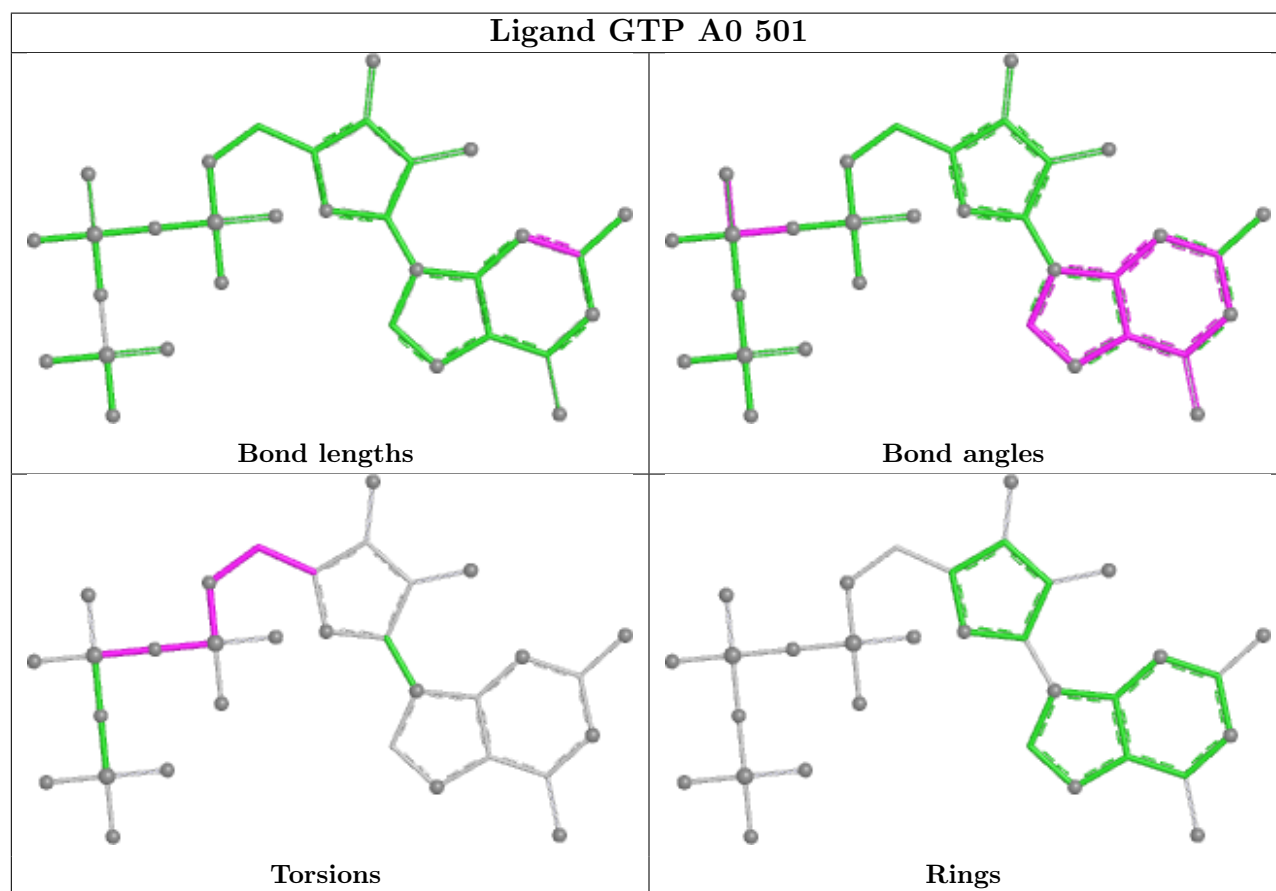
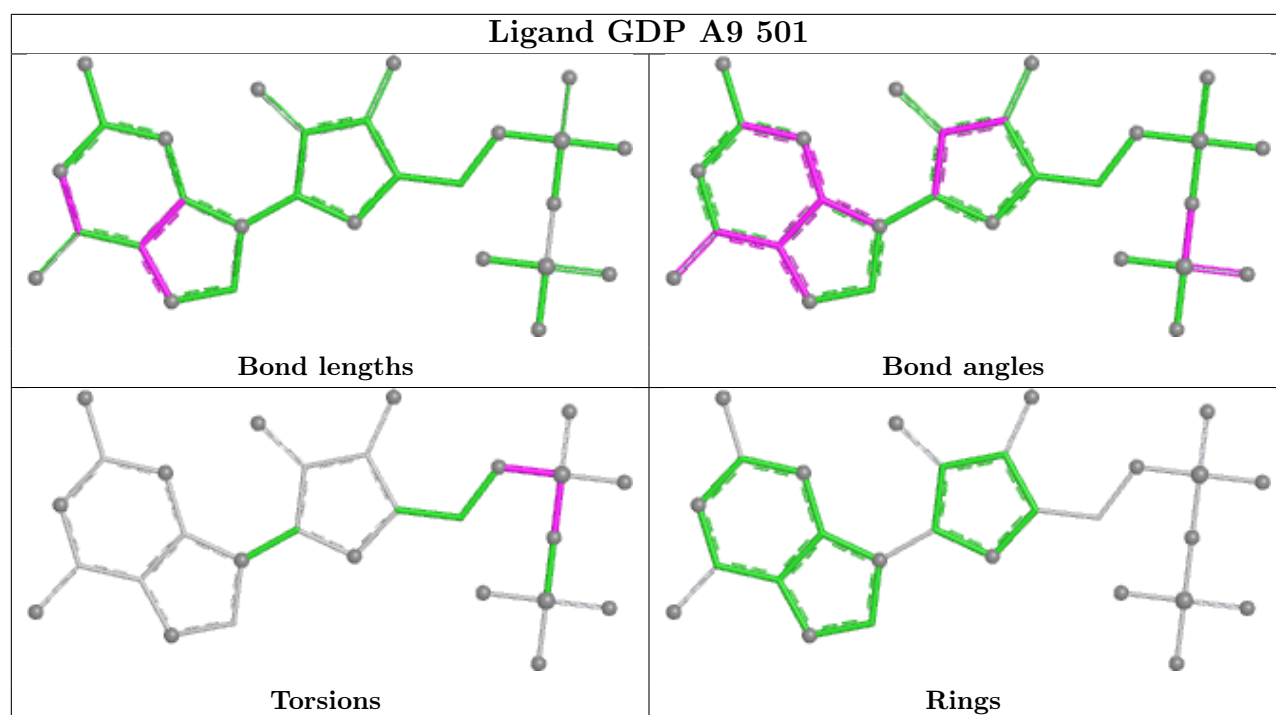


## Ligand GTP D4 501

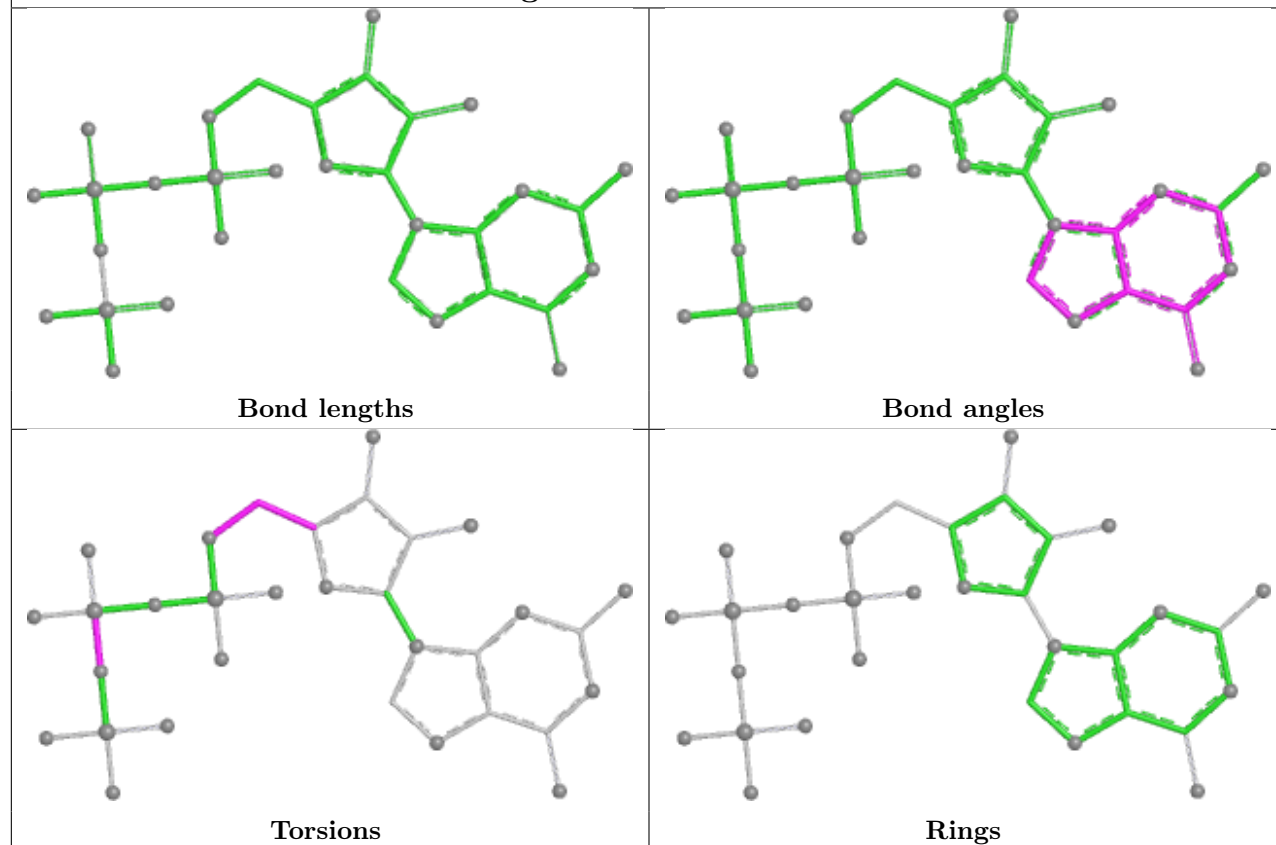


## Ligand GTP F0 501

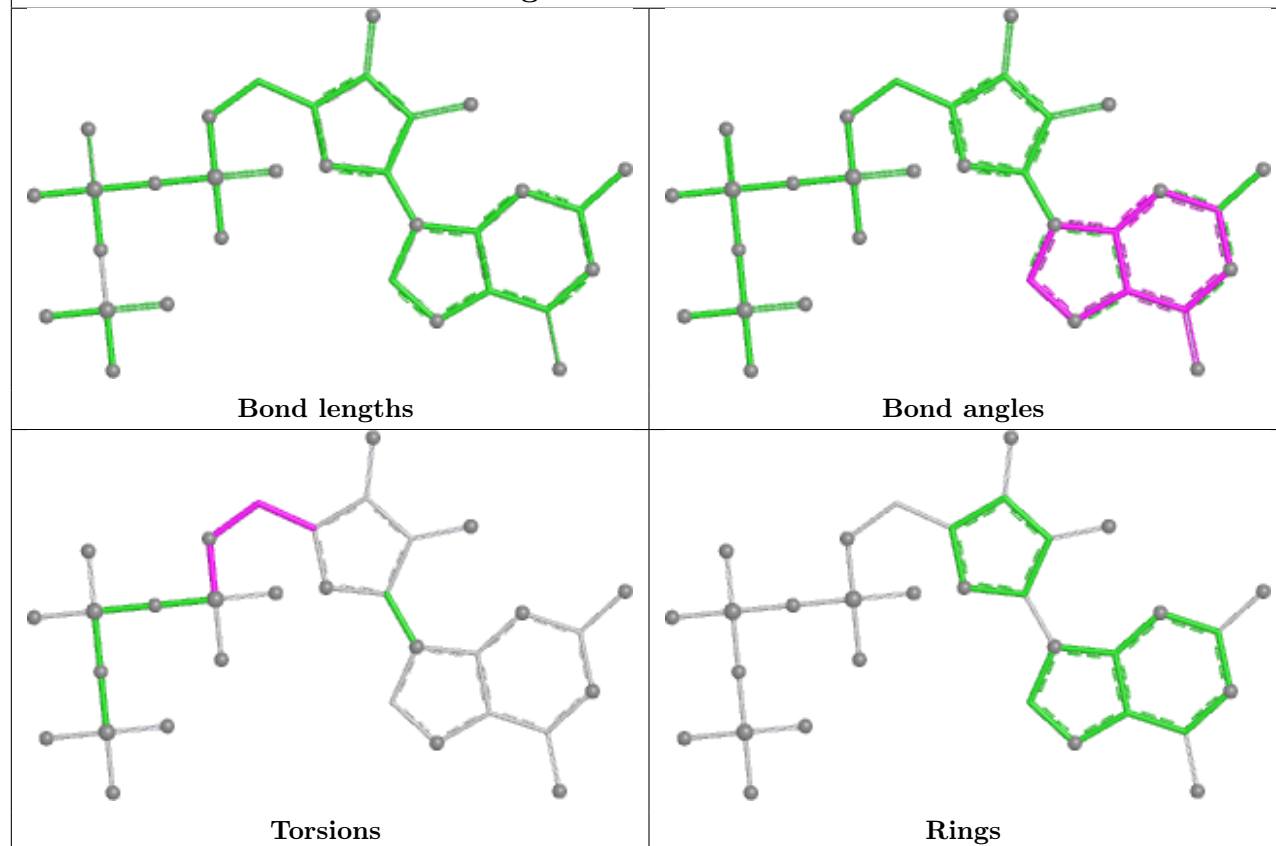




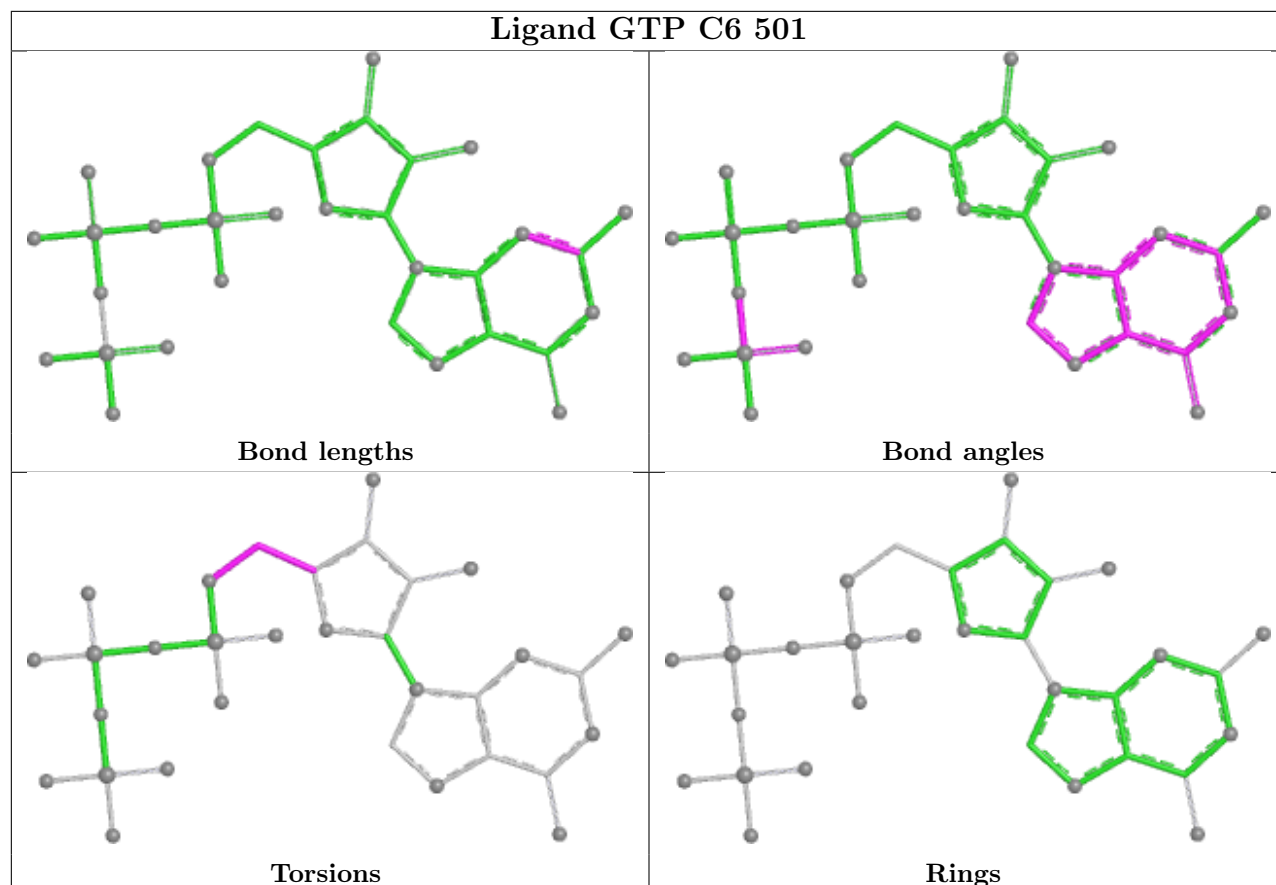
## Ligand GTP D6 501



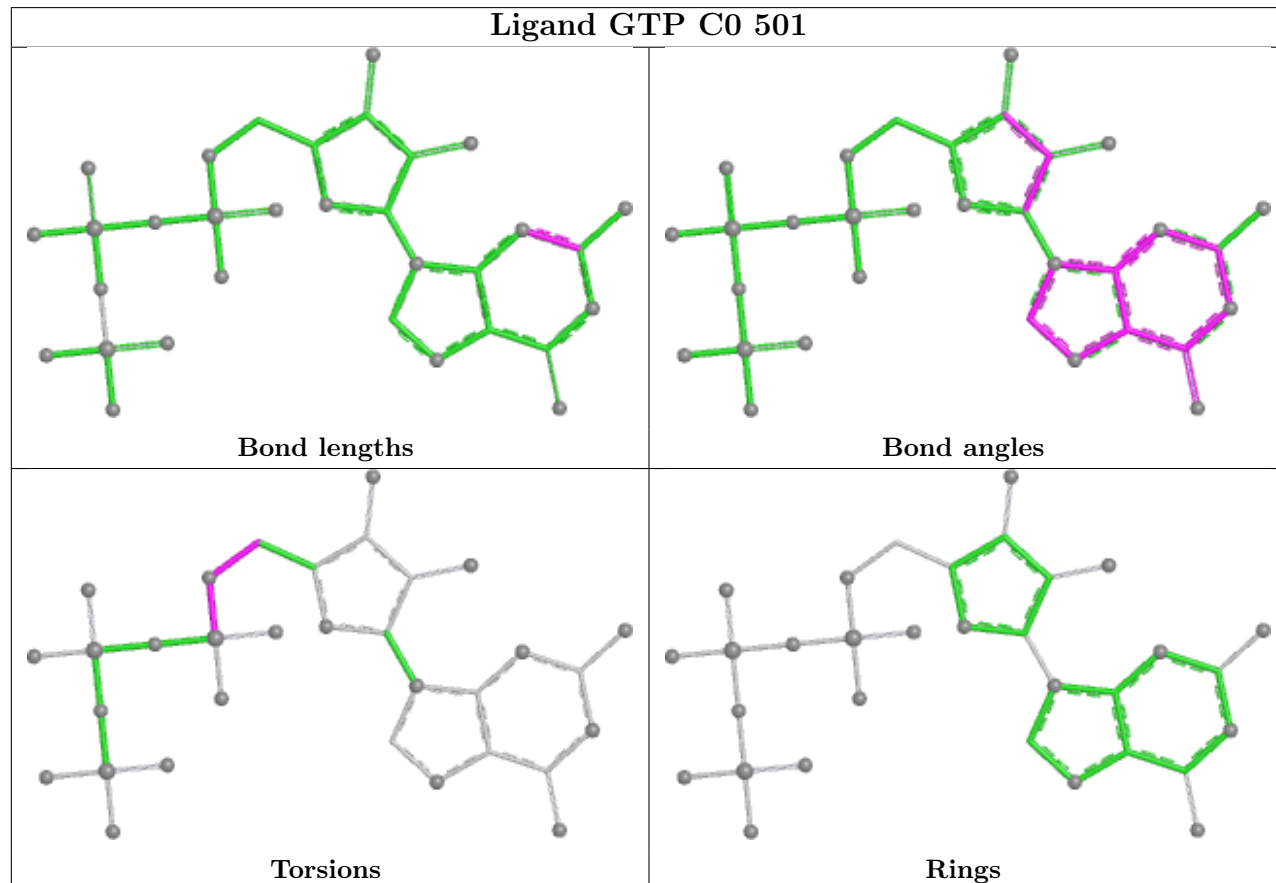
## Ligand GTP A4 501

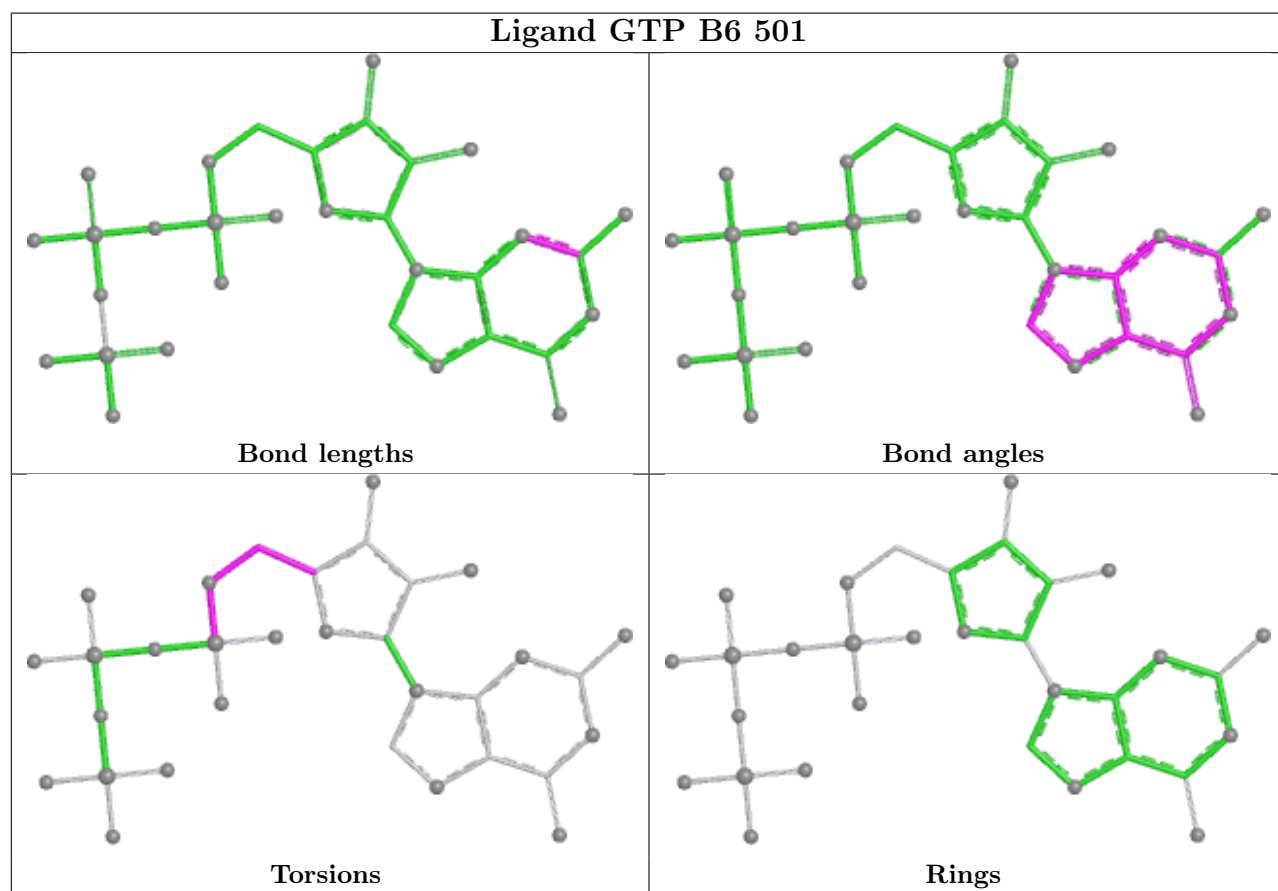
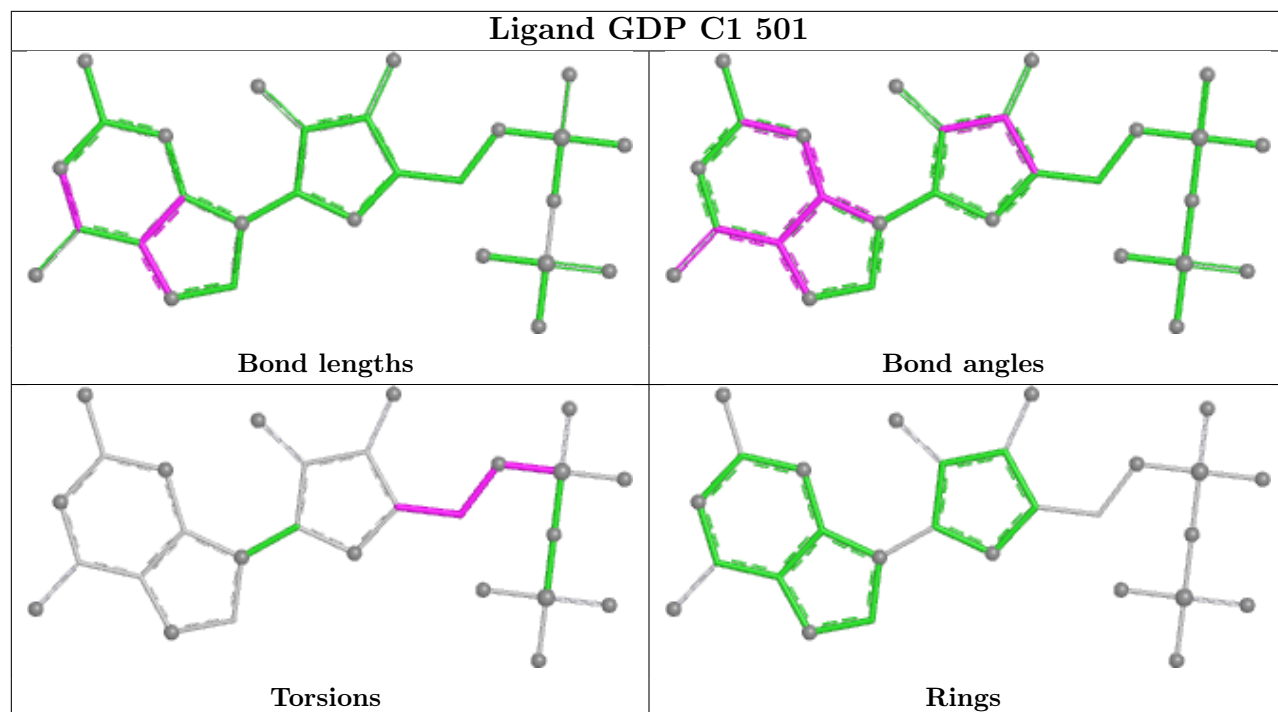


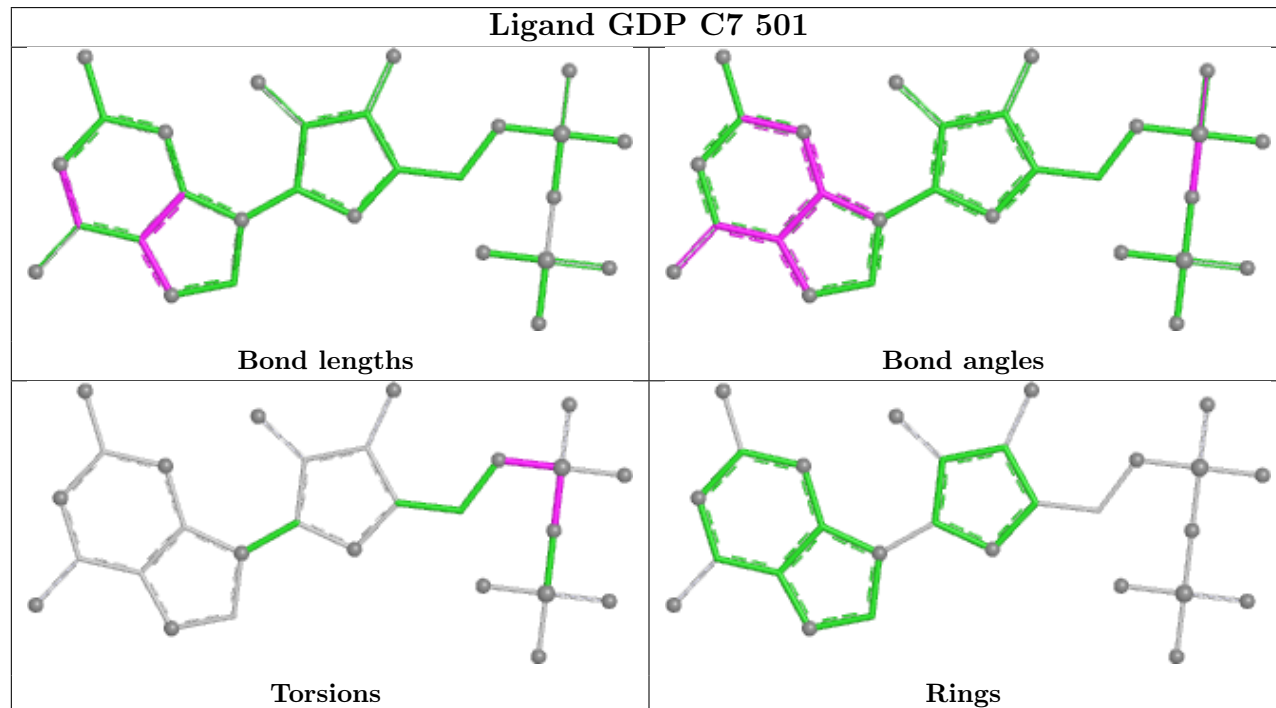
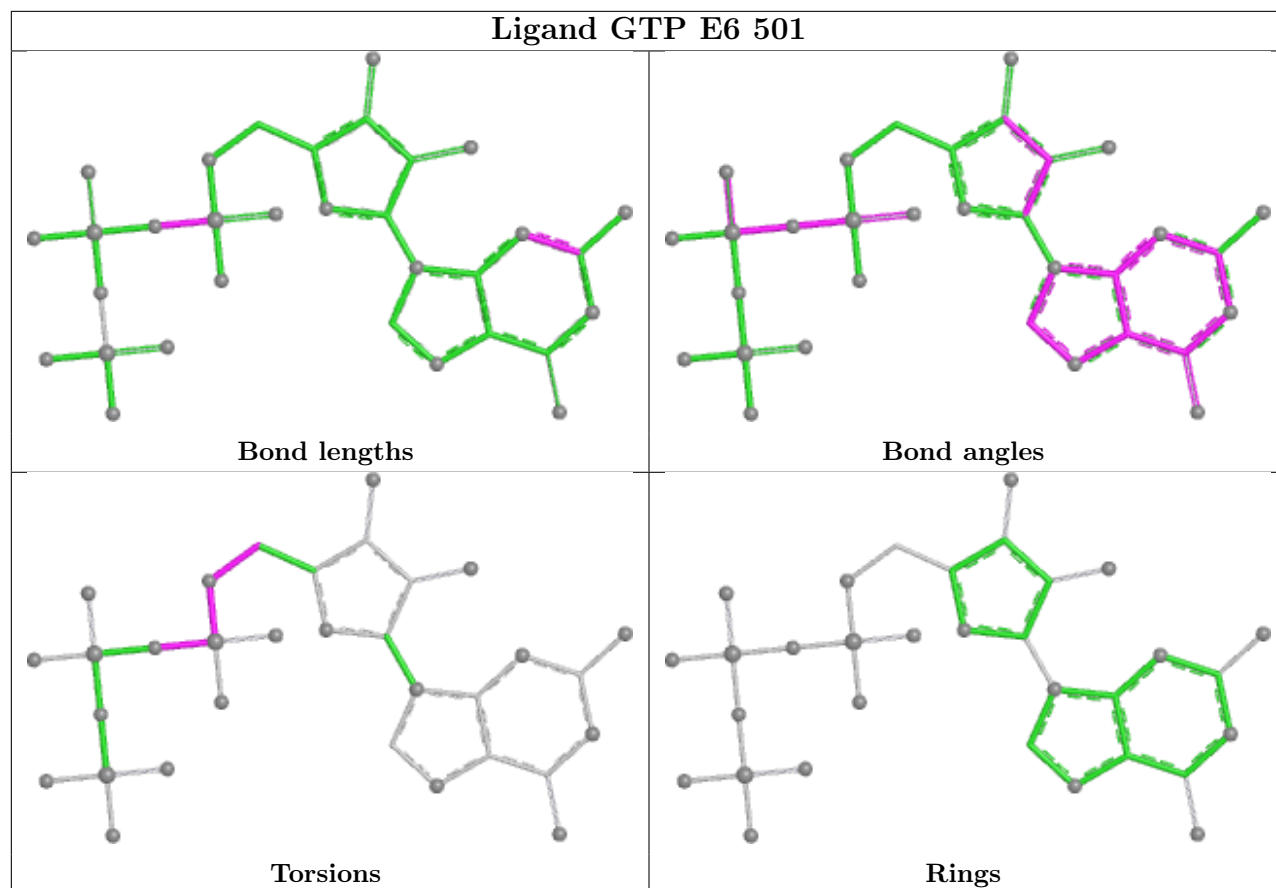
## Ligand GTP C6 501

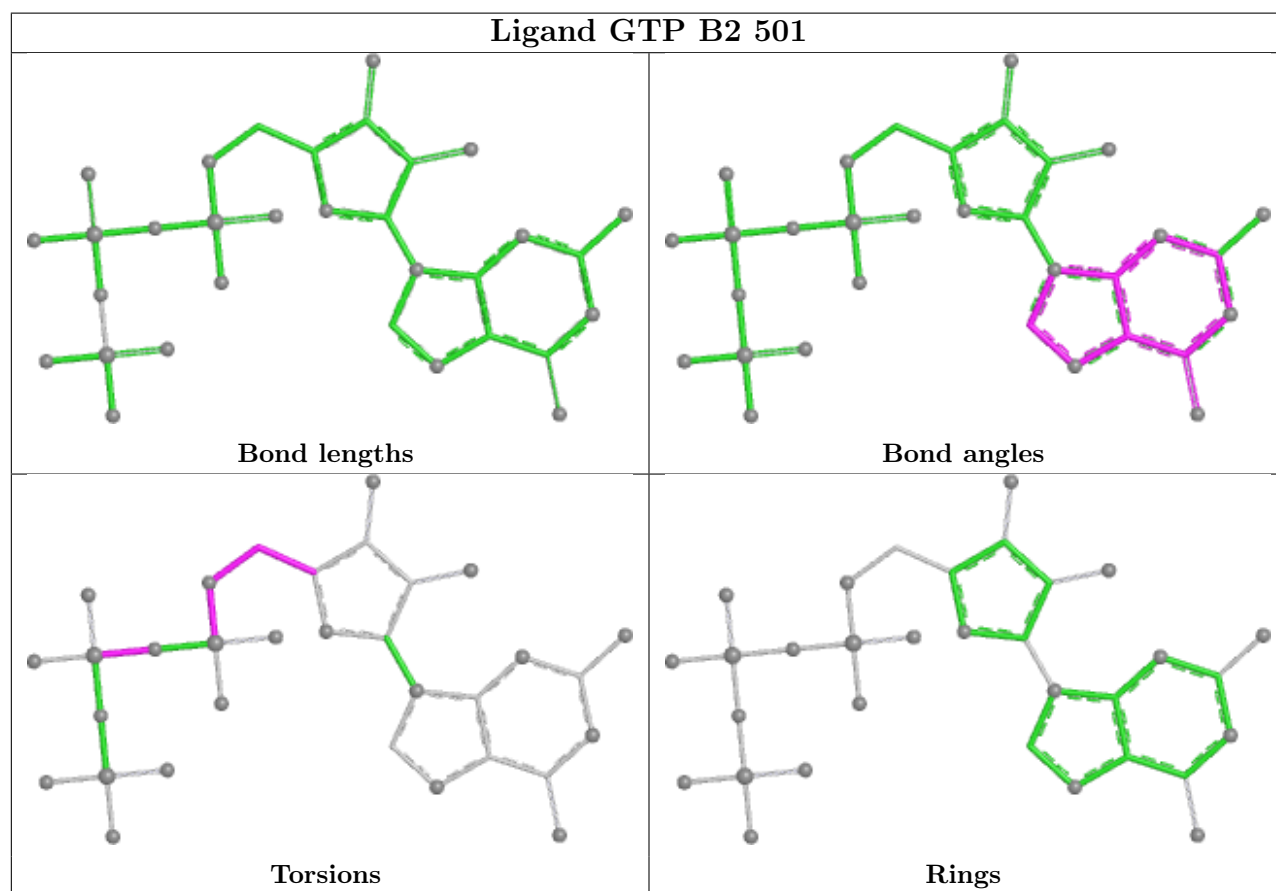
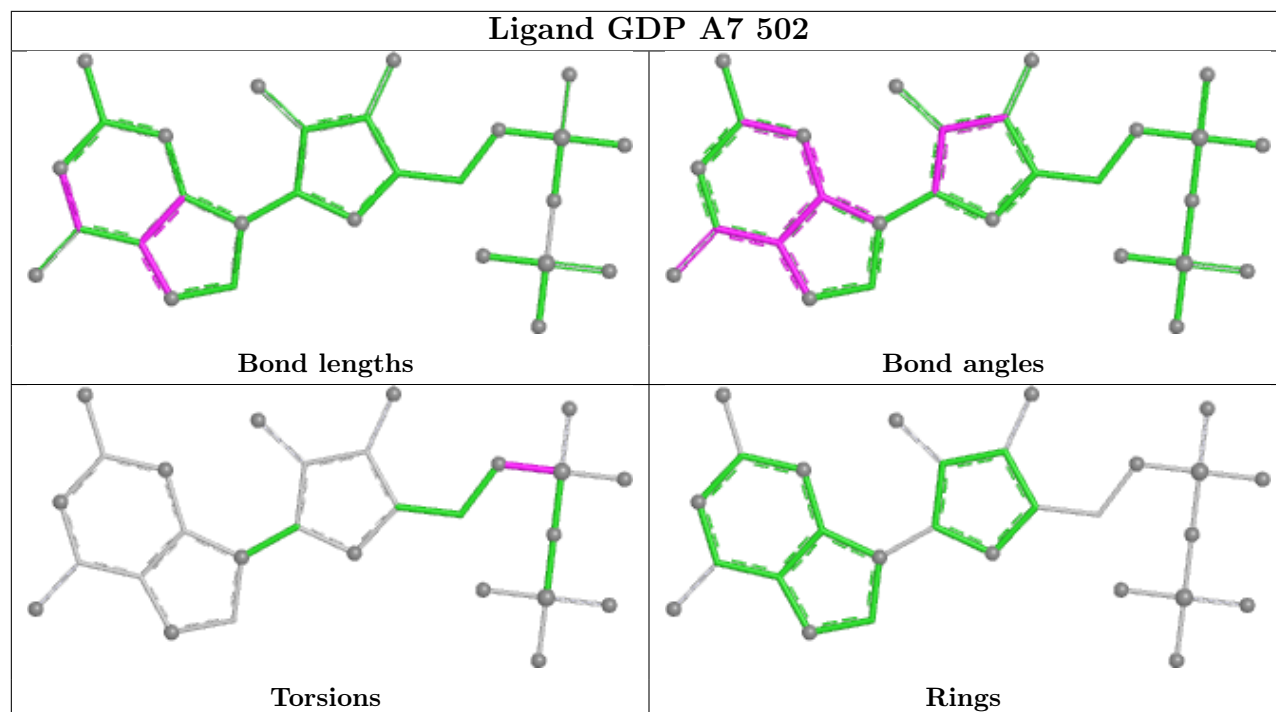


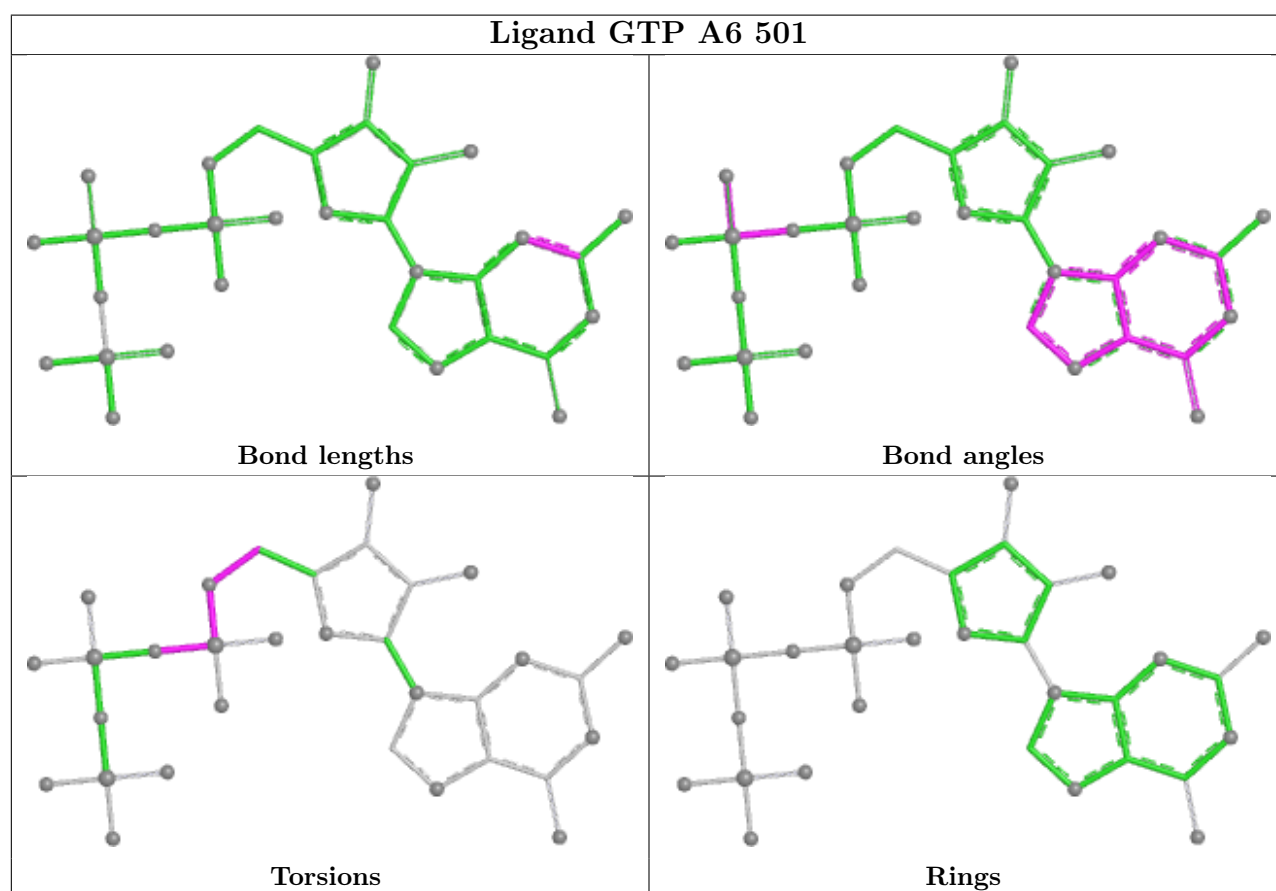
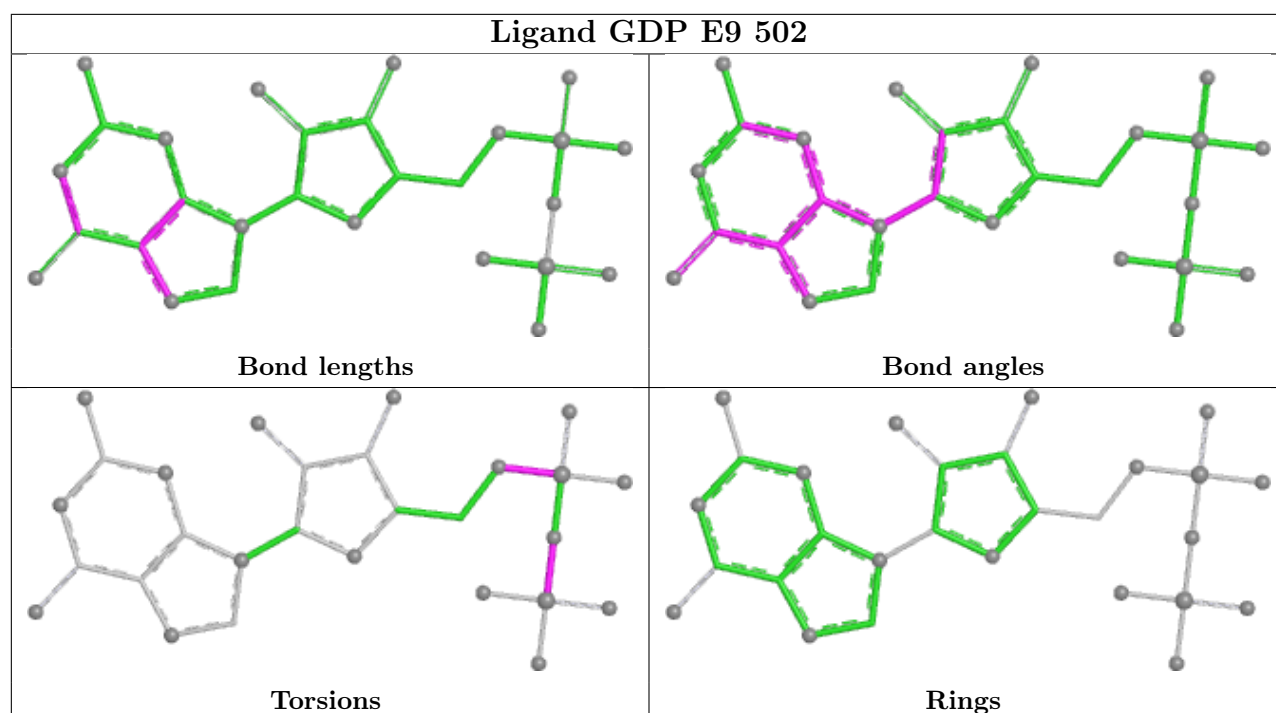
## Ligand GTP C0 501

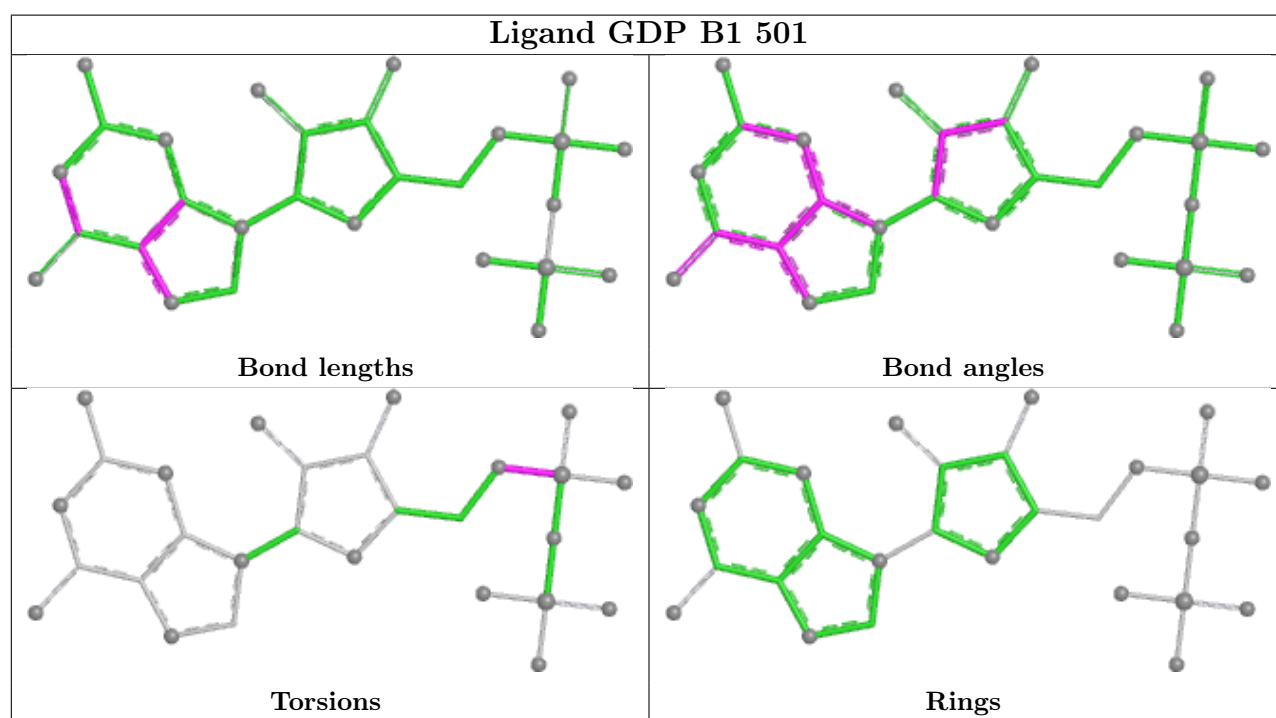
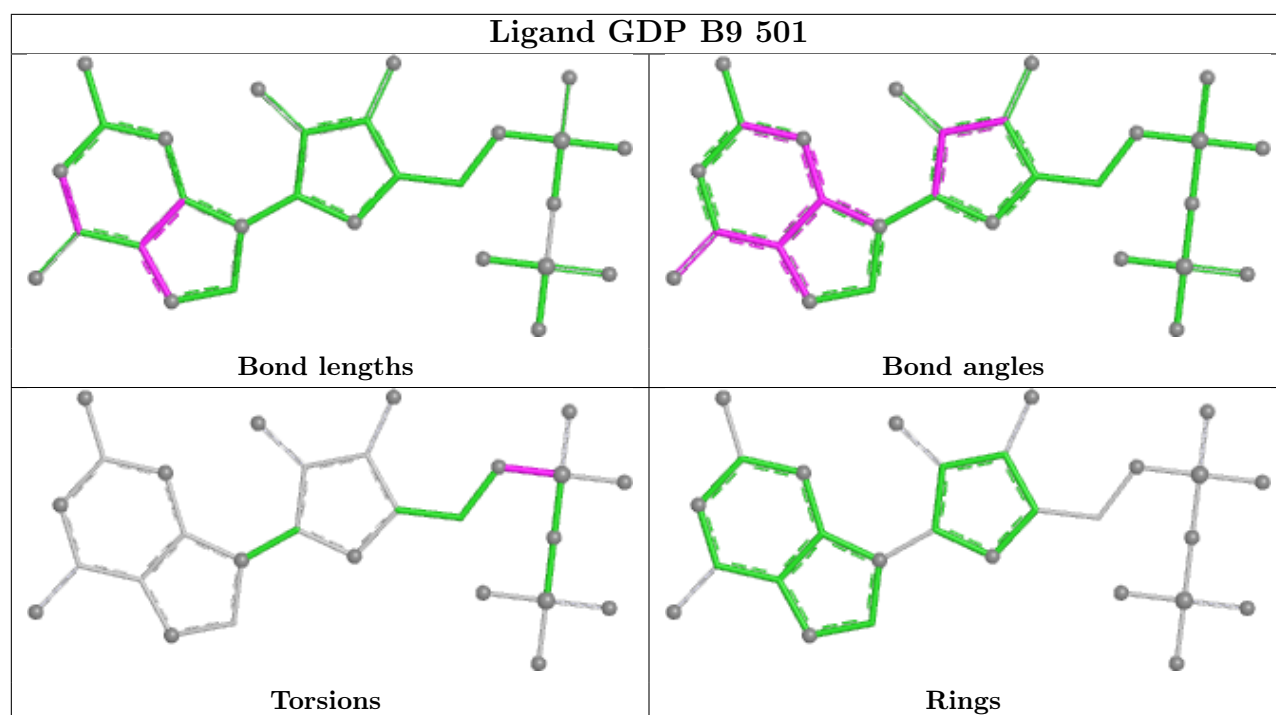


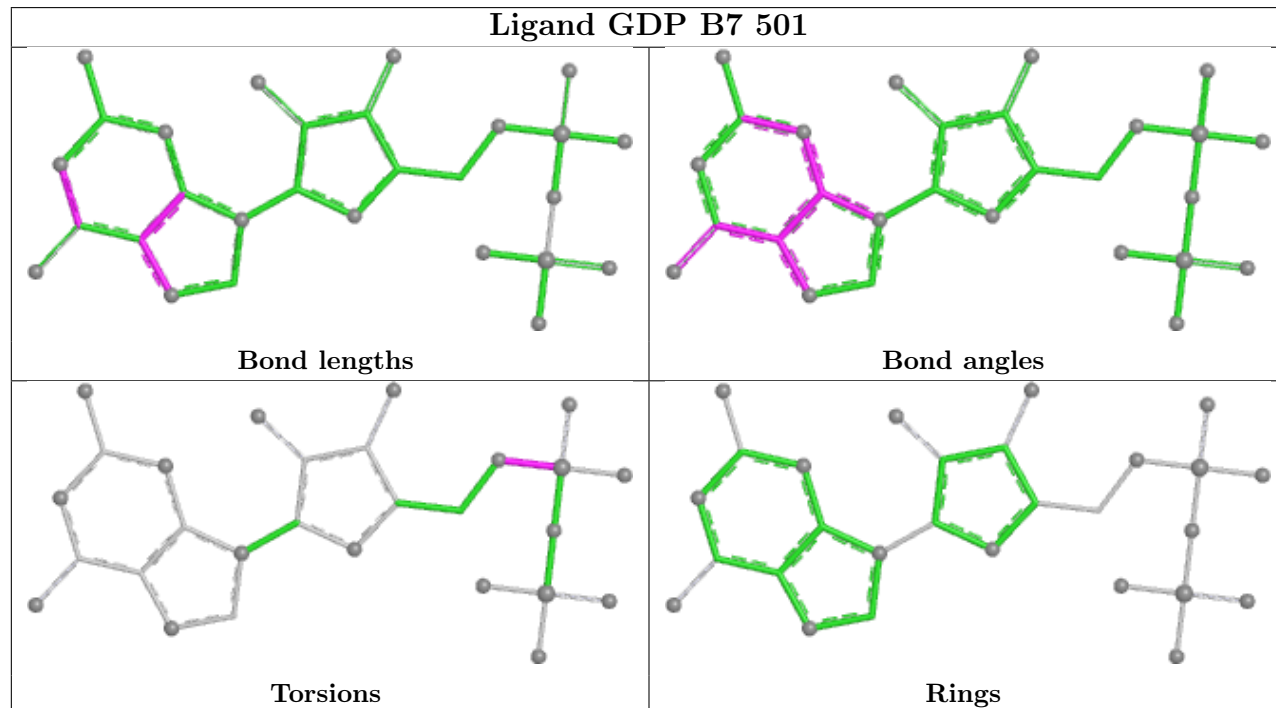
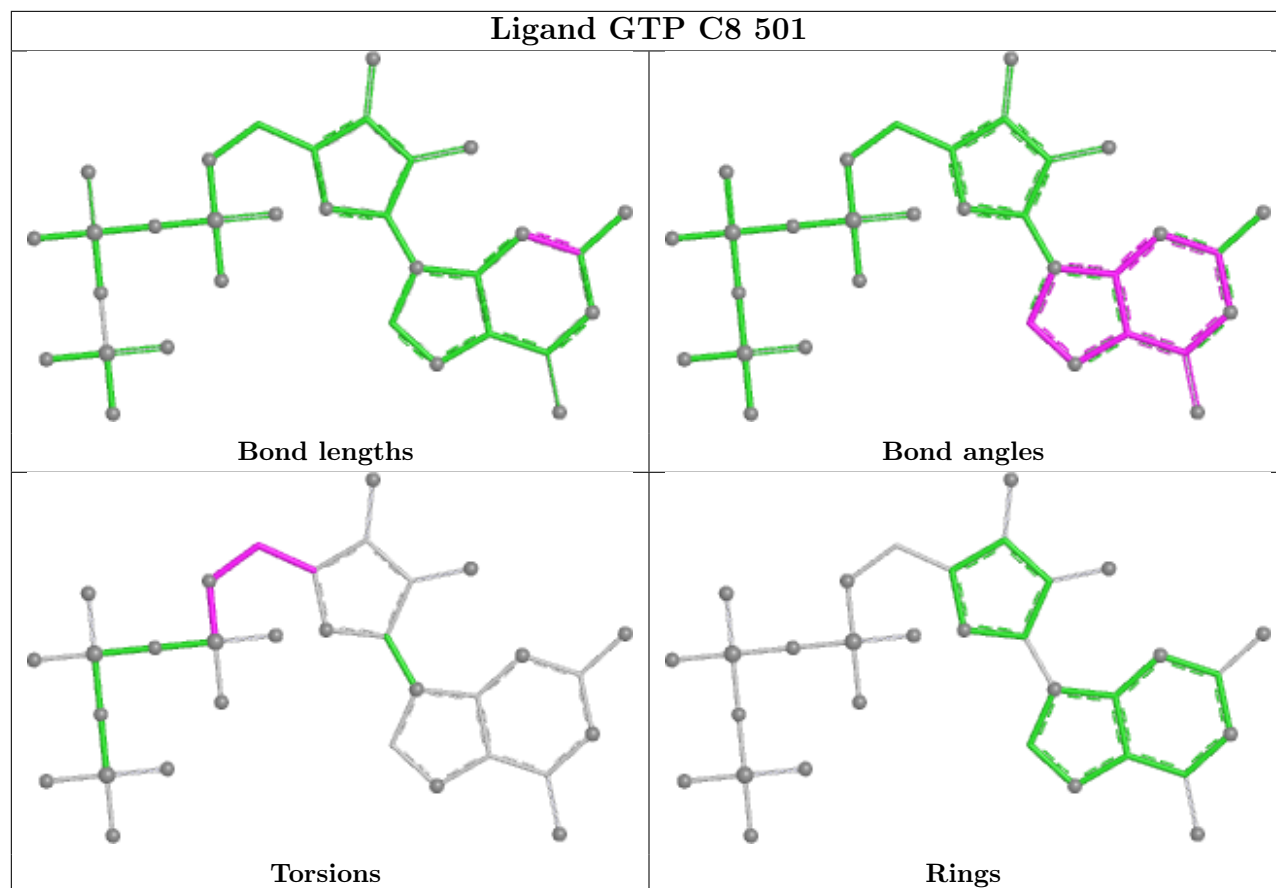


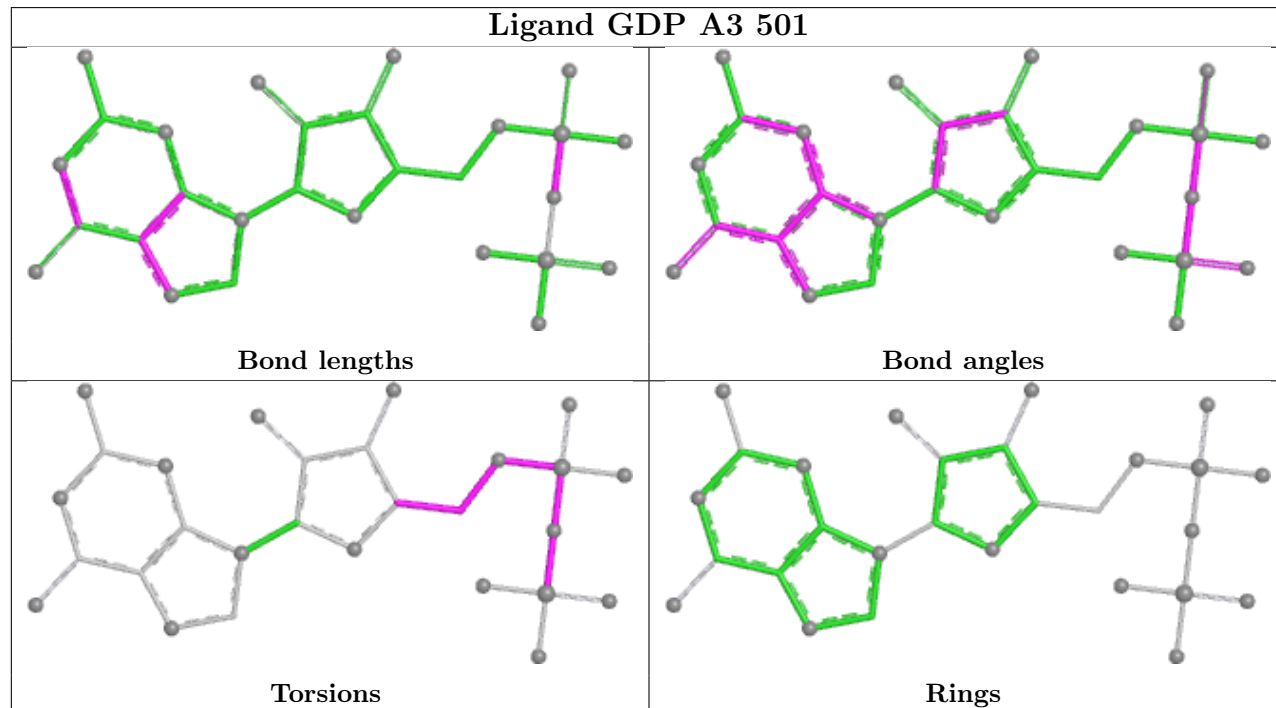
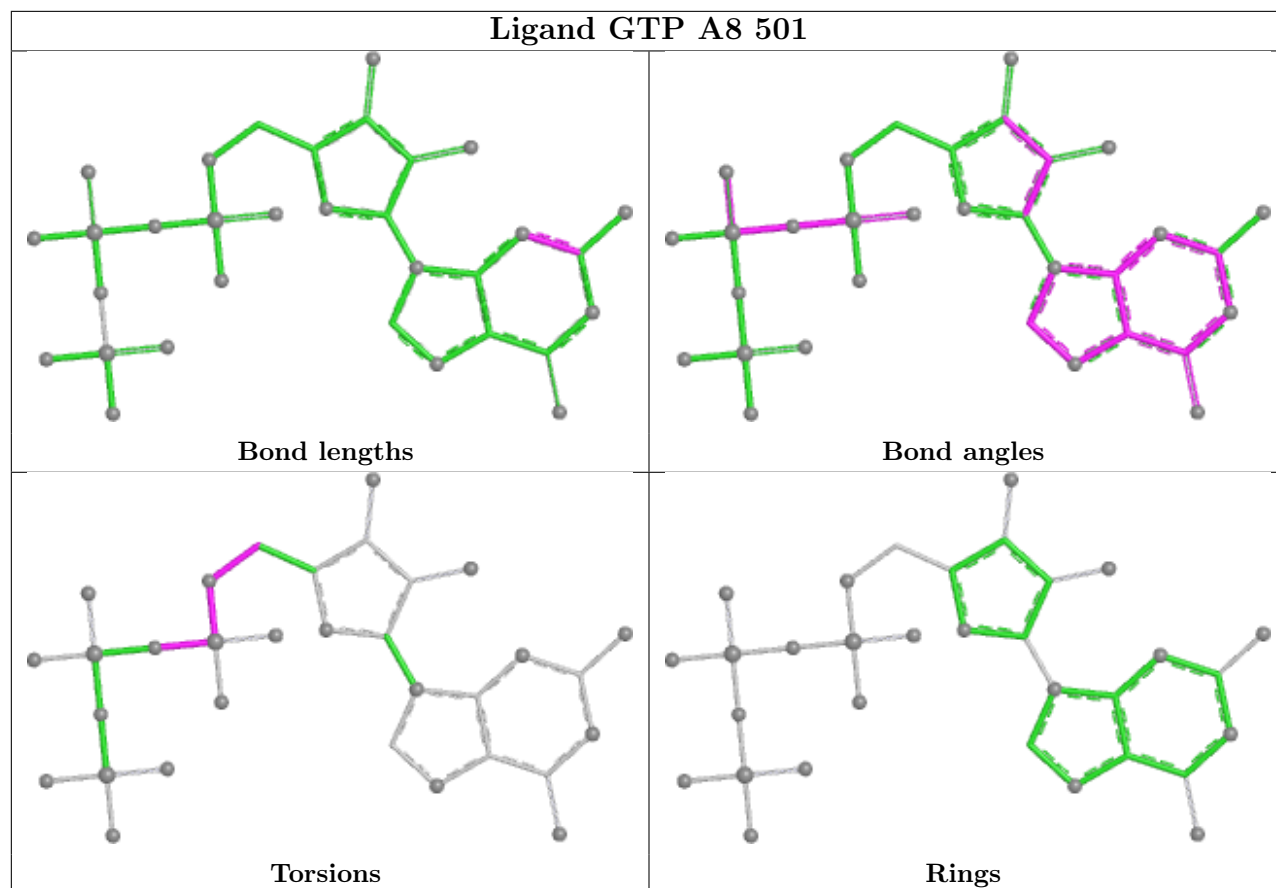


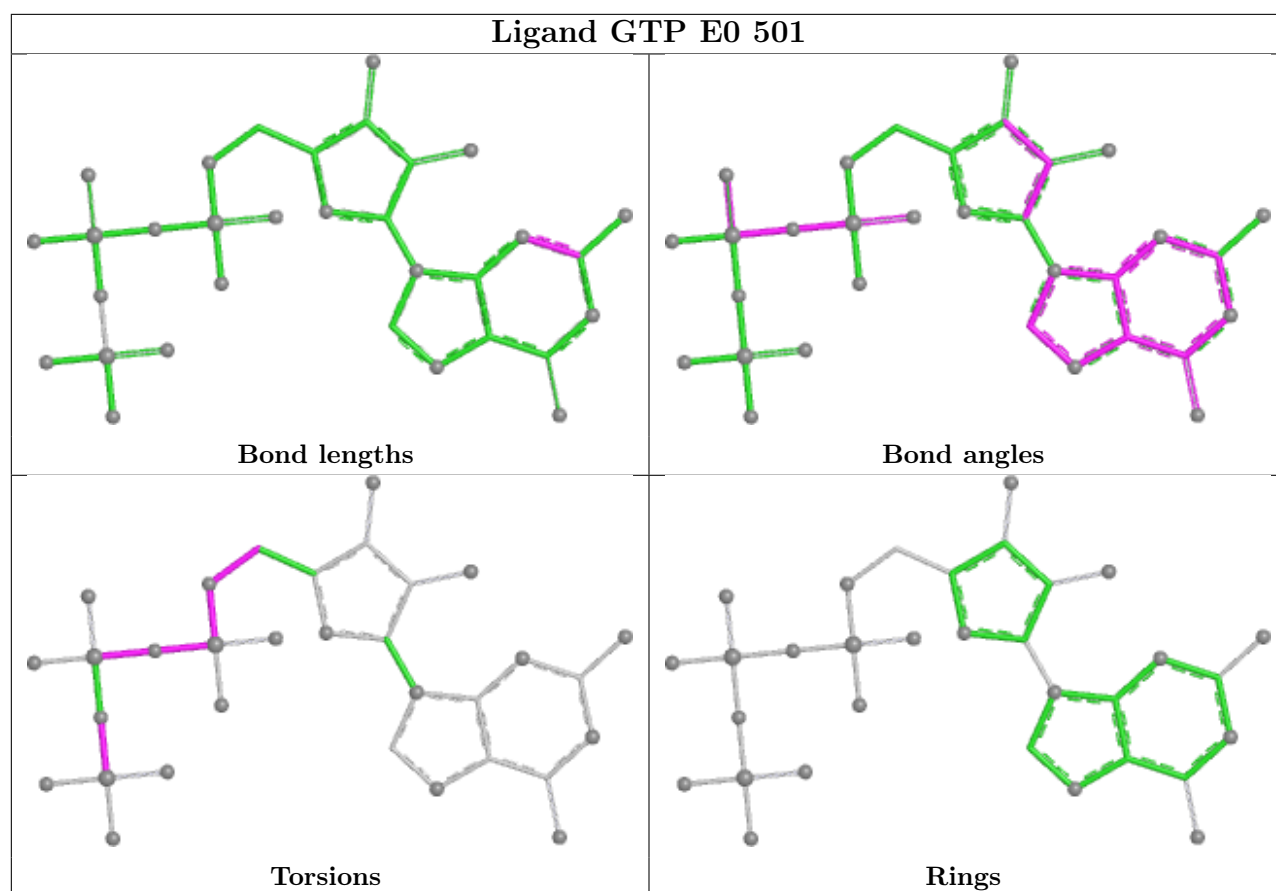












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

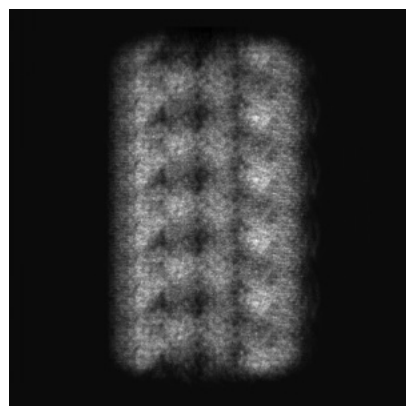
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72718. These allow visual inspection of the internal detail of the map and identification of artifacts.

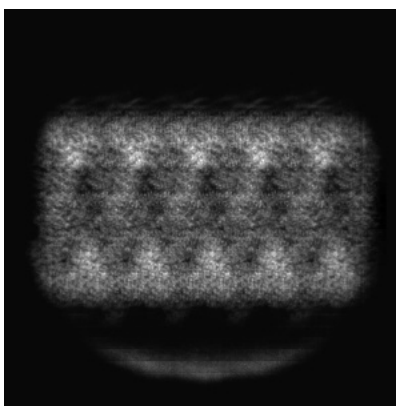
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

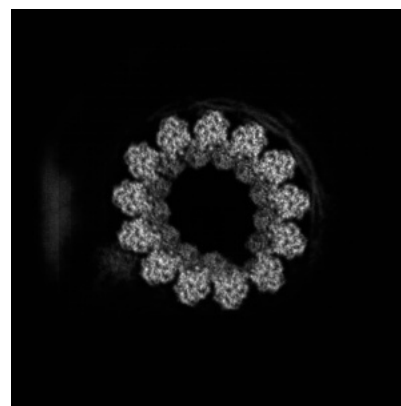
#### 6.1.1 Primary map



X

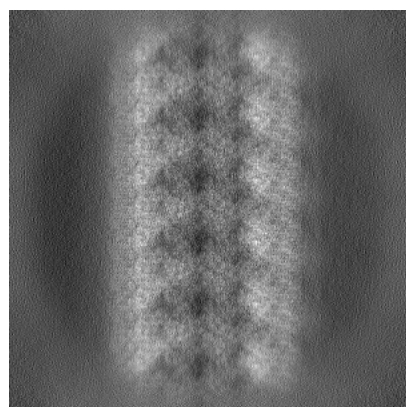


Y

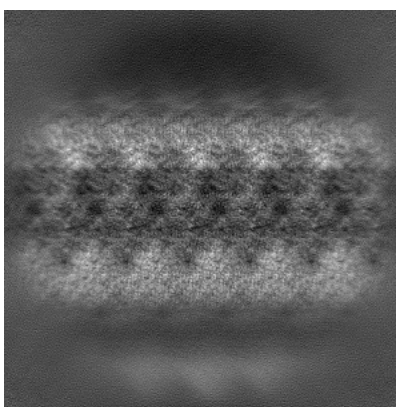


Z

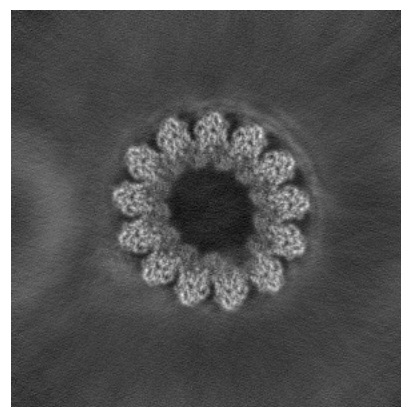
#### 6.1.2 Raw map



X



Y

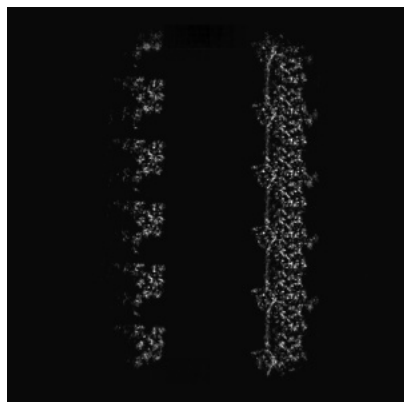


Z

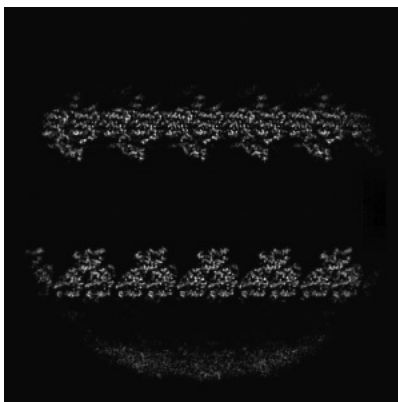
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

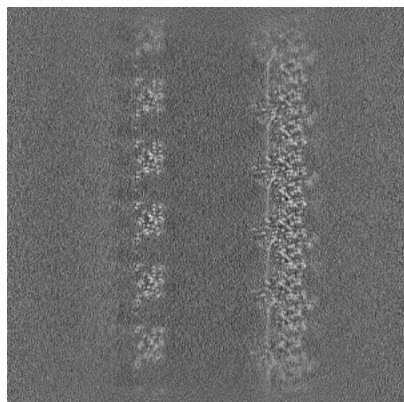


Y Index: 200

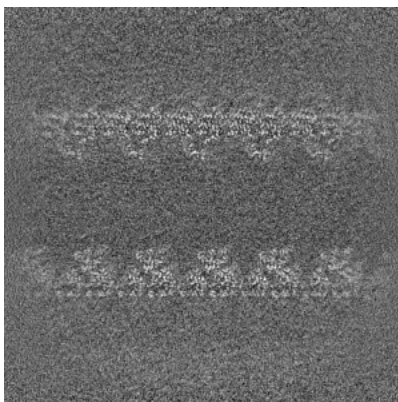


Z Index: 200

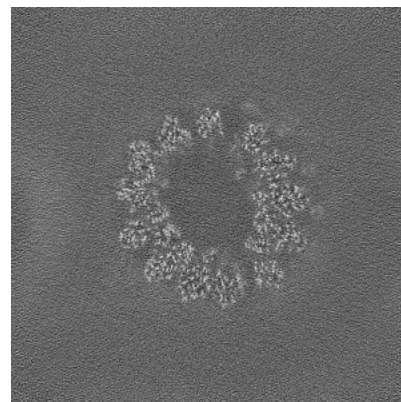
### 6.2.2 Raw map



X Index: 200



Y Index: 200

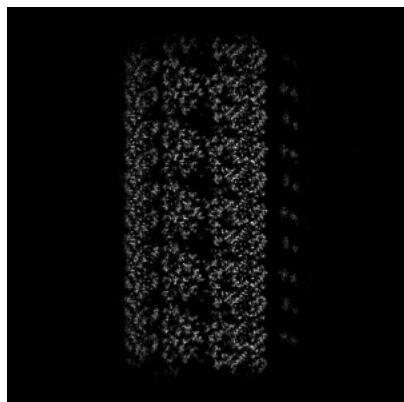


Z Index: 200

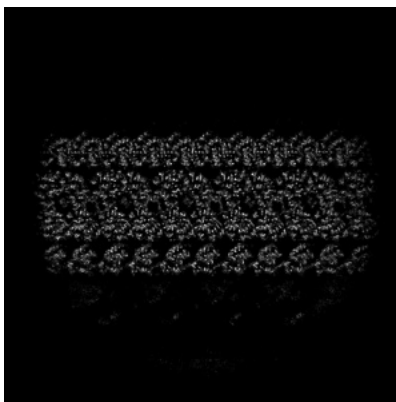
The images above show central slices of the map in three orthogonal directions.

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

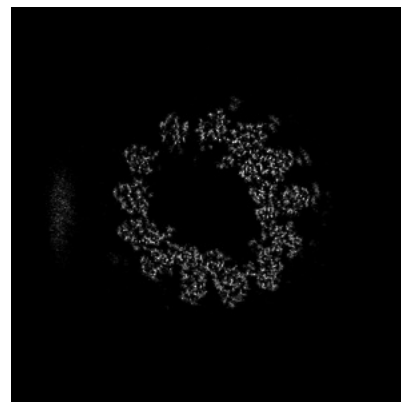
### 6.3.1 Primary map



X Index: 265

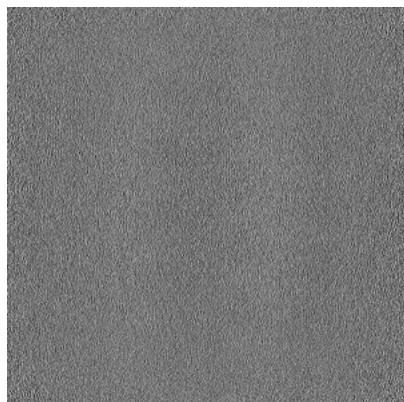


Y Index: 129

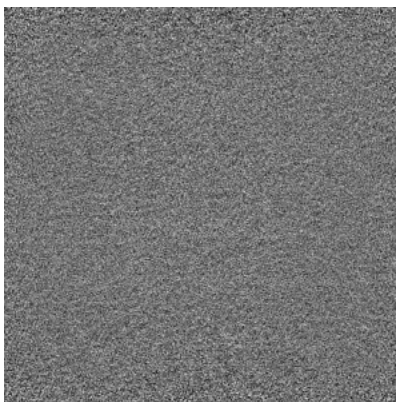


Z Index: 126

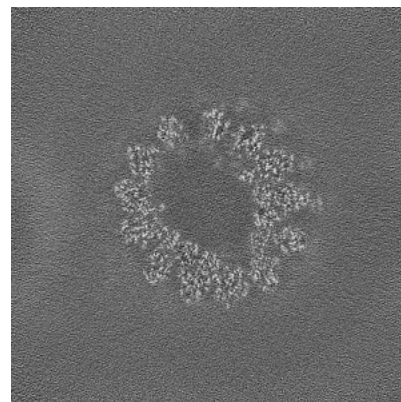
### 6.3.2 Raw map



X Index: 0



Y Index: 1

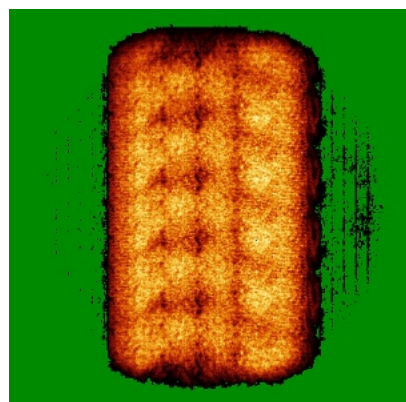


Z Index: 194

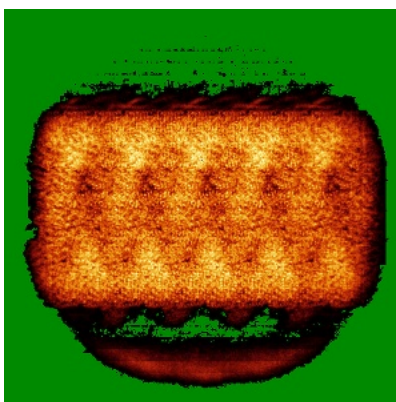
The images above show the largest variance slices of the map in three orthogonal directions.

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

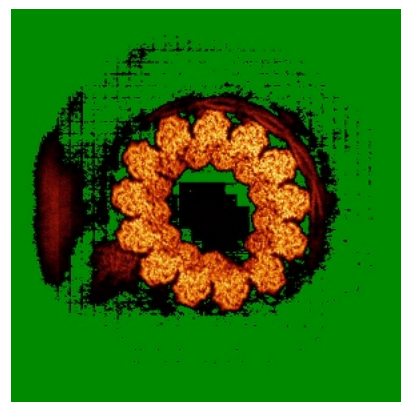
### 6.4.1 Primary map



X

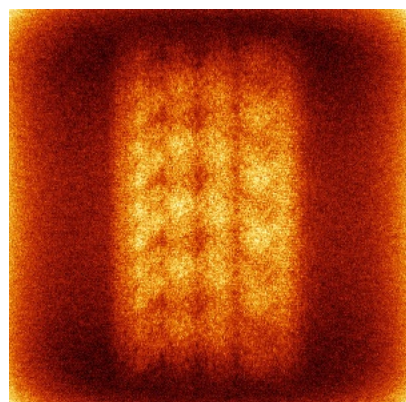


Y

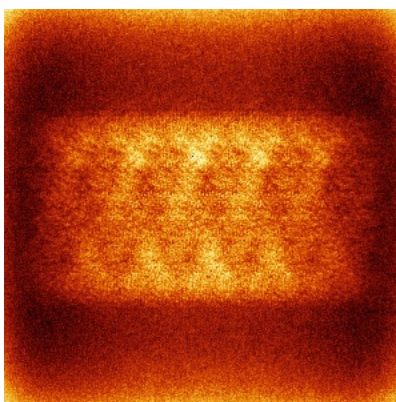


Z

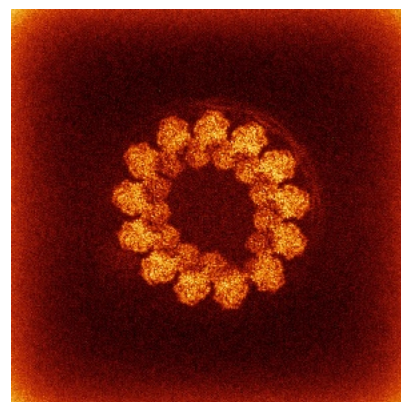
### 6.4.2 Raw map



X



Y

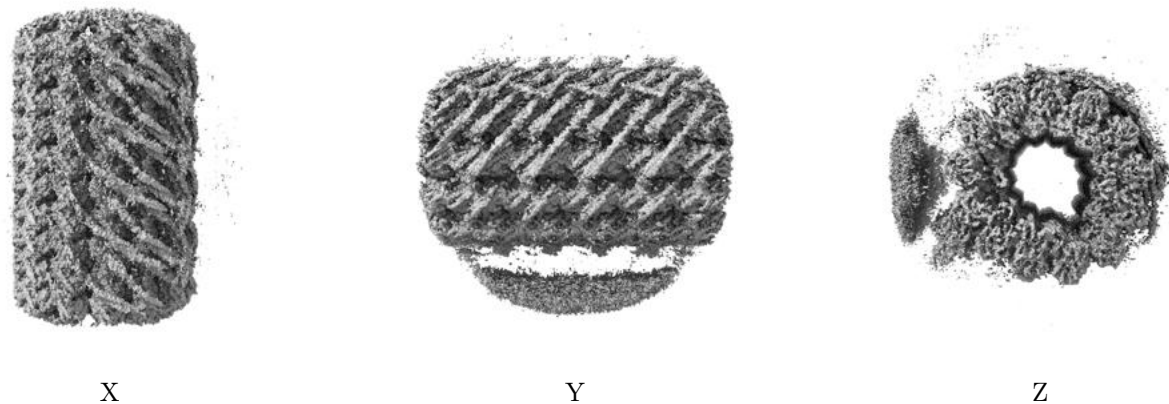


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

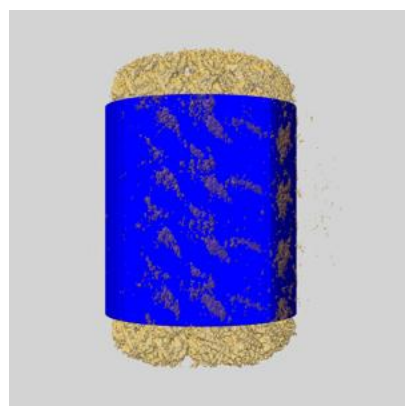
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

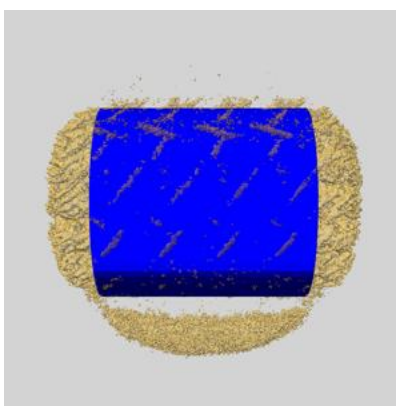
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

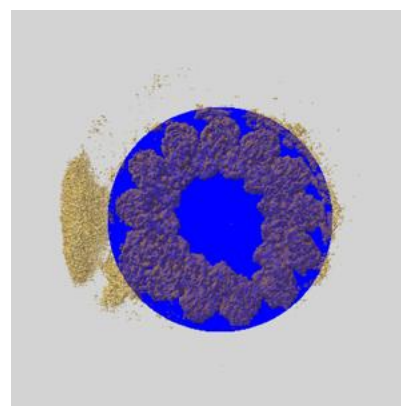
### 6.6.1 emd\_72718\_msk\_1.map [i](#)



X



Y

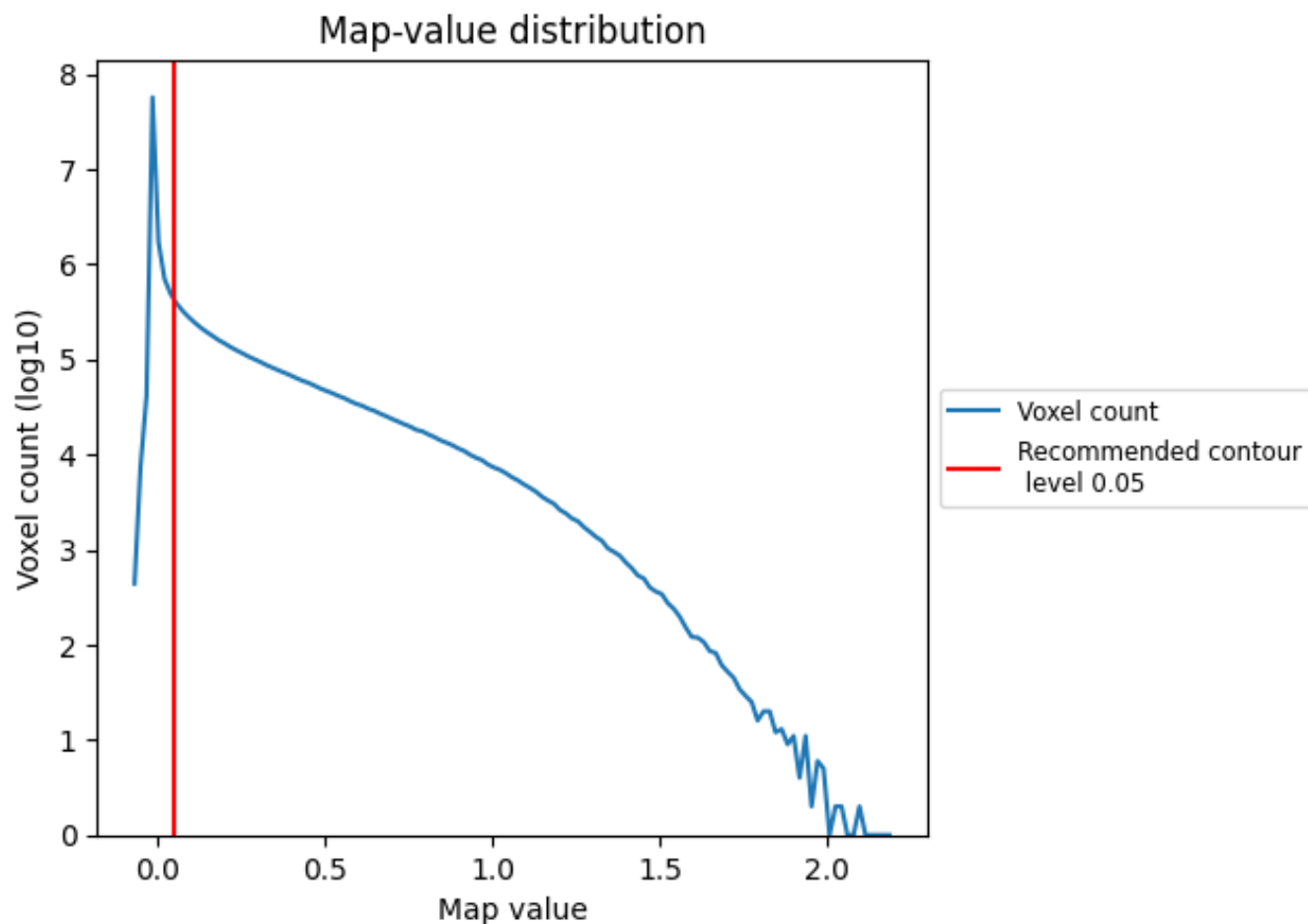


Z

## 7 Map analysis [i](#)

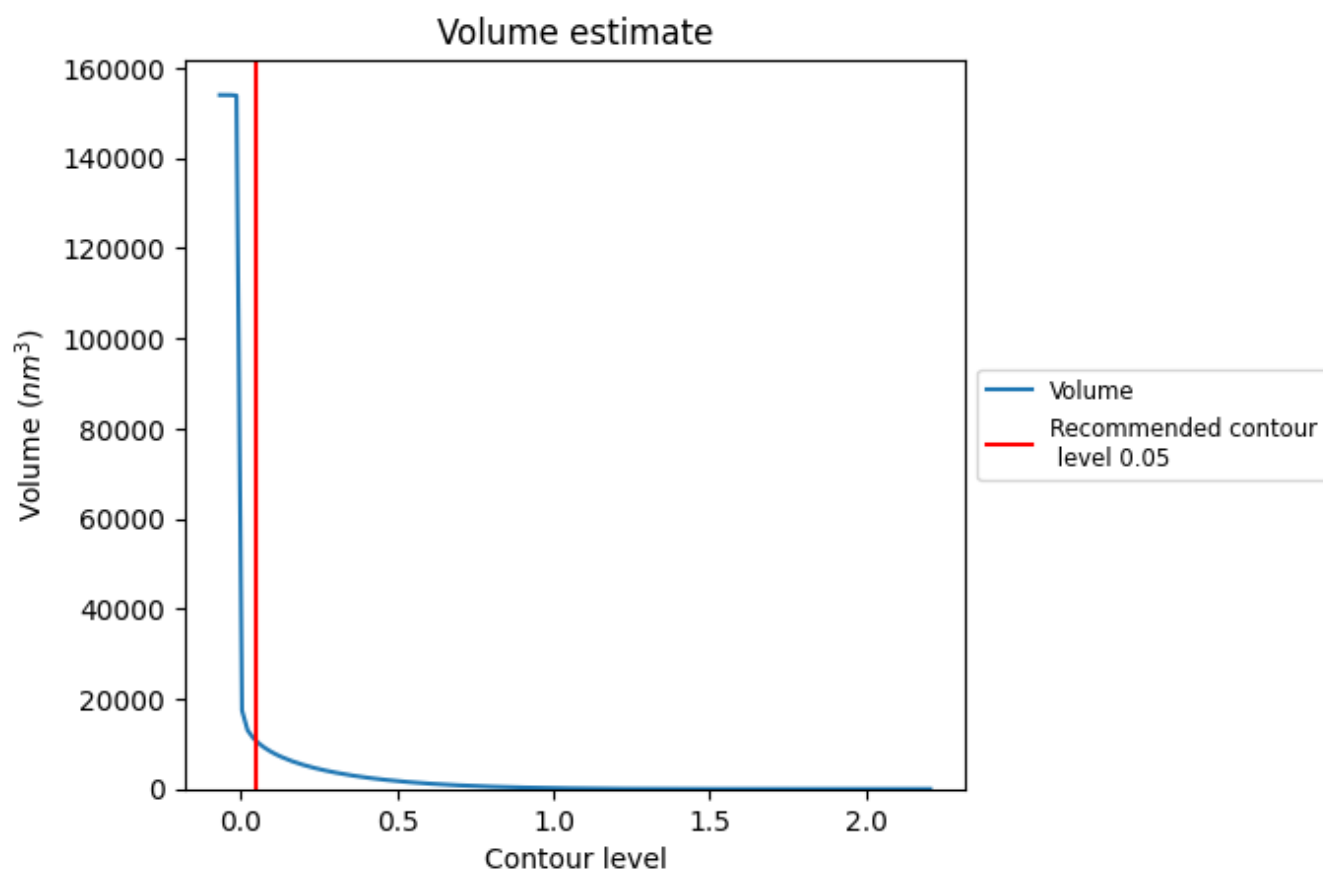
This section contains the results of statistical analysis of the map.

### 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.

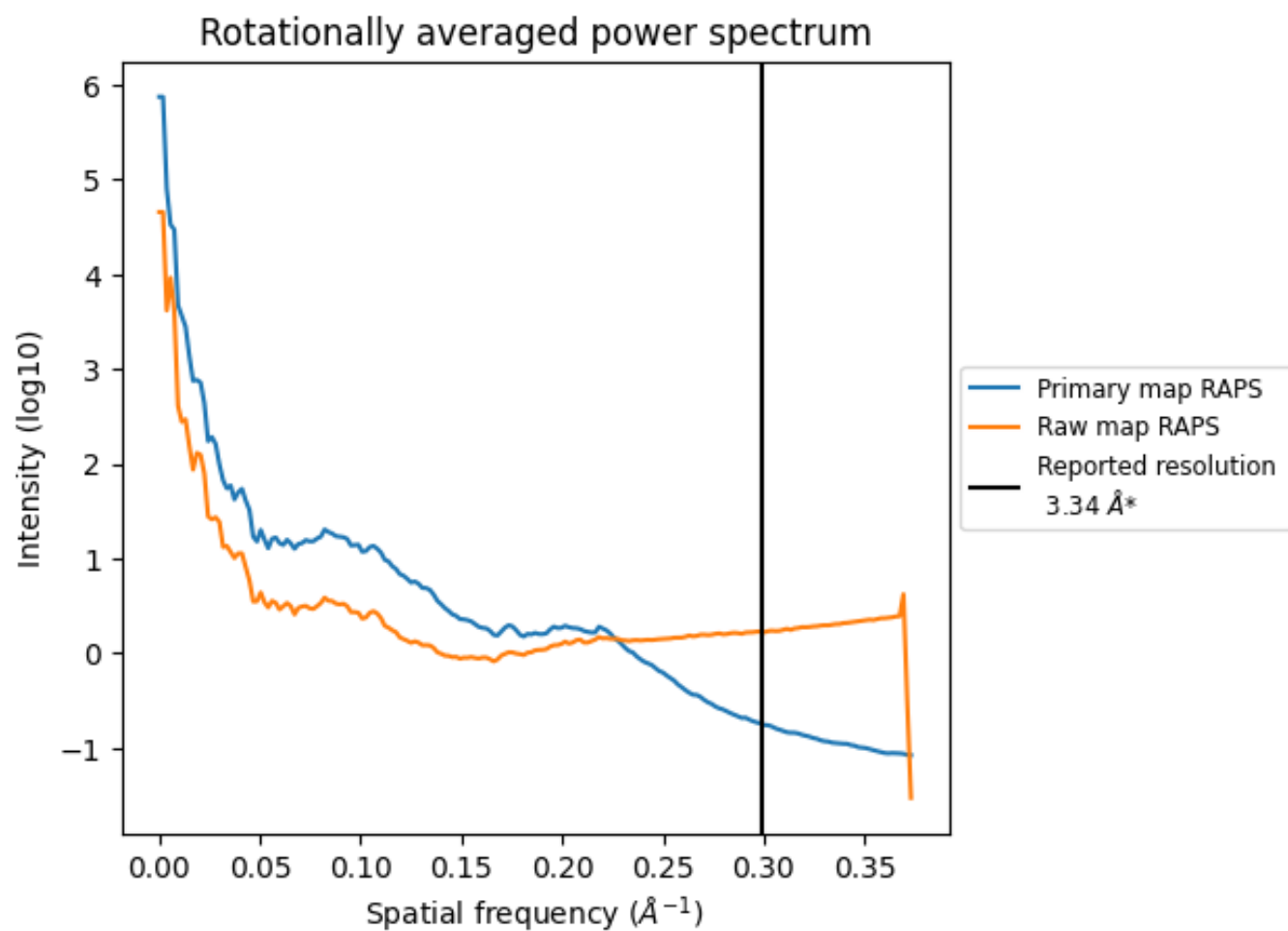
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 10584  $\text{nm}^3$ ; this corresponds to an approximate mass of 9561 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 ⓘ

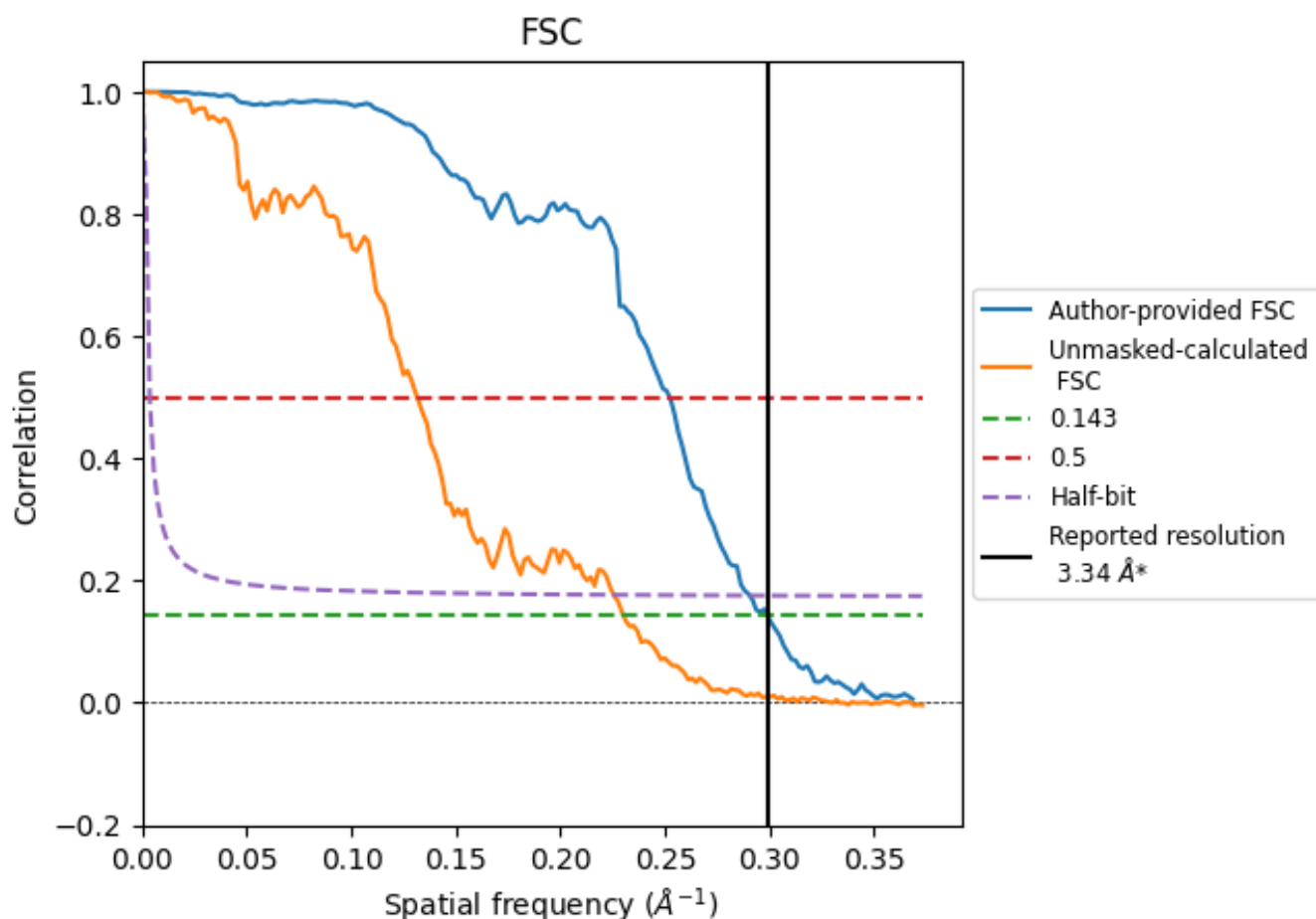


\*Reported resolution corresponds to spatial frequency of 0.299 Å<sup>-1</sup>

## 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 0.299  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

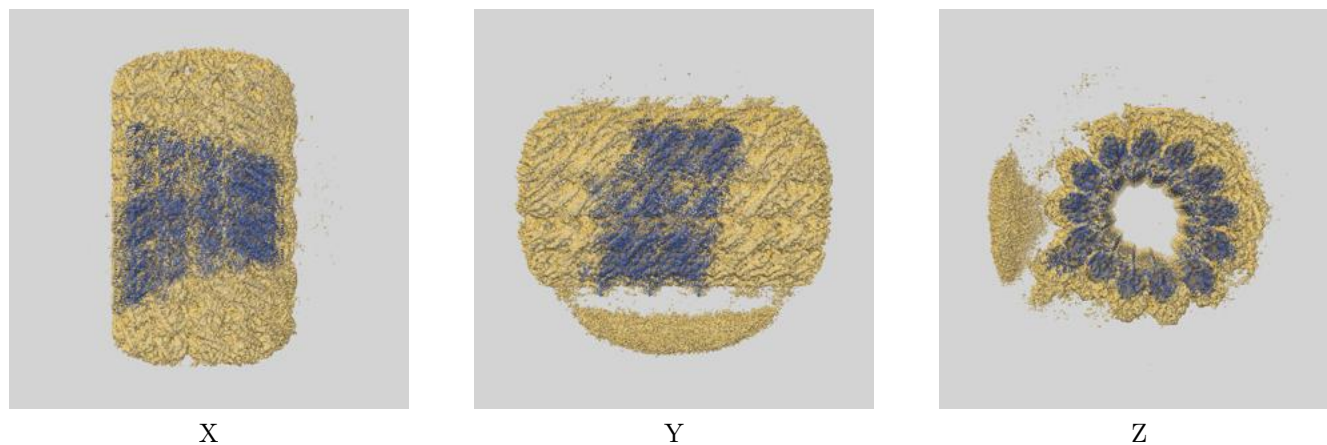
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.34                               | -    | -        |
| Author-provided FSC curve | 3.34                               | 3.96 | 3.44     |
| Unmasked-calculated*      | 4.34                               | 7.60 | 4.43     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.34 by more than 10 %

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

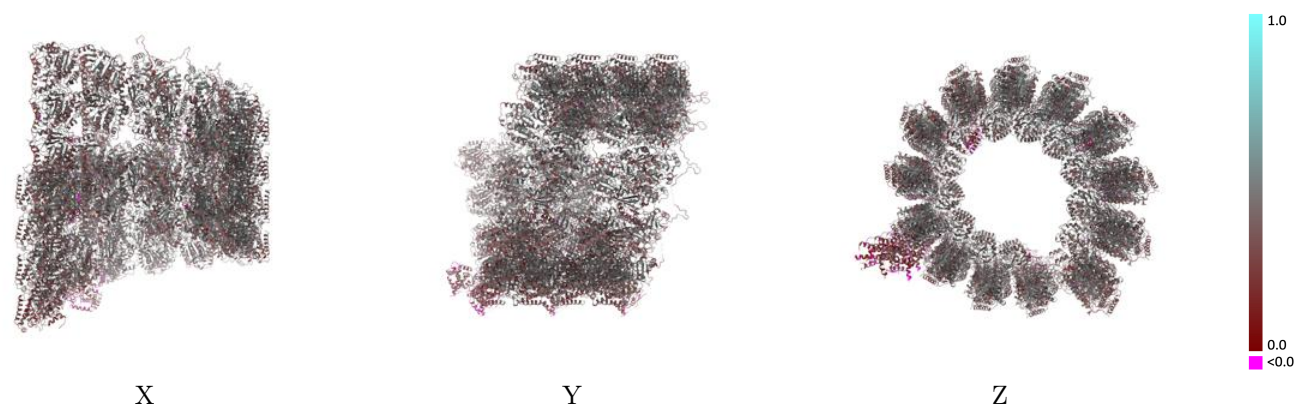
This section contains information regarding the fit between EMDB map EMD-72718 and PDB model 9YA2. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



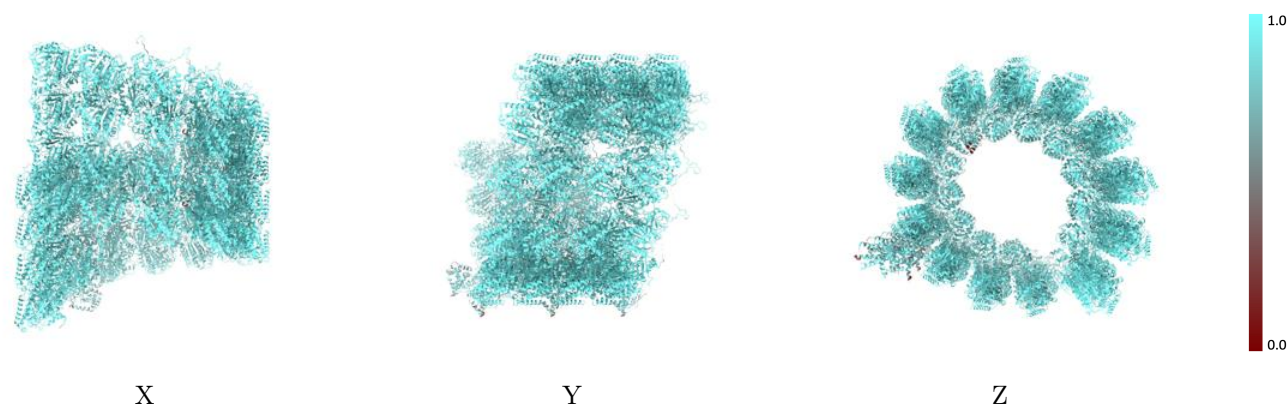
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



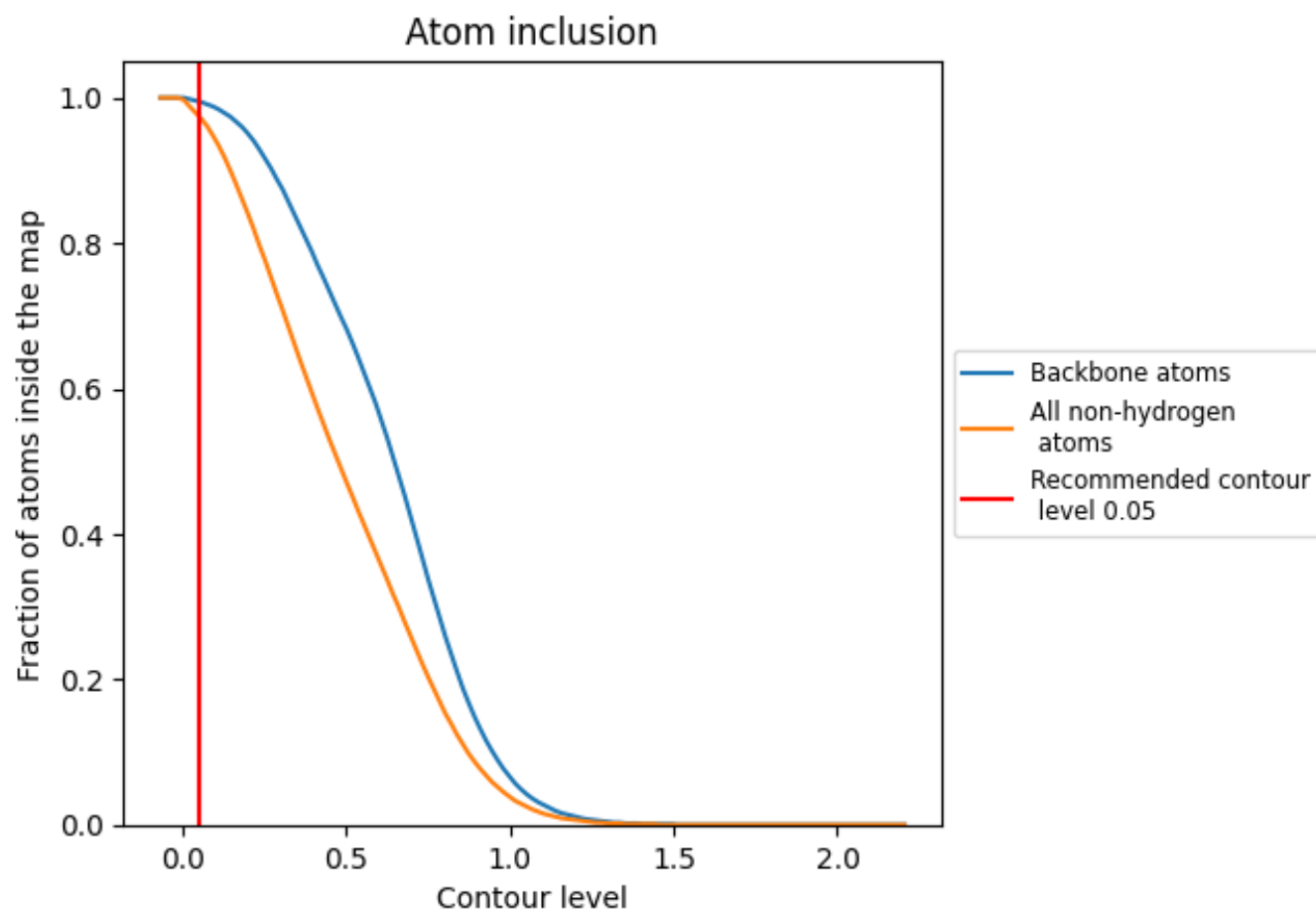
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9740   |  0.3950   |
| A     |  0.9580   |  0.3710   |
| A0    |  0.9900   |  0.4020   |
| A1    |  0.9850   |  0.3950   |
| A2    |  0.9910   |  0.3960   |
| A3    |  0.9710   |  0.3350   |
| A4    |  0.9910   |  0.4120   |
| A5    |  0.9890   |  0.4100   |
| A6    |  0.9890   |  0.4060   |
| A7    |  0.9810   |  0.3730   |
| A8    |  0.9830   |  0.4030   |
| A9    |  0.9880   |  0.4070   |
| B     |  0.9420   |  0.3870   |
| B0    |  0.9860   |  0.4020   |
| B1    |  0.9860  |  0.3890  |
| B2    |  0.9890 |  0.4080 |
| B3    |  0.9860 |  0.4130 |
| B4    |  0.9860 |  0.4090 |
| B5    |  0.9840 |  0.3900 |
| B6    |  0.9870 |  0.4070 |
| B7    |  0.9850 |  0.4110 |
| B8    |  0.9840 |  0.4030 |
| B9    |  0.9840 |  0.3960 |
| C     |  0.9160 |  0.3690 |
| C0    |  0.9900 |  0.4160 |
| C1    |  0.9830 |  0.3990 |
| C2    |  0.9850 |  0.4010 |
| C3    |  0.9800 |  0.3760 |
| C4    |  0.9850 |  0.4030 |
| C5    |  0.9830 |  0.4080 |
| C6    |  0.9860 |  0.3990 |
| C7    |  0.9830 |  0.3920 |
| C8    |  0.9890 |  0.4340 |
| C9    |  0.9860 |  0.4330 |
| D     |  0.8810 |  0.1270 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| D0    |  0.9900   |  0.4380   |
| D1    |  0.9880   |  0.4310   |
| D2    |  0.9910   |  0.4360   |
| D3    |  0.9890   |  0.4410   |
| D4    |  0.9910   |  0.4340   |
| D5    |  0.9900   |  0.4430   |
| D6    |  0.9910   |  0.4340   |
| D7    |  0.9890   |  0.4390   |
| D8    |  0.9900   |  0.4290   |
| D9    |  0.9890   |  0.4330   |
| E     |  0.9160   |  0.3410   |
| E0    |  0.9920   |  0.4210   |
| E1    |  0.9940   |  0.4240   |
| E2    |  0.9910   |  0.4240   |
| E3    |  0.9920   |  0.4280   |
| E4    |  0.9880   |  0.4020   |
| E5    |  0.9900   |  0.4200   |
| E6    |  0.9940  |  0.4230  |
| E7    |  0.9900 |  0.4180 |
| E8    |  0.9830 |  0.3910 |
| E9    |  0.9870 |  0.4100 |
| F     |  0.9140 |  0.3570 |
| F0    |  0.9840 |  0.3850 |
| F1    |  0.9910 |  0.4070 |
| G     |  0.9290 |  0.3540 |
| H     |  0.9460 |  0.3580 |
| I     |  0.8660 |  0.3380 |
| J     |  0.9610 |  0.3750 |
| K     |  0.9570 |  0.3820 |
| L     |  0.7910 |  0.2090 |
| M     |  0.7520 |  0.1490 |
| N     |  0.7980 |  0.1980 |
| O     |  0.9200 |  0.3270 |
| P     |  0.9100 |  0.3050 |
| Q     |  0.7850 |  0.1870 |
| R     |  0.9170 |  0.3060 |
| S     |  0.9420 |  0.3510 |
| T     |  0.9240 |  0.3170 |
| U     |  0.9260 |  0.3230 |
| V     |  0.7790 |  0.1570 |
| W     |  0.8070 |  0.1890 |
| a     |  0.9850 |  0.3830 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| b     |  0.9780   |  0.3730   |
| c     |  0.9780   |  0.4050   |
| d     |  0.9790   |  0.3920   |
| e     |  0.9800   |  0.4010   |
| f     |  0.9830   |  0.3910   |
| g     |  0.9830   |  0.3980   |
| h     |  0.9780   |  0.3990   |
| i     |  0.9750   |  0.3920   |
| j     |  0.9760   |  0.3830   |
| k     |  0.9410   |  0.3150   |
| l     |  0.9630   |  0.3320   |
| m     |  0.8950   |  0.3390   |
| n     |  0.8940   |  0.3260   |
| o     |  0.9810   |  0.4180   |
| p     |  0.9820   |  0.4260   |
| q     |  0.9750   |  0.4330   |
| r     |  0.9830   |  0.4250   |
| s     |  0.9800   |  0.4260   |
| t     |  0.9830  |  0.4300  |
| u     |  0.9800 |  0.4010 |
| v     |  0.9780 |  0.4110 |
| w     |  0.9730 |  0.3850 |
| x     |  0.9590 |  0.3910 |