



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 6O2T / pdb\_00006o2t  
EMDB ID : EMD-0615  
Title : Acetylated Microtubules  
Authors : Eshun-Wilson, L.; Zhang, R.; Portran, D.; Nachury, M.V.; Toso, D.; Lohr, T.; Vendruscolo, M.; Bonomi, M.; Fraser, J.S.; Nogales, E.  
Deposited on : 2019-02-24  
Resolution : 4.10 Å(reported)  
Based on initial model : 3JAR

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:

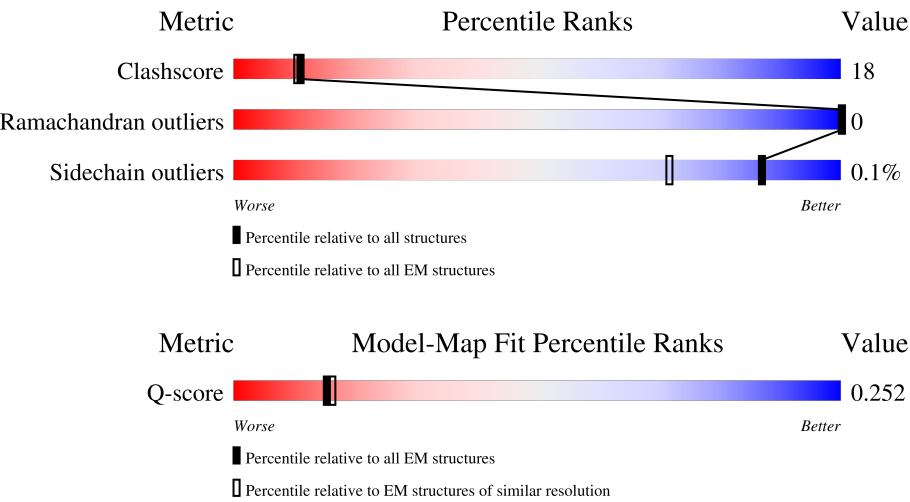
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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                       | 6458 ( 3.60 - 4.60 )                                     |

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   | 1A    | 451    | <div><div>21%</div><div>70%</div><div>27%</div><div>.</div></div> |
| 1   | 1B    | 451    | <div><div>21%</div><div>71%</div><div>26%</div><div>.</div></div> |
| 1   | 1C    | 451    | <div><div>23%</div><div>69%</div><div>27%</div><div>.</div></div> |
| 1   | 1D    | 451    | <div><div>28%</div><div>69%</div><div>28%</div><div>.</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 1E    | 451    |                  |
| 1   | 1F    | 451    |                  |
| 1   | 1G    | 451    |                  |
| 1   | 1I    | 451    |                  |
| 1   | 1J    | 451    |                  |
| 1   | 1K    | 451    |                  |
| 1   | 1L    | 451    |                  |
| 1   | 1M    | 451    |                  |
| 1   | 1N    | 451    |                  |
| 1   | 2A    | 451    |                  |
| 1   | 2B    | 451    |                  |
| 1   | 2C    | 451    |                  |
| 1   | 2D    | 451    |                  |
| 1   | 2E    | 451    |                  |
| 1   | 2F    | 451    |                  |
| 1   | 2G    | 451    |                  |
| 1   | 2I    | 451    |                  |
| 1   | 2J    | 451    |                  |
| 1   | 2K    | 451    |                  |
| 1   | 2L    | 451    |                  |
| 1   | 2M    | 451    |                  |
| 1   | 2N    | 451    |                  |
| 1   | 3A    | 451    |                  |
| 1   | 3B    | 451    |                  |
| 1   | 3C    | 451    |                  |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | 3D    | 451    | <div> <div>41%</div> <div>70%</div> <div>27%</div> </div> |
| 1   | 3E    | 451    | <div> <div>34%</div> <div>71%</div> <div>26%</div> </div> |
| 1   | 3F    | 451    | <div> <div>38%</div> <div>70%</div> <div>27%</div> </div> |
| 1   | 3G    | 451    | <div> <div>36%</div> <div>70%</div> <div>27%</div> </div> |
| 1   | 3I    | 451    | <div> <div>40%</div> <div>71%</div> <div>26%</div> </div> |
| 1   | 3J    | 451    | <div> <div>35%</div> <div>71%</div> <div>26%</div> </div> |
| 1   | 3K    | 451    | <div> <div>36%</div> <div>72%</div> <div>25%</div> </div> |
| 1   | 3L    | 451    | <div> <div>34%</div> <div>71%</div> <div>26%</div> </div> |
| 1   | 3M    | 451    | <div> <div>41%</div> <div>72%</div> <div>25%</div> </div> |
| 1   | 3N    | 451    | <div> <div>62%</div> <div>73%</div> <div>24%</div> </div> |
| 1   | 4A    | 451    | <div> <div>53%</div> <div>76%</div> <div>20%</div> </div> |
| 1   | 4B    | 451    | <div> <div>50%</div> <div>78%</div> <div>19%</div> </div> |
| 1   | 4C    | 451    | <div> <div>49%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4D    | 451    | <div> <div>51%</div> <div>76%</div> <div>21%</div> </div> |
| 1   | 4E    | 451    | <div> <div>51%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4F    | 451    | <div> <div>51%</div> <div>76%</div> <div>20%</div> </div> |
| 1   | 4G    | 451    | <div> <div>49%</div> <div>76%</div> <div>21%</div> </div> |
| 1   | 4I    | 451    | <div> <div>51%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4J    | 451    | <div> <div>53%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4K    | 451    | <div> <div>59%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4L    | 451    | <div> <div>85%</div> <div>77%</div> <div>20%</div> </div> |
| 1   | 4M    | 451    | <div> <div>95%</div> <div>78%</div> <div>19%</div> </div> |
| 1   | 4N    | 451    | <div> <div>59%</div> <div>79%</div> <div>18%</div> </div> |
| 2   | 1H    | 445    | <div> <div>20%</div> <div>71%</div> <div>26%</div> </div> |
| 2   | 1O    | 445    | <div> <div>21%</div> <div>71%</div> <div>26%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | 1P    | 445    |                  |
| 2   | 1Q    | 445    |                  |
| 2   | 1R    | 445    |                  |
| 2   | 1S    | 445    |                  |
| 2   | 1T    | 445    |                  |
| 2   | 1U    | 445    |                  |
| 2   | 1V    | 445    |                  |
| 2   | 1W    | 445    |                  |
| 2   | 1X    | 445    |                  |
| 2   | 1Y    | 445    |                  |
| 2   | 1Z    | 445    |                  |
| 2   | 2H    | 445    |                  |
| 2   | 2O    | 445    |                  |
| 2   | 2P    | 445    |                  |
| 2   | 2Q    | 445    |                  |
| 2   | 2R    | 445    |                  |
| 2   | 2S    | 445    |                  |
| 2   | 2T    | 445    |                  |
| 2   | 2U    | 445    |                  |
| 2   | 2V    | 445    |                  |
| 2   | 2W    | 445    |                  |
| 2   | 2X    | 445    |                  |
| 2   | 2Y    | 445    |                  |
| 2   | 2Z    | 445    |                  |
| 2   | 3H    | 445    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | 3O    | 445    | 77%<br>74% 22% . |
| 2   | 3P    | 445    | 68%<br>73% 23% . |
| 2   | 3Q    | 445    | 59%<br>73% 23% . |
| 2   | 3R    | 445    | 50%<br>74% 22% . |
| 2   | 3S    | 445    | 43%<br>73% 23% . |
| 2   | 3T    | 445    | 41%<br>74% 22% . |
| 2   | 3U    | 445    | 39%<br>74% 22% . |
| 2   | 3V    | 445    | 33%<br>74% 22% . |
| 2   | 3W    | 445    | 36%<br>74% 22% . |
| 2   | 3X    | 445    | 38%<br>74% 22% . |
| 2   | 3Y    | 445    | 45%<br>73% 23% . |
| 2   | 3Z    | 445    | 91%<br>74% 22% . |
| 2   | 4H    | 445    | 34%<br>68% 28% . |
| 2   | 4O    | 445    | 36%<br>68% 29% . |
| 2   | 4P    | 445    | 36%<br>67% 30% . |
| 2   | 4Q    | 445    | 39%<br>67% 30% . |
| 2   | 4R    | 445    | 36%<br>67% 29% . |
| 2   | 4S    | 445    | 36%<br>67% 29% . |
| 2   | 4T    | 445    | 36%<br>68% 29% . |
| 2   | 4U    | 445    | 34%<br>67% 29% . |
| 2   | 4V    | 445    | 34%<br>69% 27% . |
| 2   | 4W    | 445    | 36%<br>69% 27% . |
| 2   | 4X    | 445    | 57%<br>69% 28% . |
| 2   | 4Y    | 445    | 92%<br>68% 28% . |
| 2   | 4Z    | 445    | 37%<br>69% 27% . |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | GDP  | 4O    | 501 | -         | -        | X       | -                |
| 5   | GDP  | 4P    | 501 | -         | -        | X       | -                |
| 5   | GDP  | 4Q    | 501 | -         | -        | X       | -                |
| 5   | GDP  | 4R    | 501 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 355888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 1A    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1B    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1C    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1D    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1E    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1F    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1G    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1I    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1J    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1K    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1L    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1M    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 1N    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2A    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2B    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2C    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2D    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 2E    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2F    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2G    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2I    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2J    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2K    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2L    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2M    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 2N    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3A    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3B    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3C    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3D    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3E    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3F    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3G    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3I    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3J    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3K    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3L    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 3M    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 3N    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4A    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4B    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4C    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4D    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4E    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4F    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4G    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4I    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4J    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4K    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4L    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4M    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |
| 1   | 4N    | 437      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3415  | 2160 | 580 | 654 | 21 |         |       |

- Molecule 2 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 1H    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 1O    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 1P    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 1Q    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 1R    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | 1S    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1T    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1U    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1V    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1W    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1X    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1Y    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 1Z    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2H    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2O    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2P    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2Q    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2R    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2S    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2T    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2U    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2V    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2W    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2X    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2Y    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 2Z    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2   | 3H    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3O    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3P    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3Q    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3R    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3S    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3T    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3U    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3V    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3W    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3X    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3Y    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 3Z    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4H    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4O    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4P    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4Q    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4R    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4S    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4T    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |
| 2   | 4U    | 429      | Total<br>3368 | C<br>2115 | N<br>578 | O<br>650 | S<br>25 | 0       | 0     |

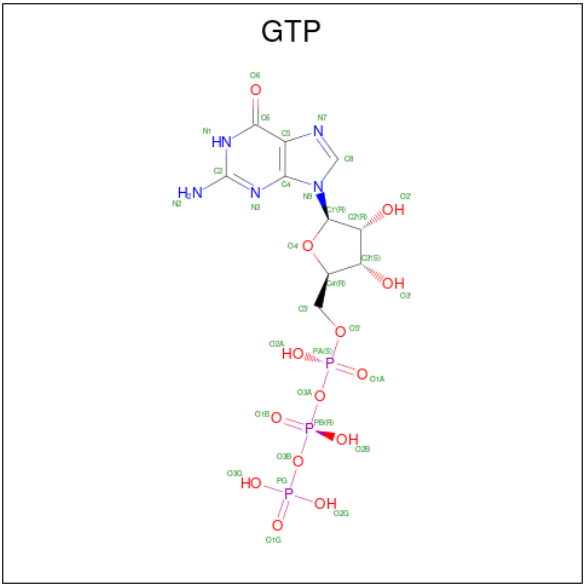
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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 4V    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 4W    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 4X    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 4Y    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |
| 2   | 4Z    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2115 | 578 | 650 | 25 |         |       |

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



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

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | 1G    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1I    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1J    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1K    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1L    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1M    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 1N    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2A    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2B    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2C    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2D    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2E    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2F    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2G    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2I    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2J    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2K    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2L    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2M    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 2N    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 3A    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 3   | 3B    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3D    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3F    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3G    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3I    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3J    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3K    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3L    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3M    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 3N    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4A    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4B    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4C    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4D    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4E    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4F    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4G    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4I    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 3   | 4J    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 3   | 4K    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 4L    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 4M    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 3   | 4N    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | 1A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1B    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1C    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1D    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1E    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1F    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1G    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1I    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1J    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1K    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1L    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1M    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 1N    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 2A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 4   | 2B    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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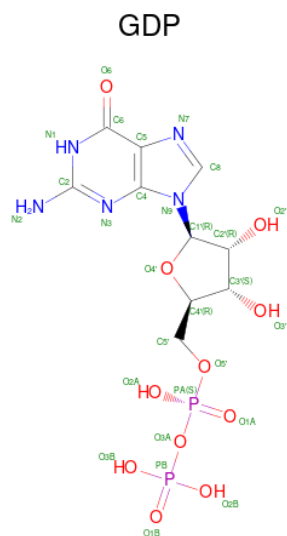
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | 2C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2D    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2F    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2G    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2I    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2J    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2K    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2L    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2M    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 2N    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3B    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3D    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3F    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3G    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3I    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3J    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3K    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | 3L    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3M    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 3N    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4A    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4B    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4C    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4D    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4E    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4F    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4G    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4I    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4J    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4K    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4L    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4M    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 4   | 4N    | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | 2O    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2P    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2Q    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2R    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2S    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2T    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2U    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2V    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2W    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2X    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2Y    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 2Z    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3H    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3O    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3P    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3Q    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3R    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3S    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3T    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3U    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3V    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

*Continued on next page...*



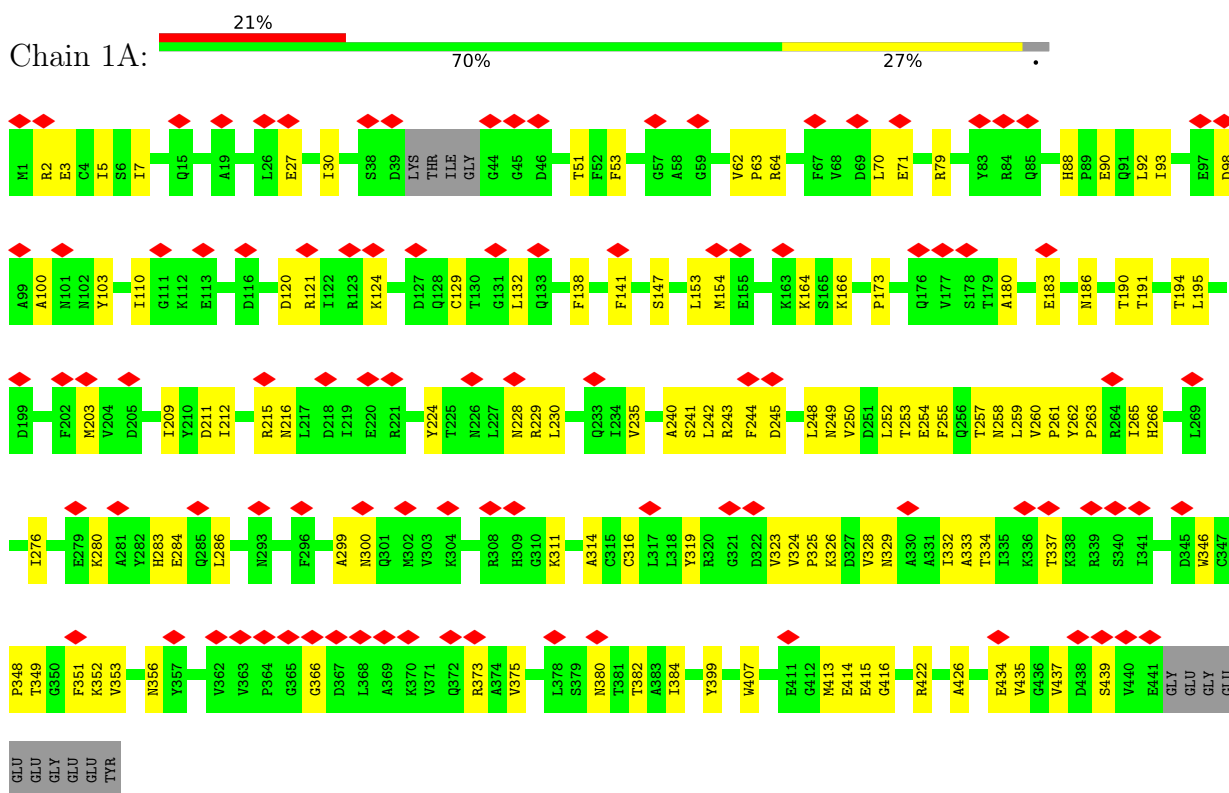
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 5   | 3W    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3X    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3Y    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 3Z    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4H    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4O    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4P    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4Q    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4R    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4S    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4T    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4U    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4V    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4W    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4X    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4Y    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 5   | 4Z    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

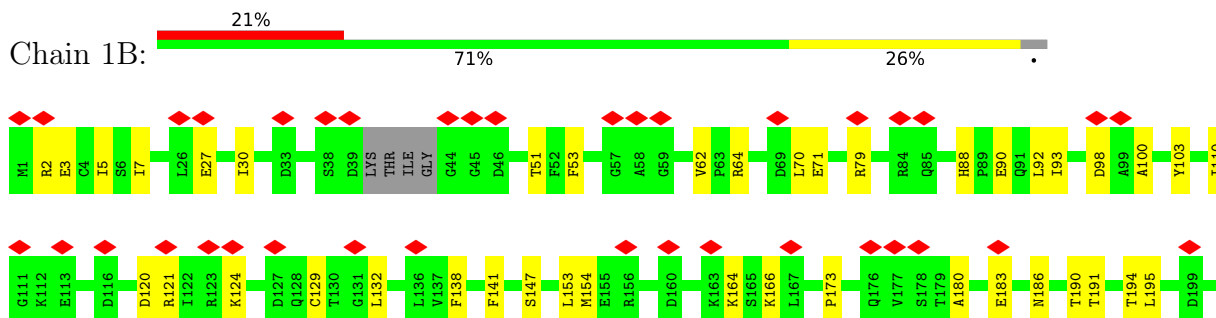
### 3 Residue-property plots

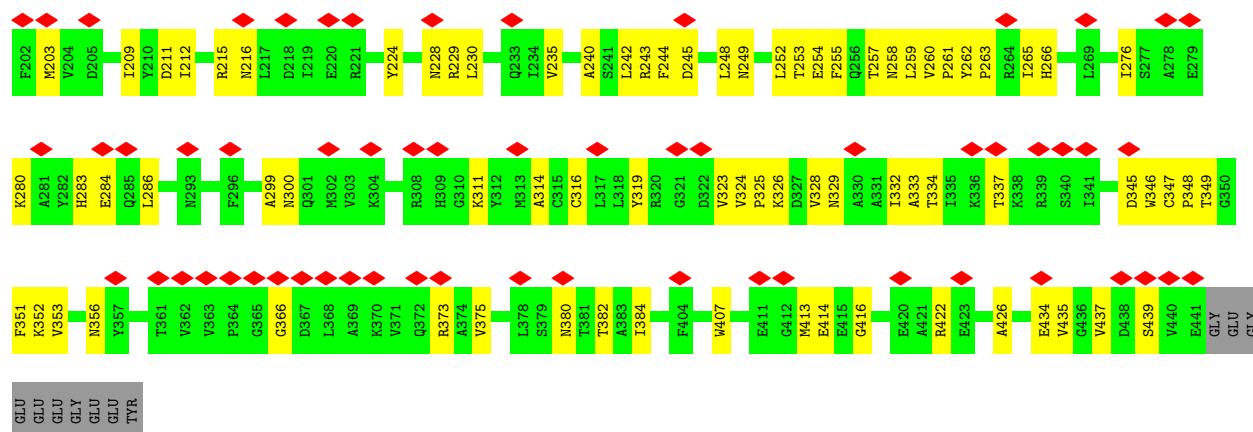
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tubulin alpha-1B chain

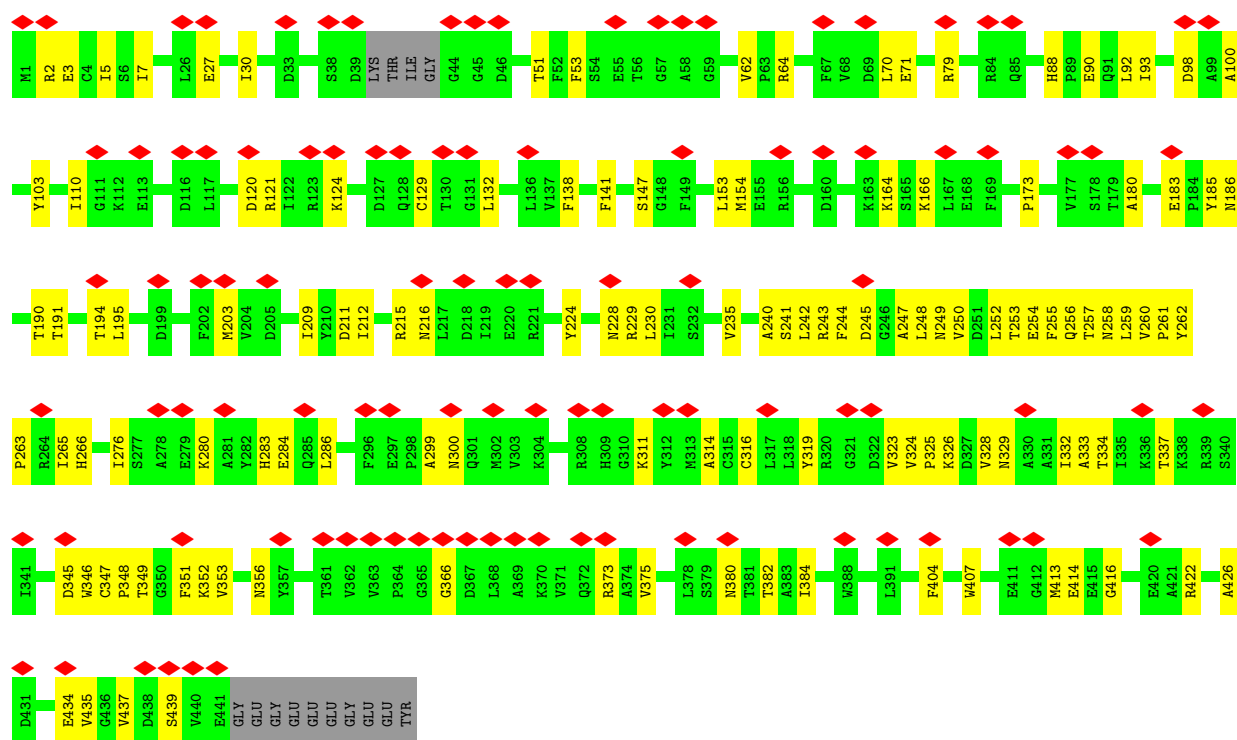


- Molecule 1: Tubulin alpha-1B chain

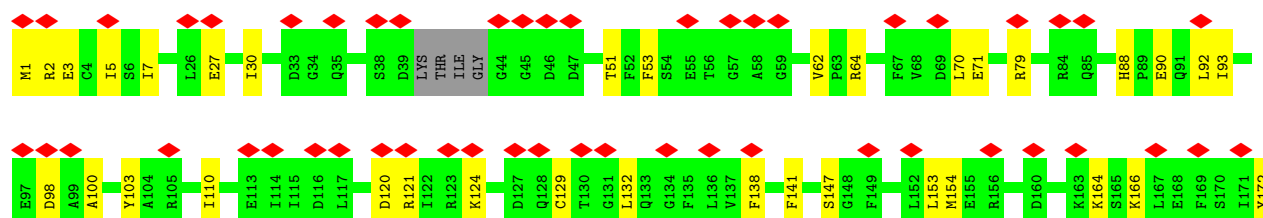


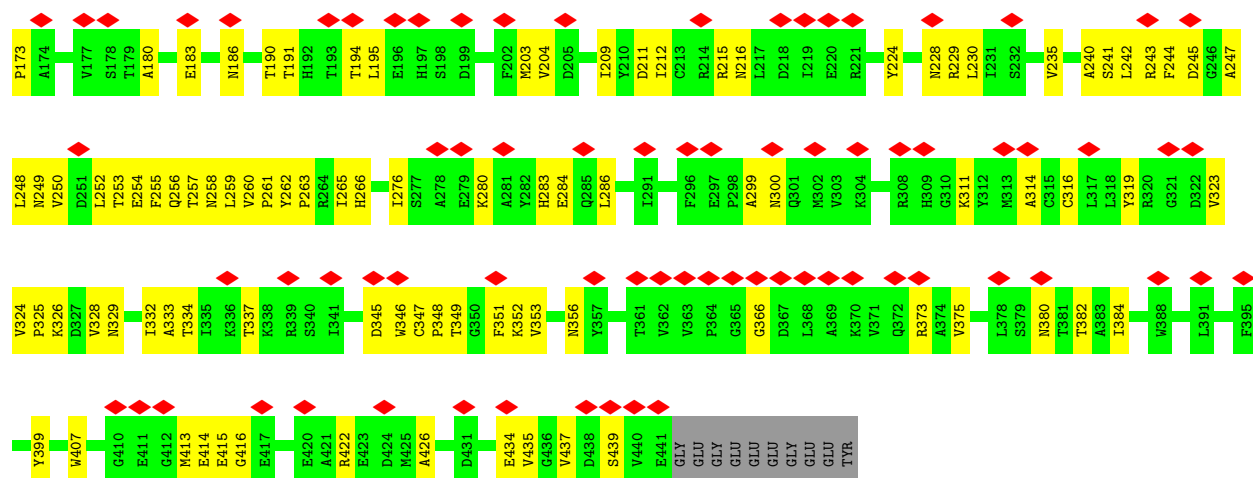


• Molecule 1: Tubulin alpha-1B chain

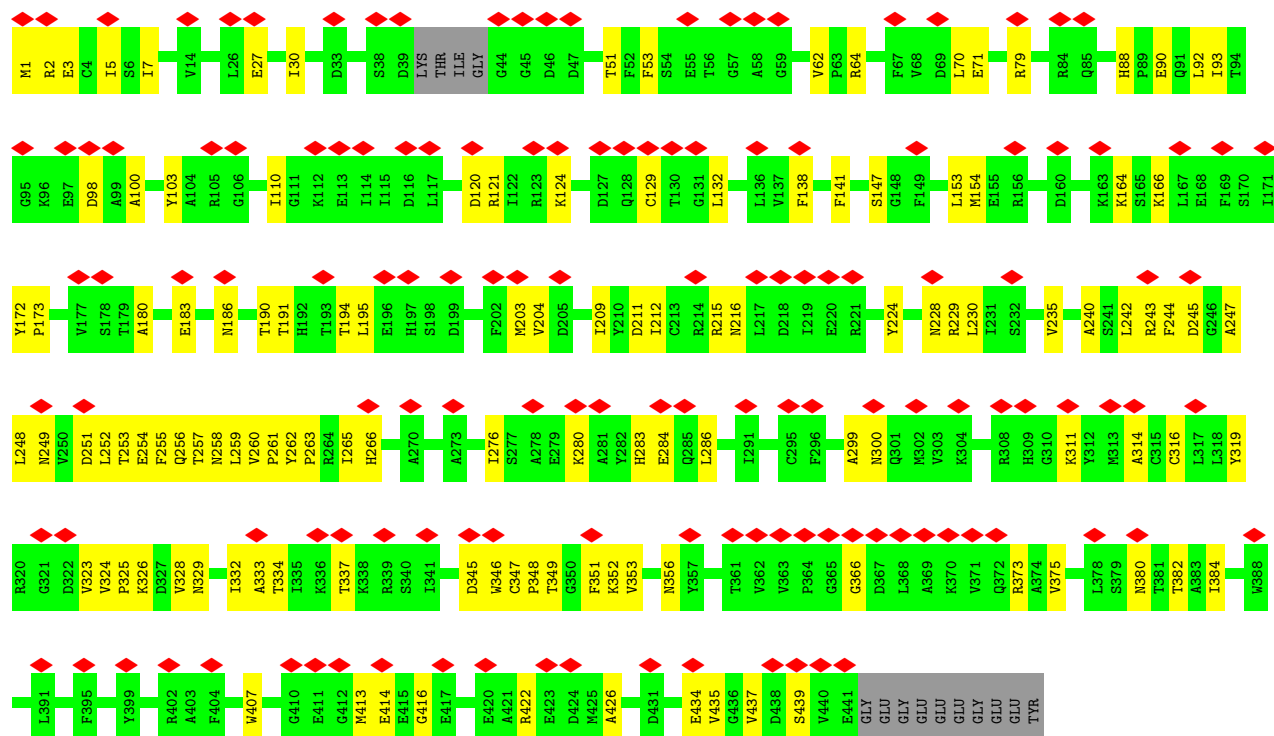


• Molecule 1: Tubulin alpha-1B chain

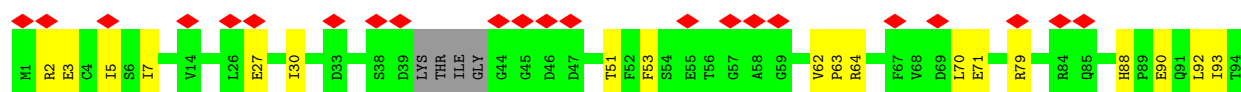


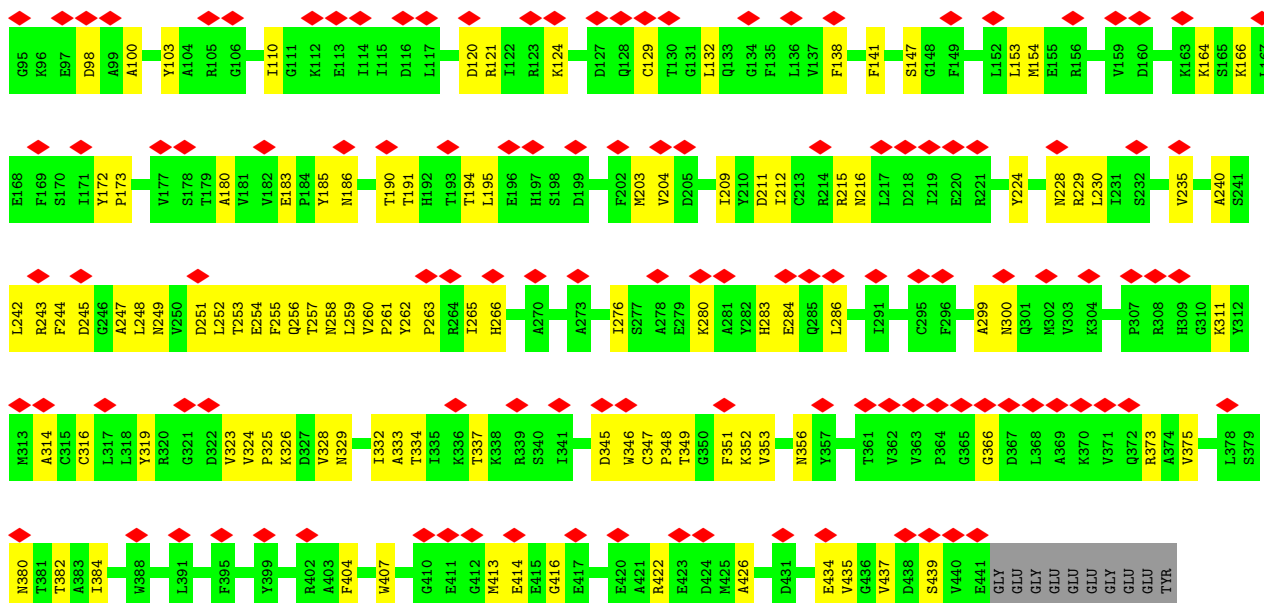


• Molecule 1: Tubulin alpha-1B chain

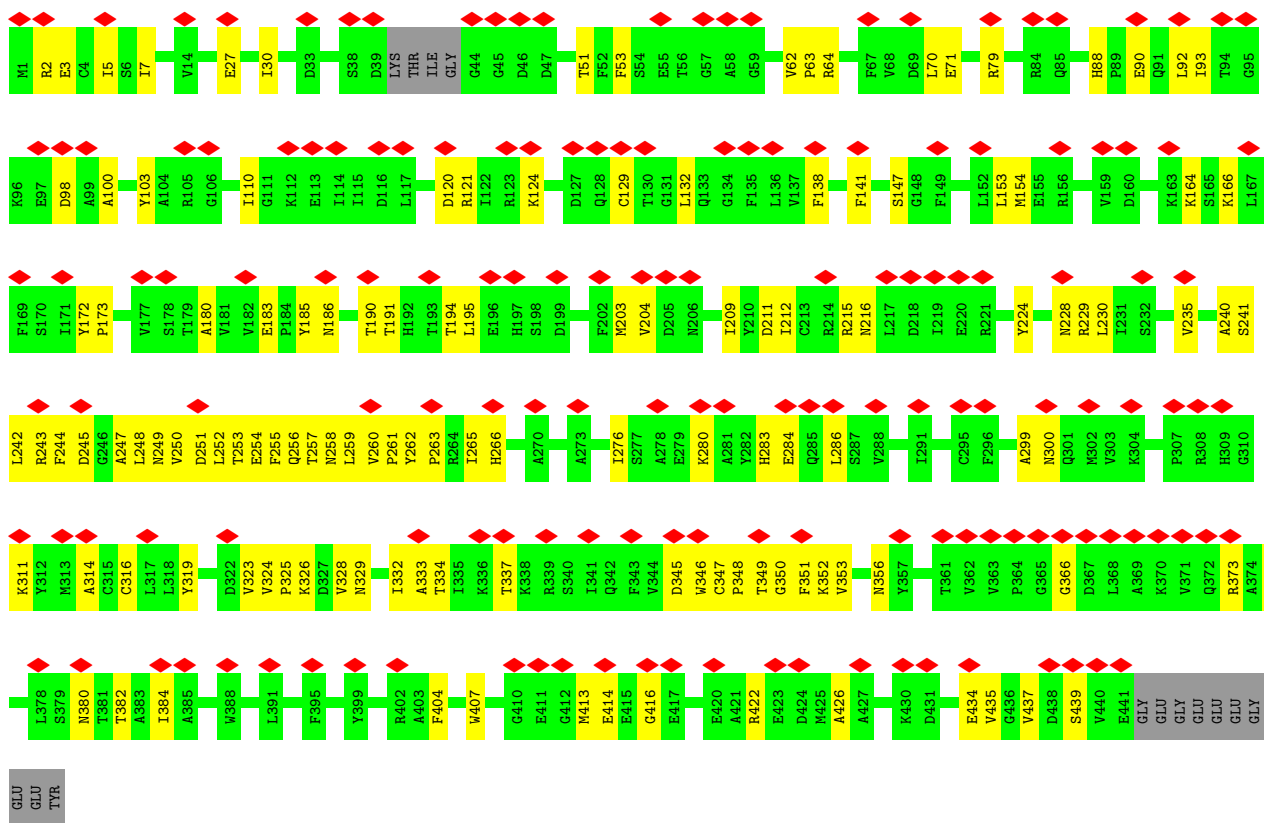


• Molecule 1: Tubulin alpha-1B chain

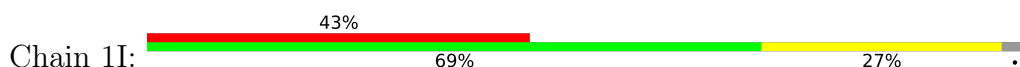


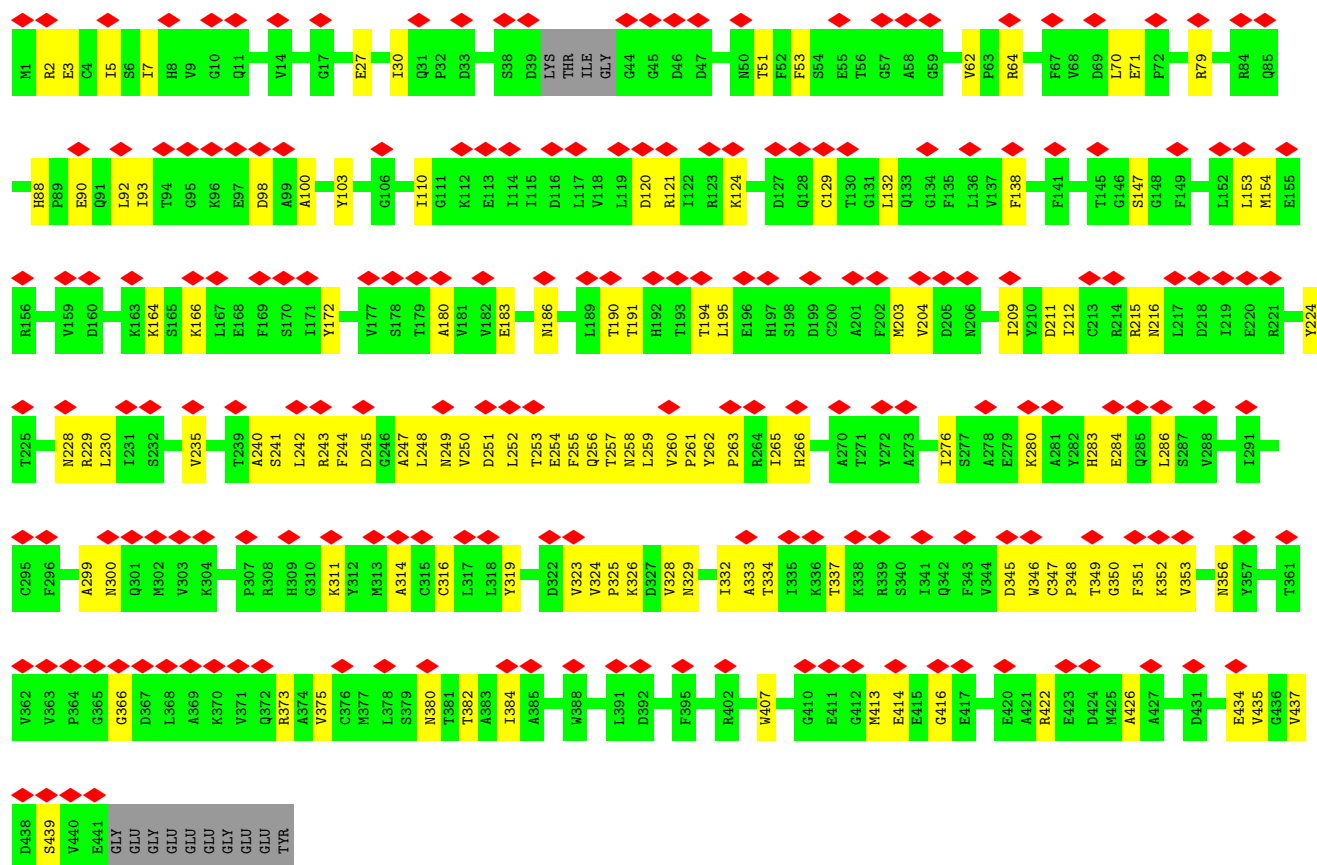


• Molecule 1: Tubulin alpha-1B chain

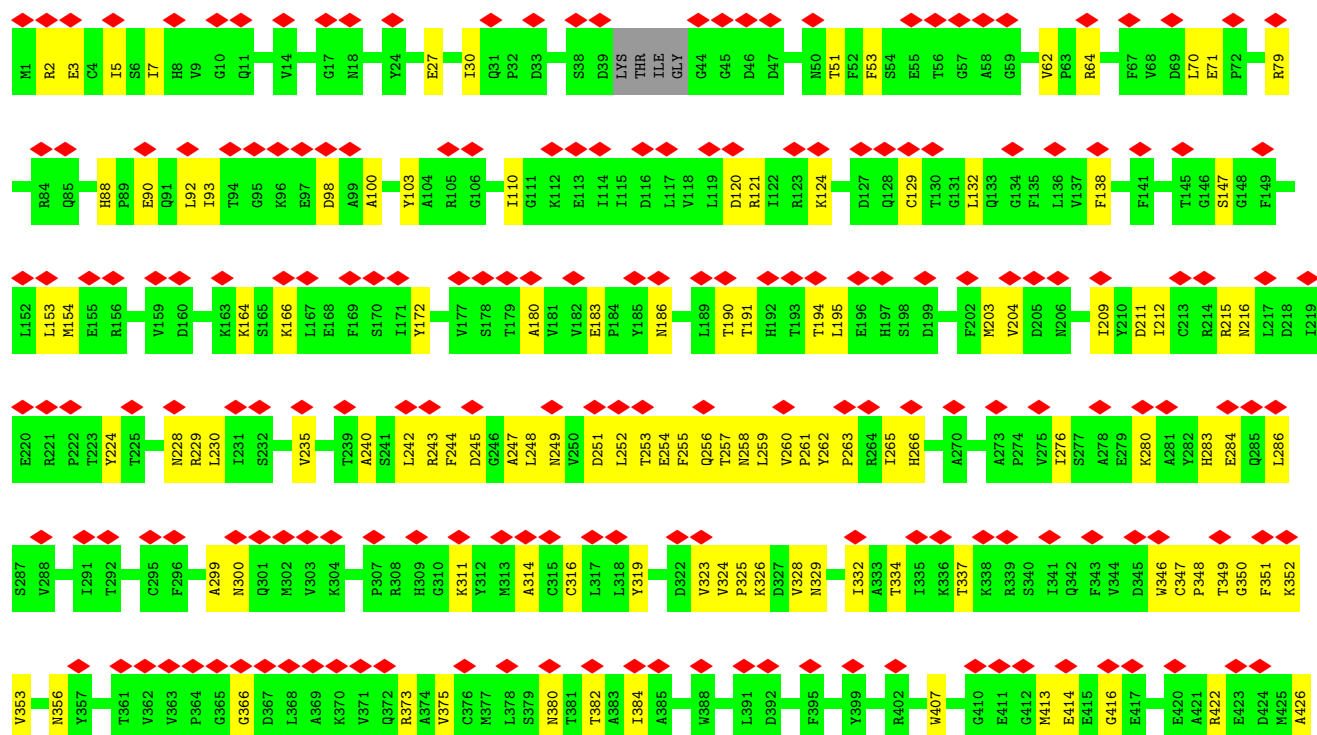


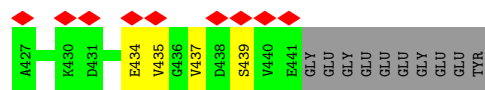
• Molecule 1: Tubulin alpha-1B chain



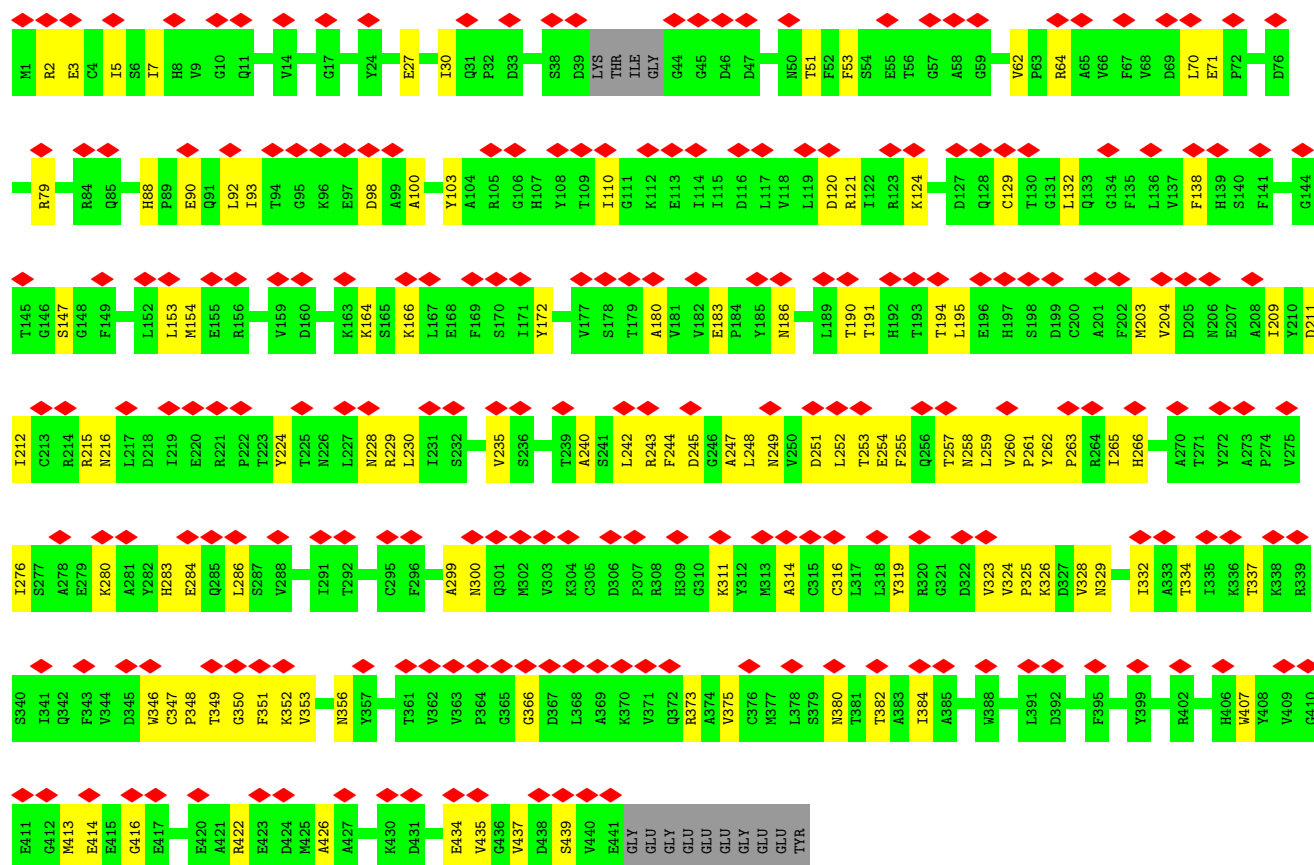
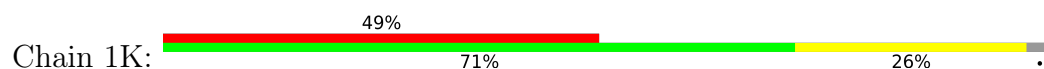


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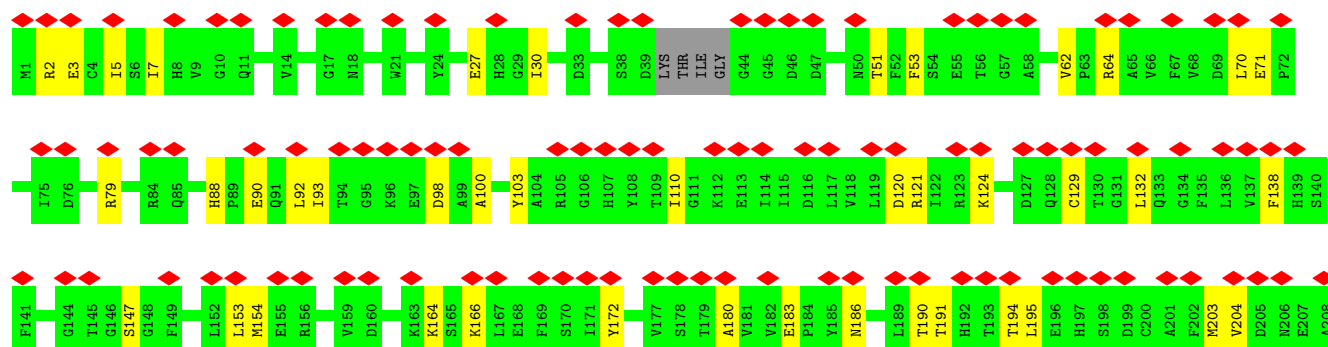


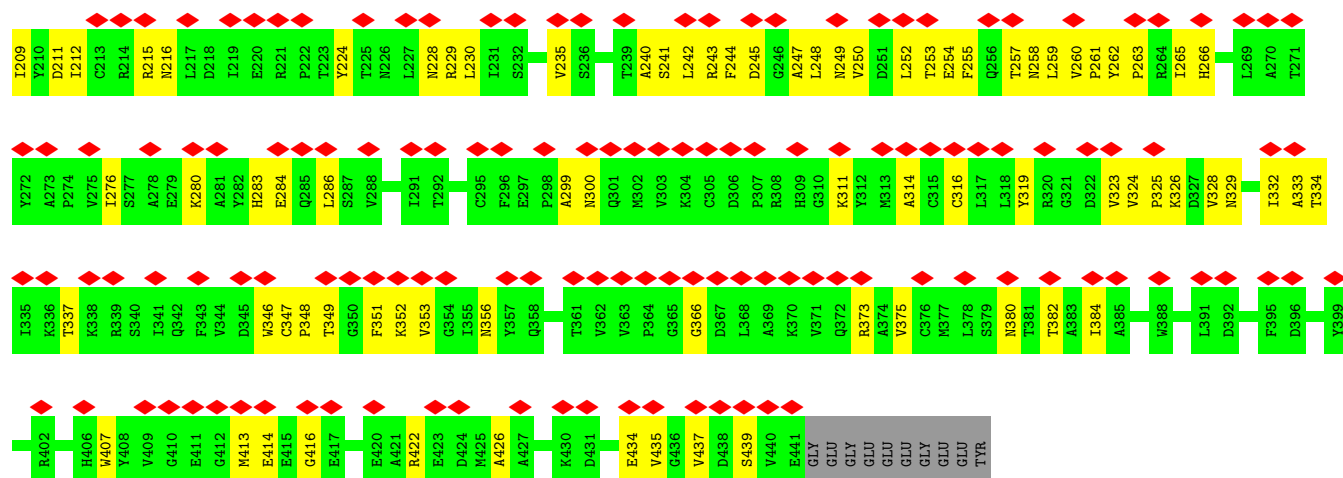


• Molecule 1: Tubulin alpha-1B chain

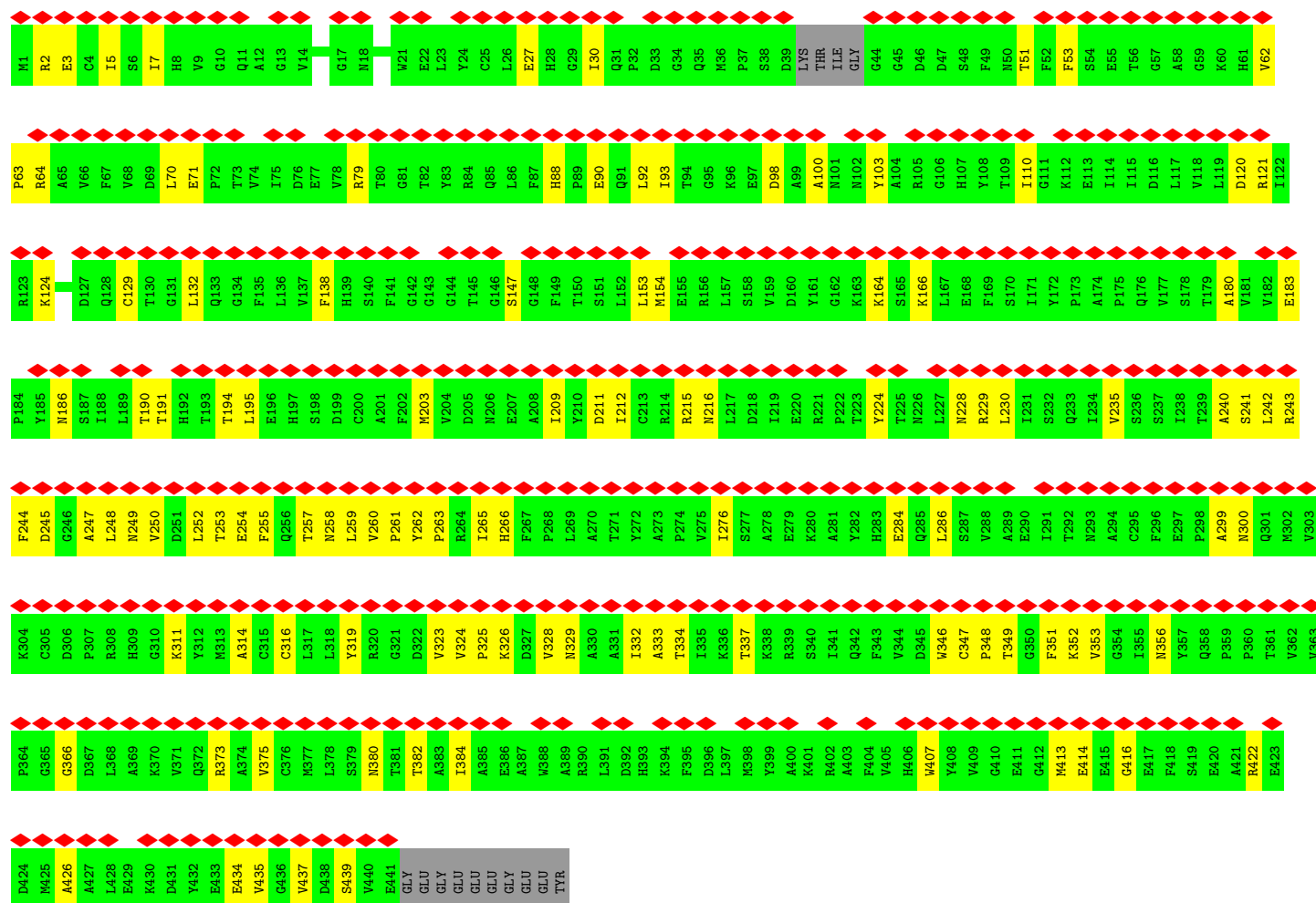
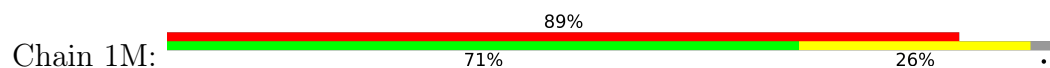


• Molecule 1: Tubulin alpha-1B chain



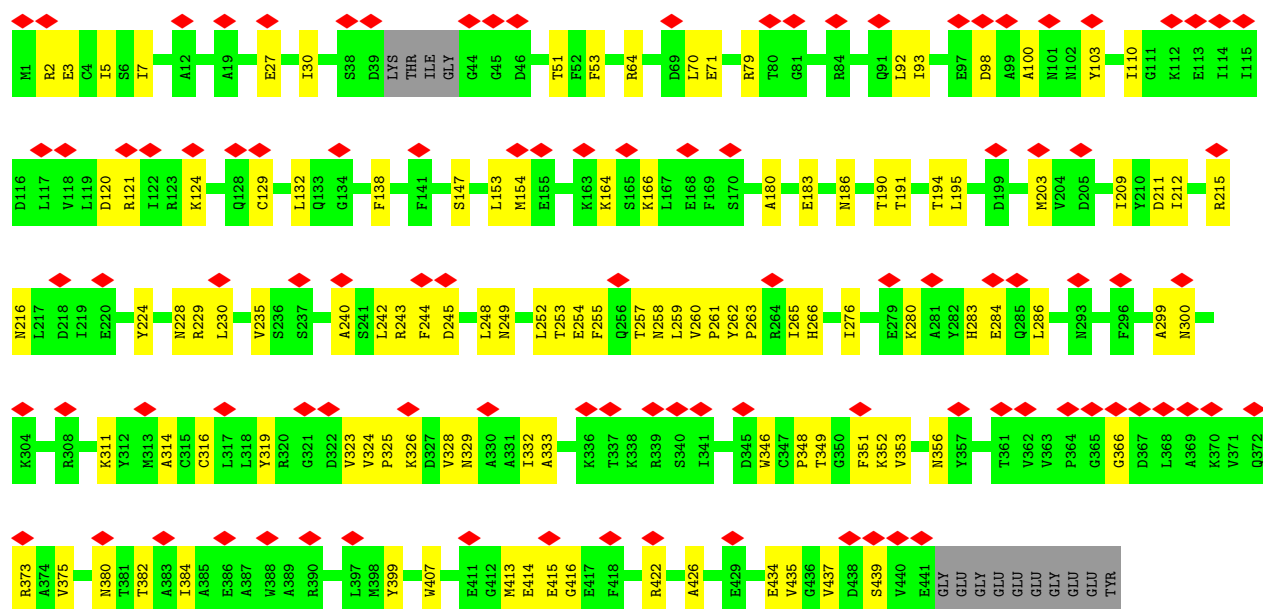
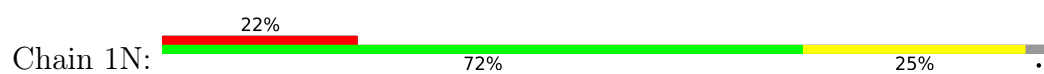


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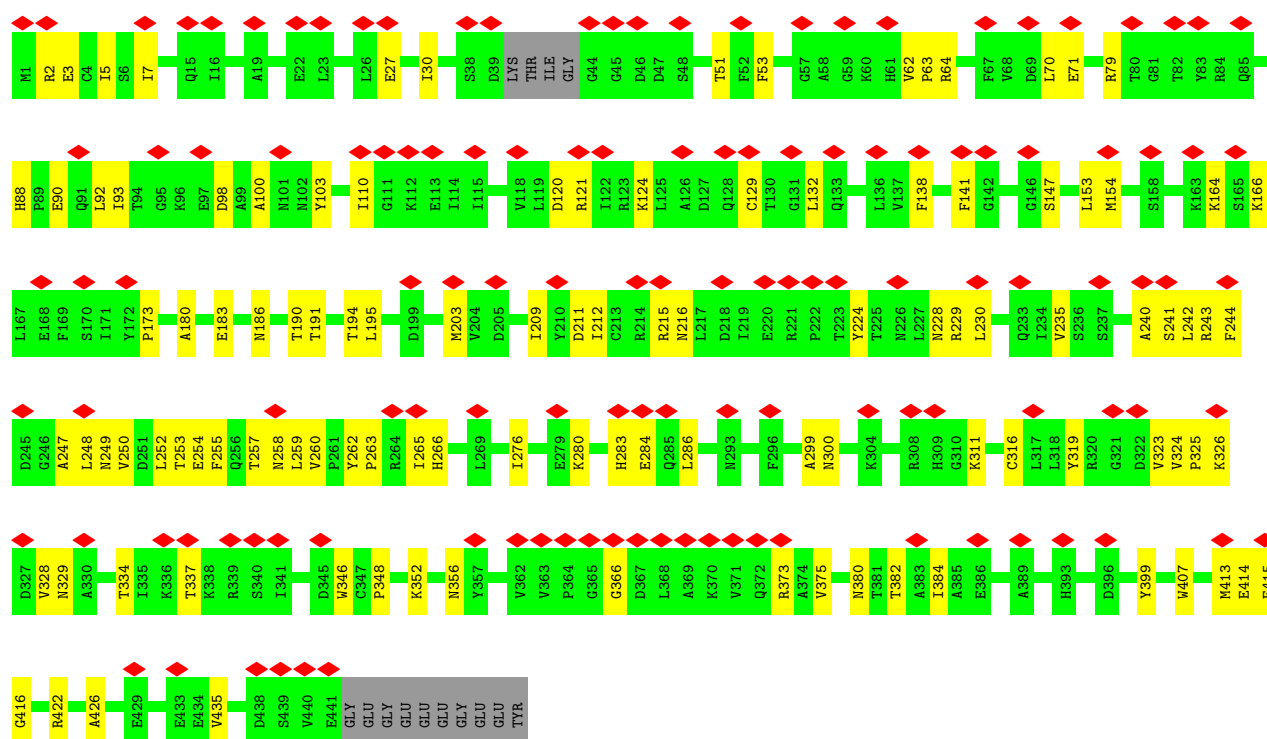
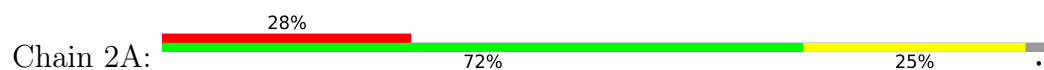


• Molecule 1: Tubulin alpha-1B chain

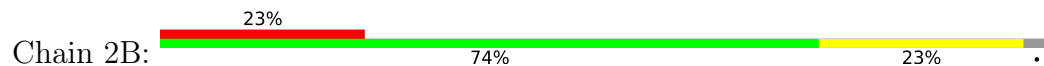


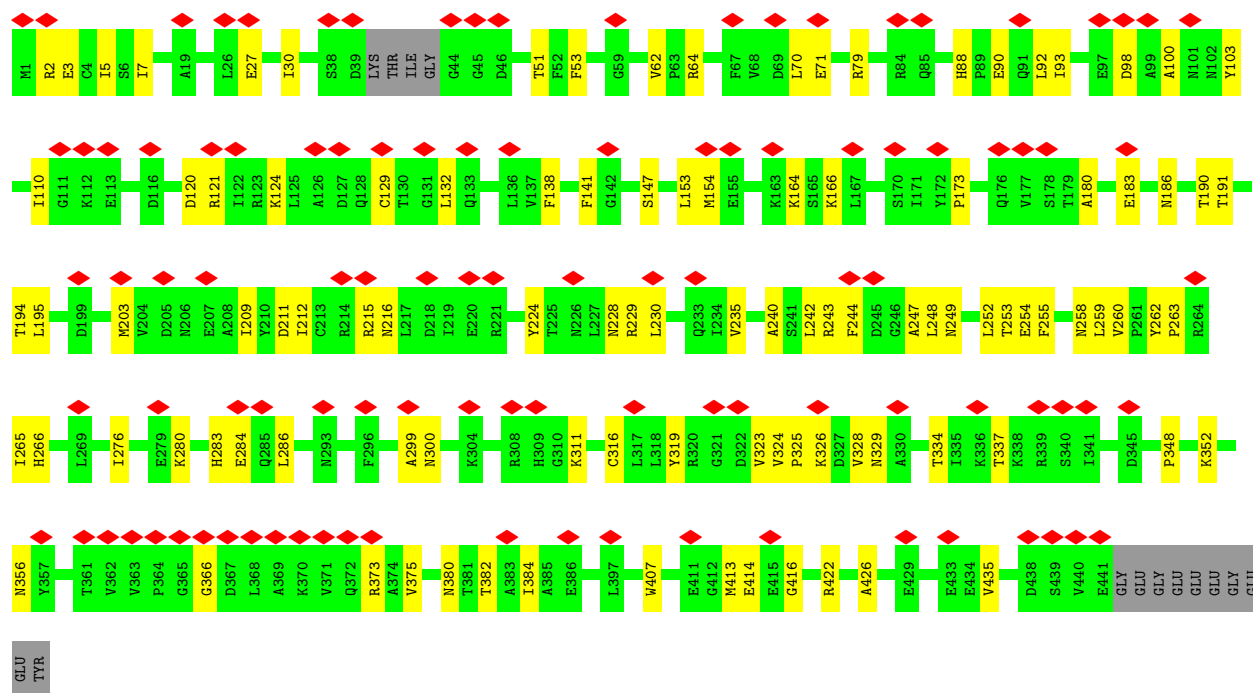


• Molecule 1: Tubulin alpha-1B chain

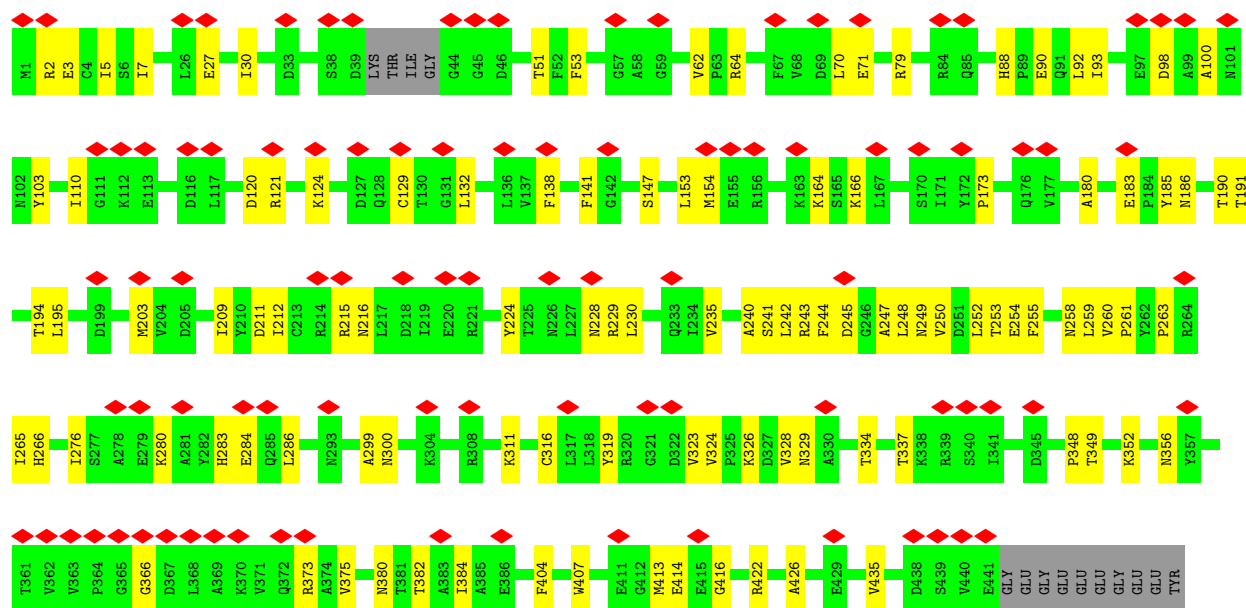
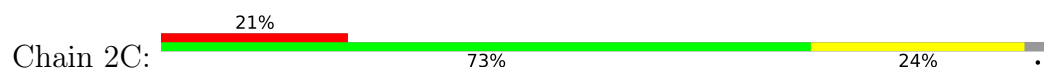


• Molecule 1: Tubulin alpha-1B chain

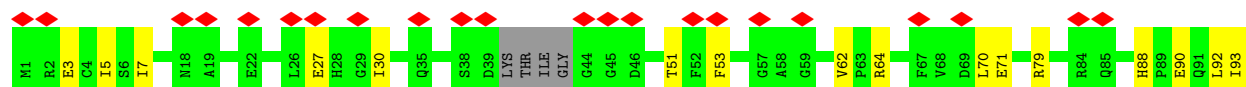
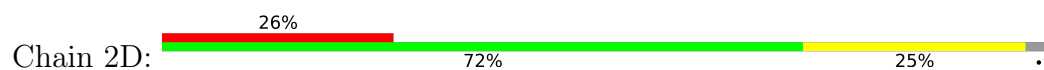


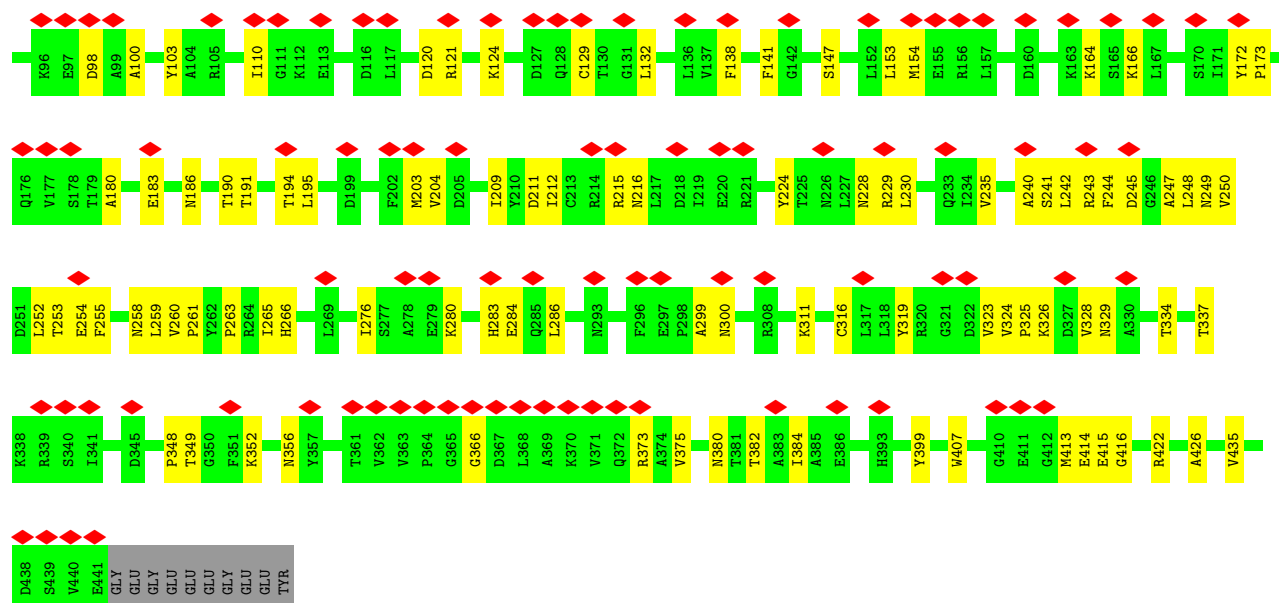


• Molecule 1: Tubulin alpha-1B chain

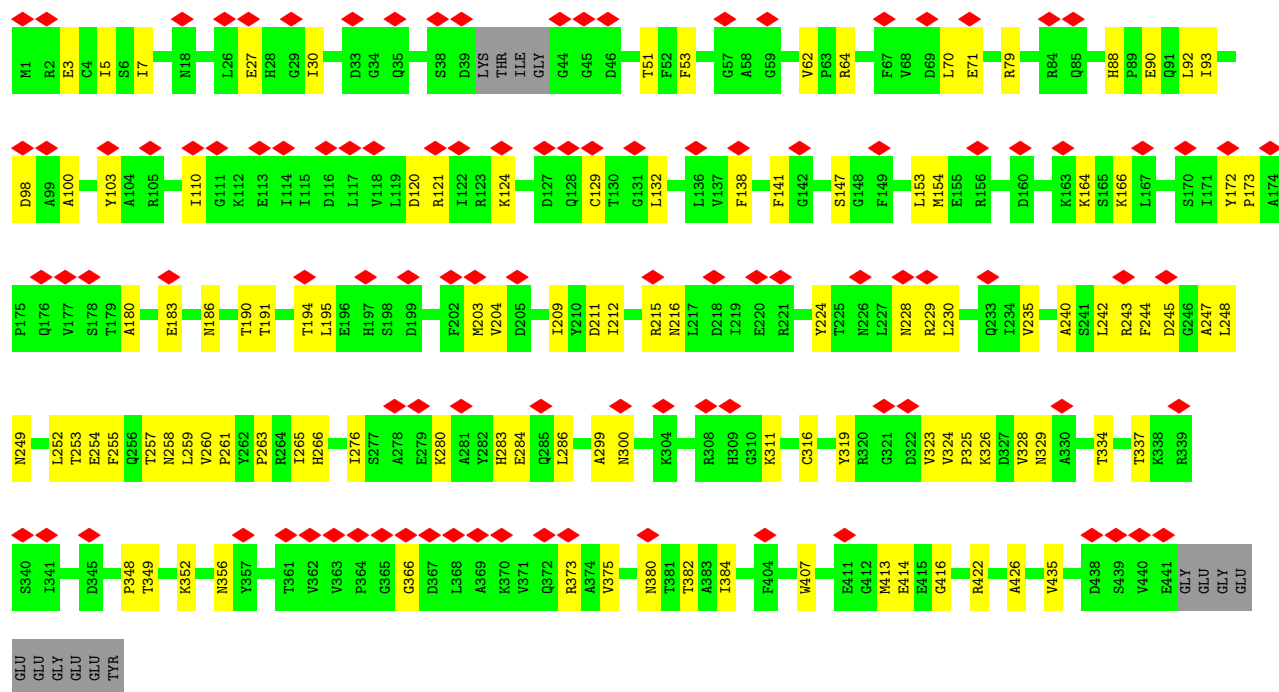
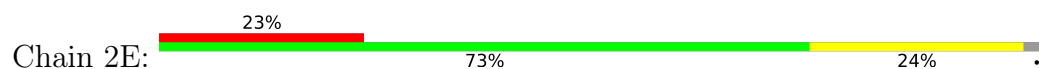


• Molecule 1: Tubulin alpha-1B chain

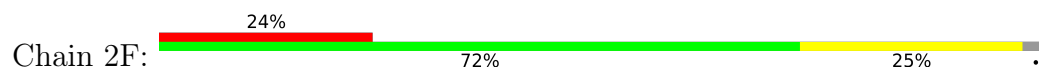


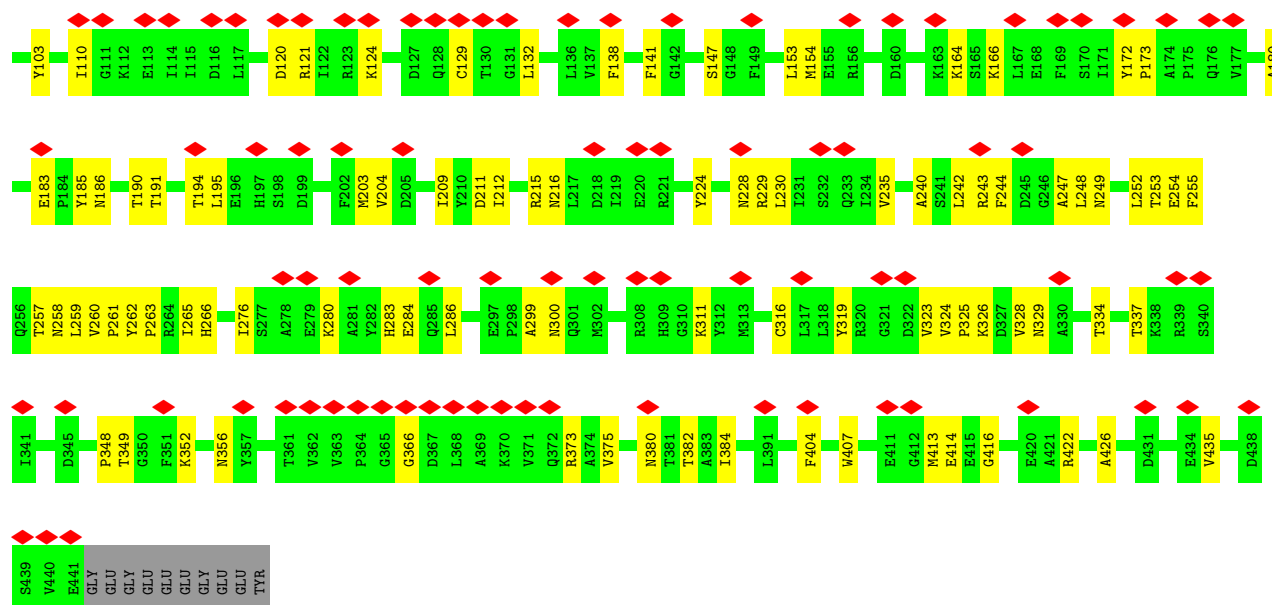


• Molecule 1: Tubulin alpha-1B chain

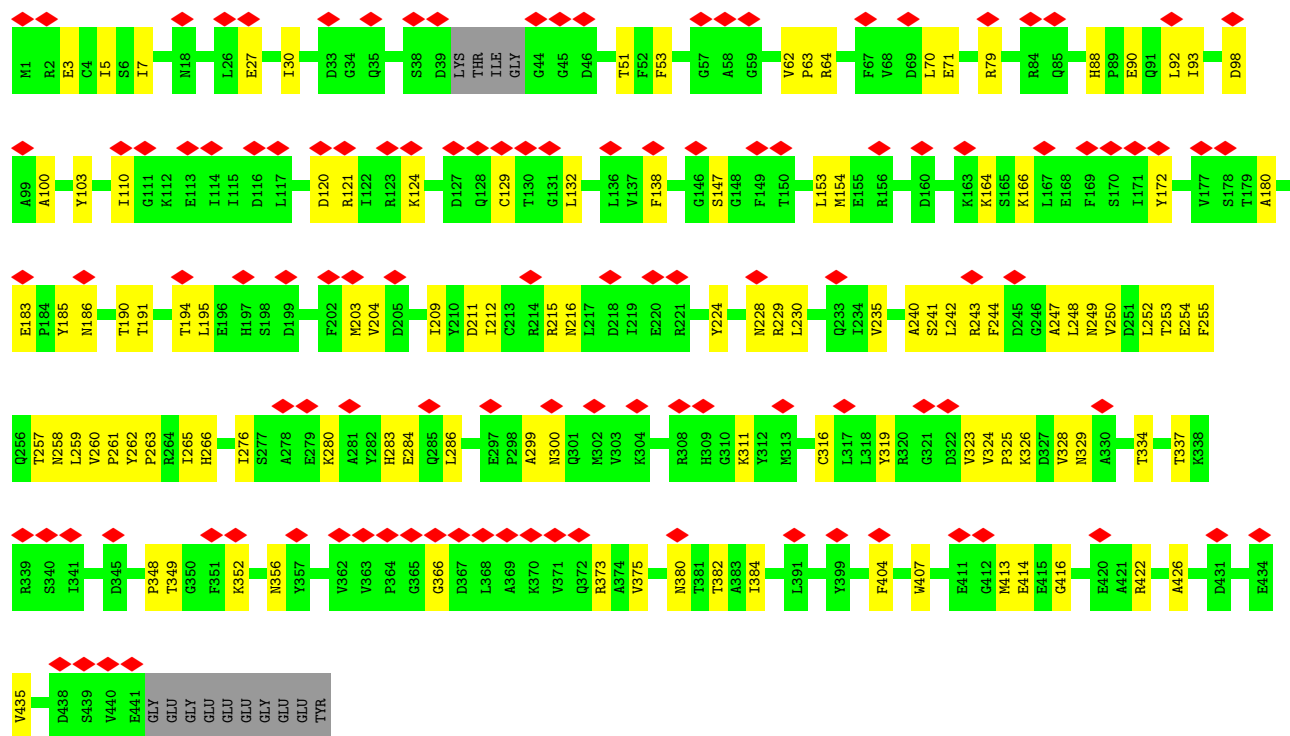
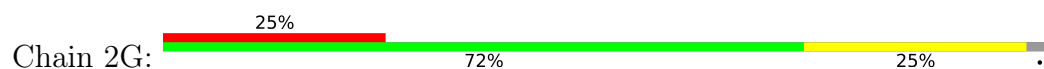


• Molecule 1: Tubulin alpha-1B chain

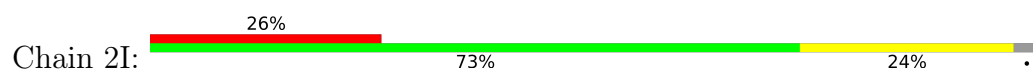


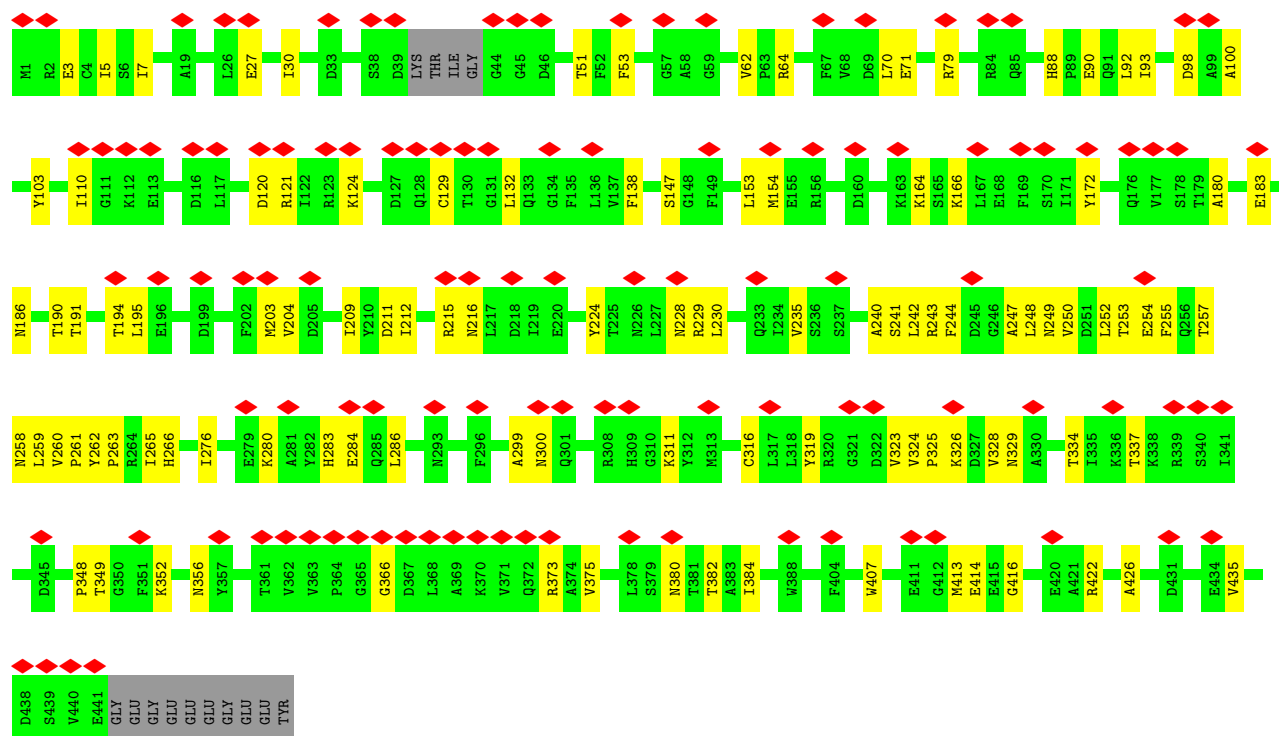


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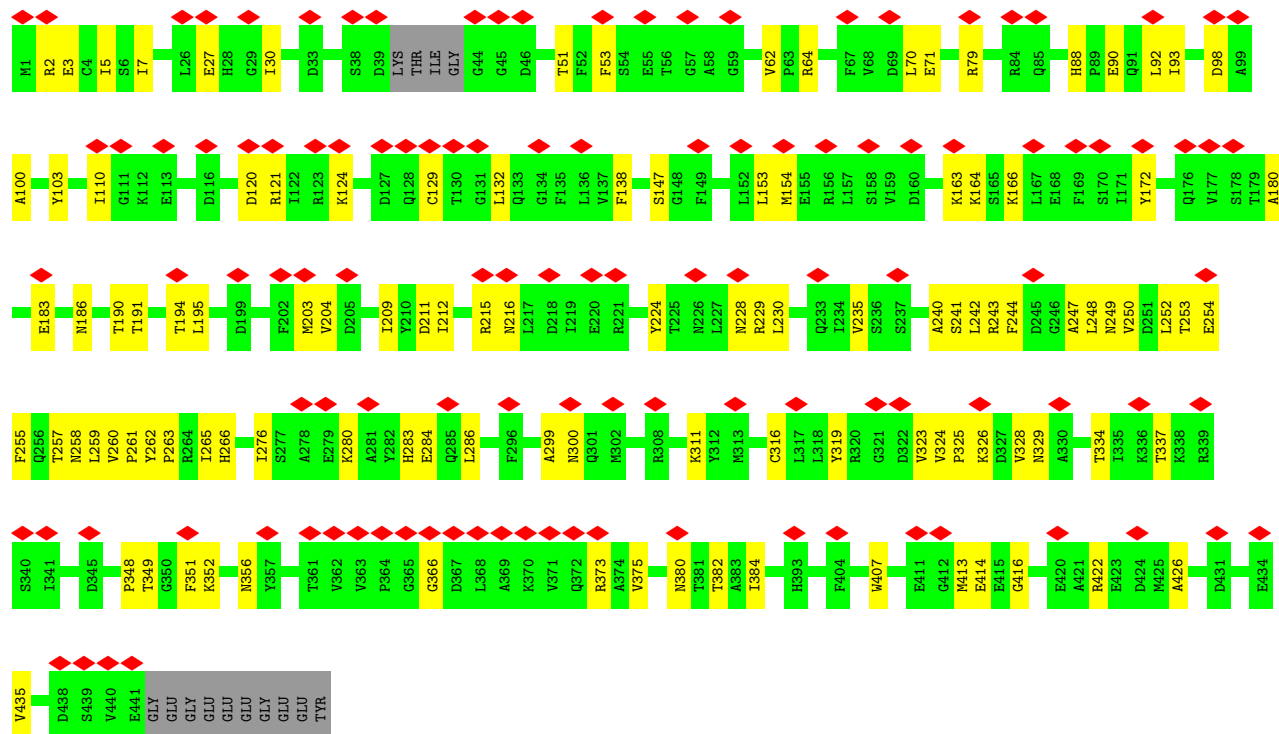
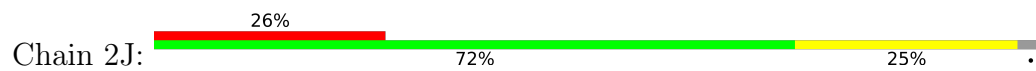


• Molecule 1: Tubulin alpha-1B chain

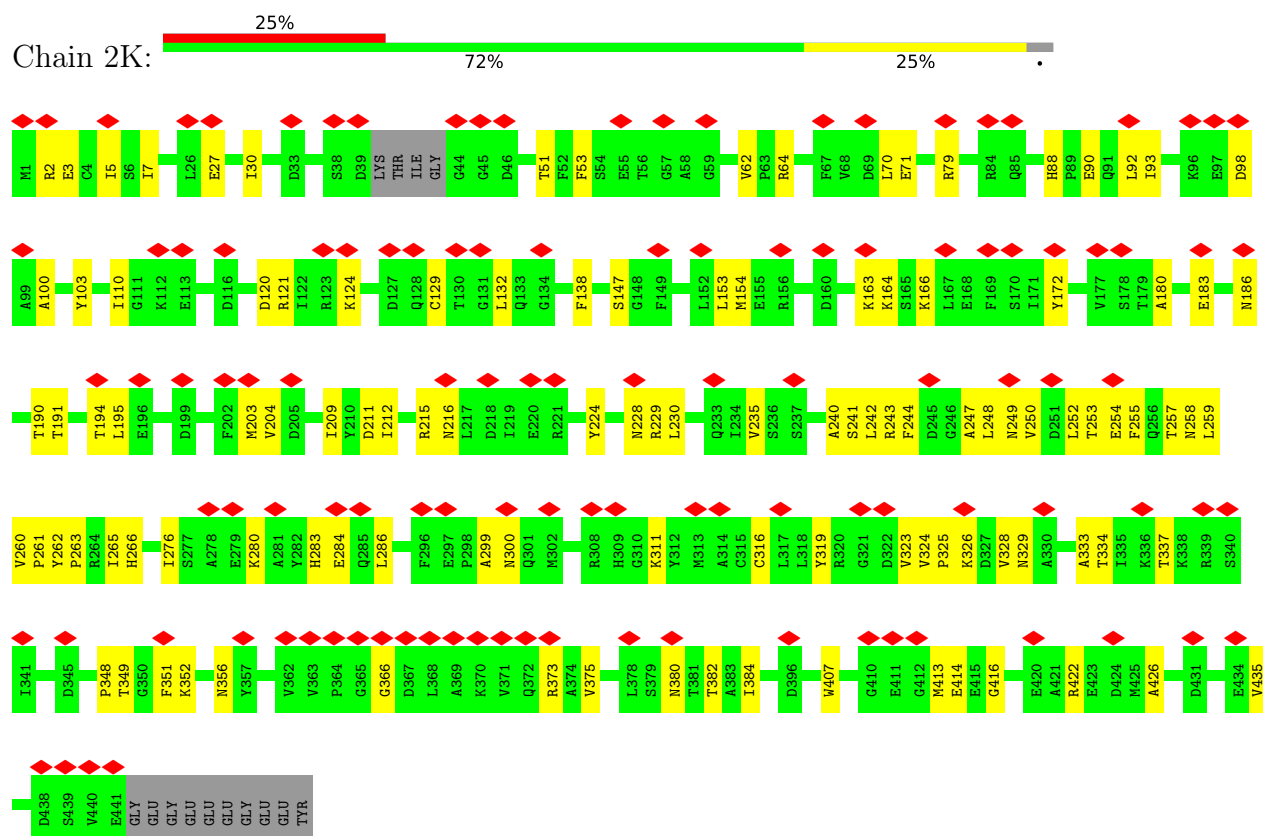




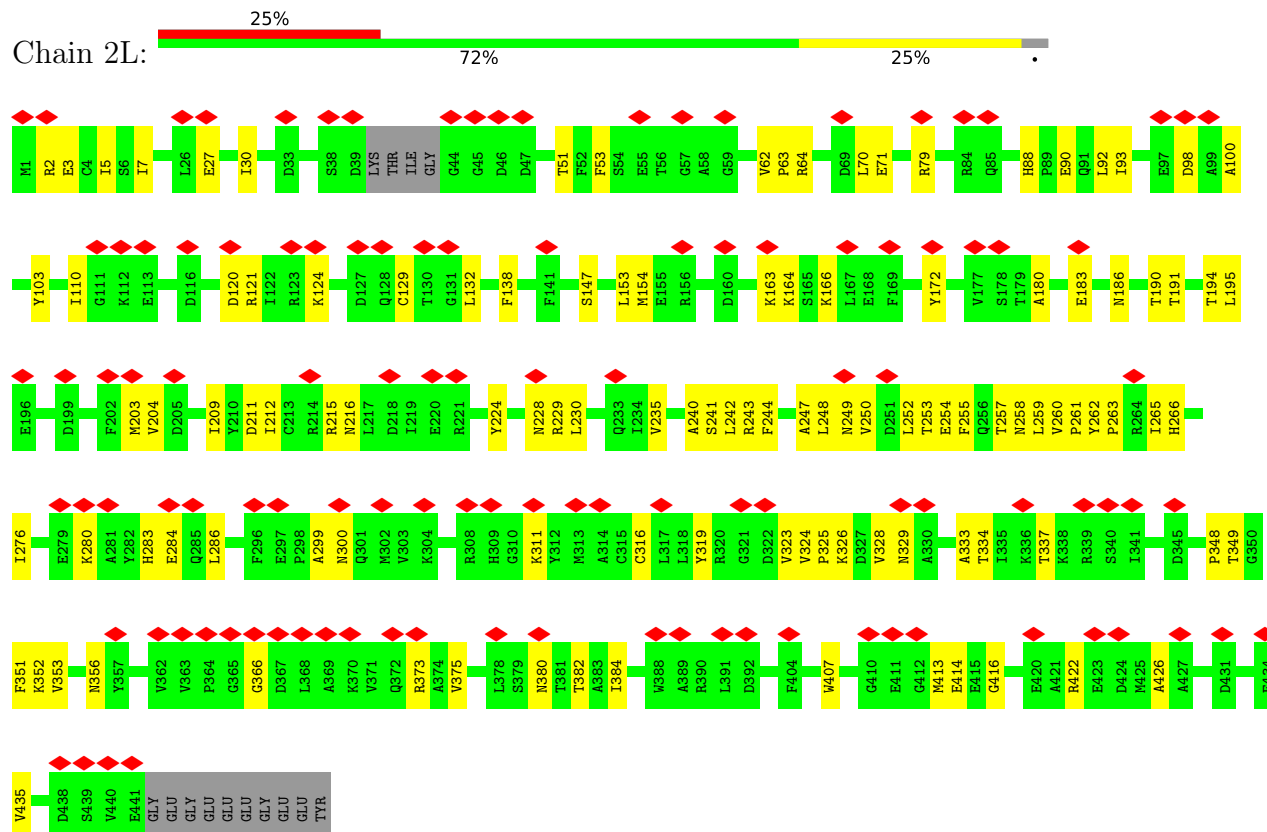
- Molecule 1: Tubulin alpha-1B chain



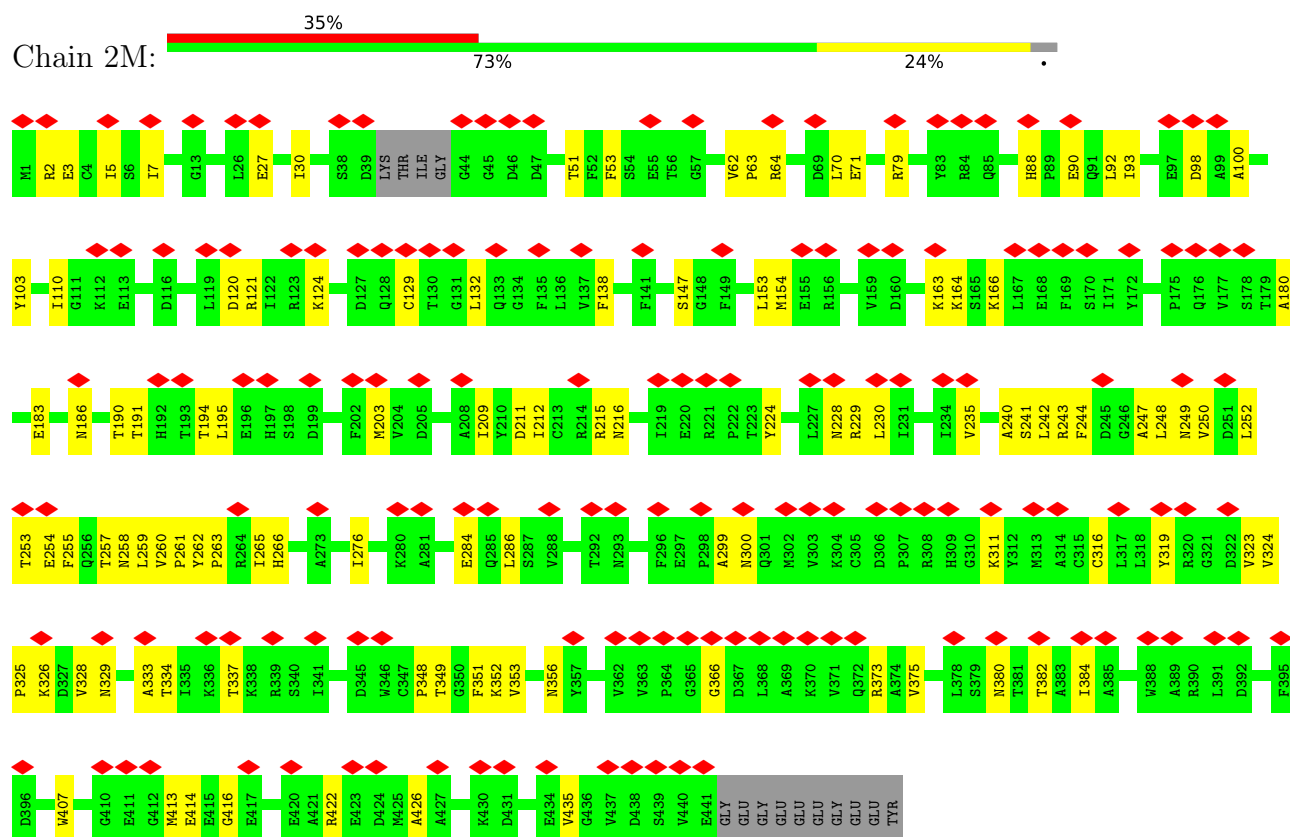
- Molecule 1: Tubulin alpha-1B chain



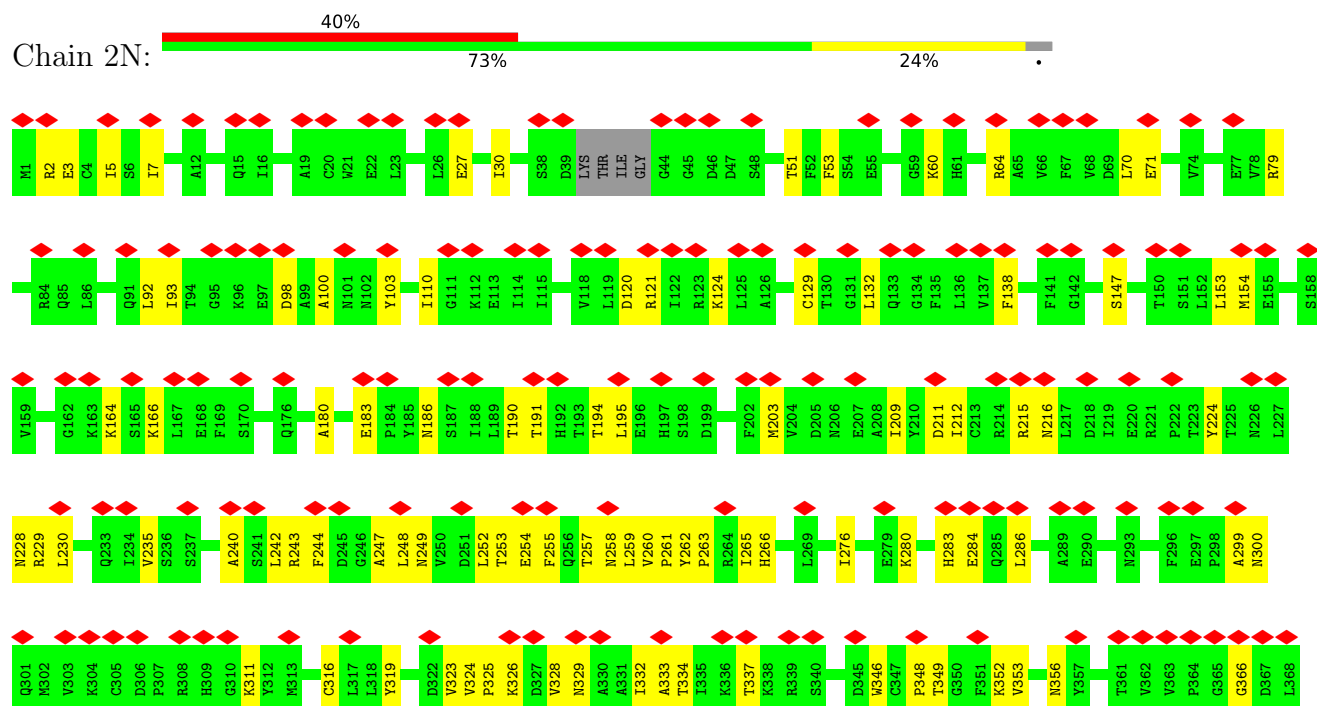
• Molecule 1: Tubulin alpha-1B chain

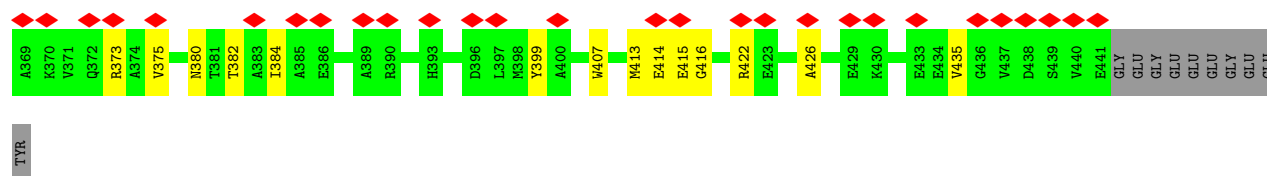


- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain





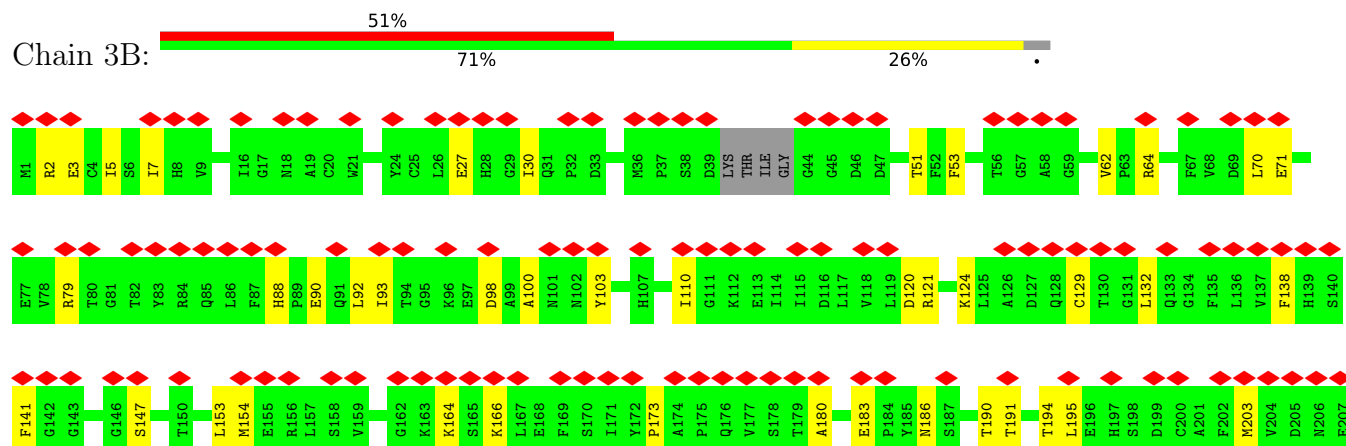
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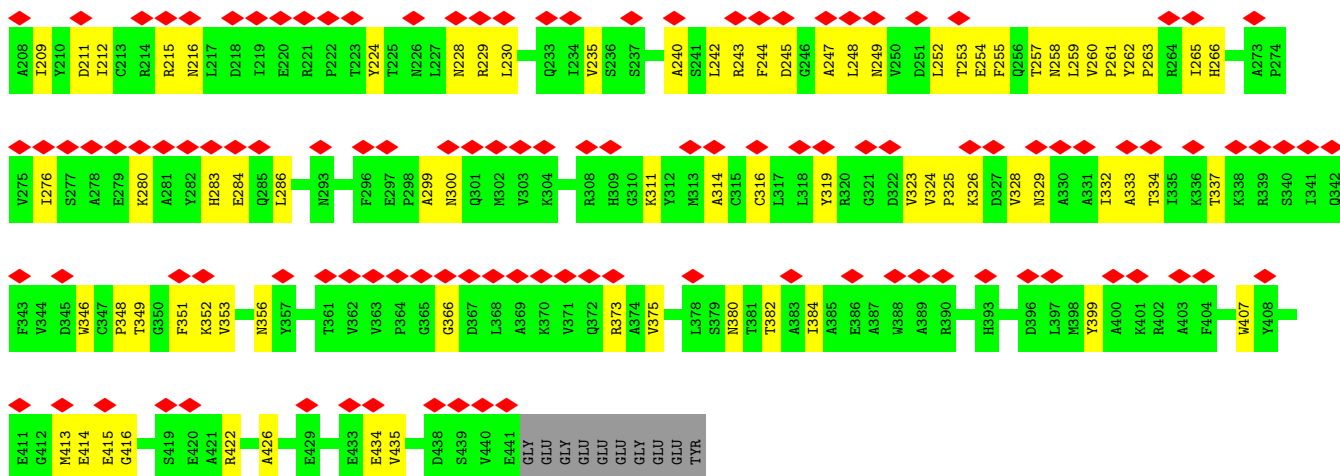


• Molecule 1: Tubulin alpha-1B chain

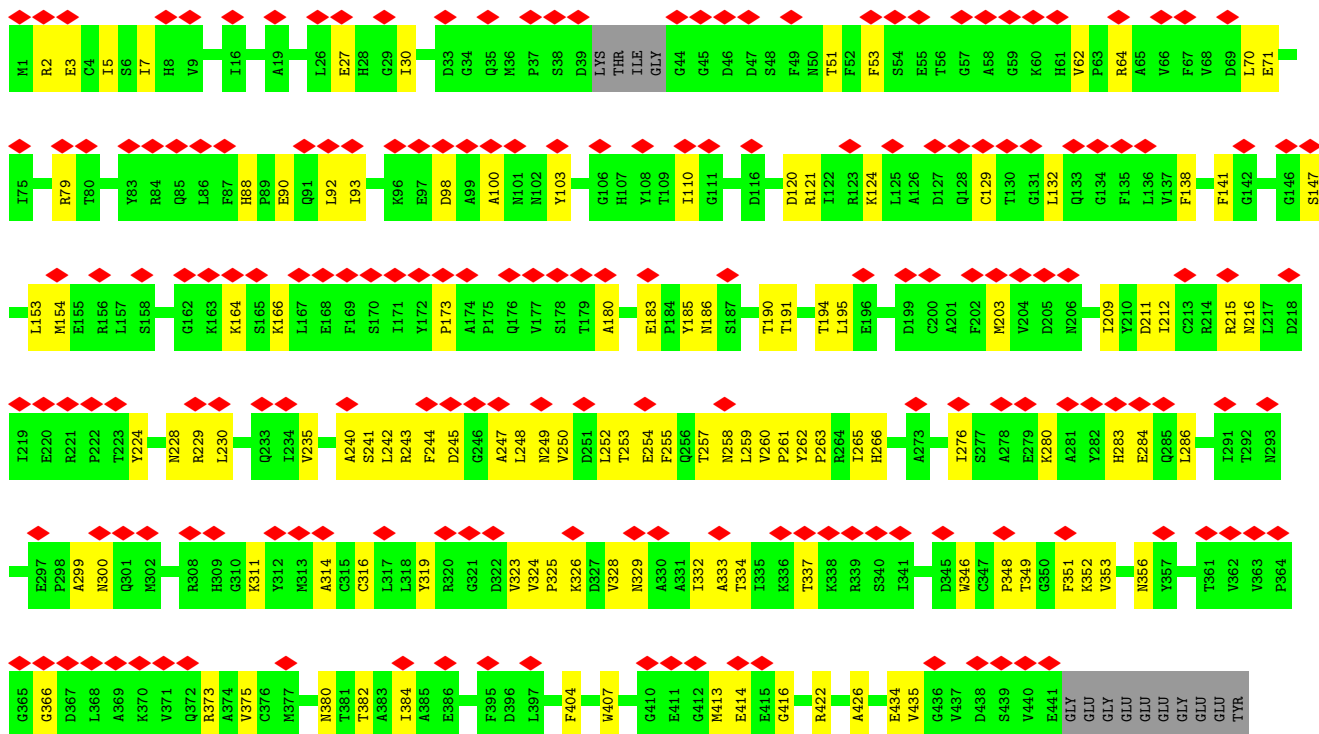
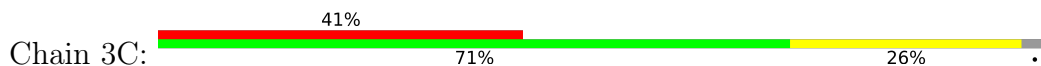
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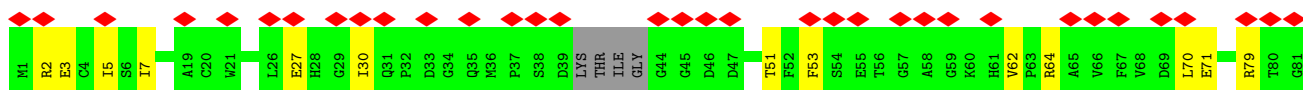
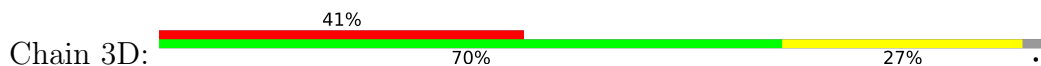


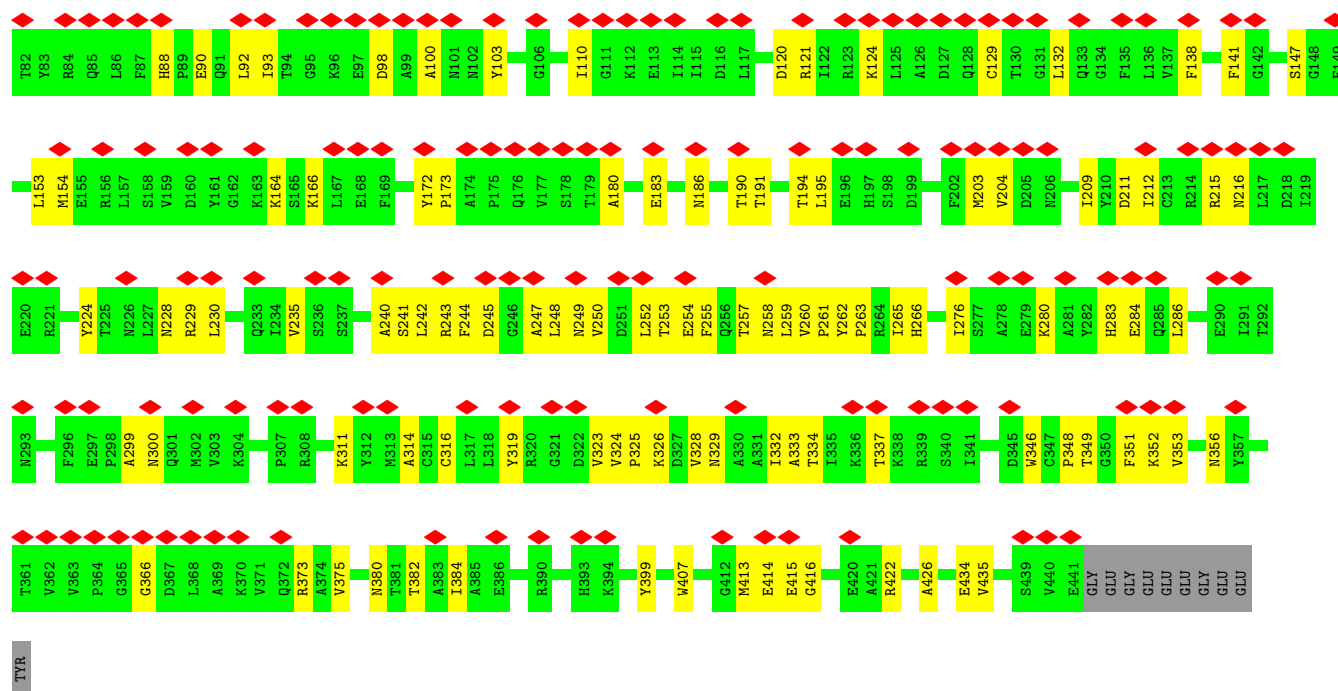


• Molecule 1: Tubulin alpha-1B chain

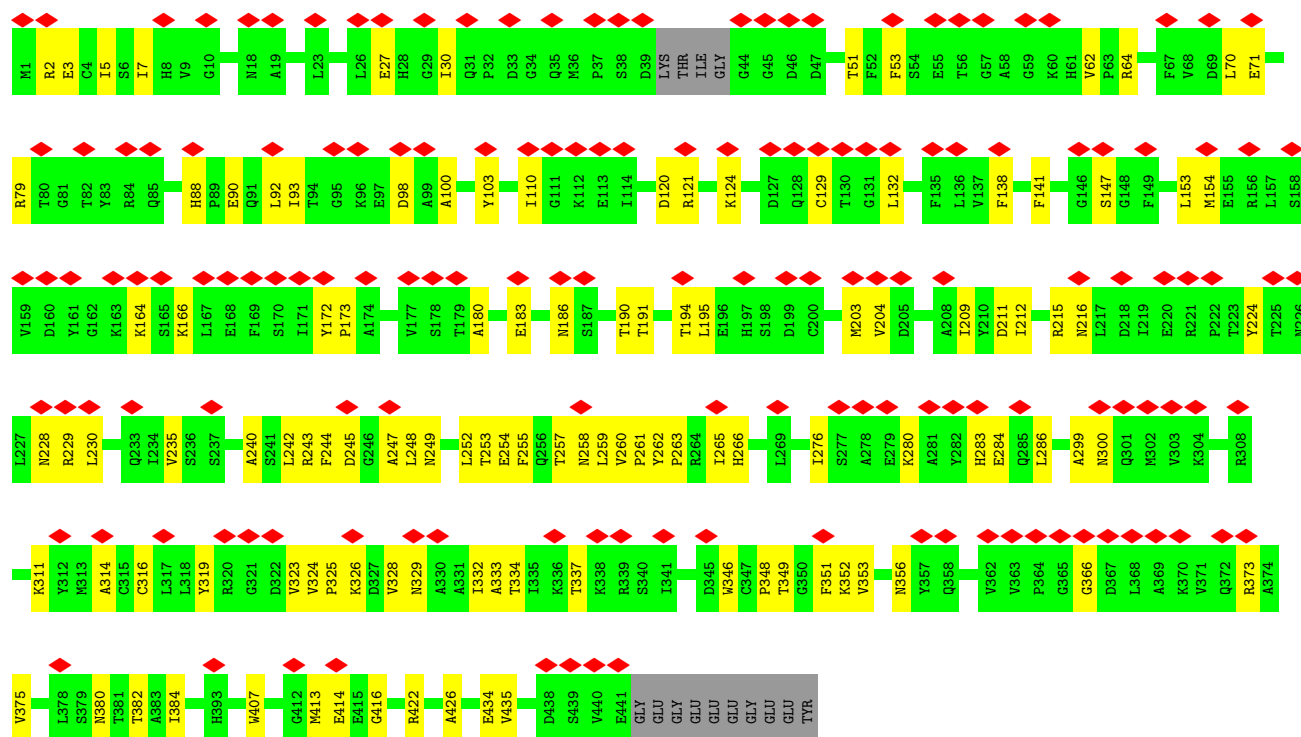


• Molecule 1: Tubulin alpha-1B chain



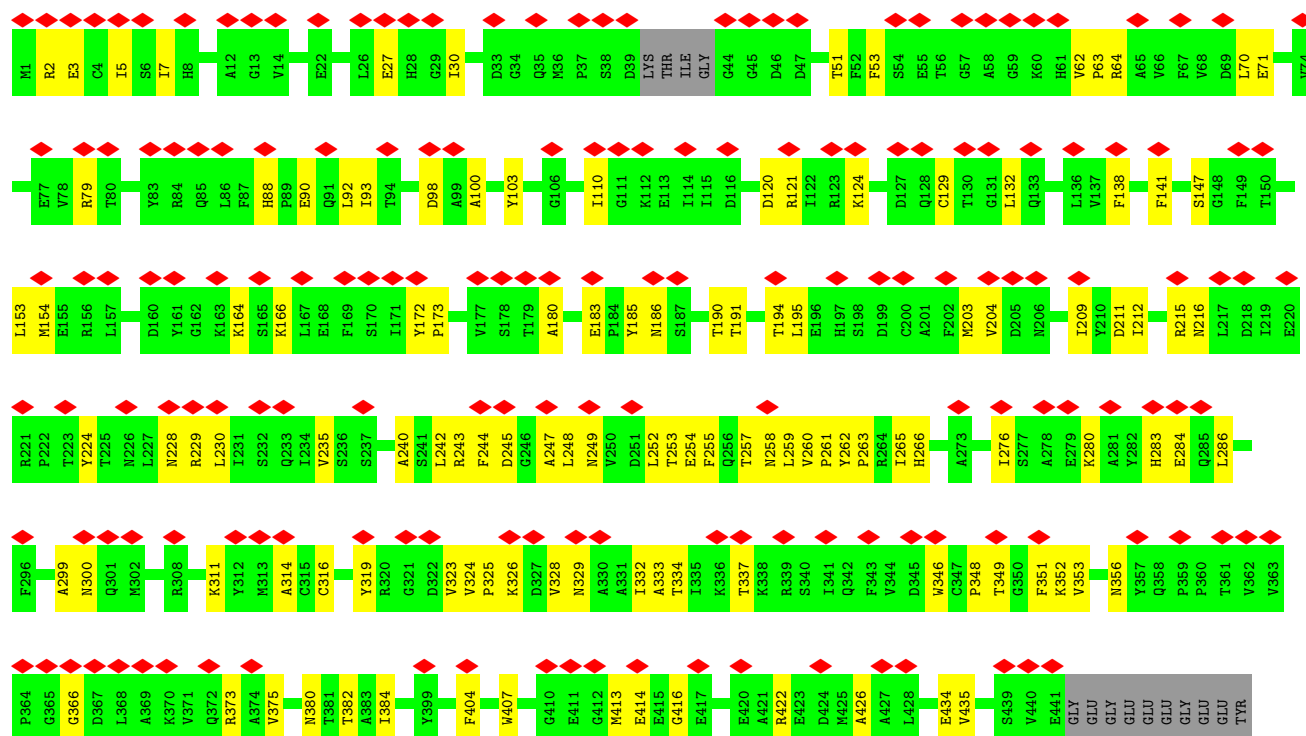


- Molecule 1: Tubulin alpha-1B chain

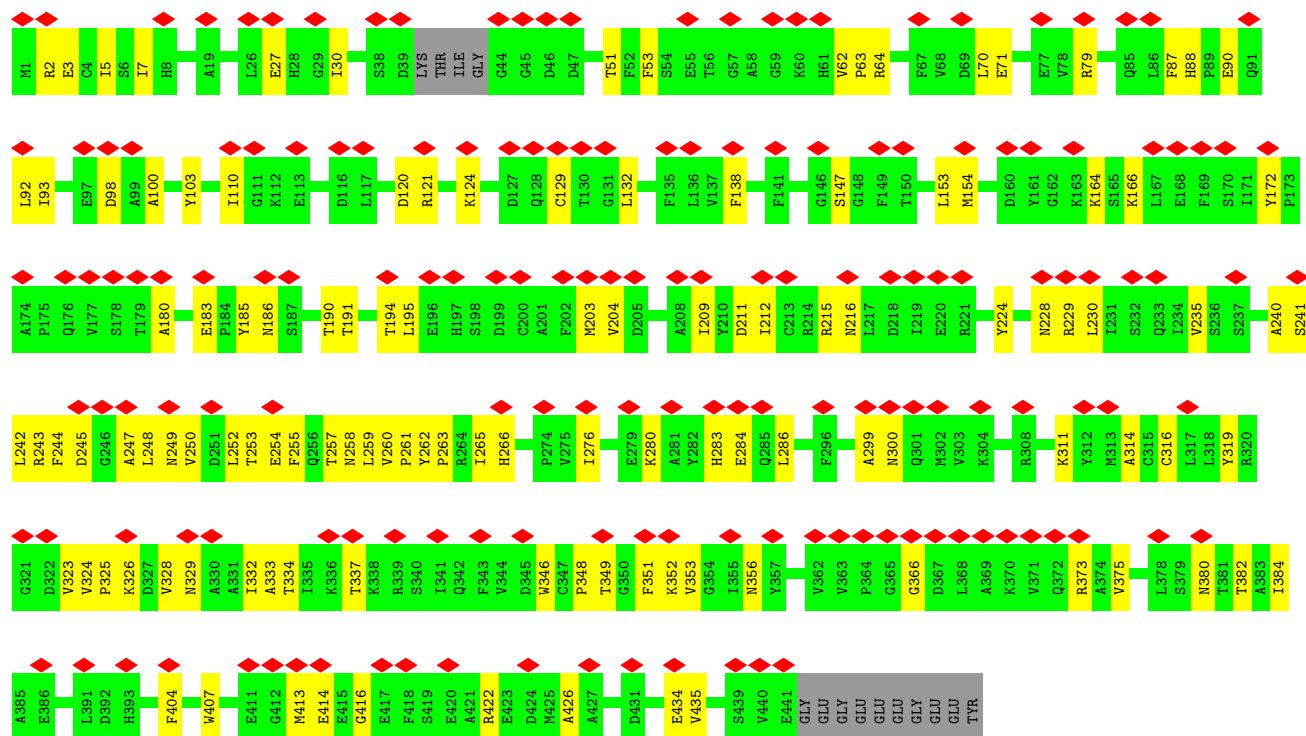
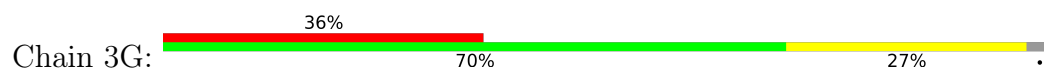


- Molecule 1: Tubulin alpha-1B chain

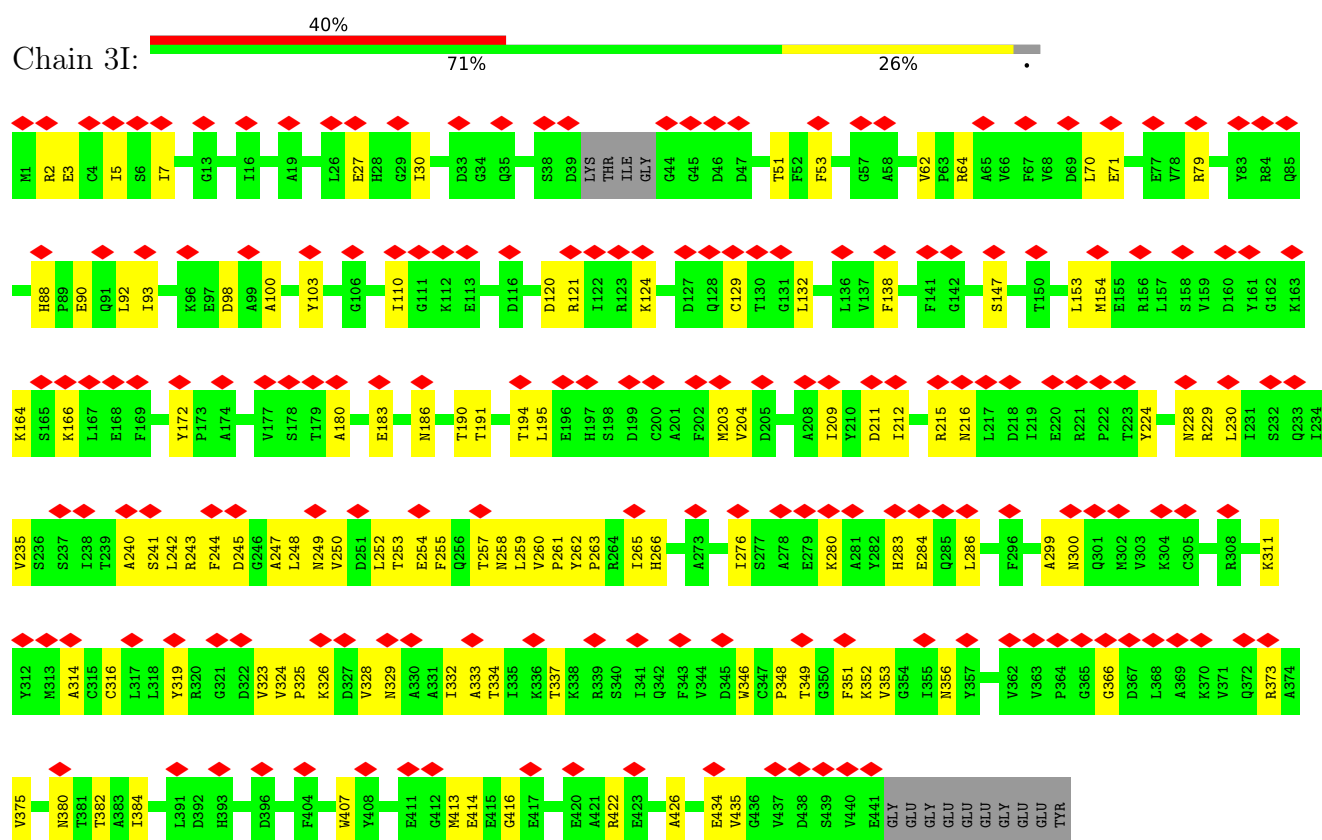




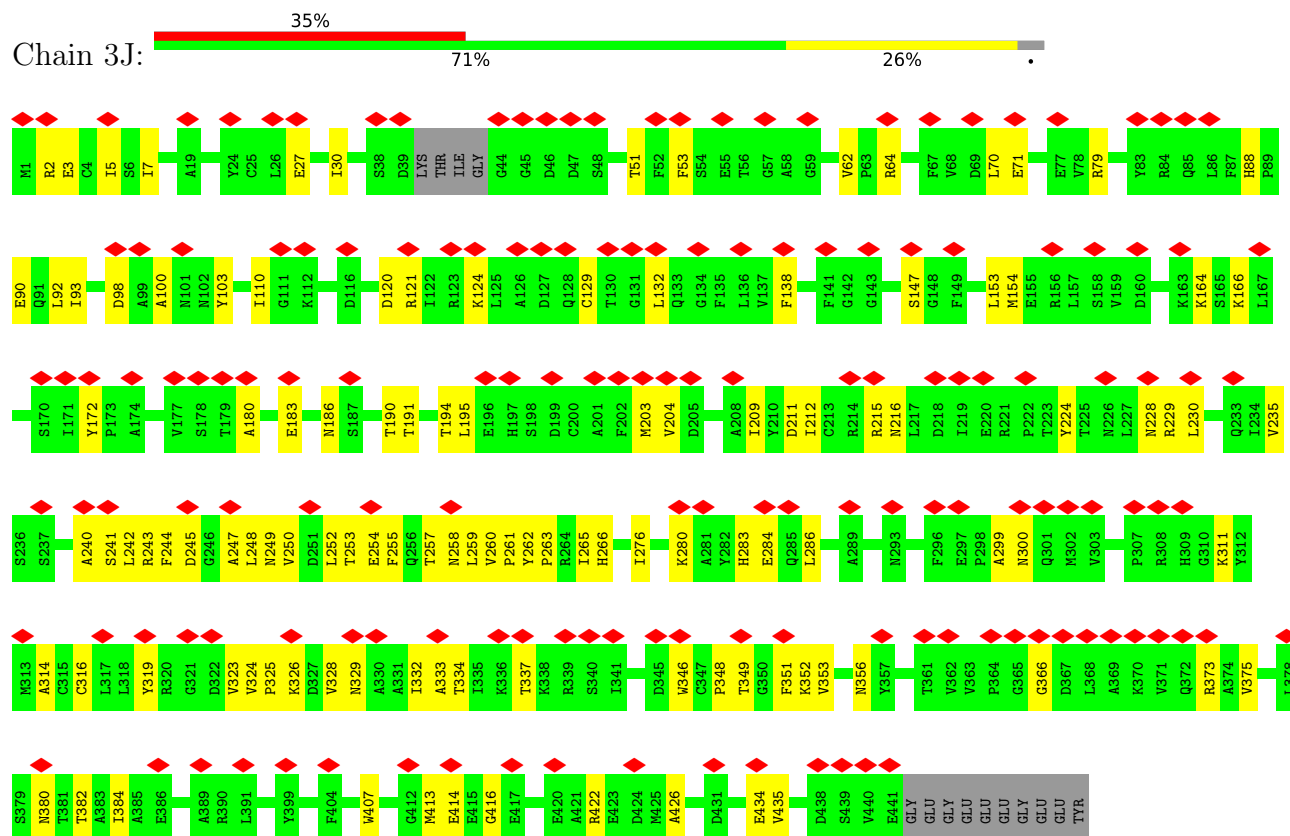
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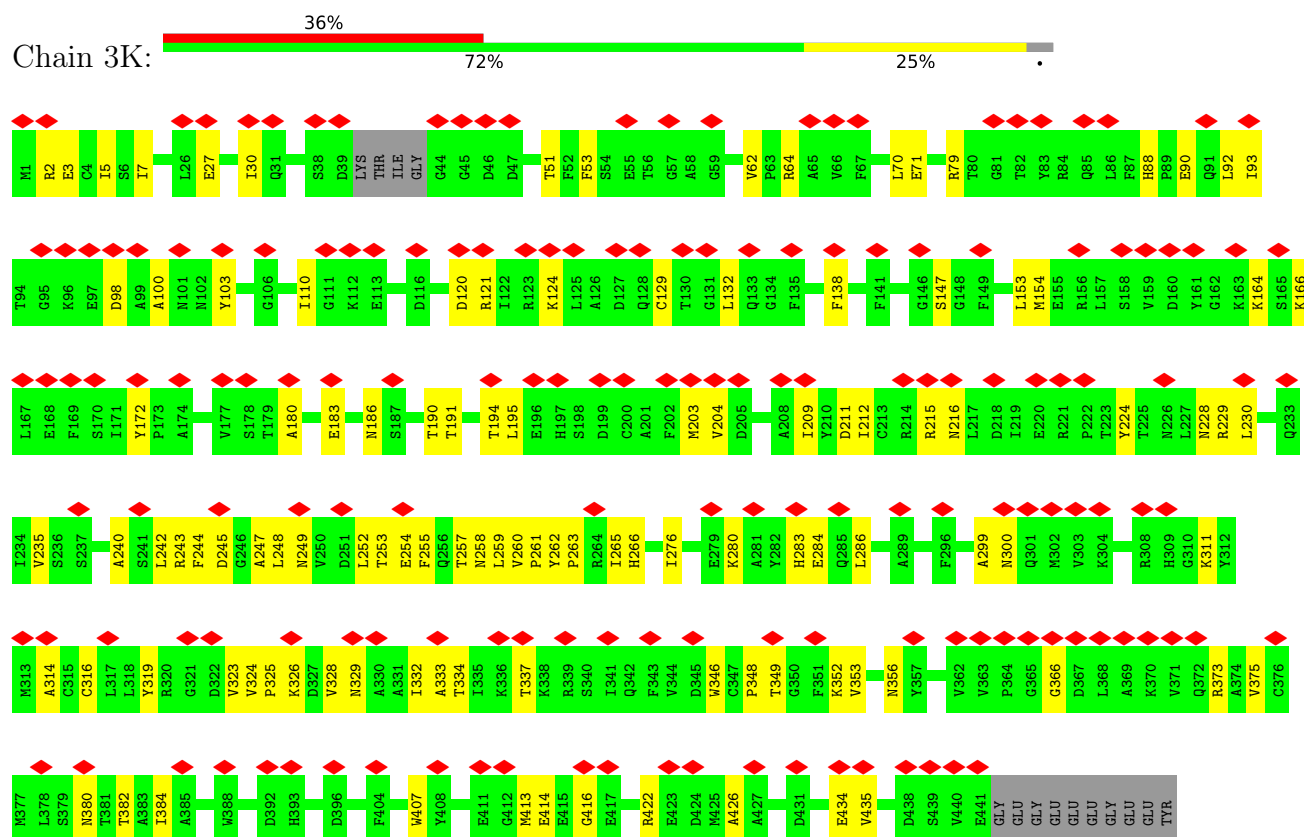
• Molecule 1: Tubulin alpha-1B chain



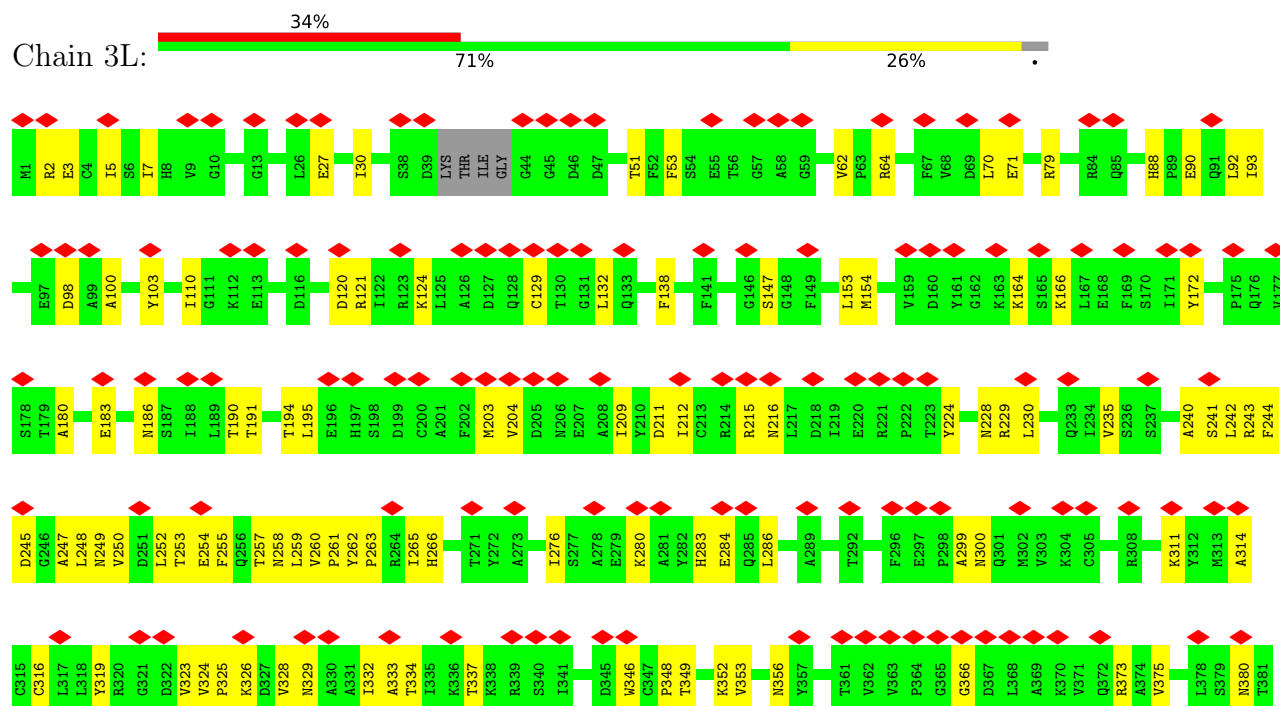
• Molecule 1: Tubulin alpha-1B chain

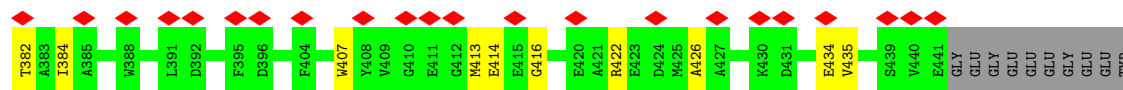


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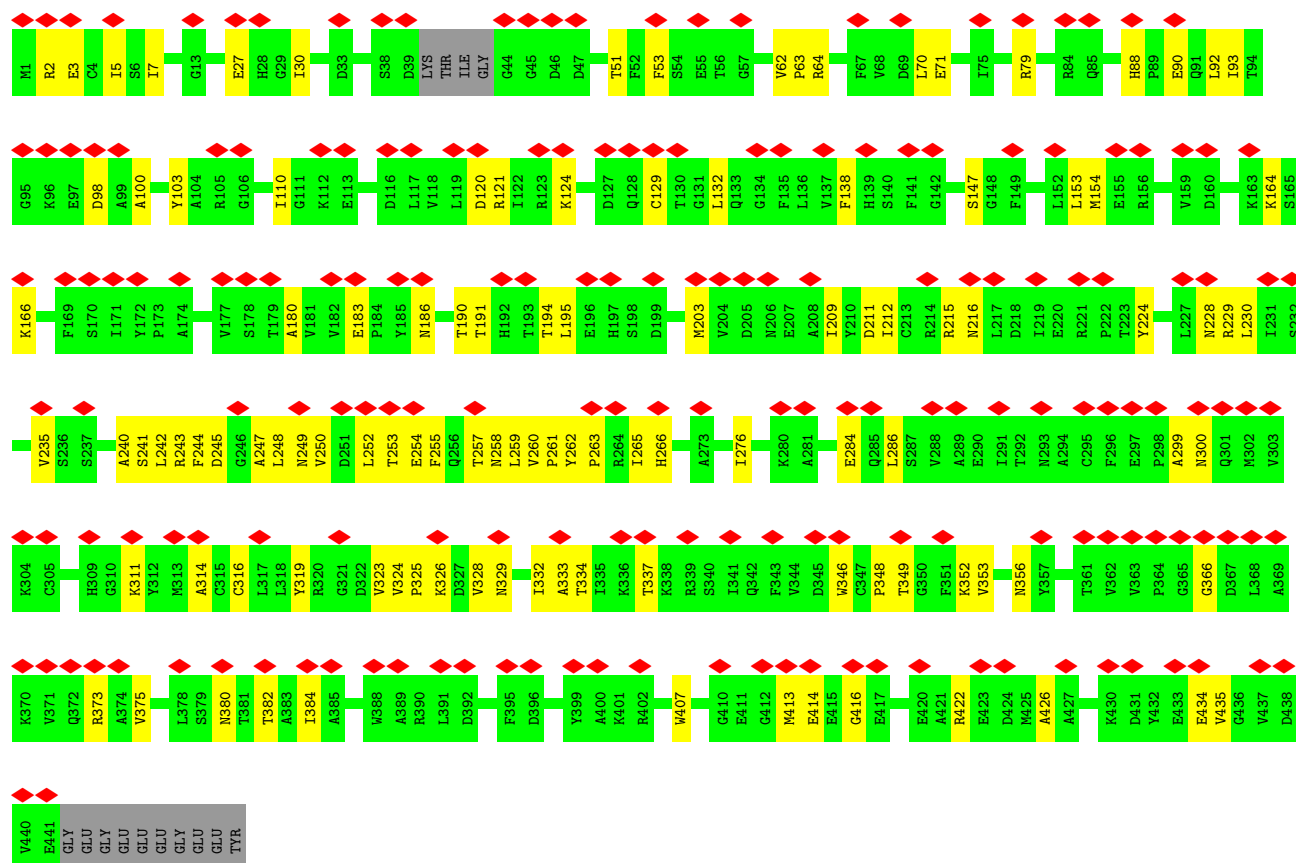
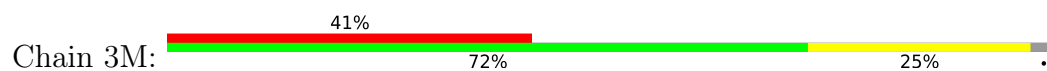


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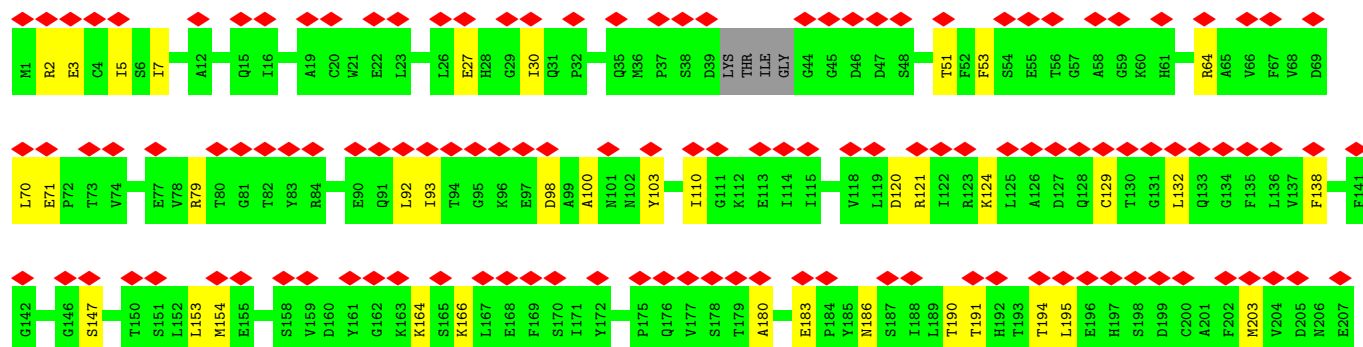
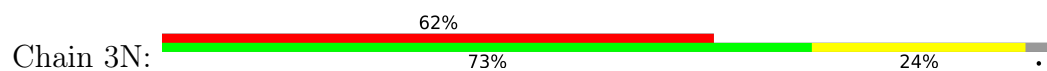


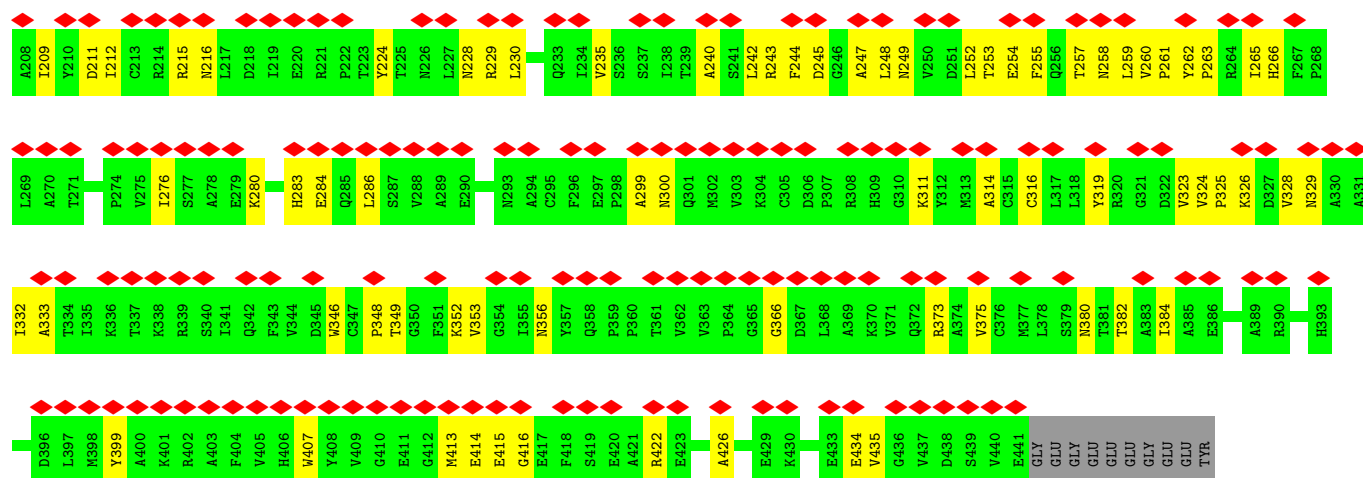


• Molecule 1: Tubulin alpha-1B chain

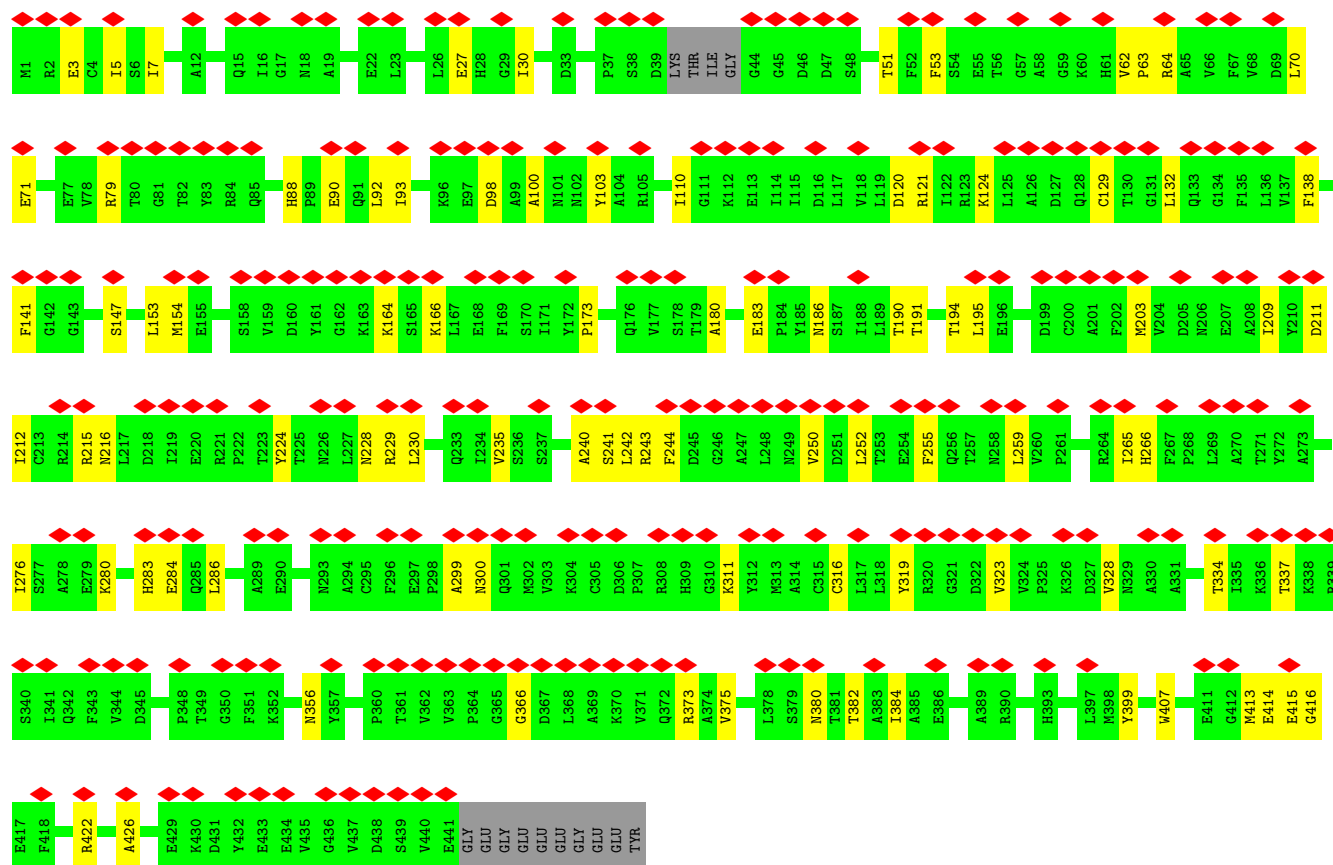
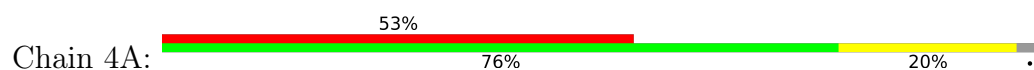


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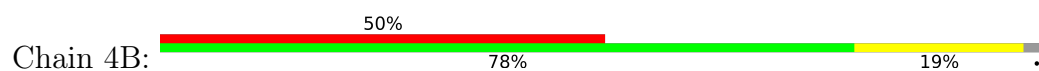


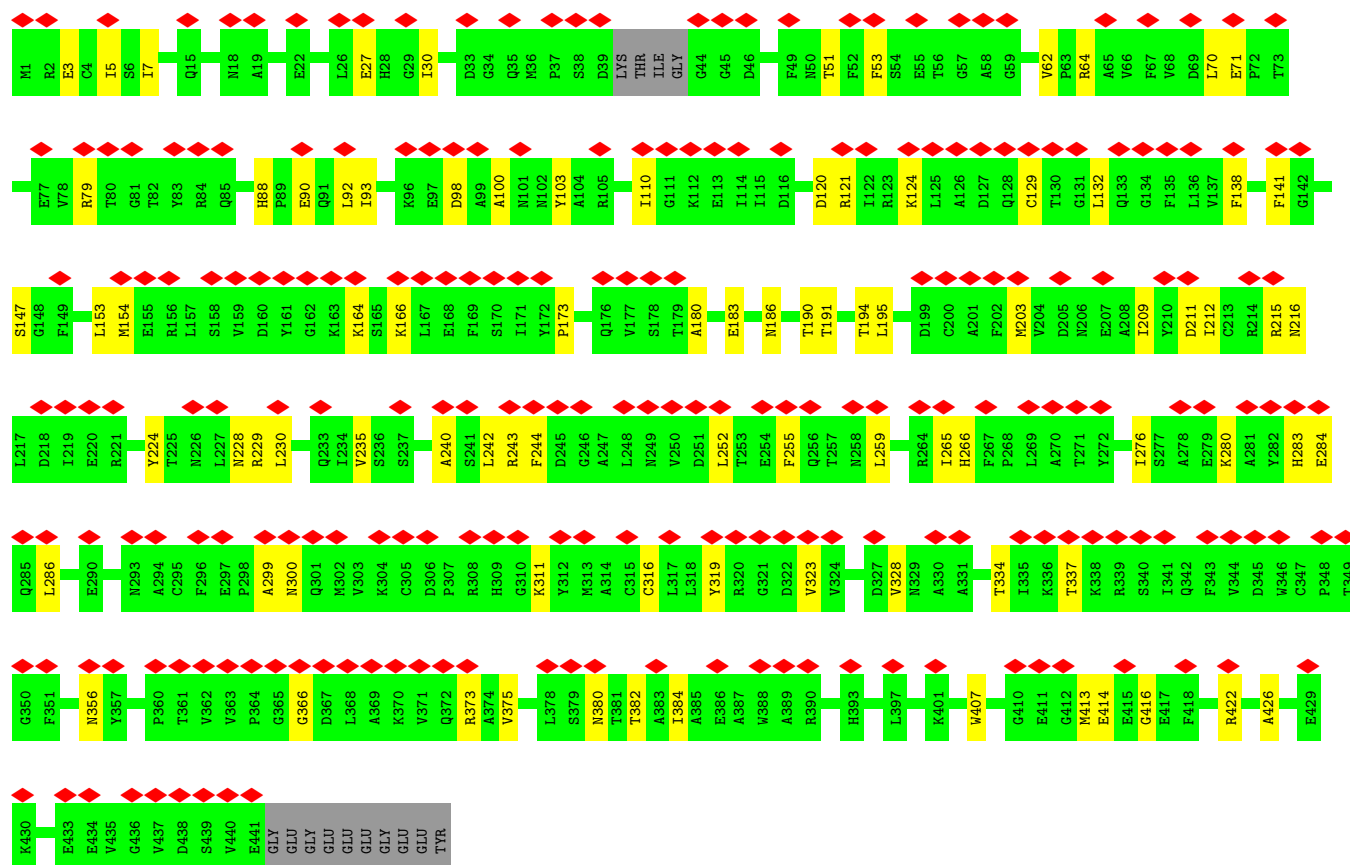


• Molecule 1: Tubulin alpha-1B chain

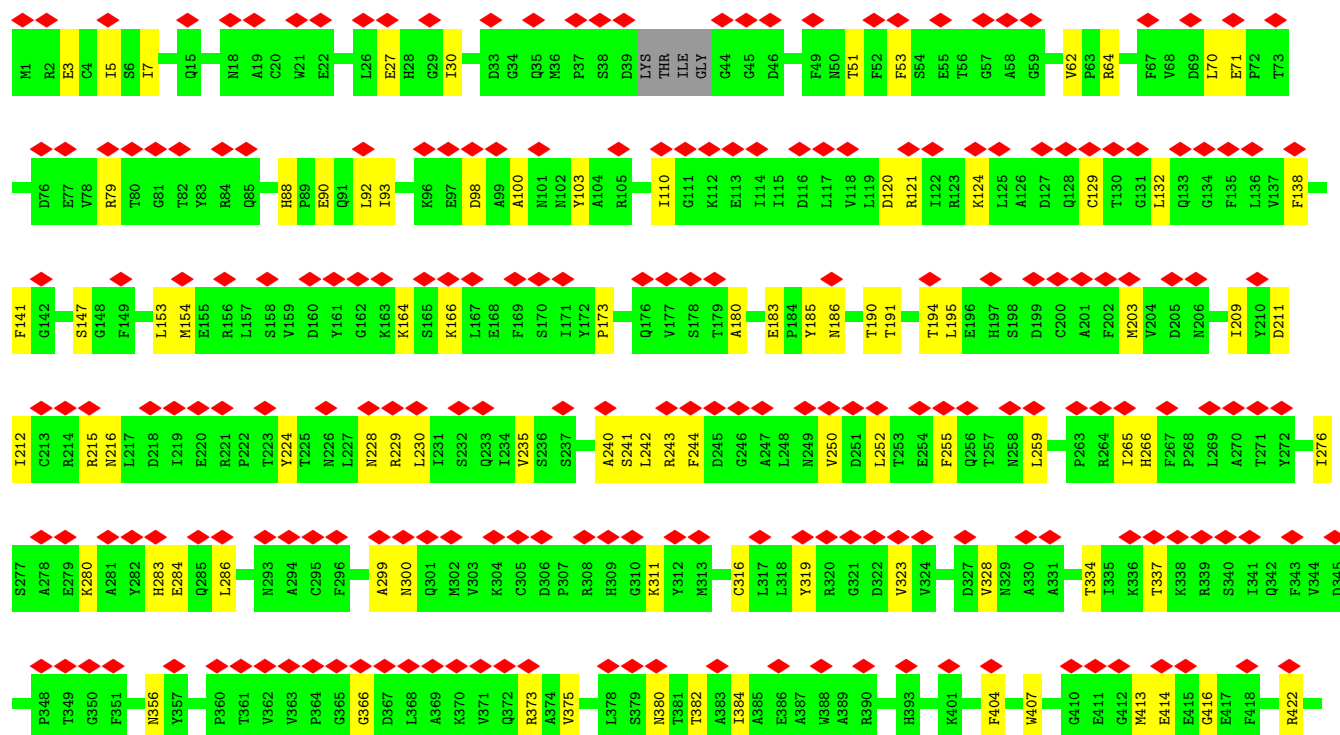
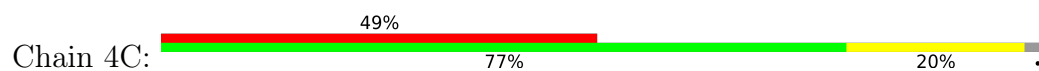


• Molecule 1: Tubulin alpha-1B chain

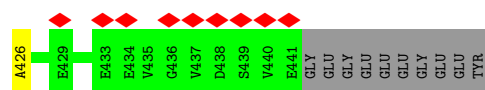




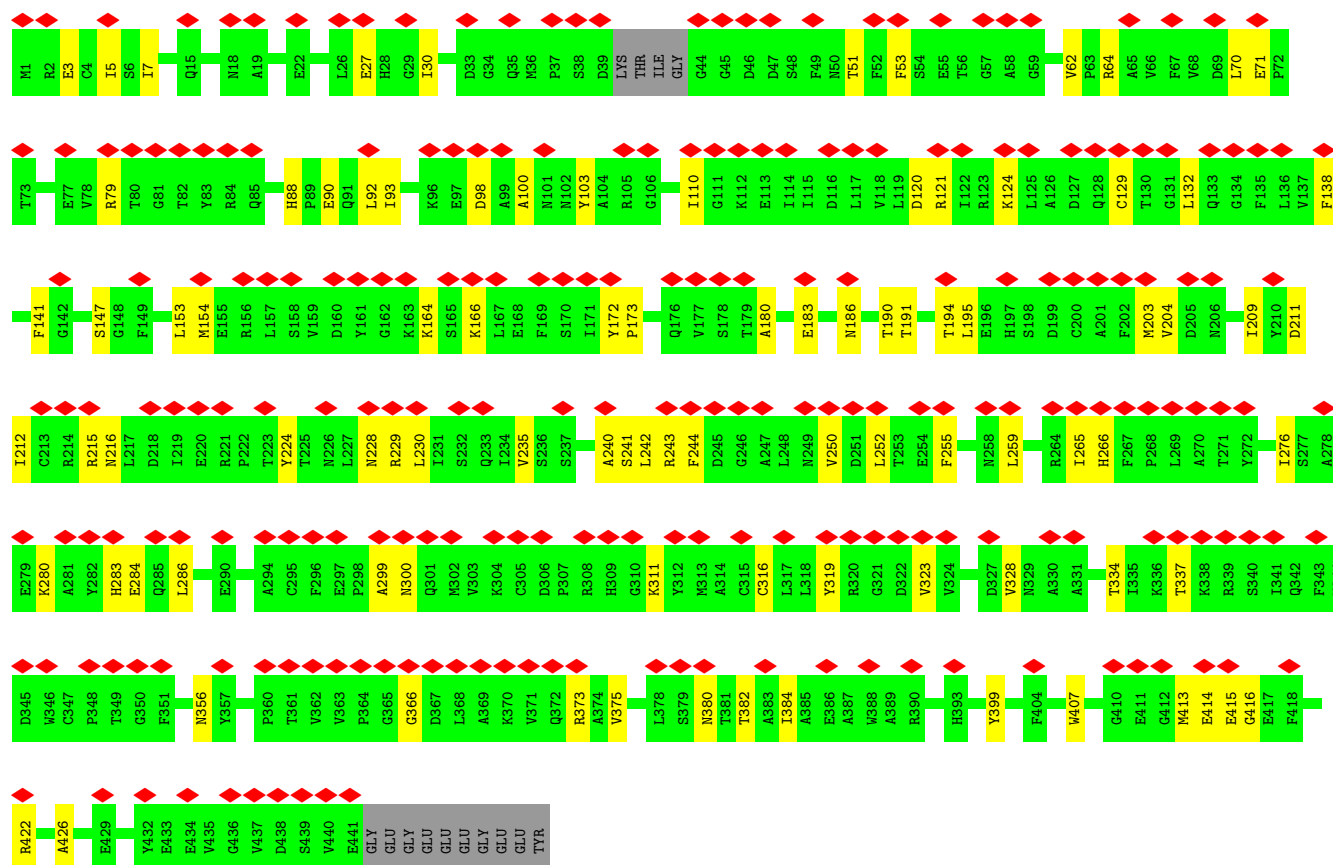
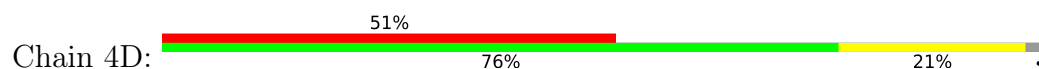
• Molecule 1: Tubulin alpha-1B chain



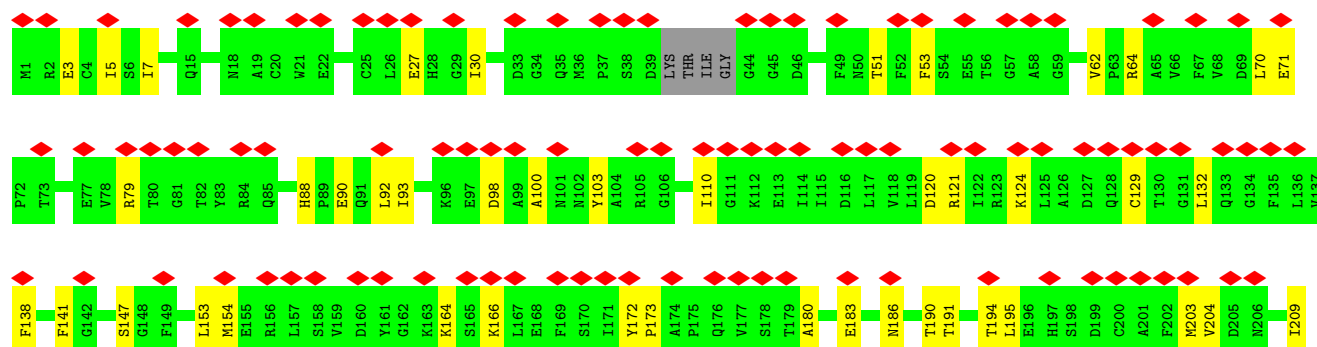
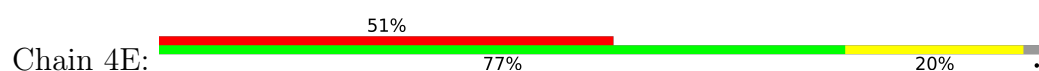


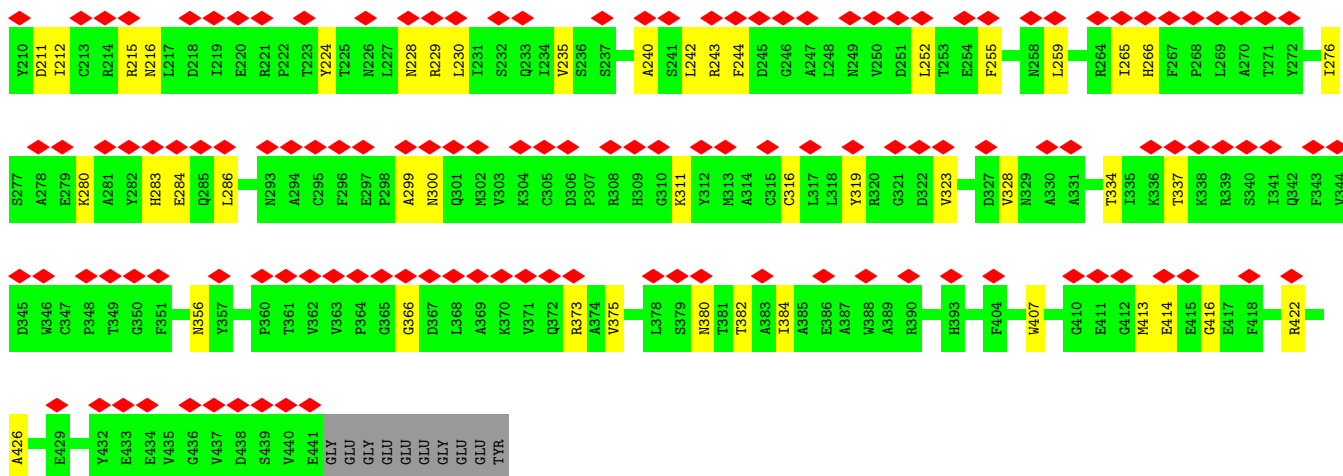


• Molecule 1: Tubulin alpha-1B chain

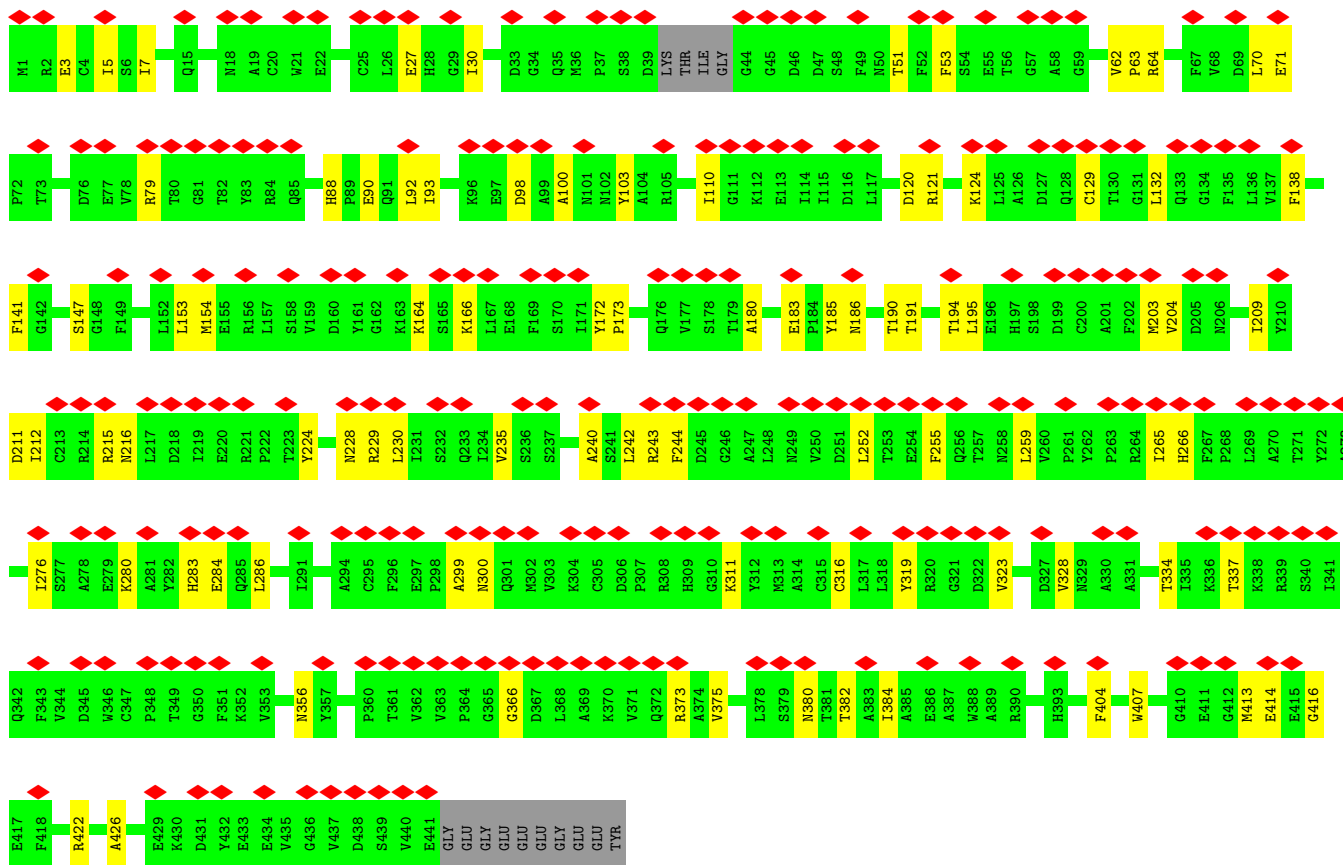
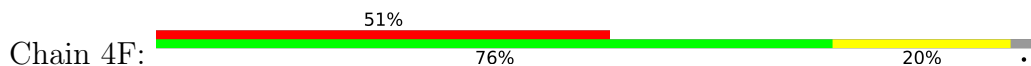


• Molecule 1: Tubulin alpha-1B chain

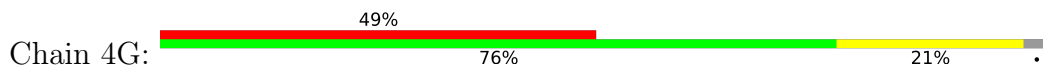


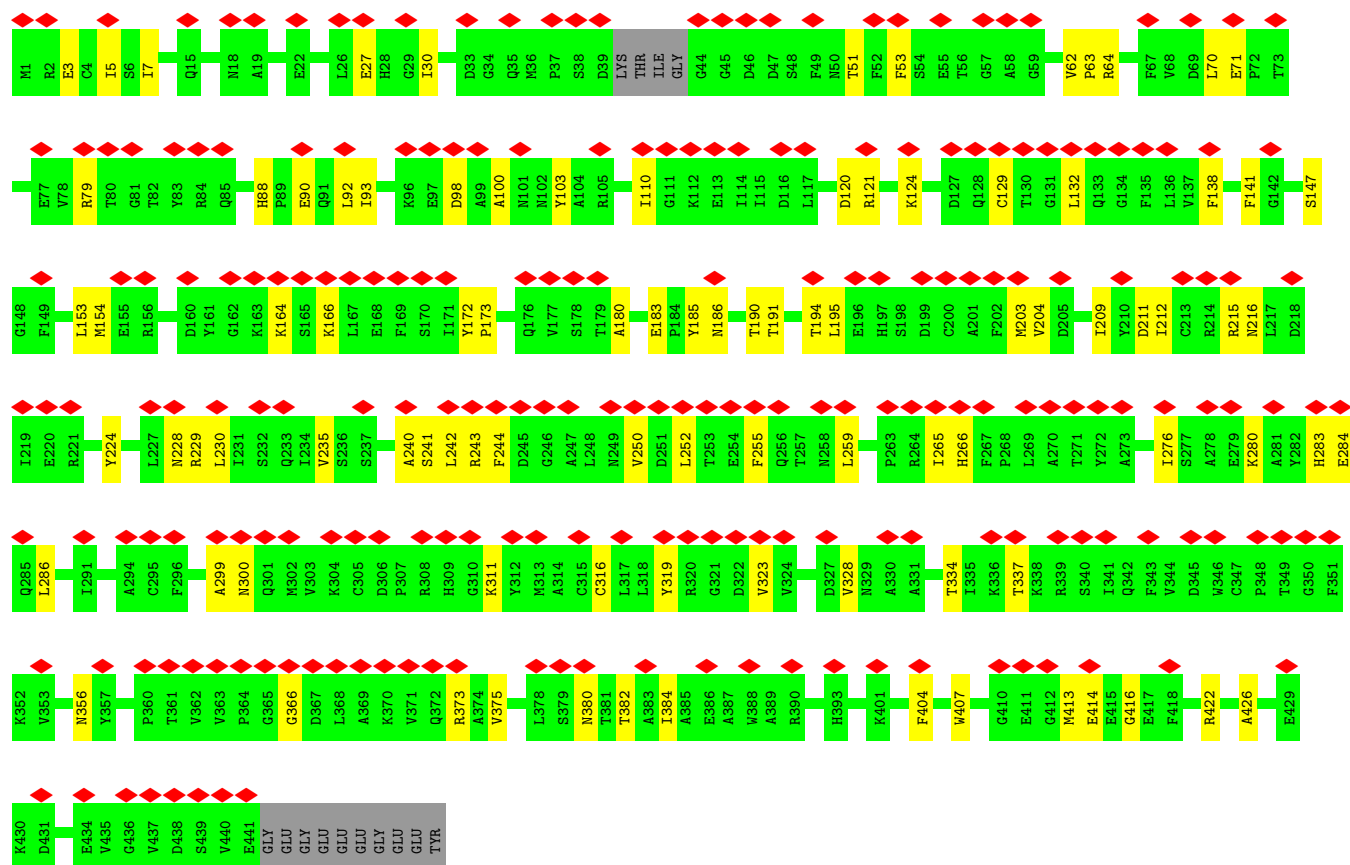


• Molecule 1: Tubulin alpha-1B chain

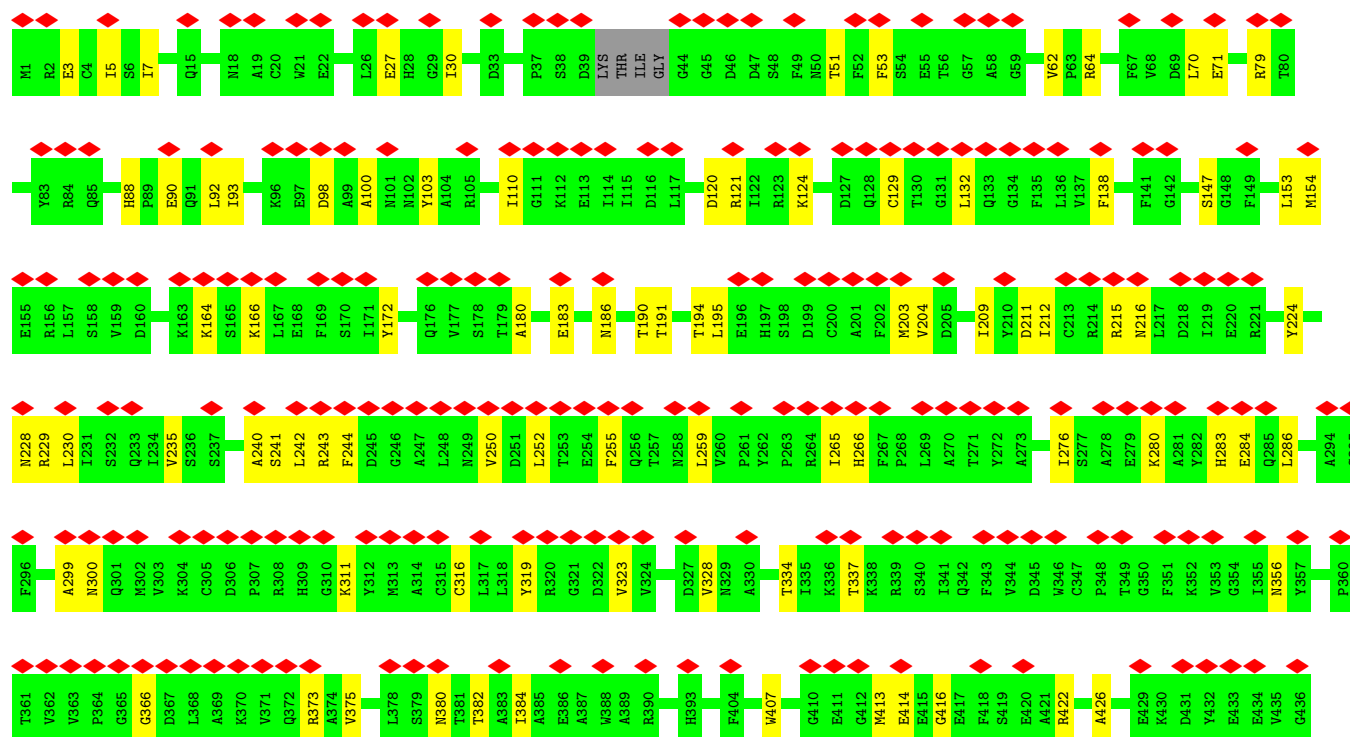
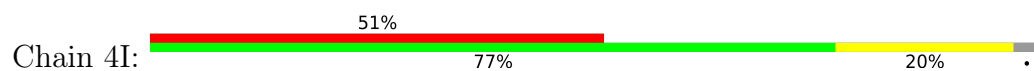


• Molecule 1: Tubulin alpha-1B chain

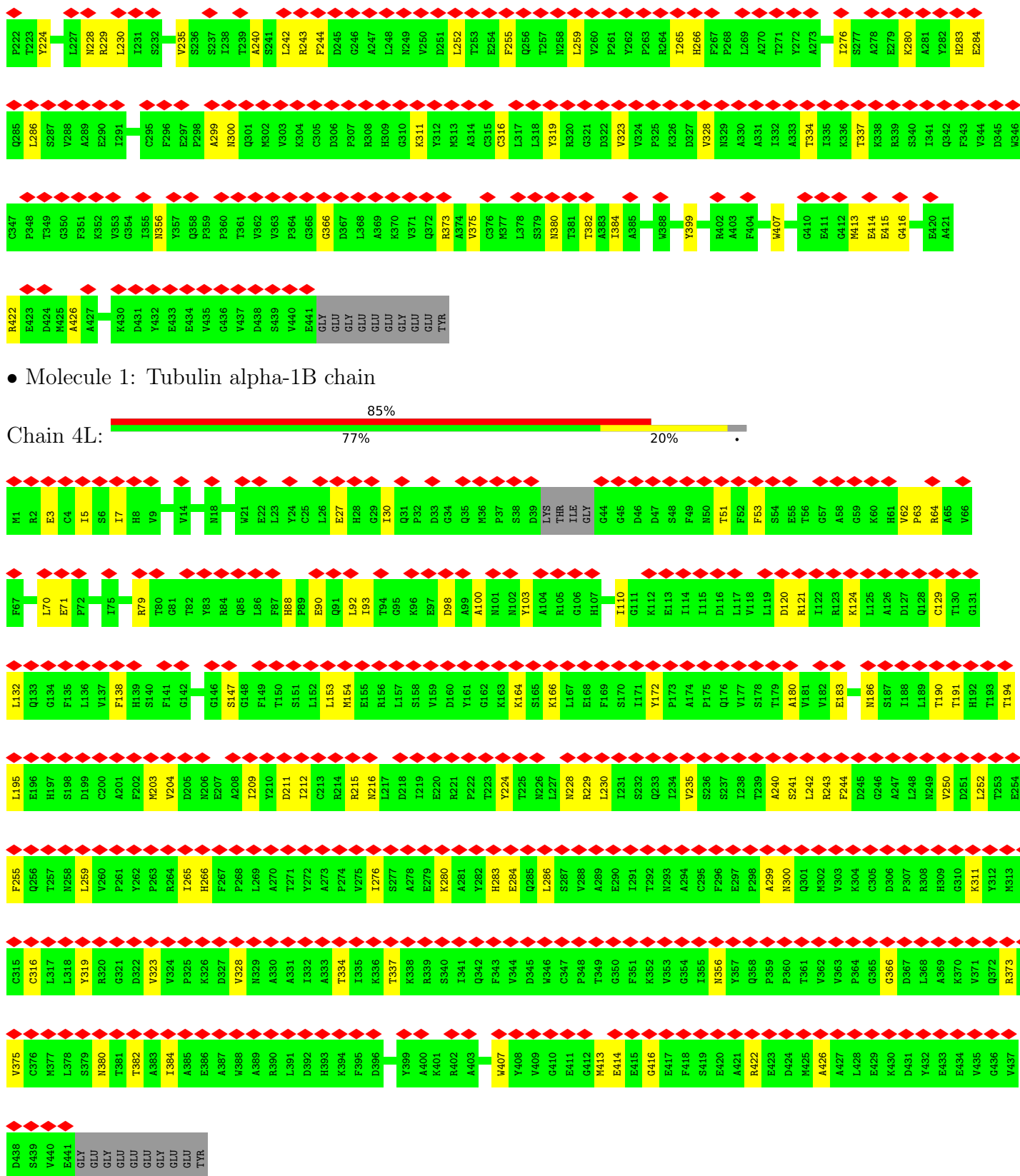




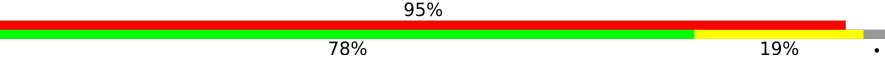
• Molecule 1: Tubulin alpha-1B chain

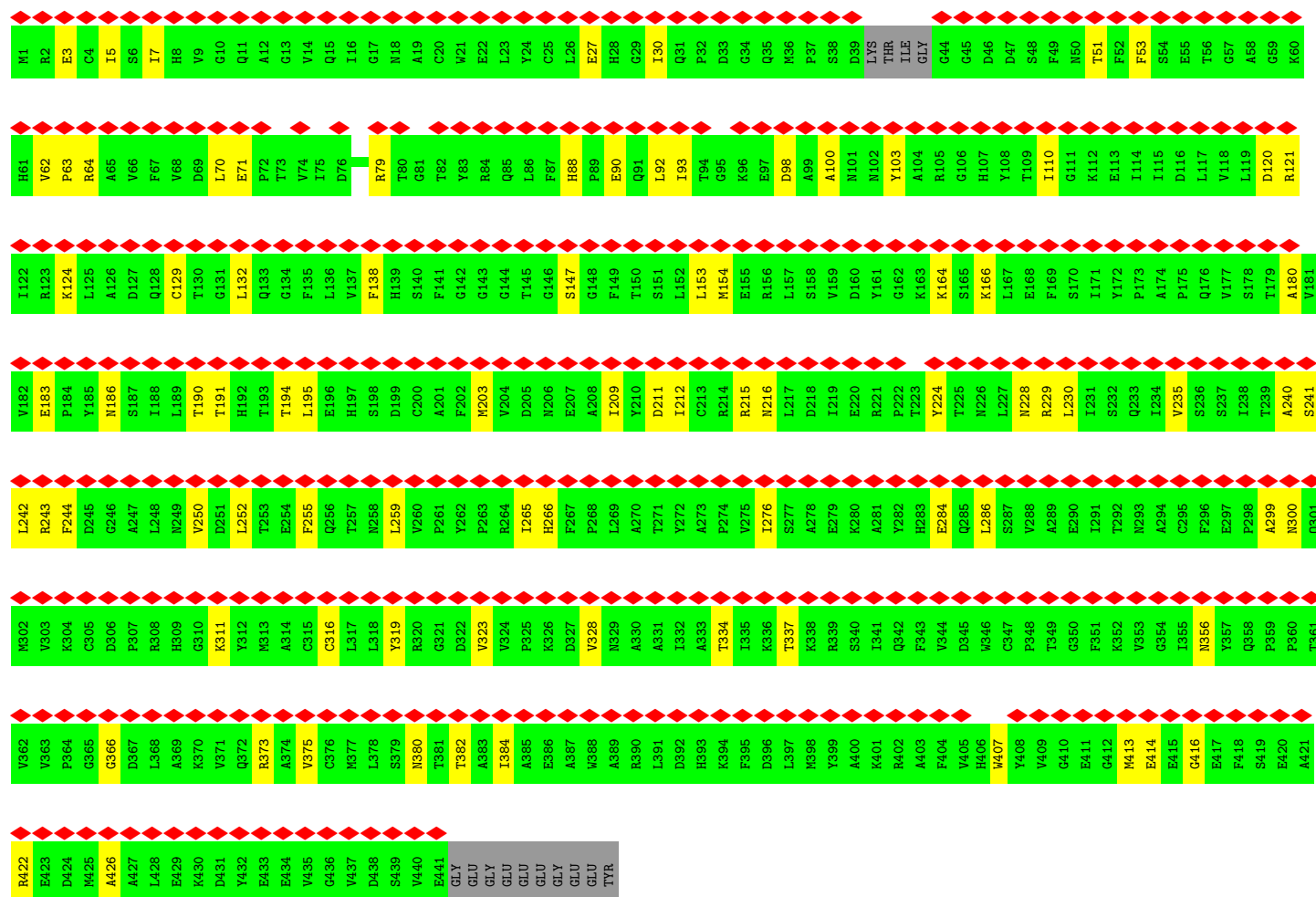






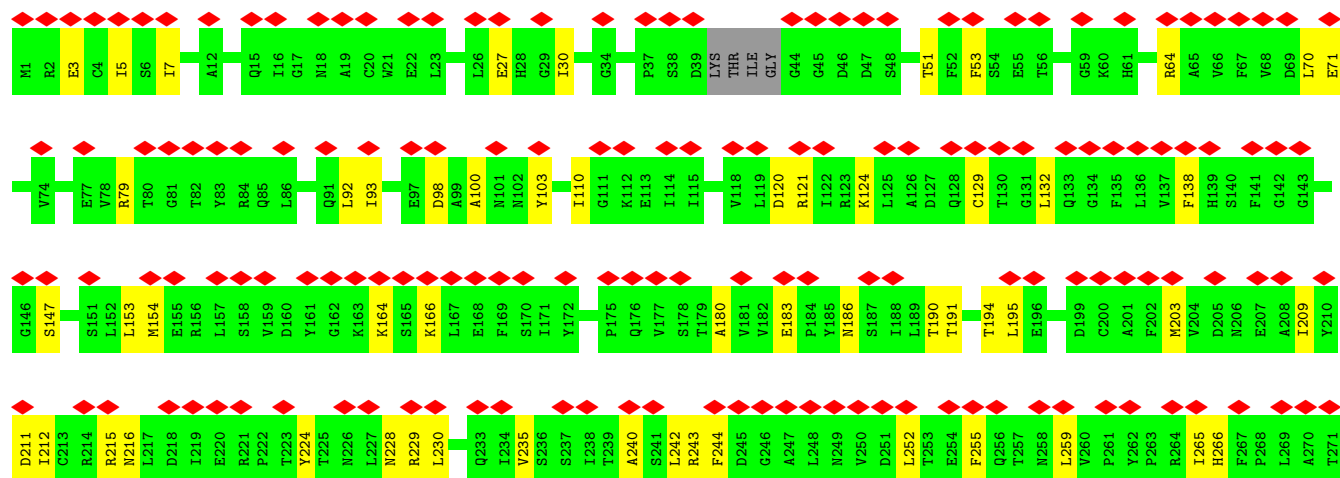
• Molecule 1: Tubulin alpha-1B chain

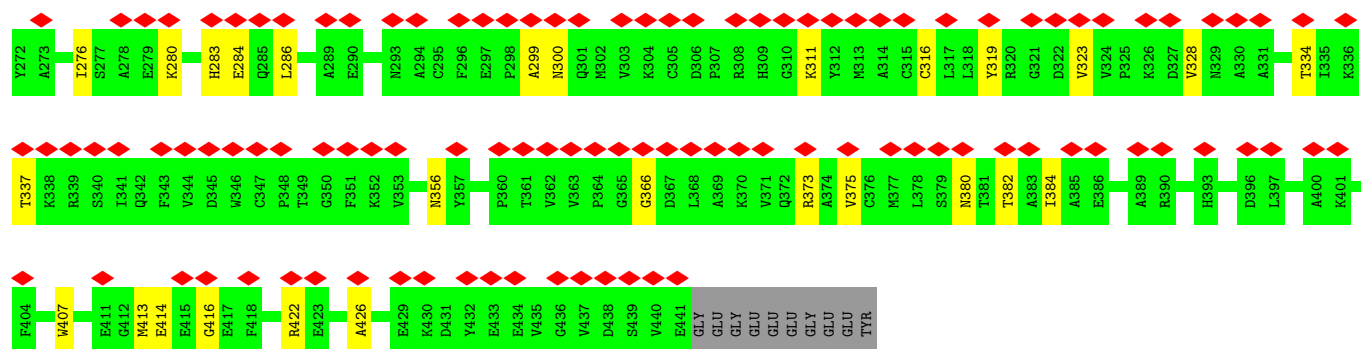
Chain 4M: 



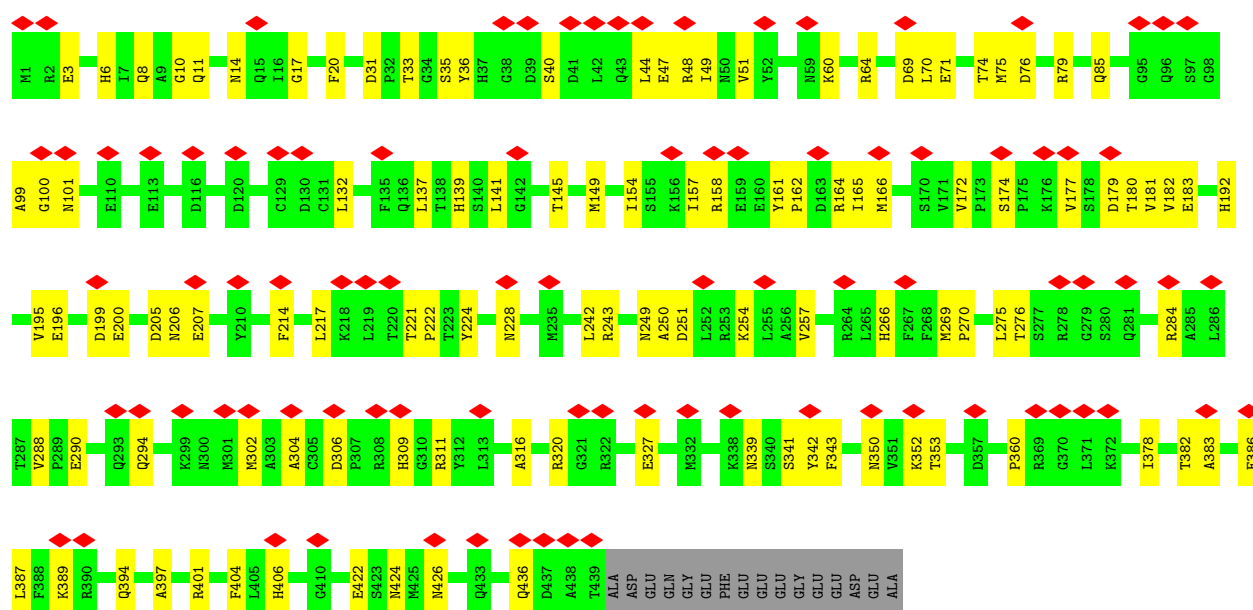
• Molecule 1: Tubulin alpha-1B chain

Chain 4N: 

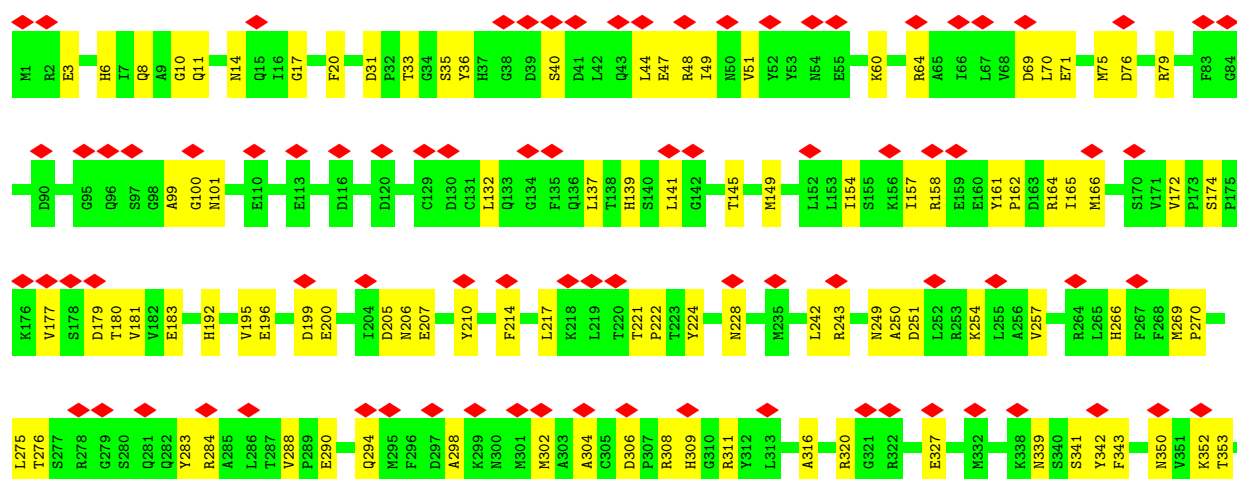




• Molecule 2: Tubulin beta chain

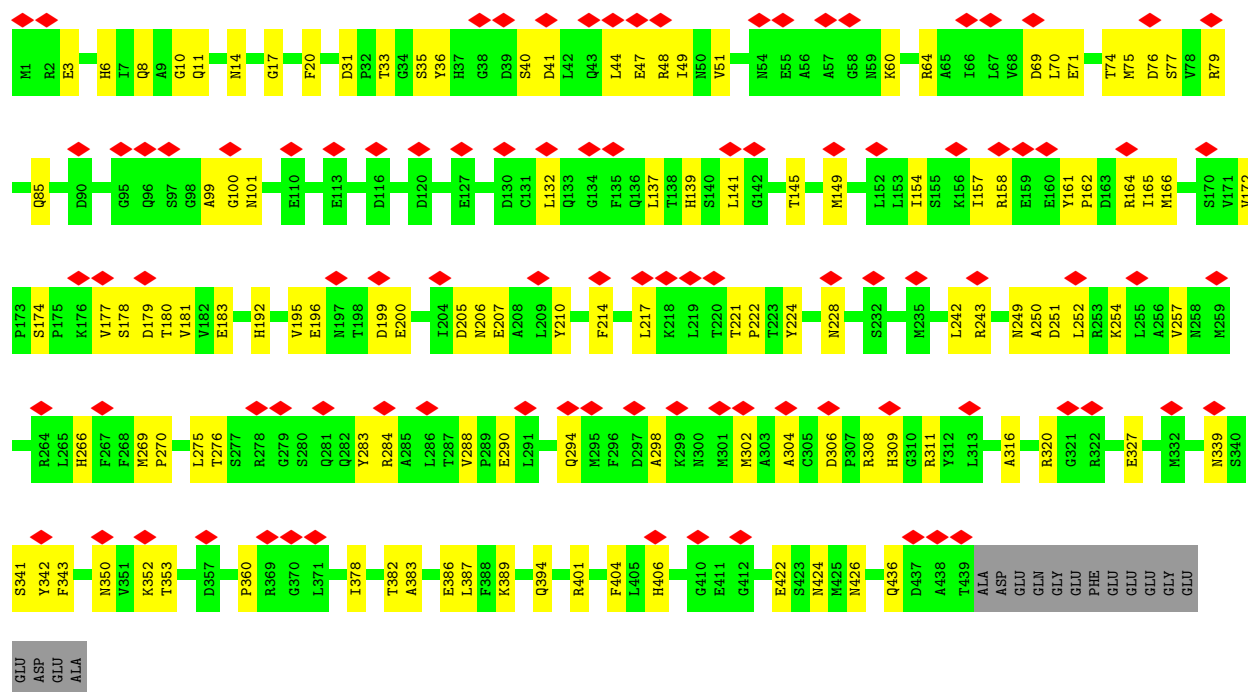


• Molecule 2: Tubulin beta chain

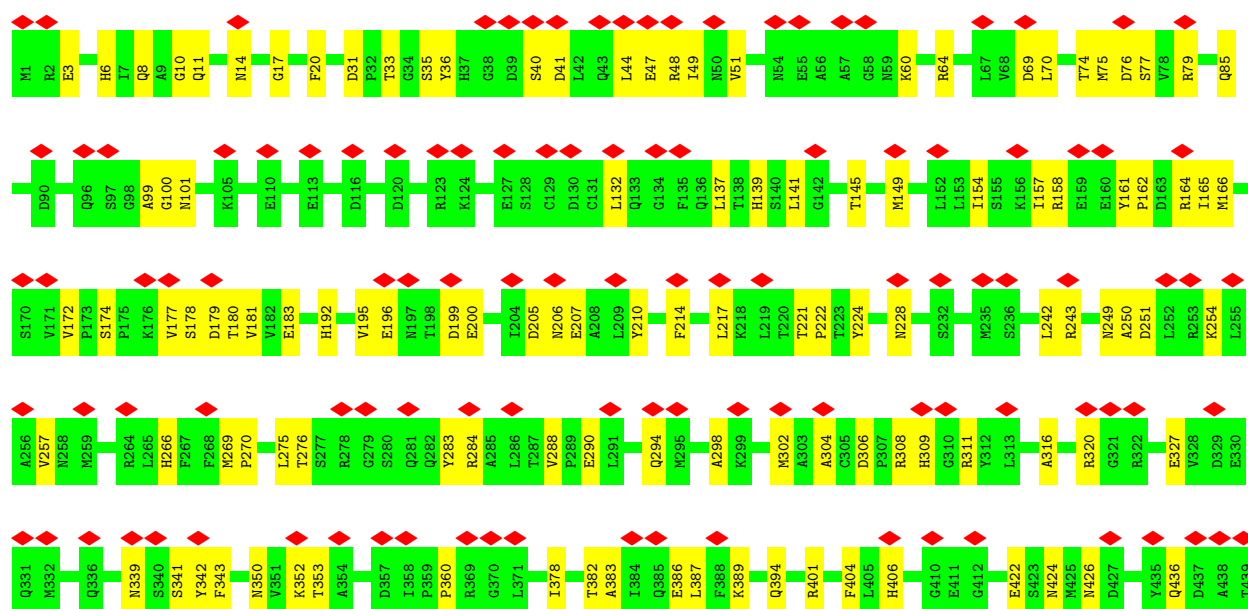




• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

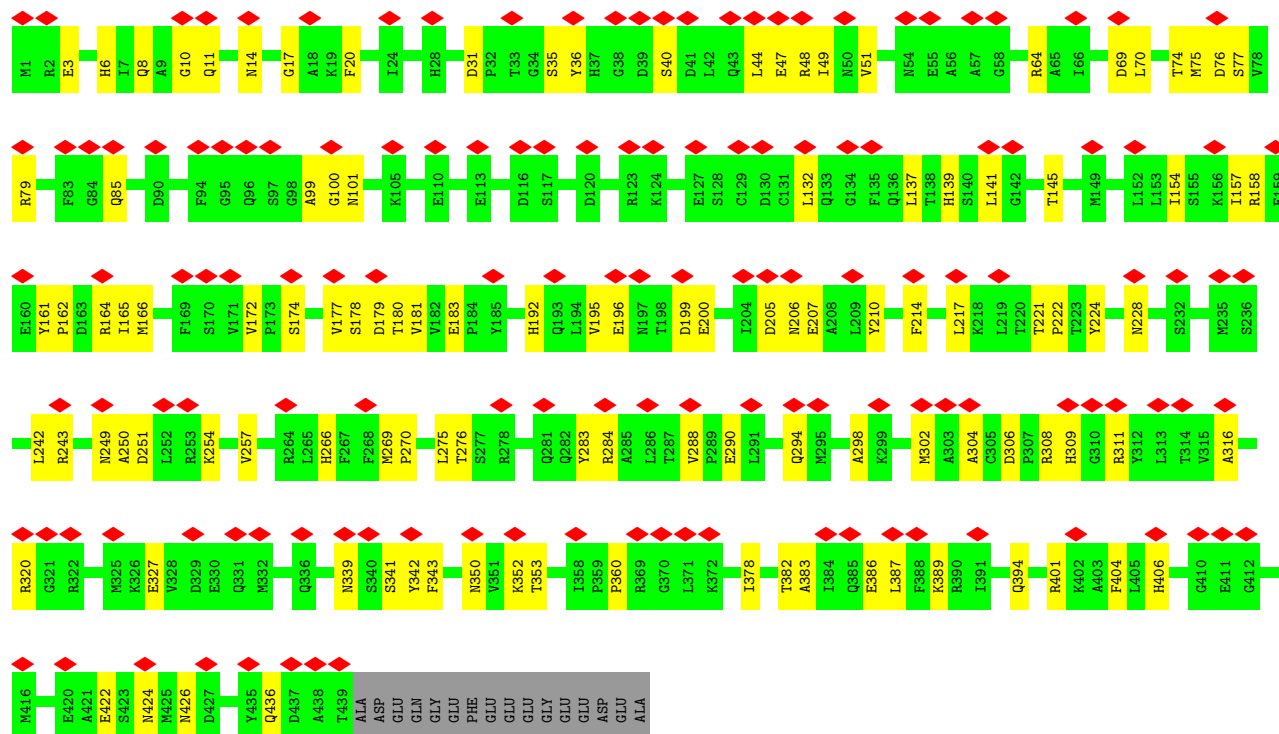




ALA  
ASP  
GLU  
GLN  
GLY  
PHE  
GLU  
GLU  
GLY  
GLY  
ASP  
GLU  
ALA

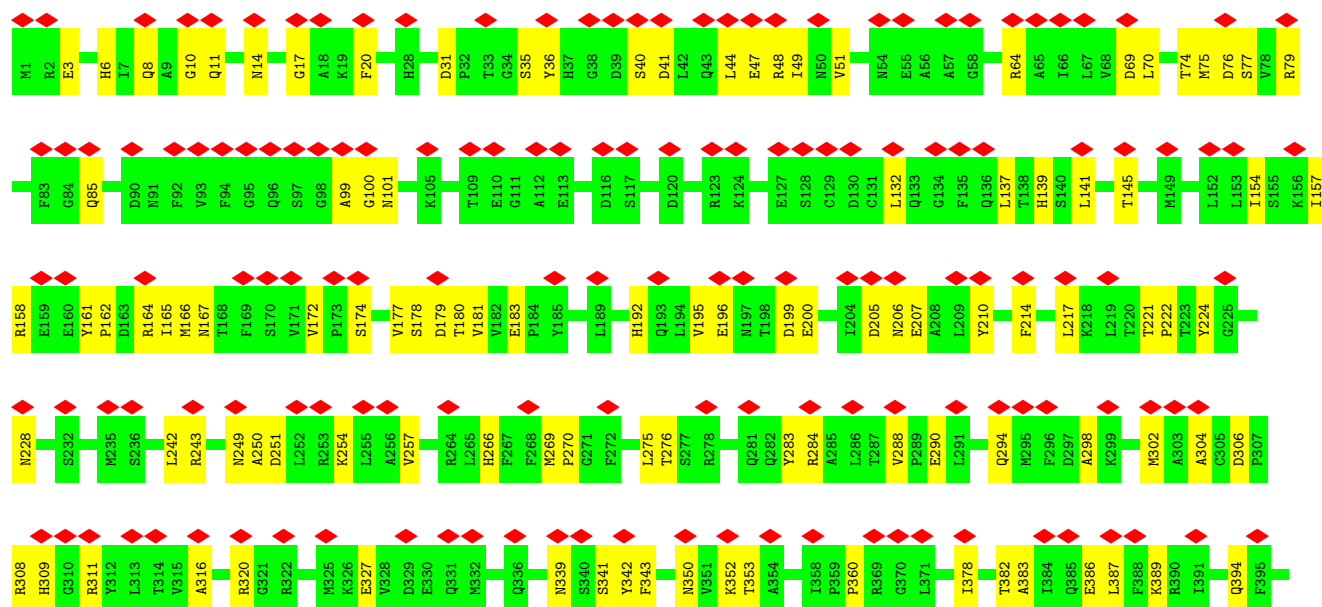
• Molecule 2: Tubulin beta chain

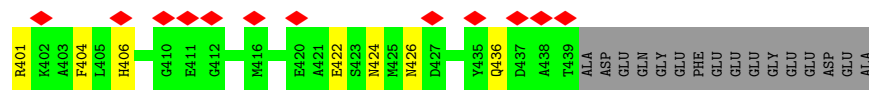
Chain 1R: 31% 71% 26%



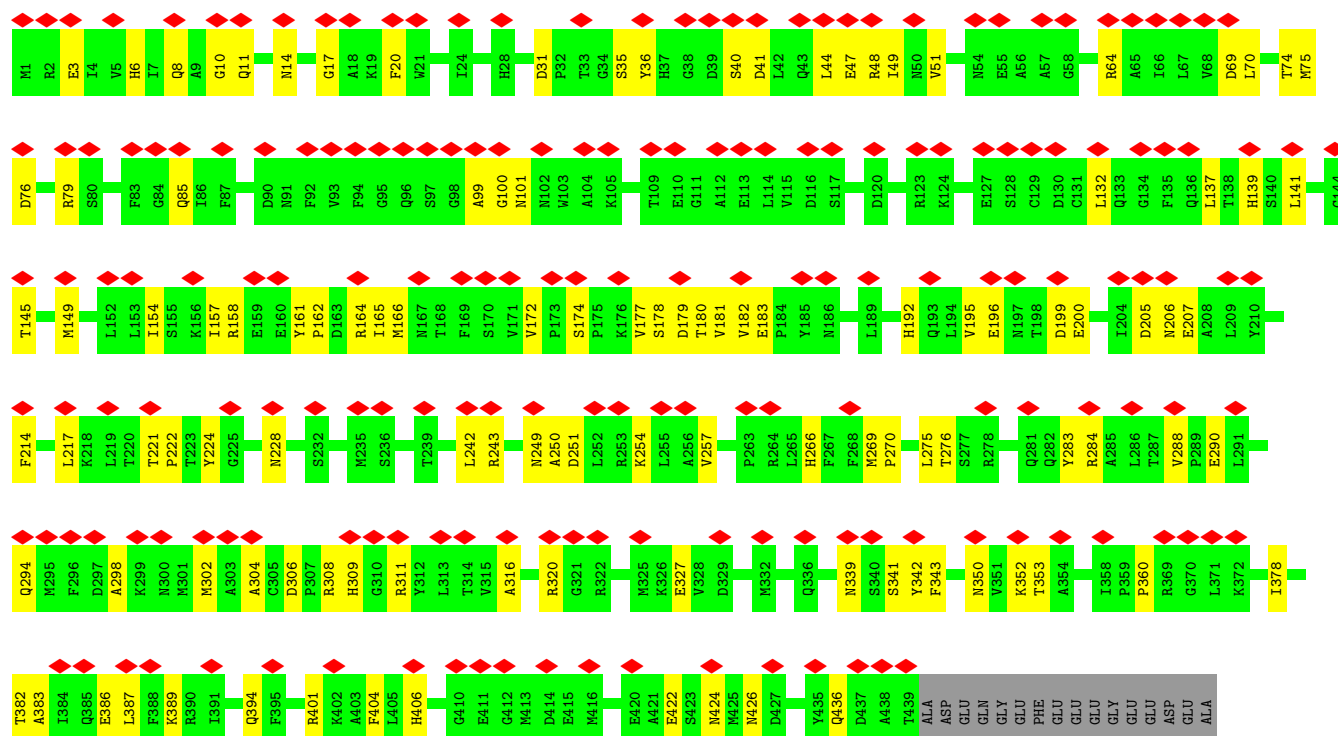
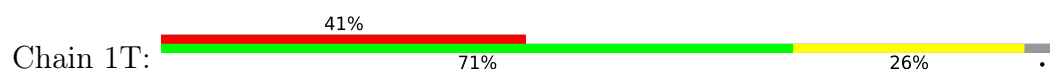
• Molecule 2: Tubulin beta chain

Chain 1S: 36% 70% 26%

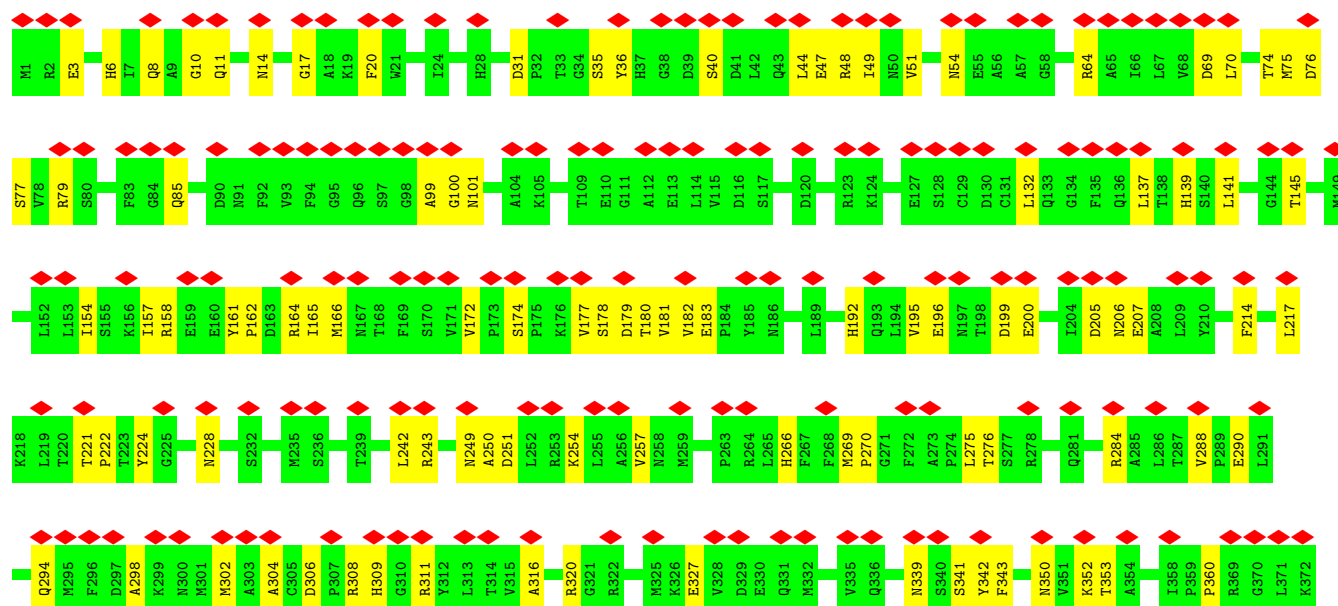
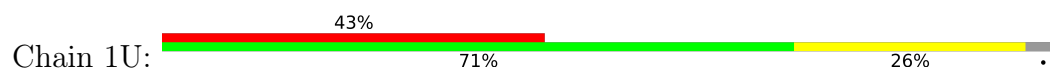


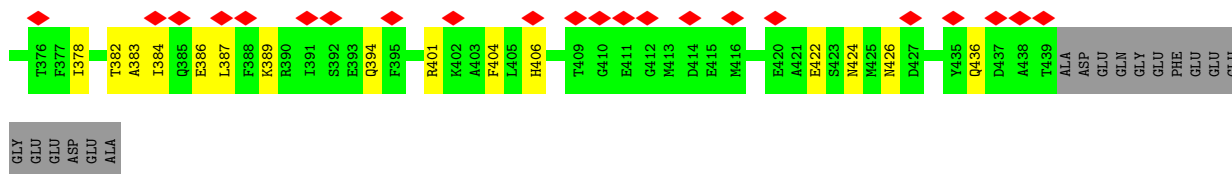


• Molecule 2: Tubulin beta chain

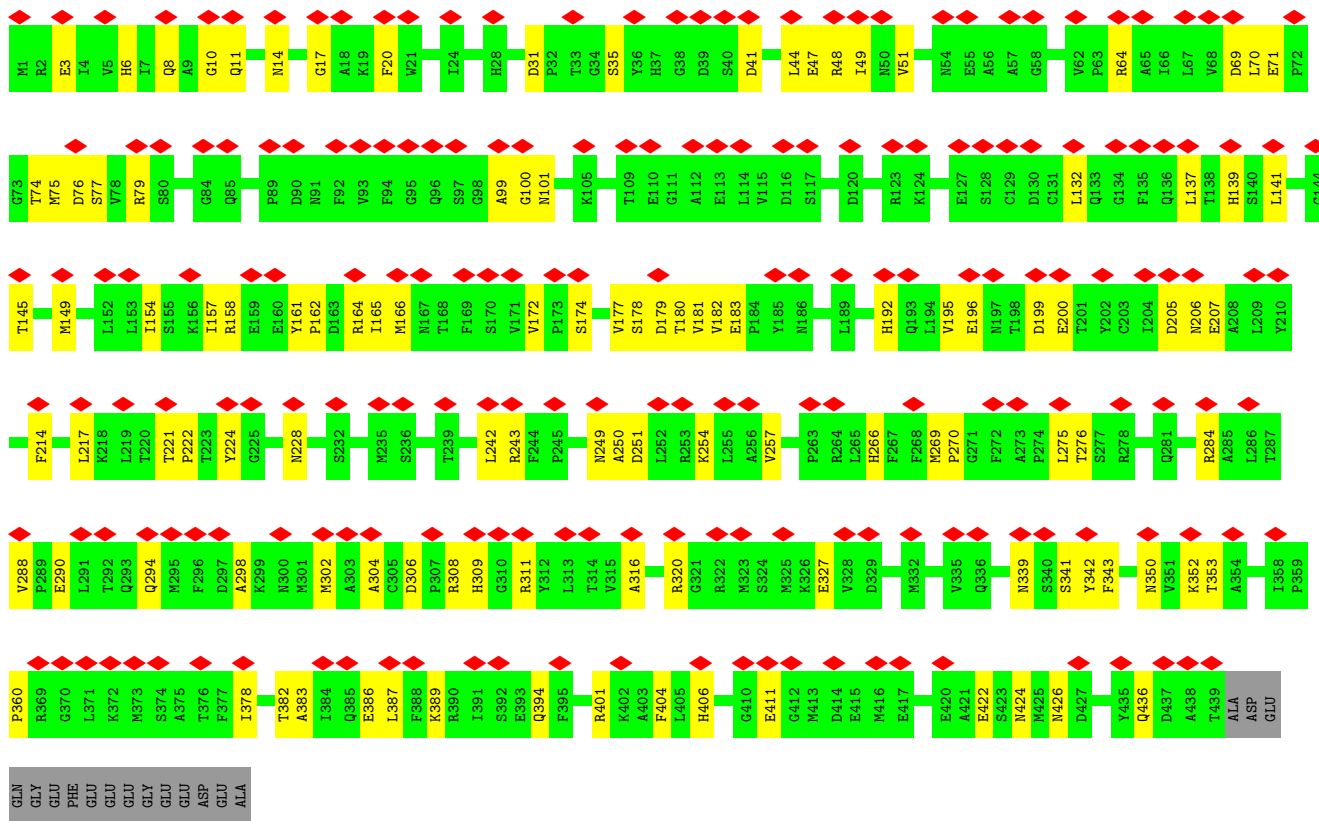
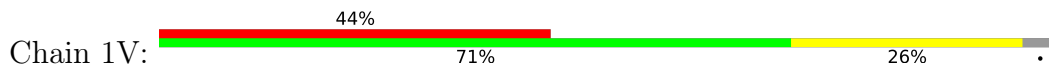


• Molecule 2: Tubulin beta chain

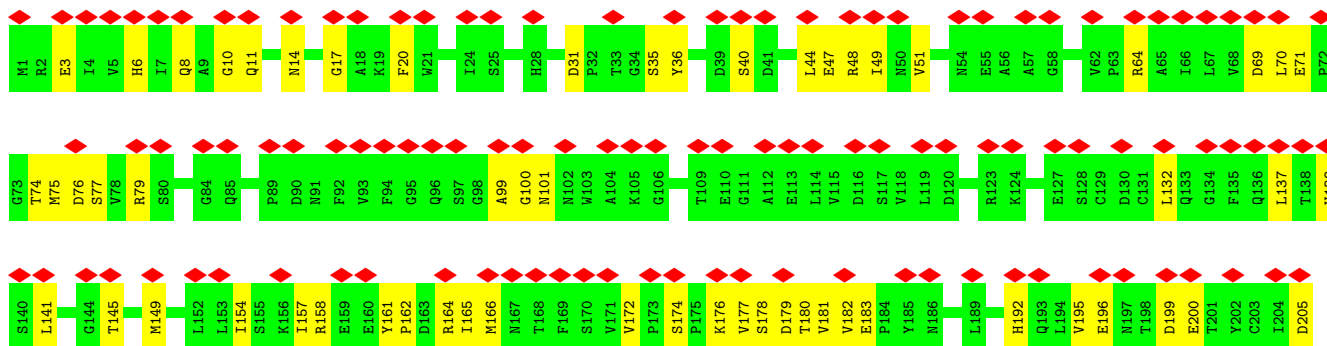
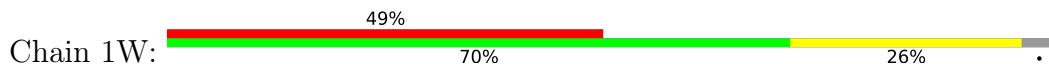




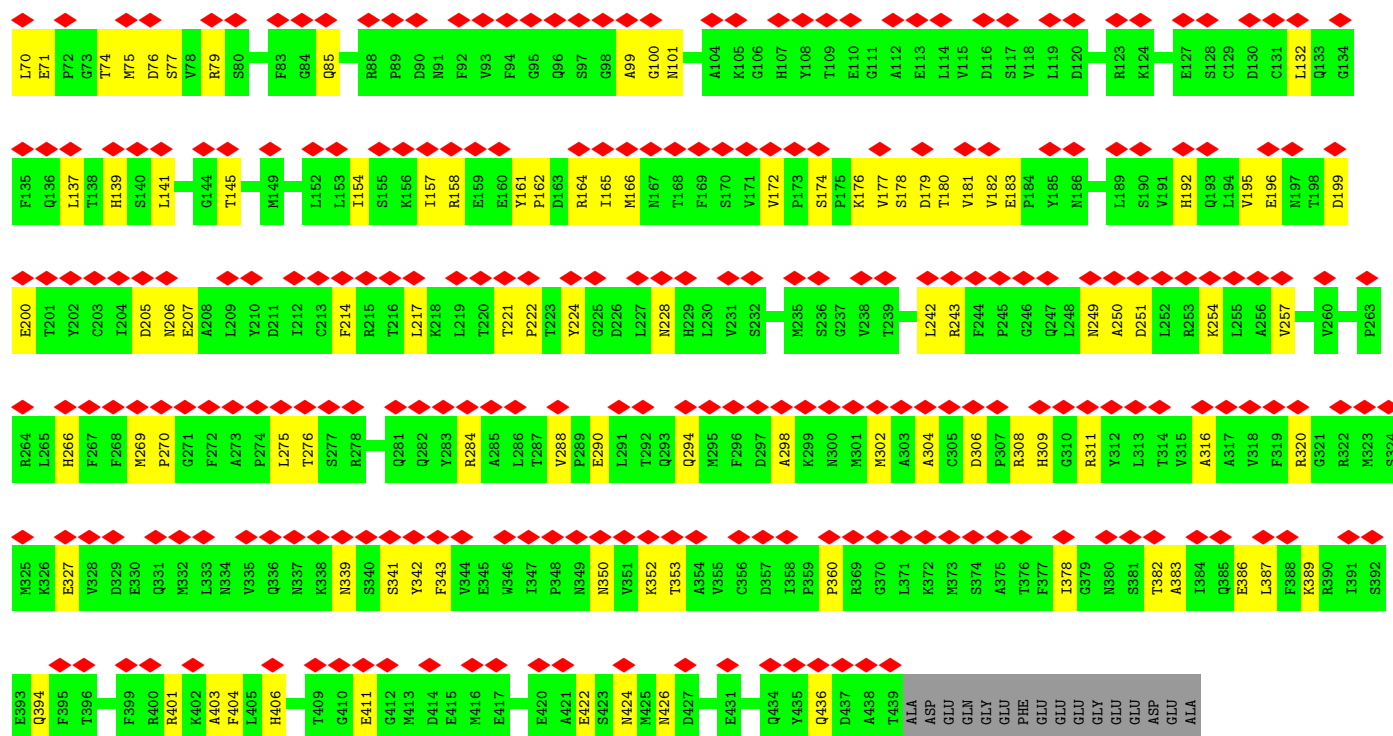
• Molecule 2: Tubulin beta chain



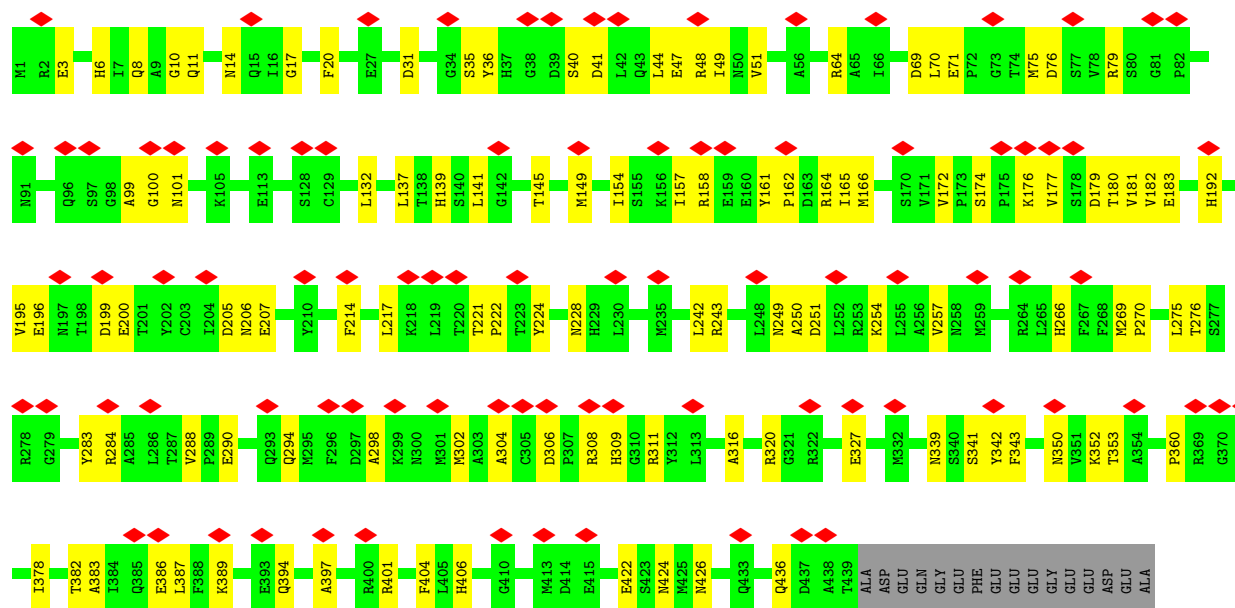
• Molecule 2: Tubulin beta chain



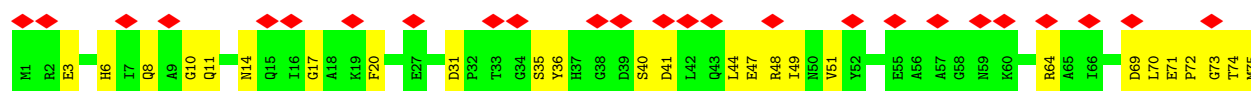


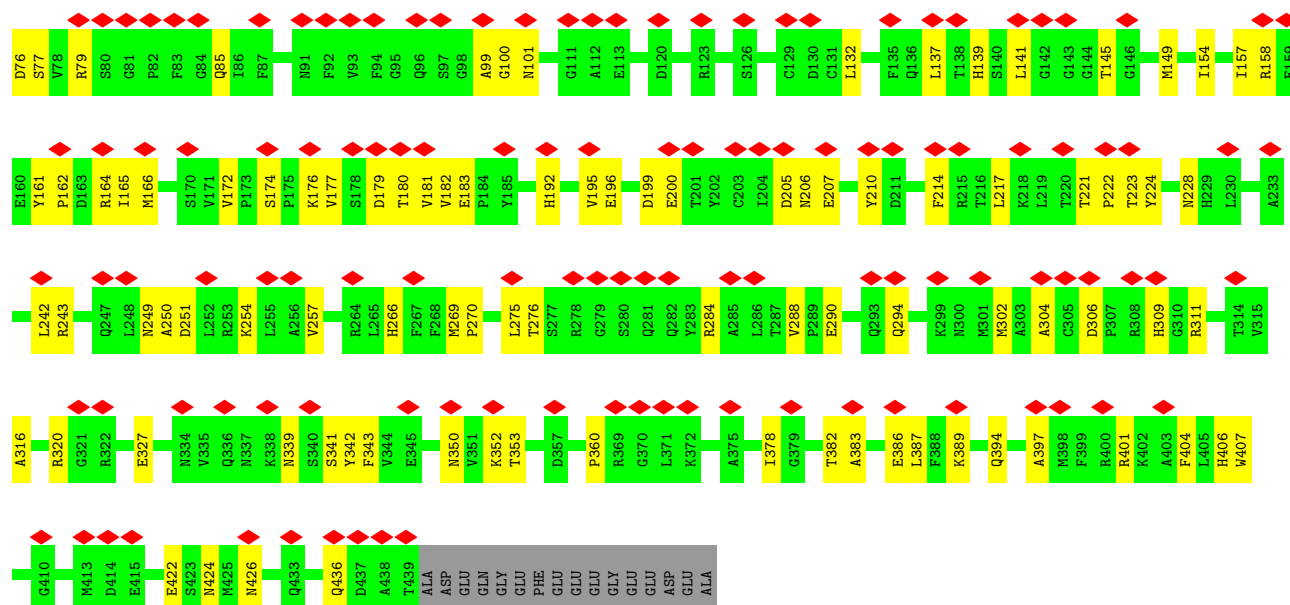


• Molecule 2: Tubulin beta chain

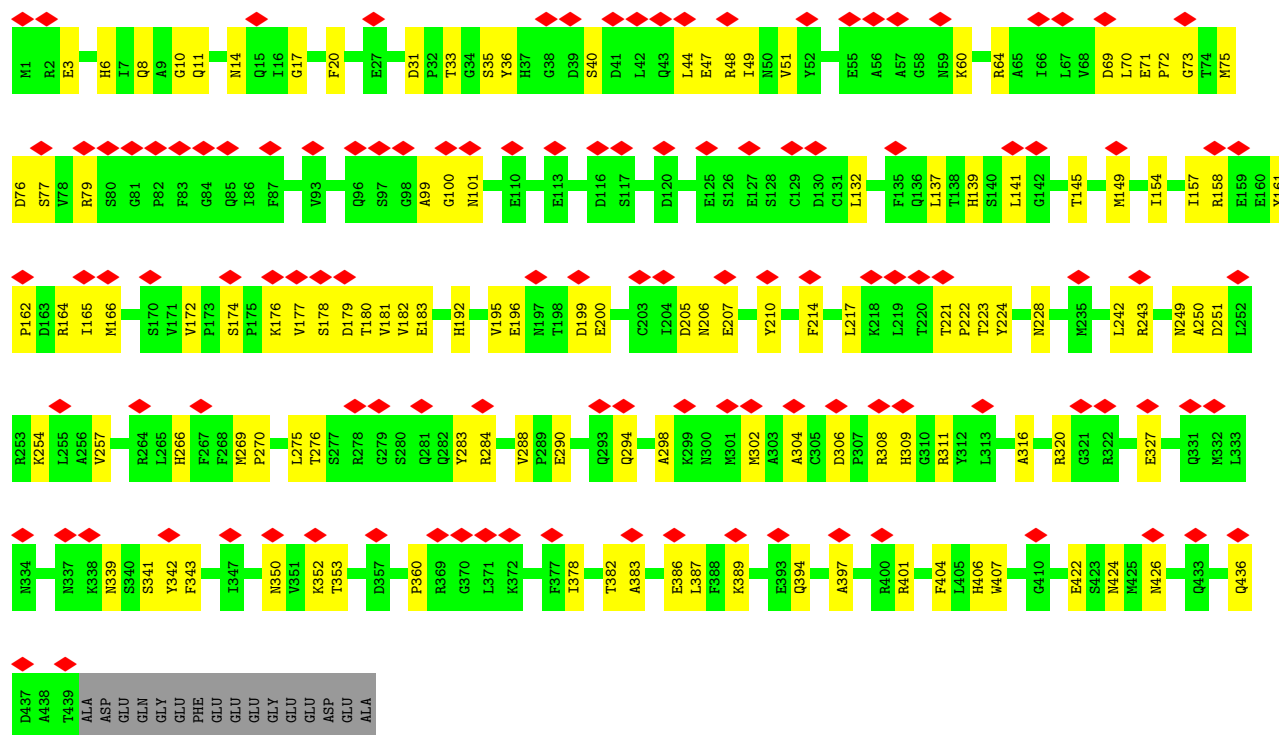


• Molecule 2: Tubulin beta chain

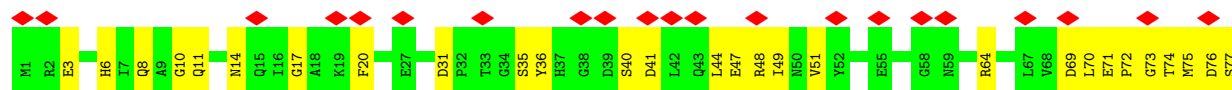


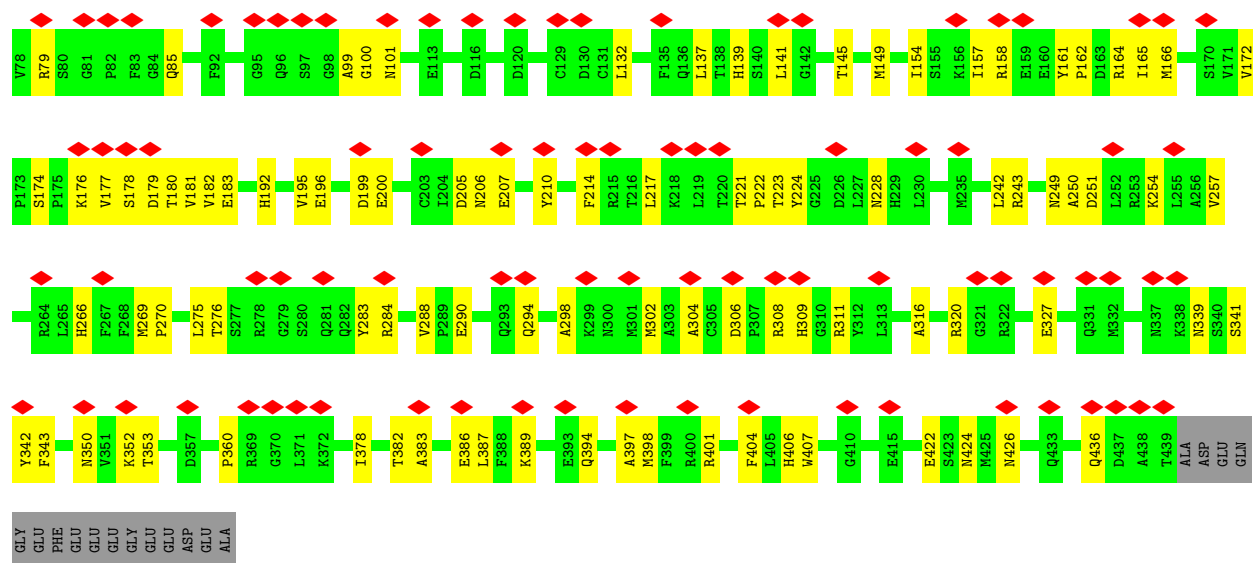


• Molecule 2: Tubulin beta chain

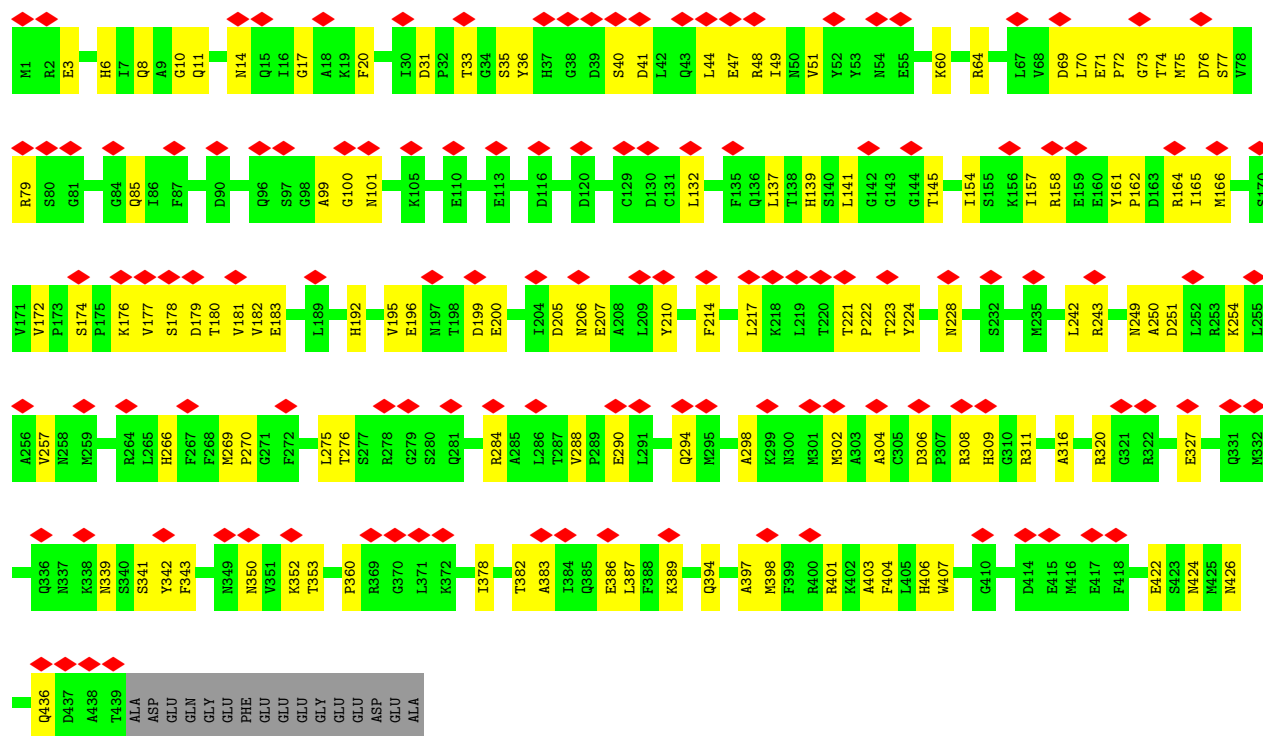


• Molecule 2: Tubulin beta chain

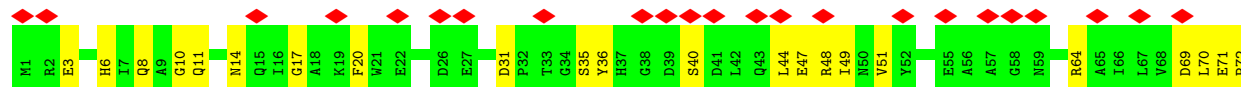


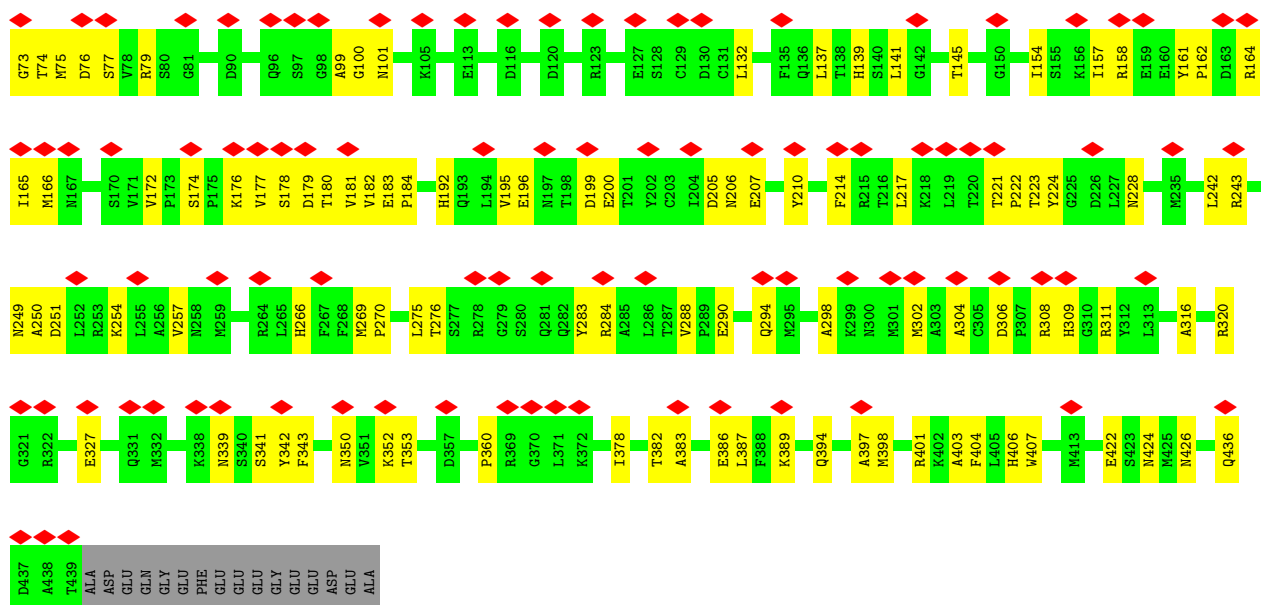


• Molecule 2: Tubulin beta chain

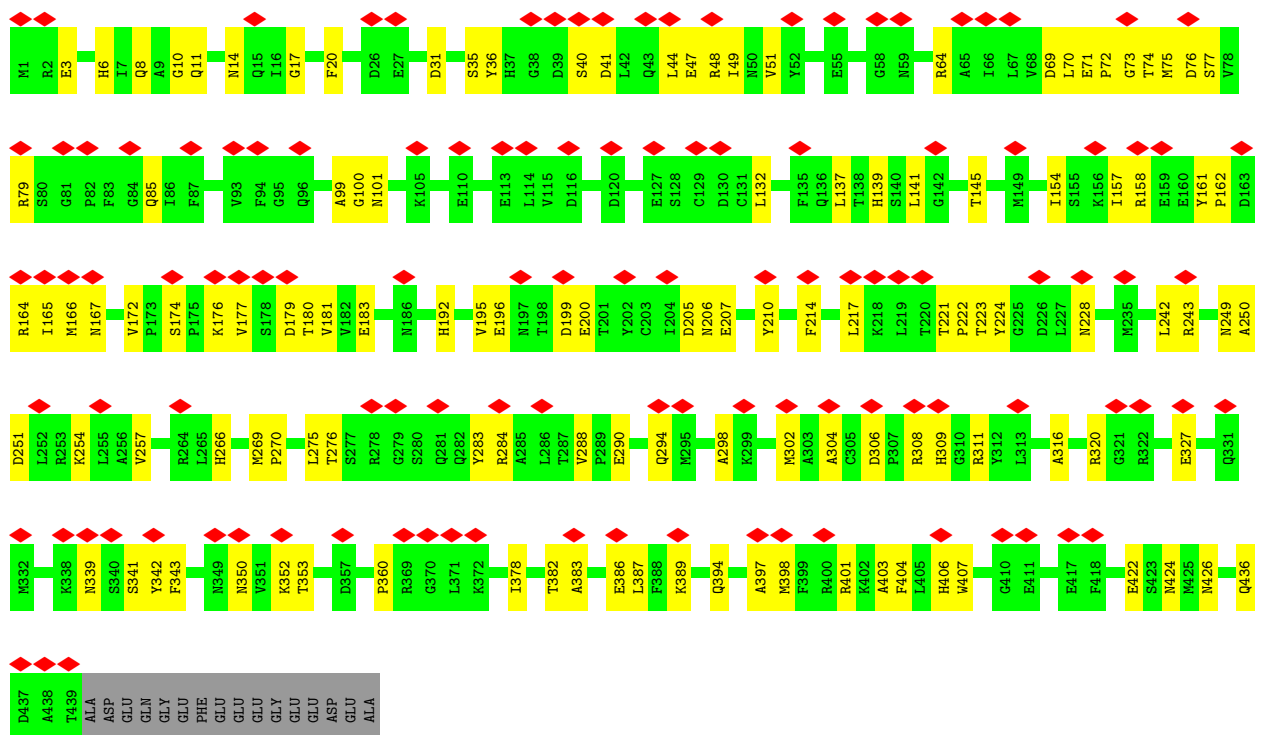


• Molecule 2: Tubulin beta chain





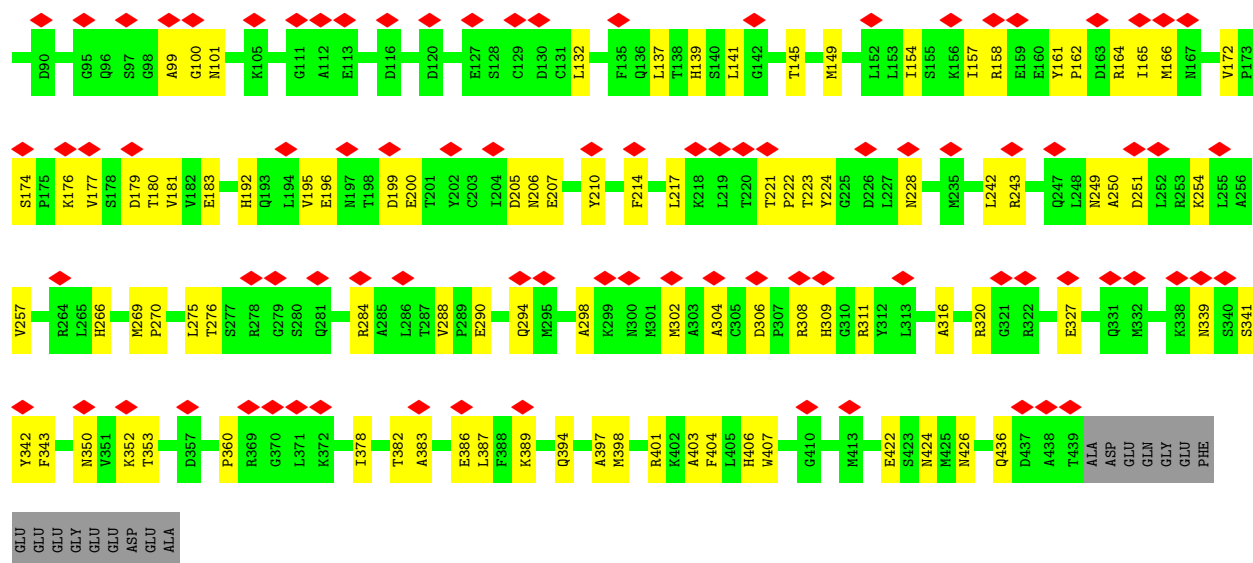
• Molecule 2: Tubulin beta chain



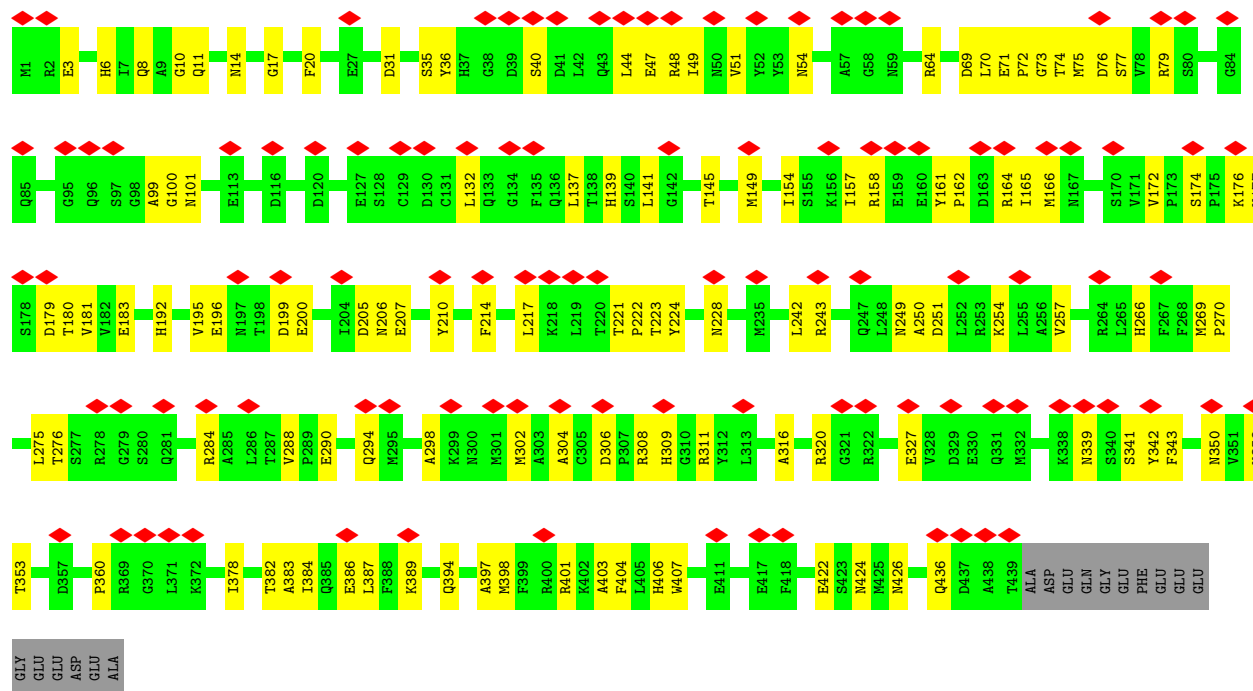
• Molecule 2: Tubulin beta chain





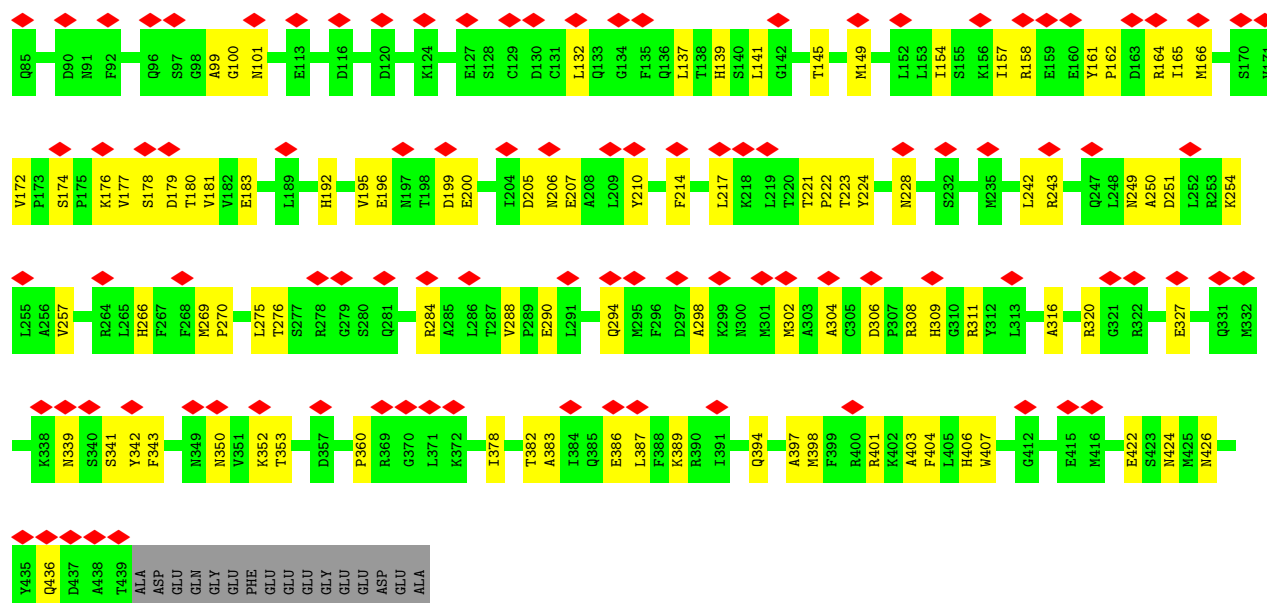


• Molecule 2: Tubulin beta chain

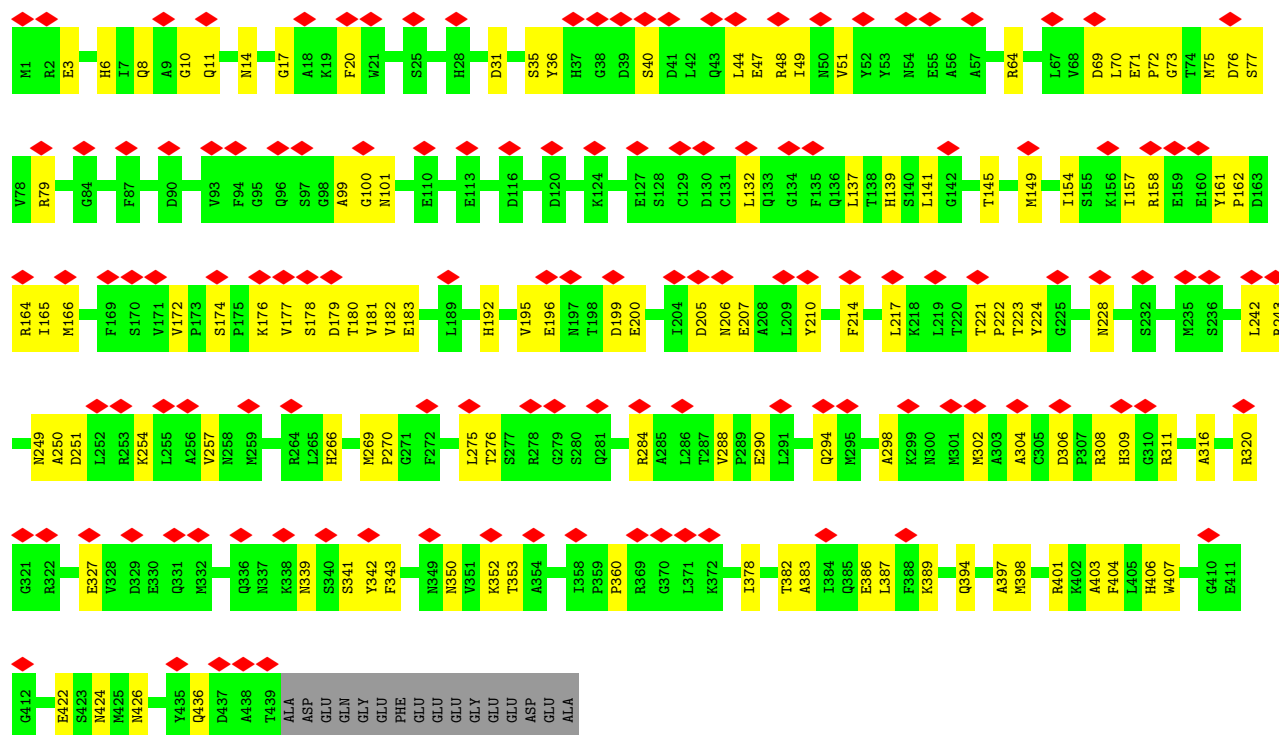


• Molecule 2: Tubulin beta chain

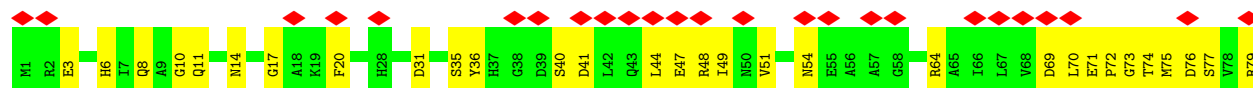


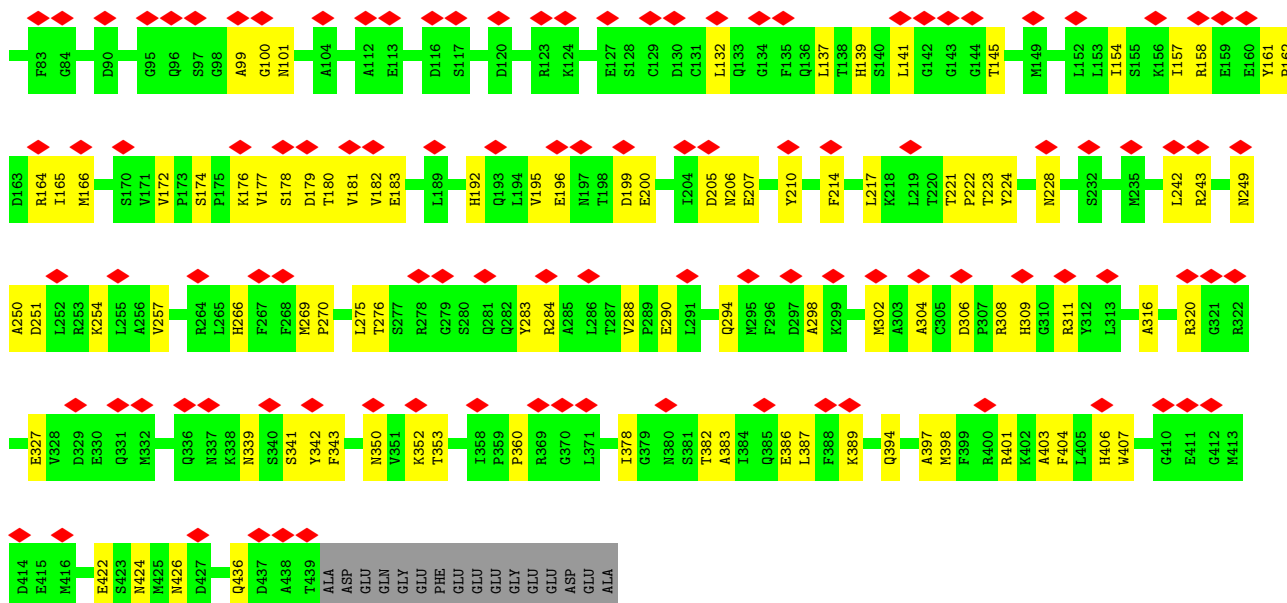


• Molecule 2: Tubulin beta chain

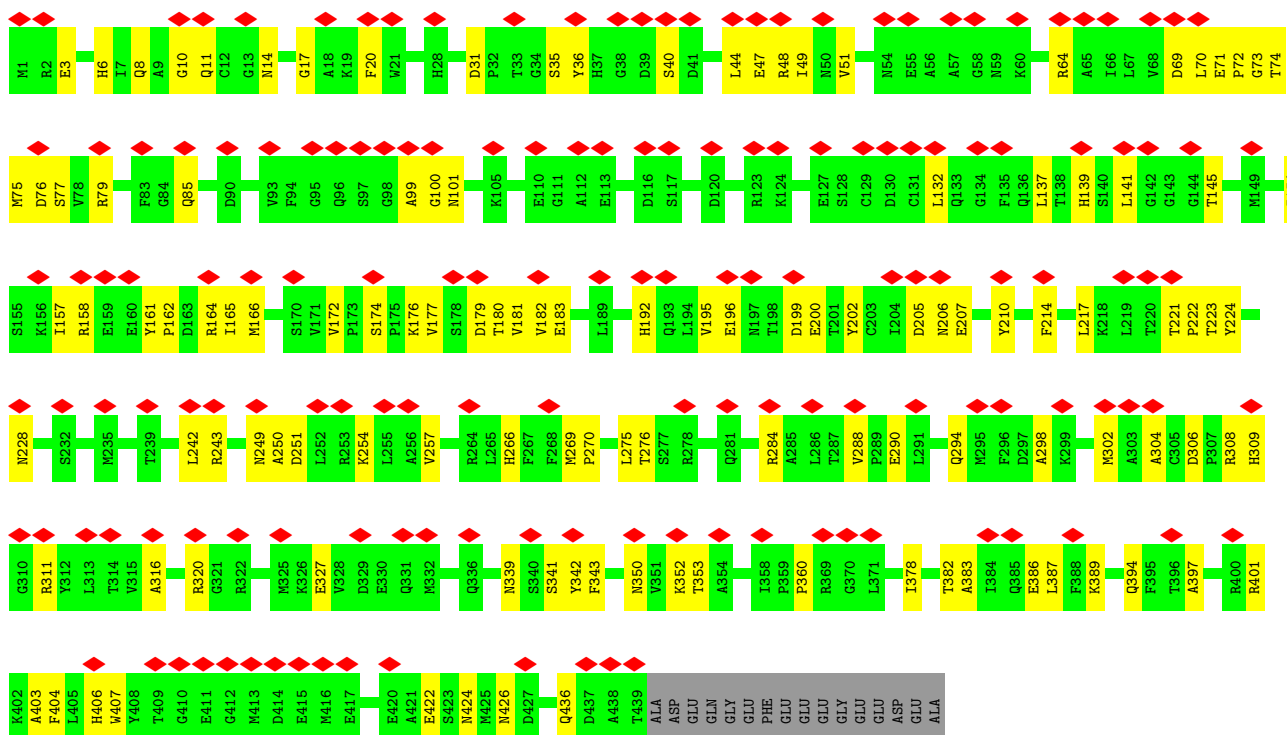


• Molecule 2: Tubulin beta chain

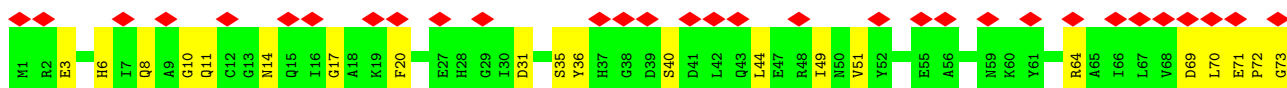
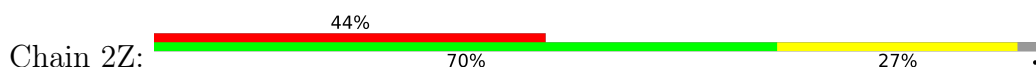


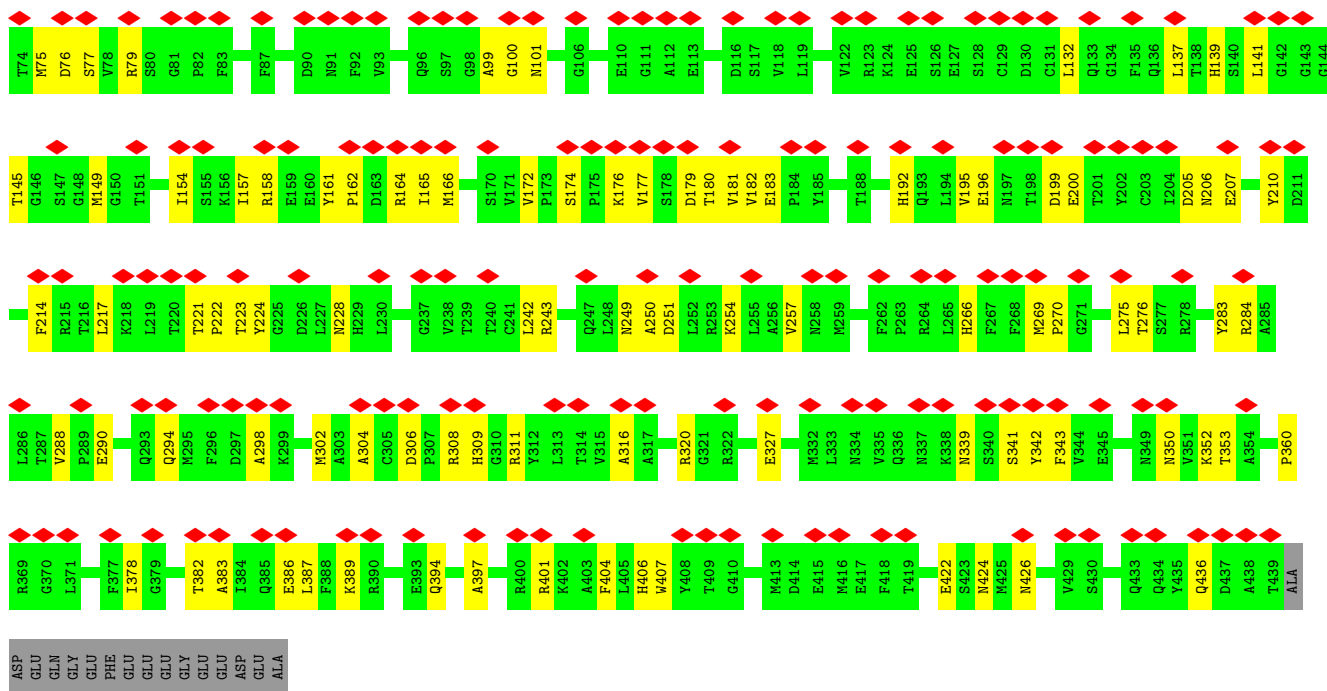


- Molecule 2: Tubulin beta chain

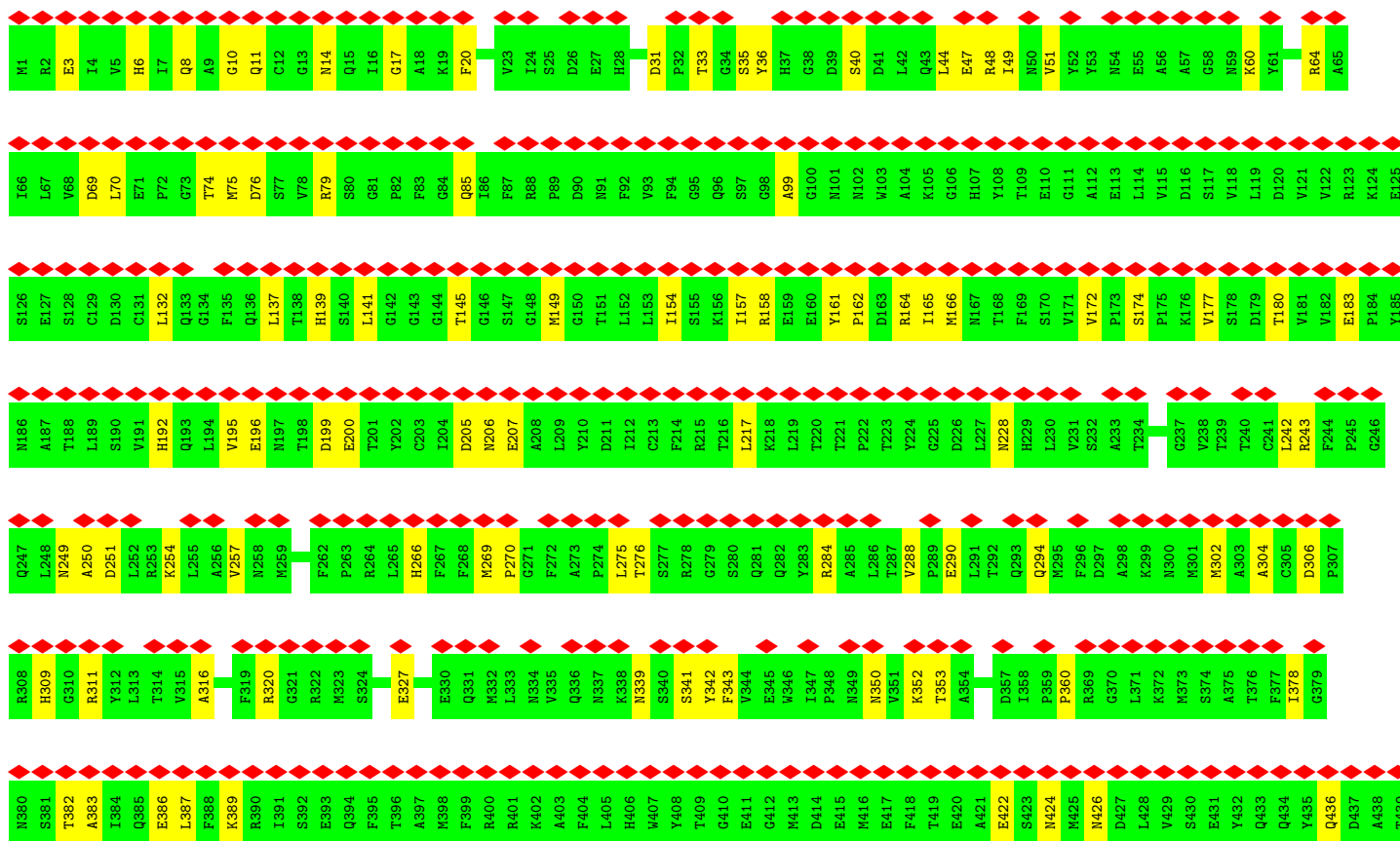
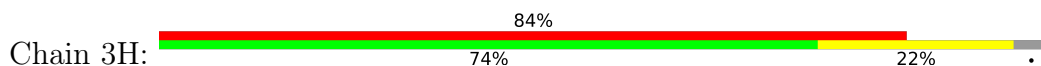


- Molecule 2: Tubulin beta chain





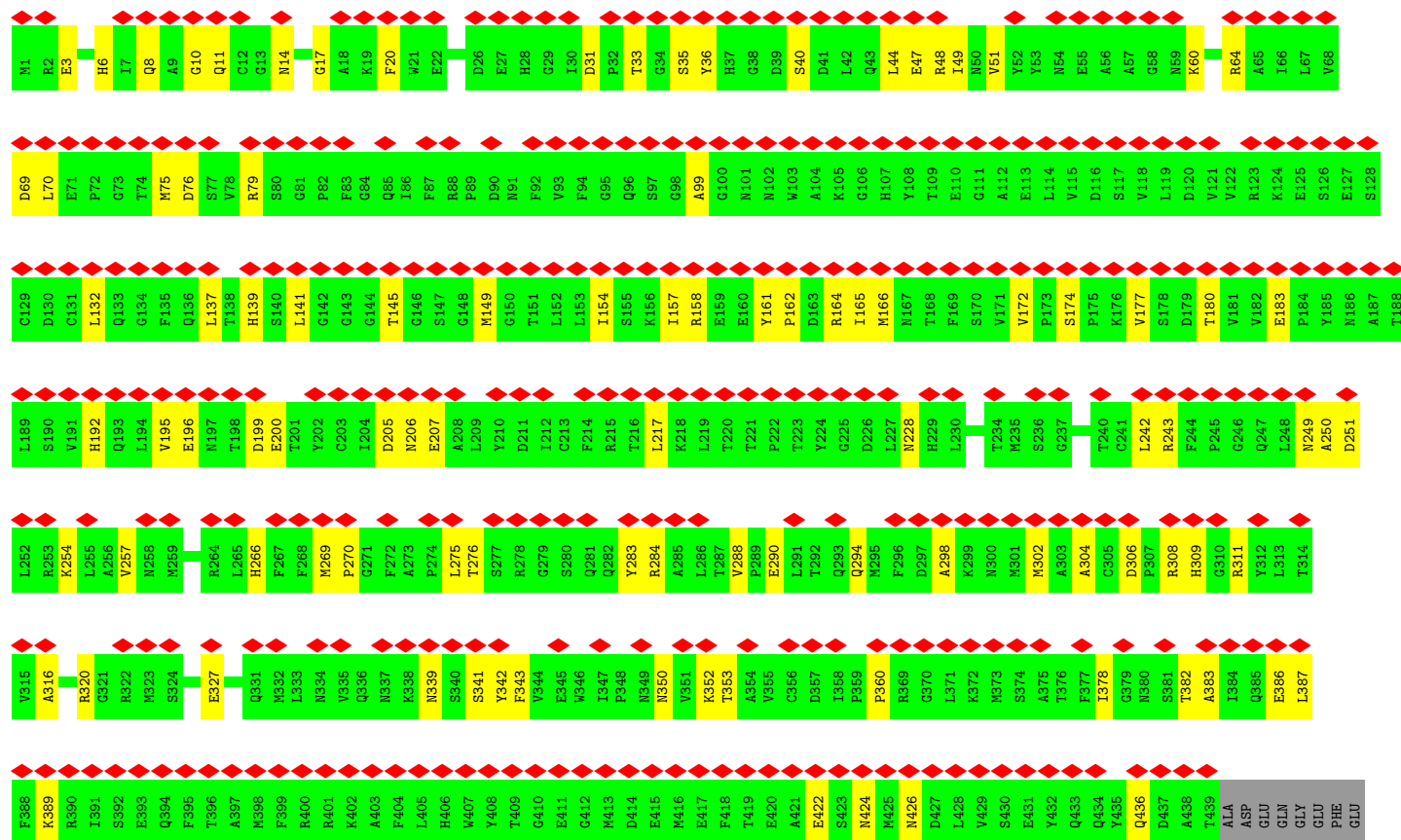
• Molecule 2: Tubulin beta chain



ALA  
ASP  
GLU  
GLN  
GLY  
PHE  
GLU  
GLU  
GLY  
GLY  
ASP  
GLU  
ALA

• Molecule 2: Tubulin beta chain

Chain 3O: 

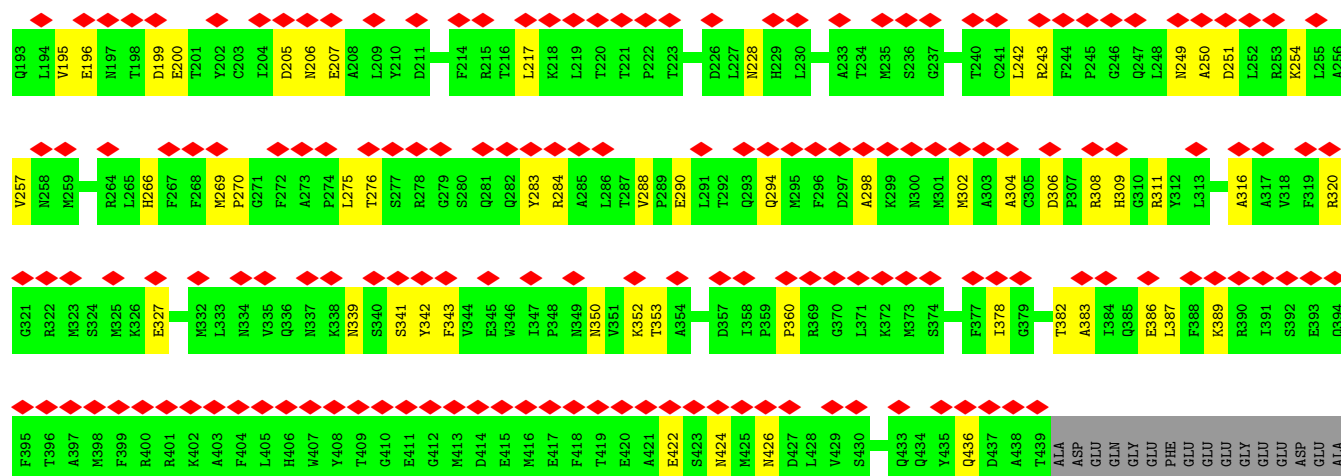


GLU  
GLU  
GLY  
GLY  
ASP  
GLU  
ALA

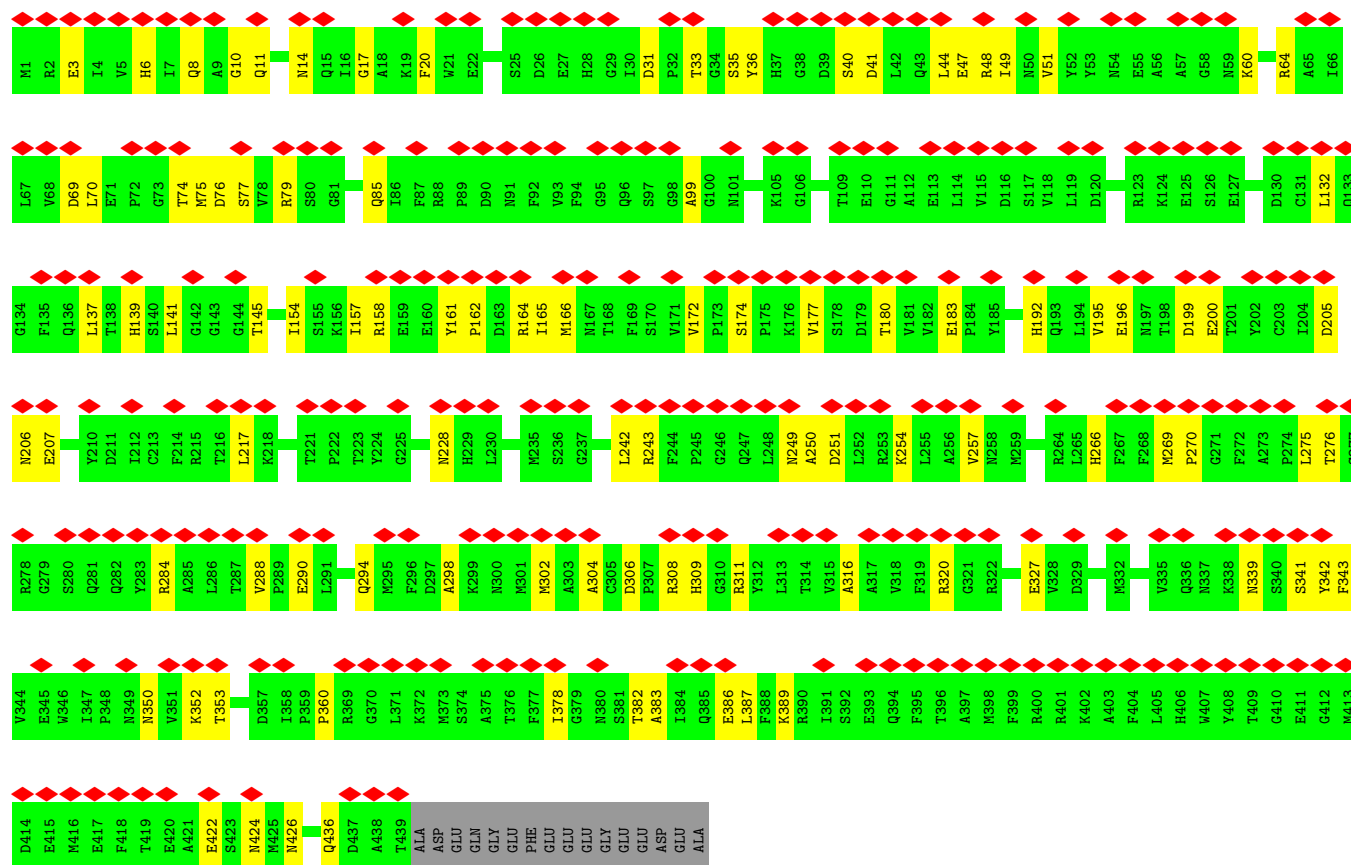
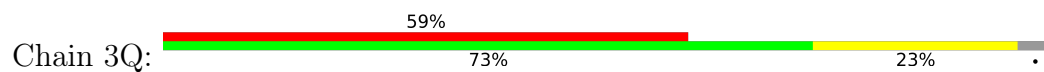
• Molecule 2: Tubulin beta chain

Chain 3P: 

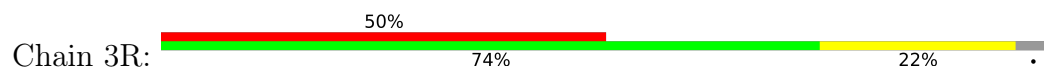


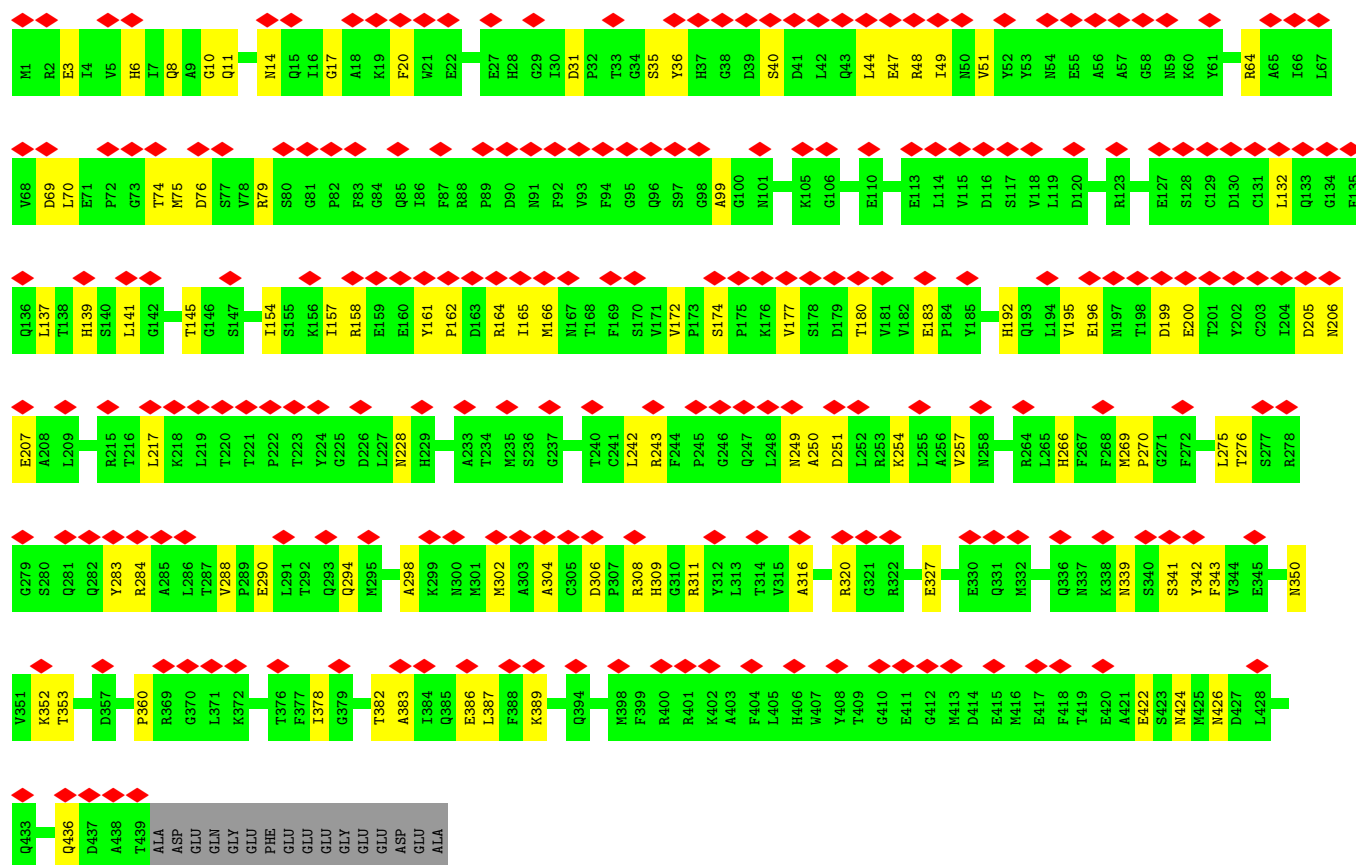


• Molecule 2: Tubulin beta chain

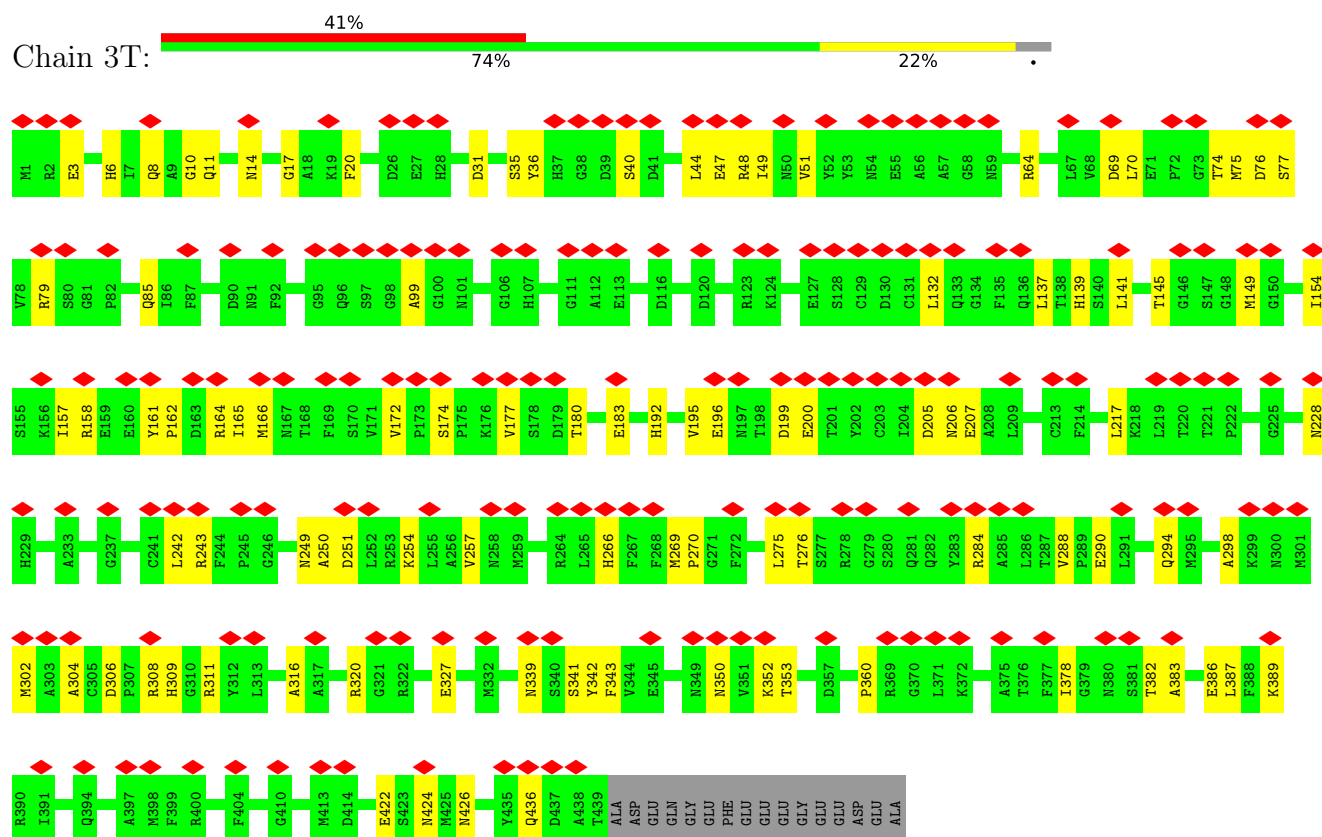


• Molecule 2: Tubulin beta chain



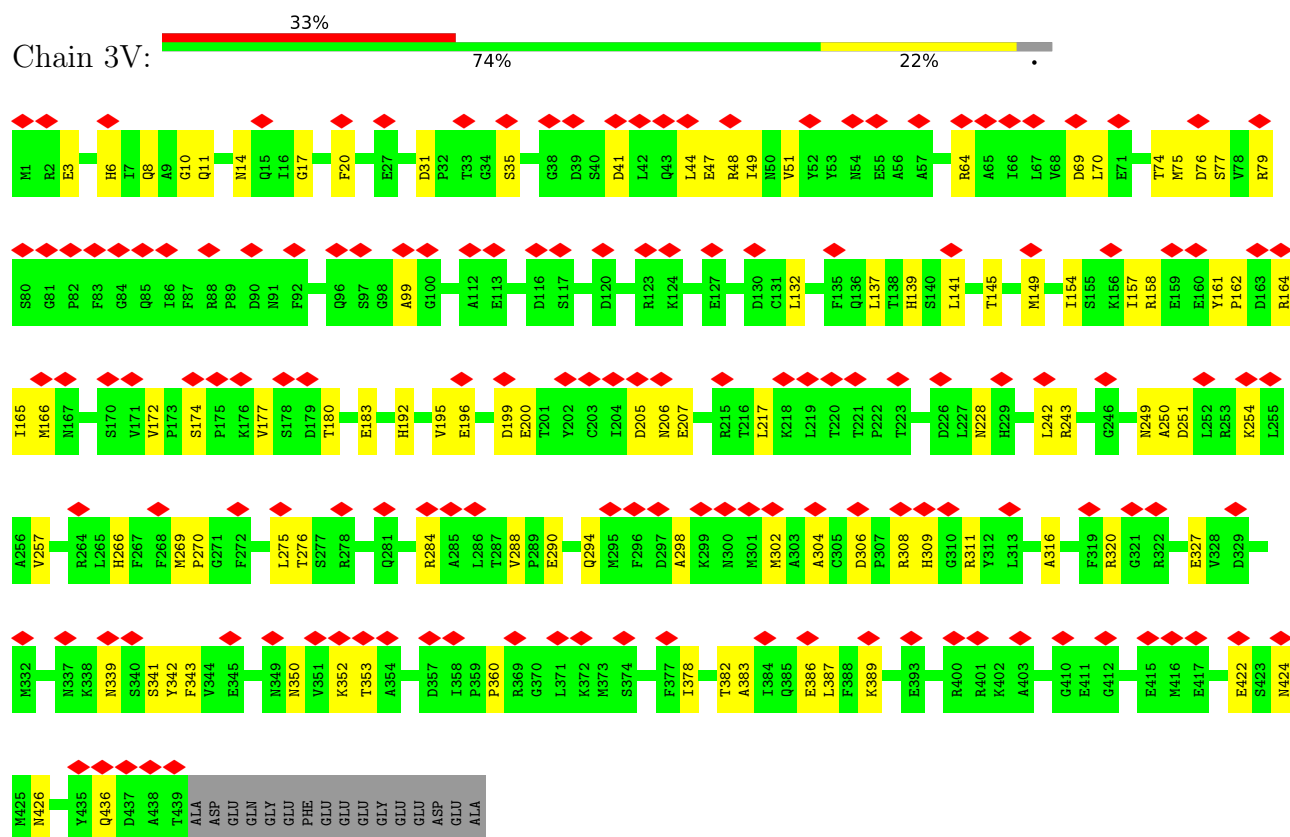


- Molecule 2: Tubulin beta chain



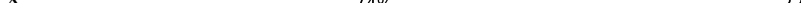


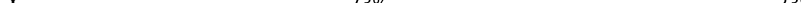
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain

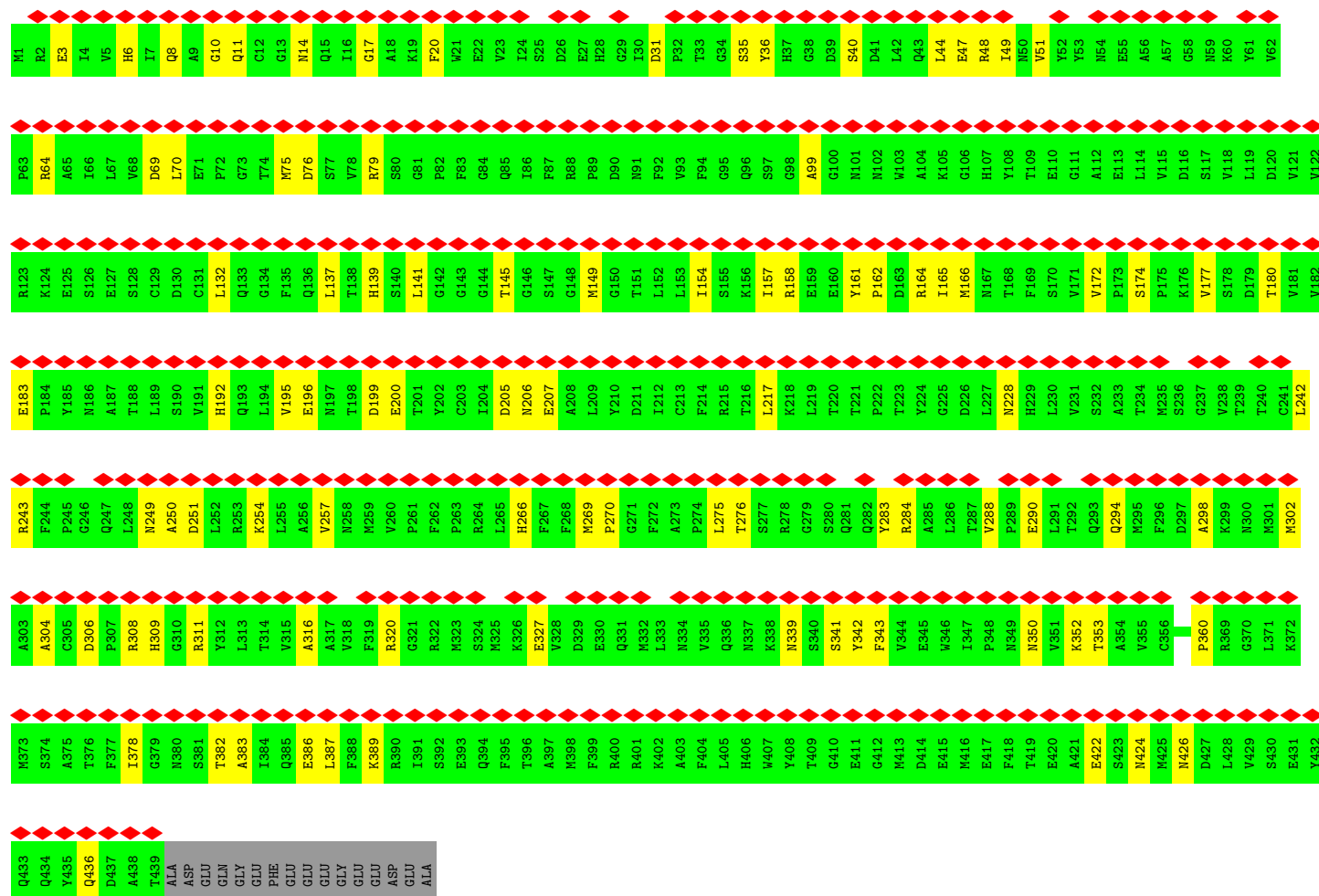
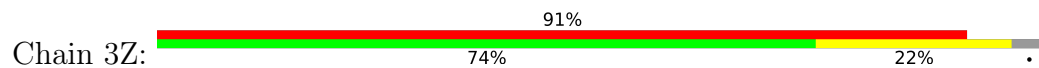


Chain 3X: 

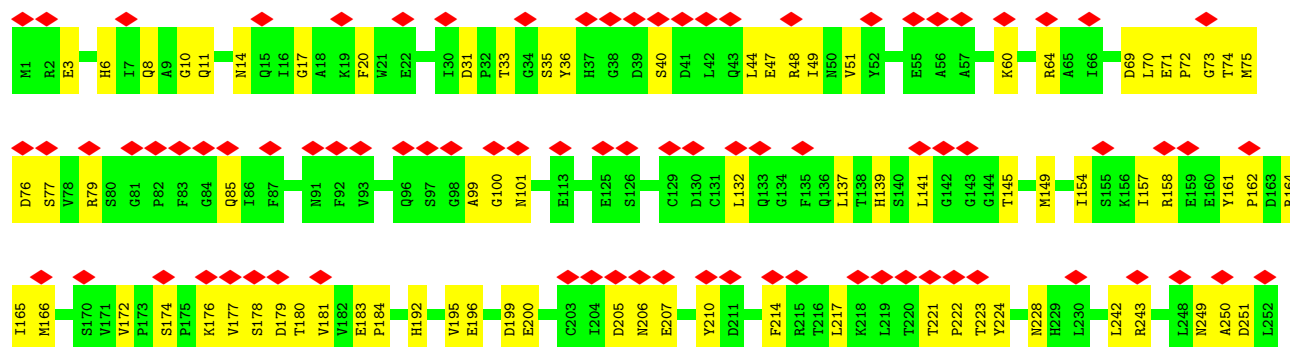
Chain 3Y:  45% 73% 23%

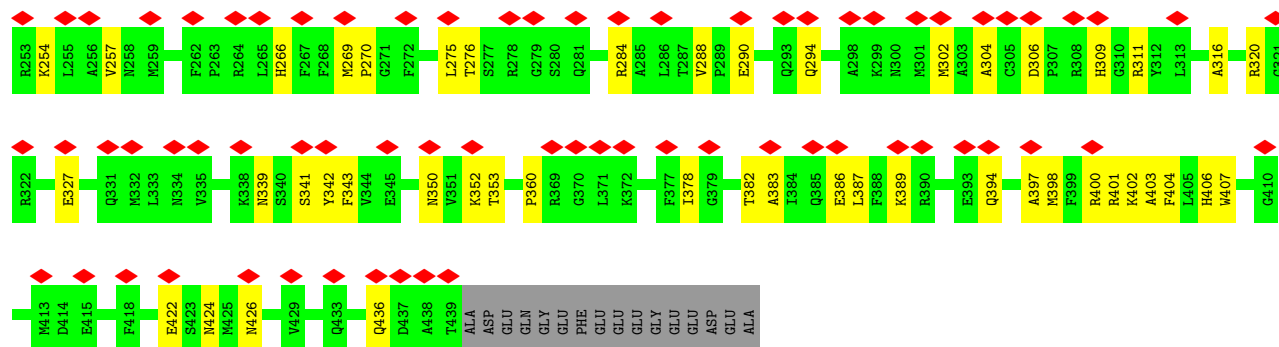
GLU  
ALA

• Molecule 2: Tubulin beta chain

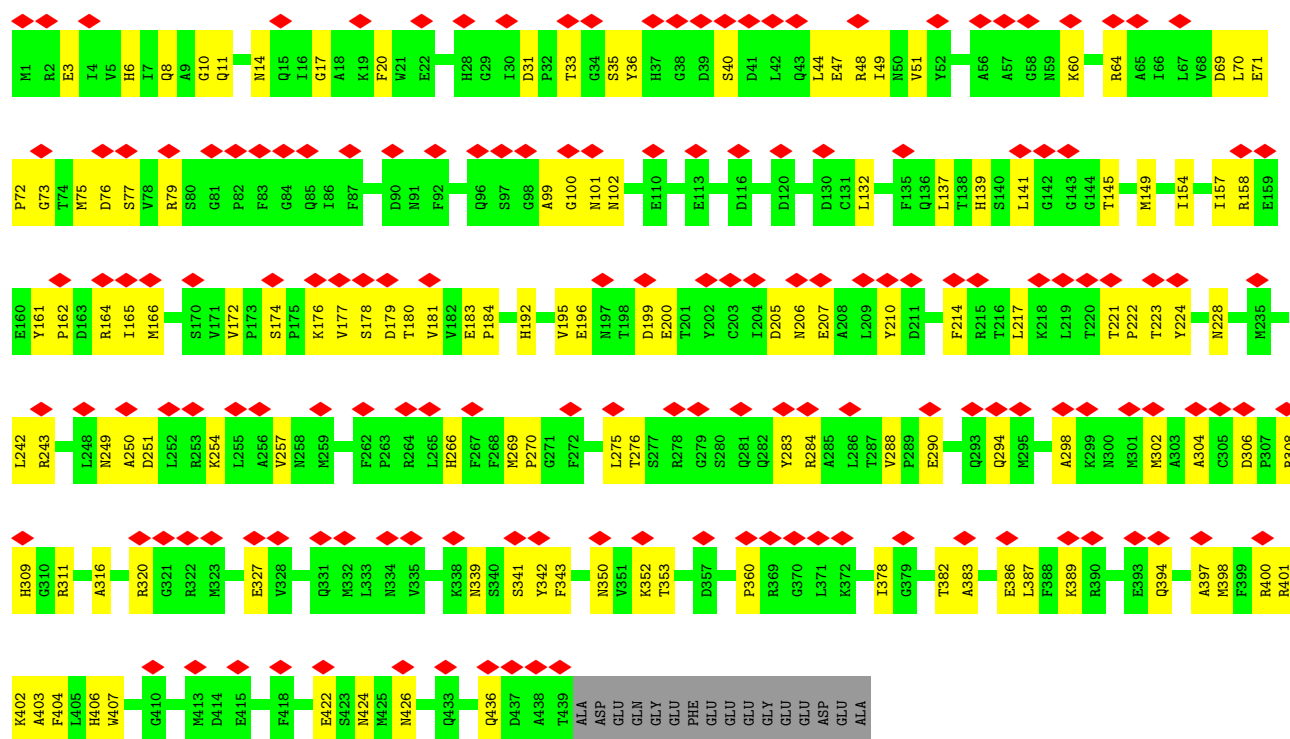


• Molecule 2: Tubulin beta chain

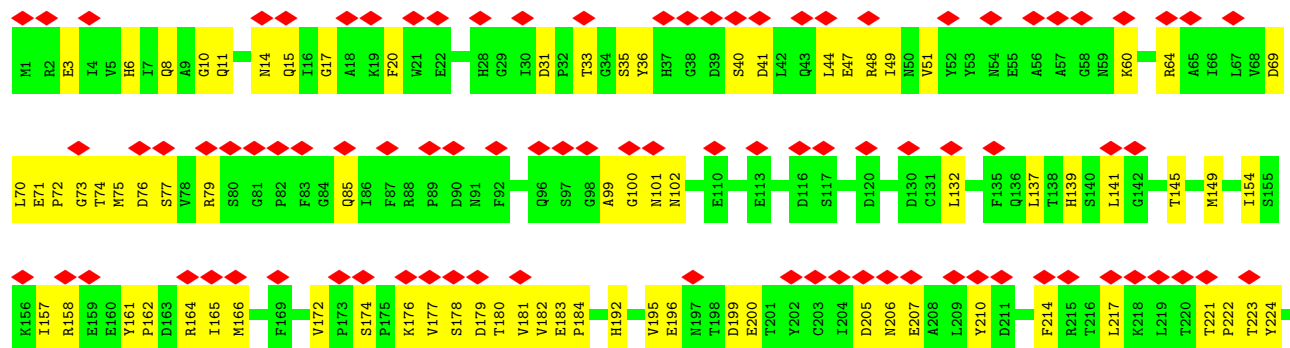


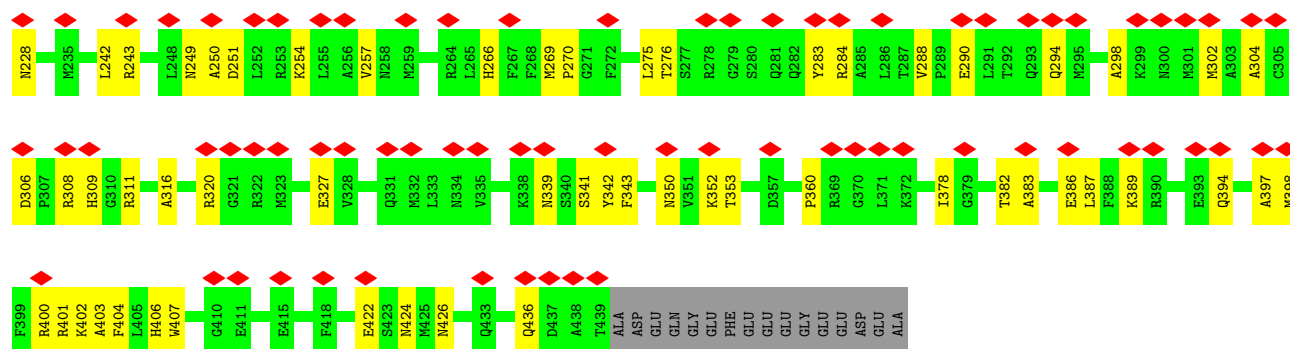


• Molecule 2: Tubulin beta chain

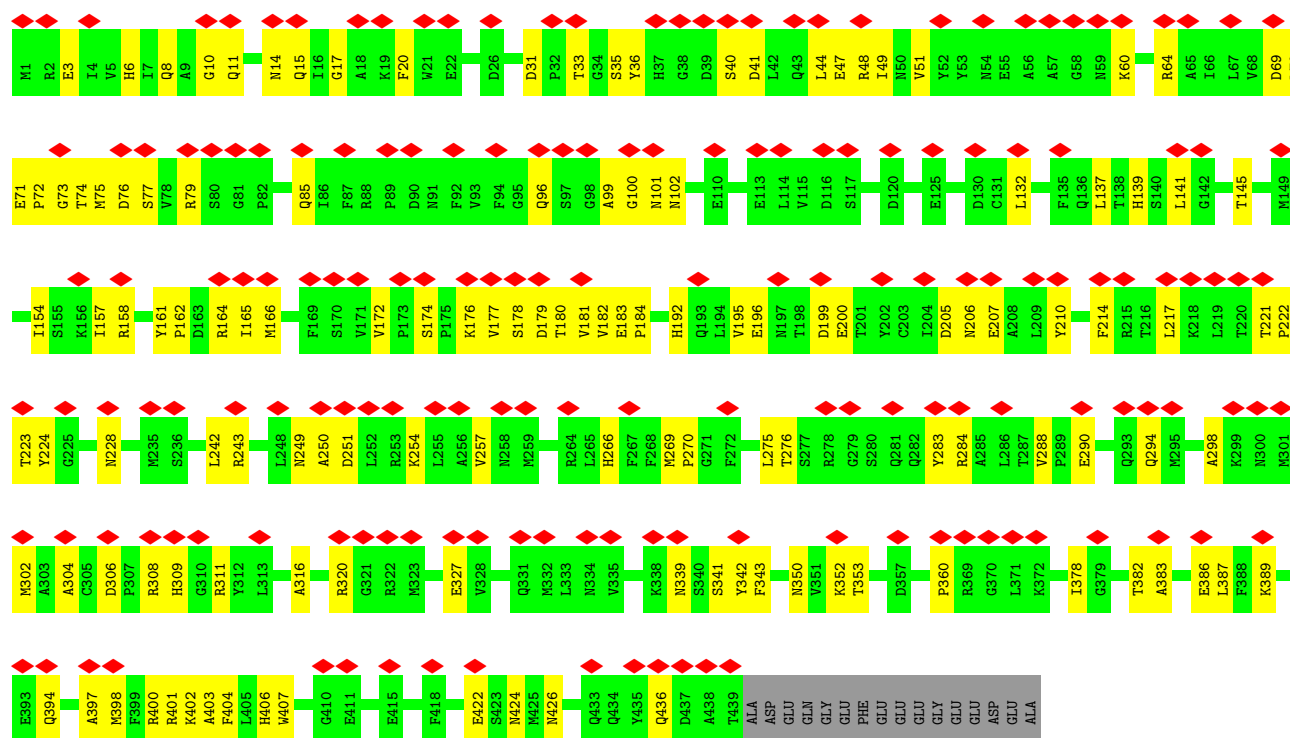


• Molecule 2: Tubulin beta chain

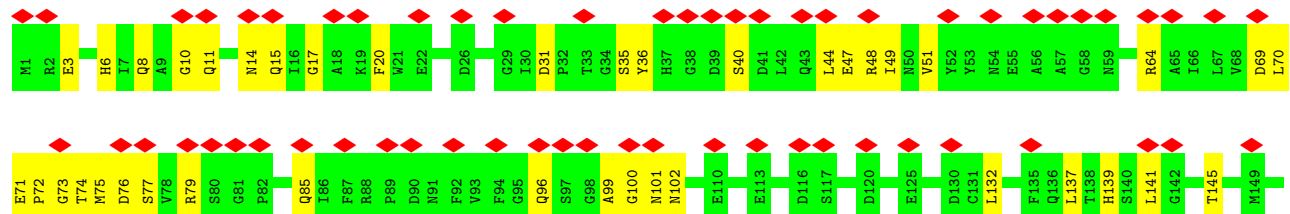


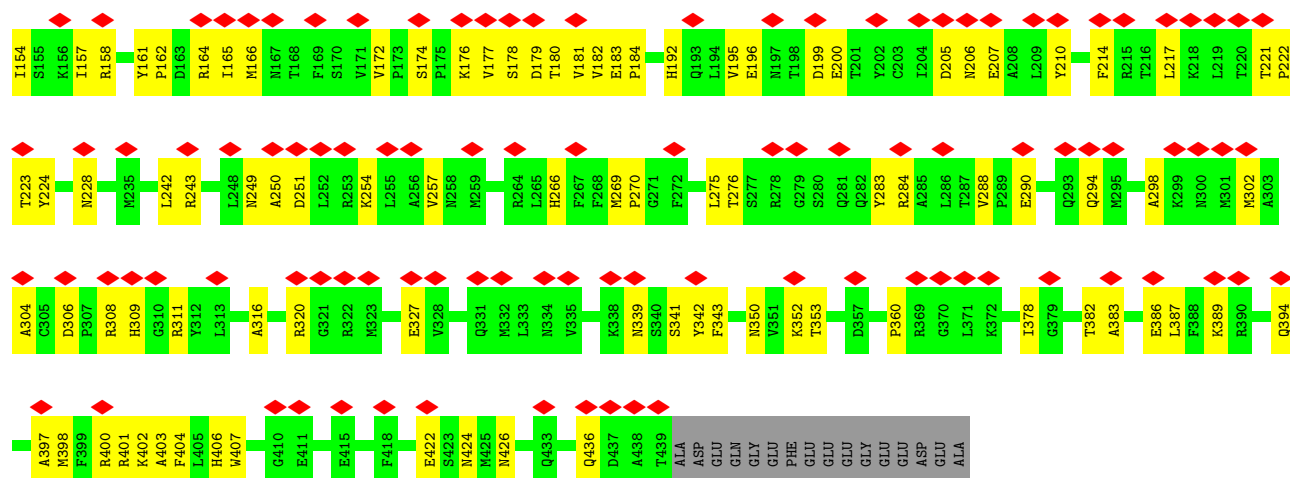


• Molecule 2: Tubulin beta chain

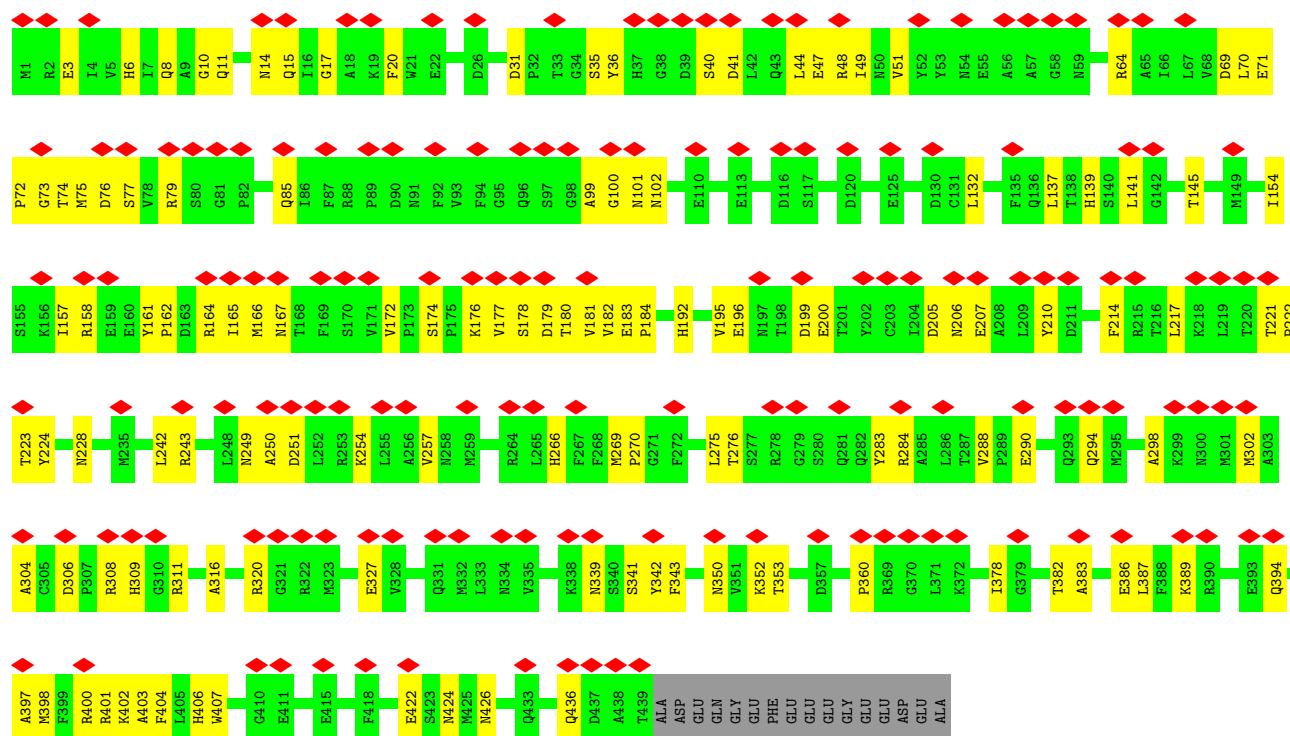


• Molecule 2: Tubulin beta chain

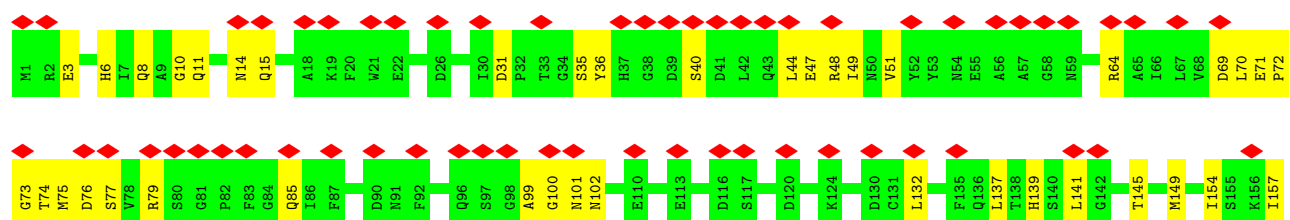


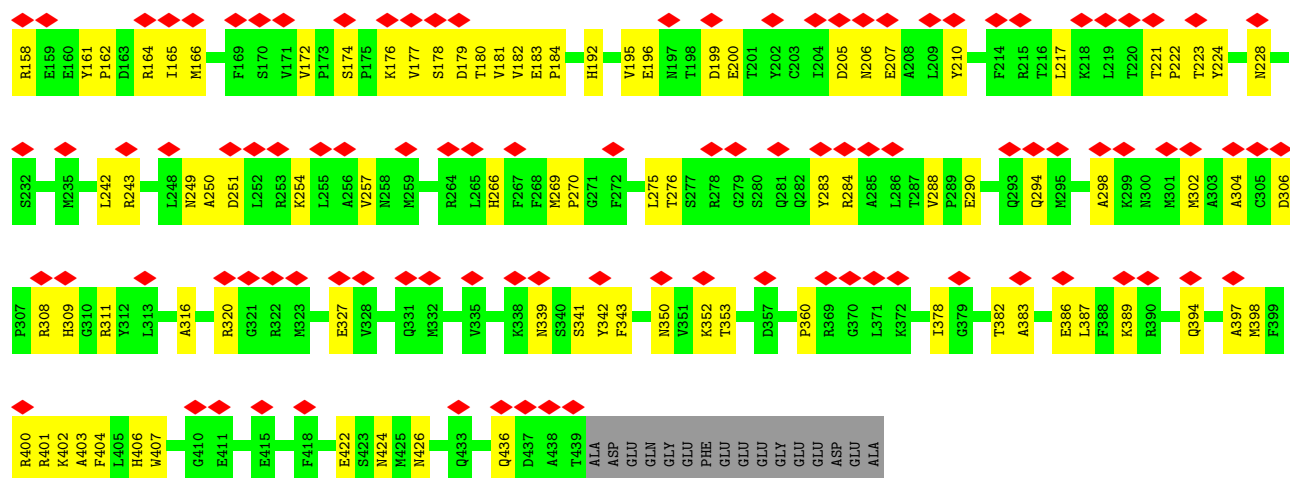


• Molecule 2: Tubulin beta chain

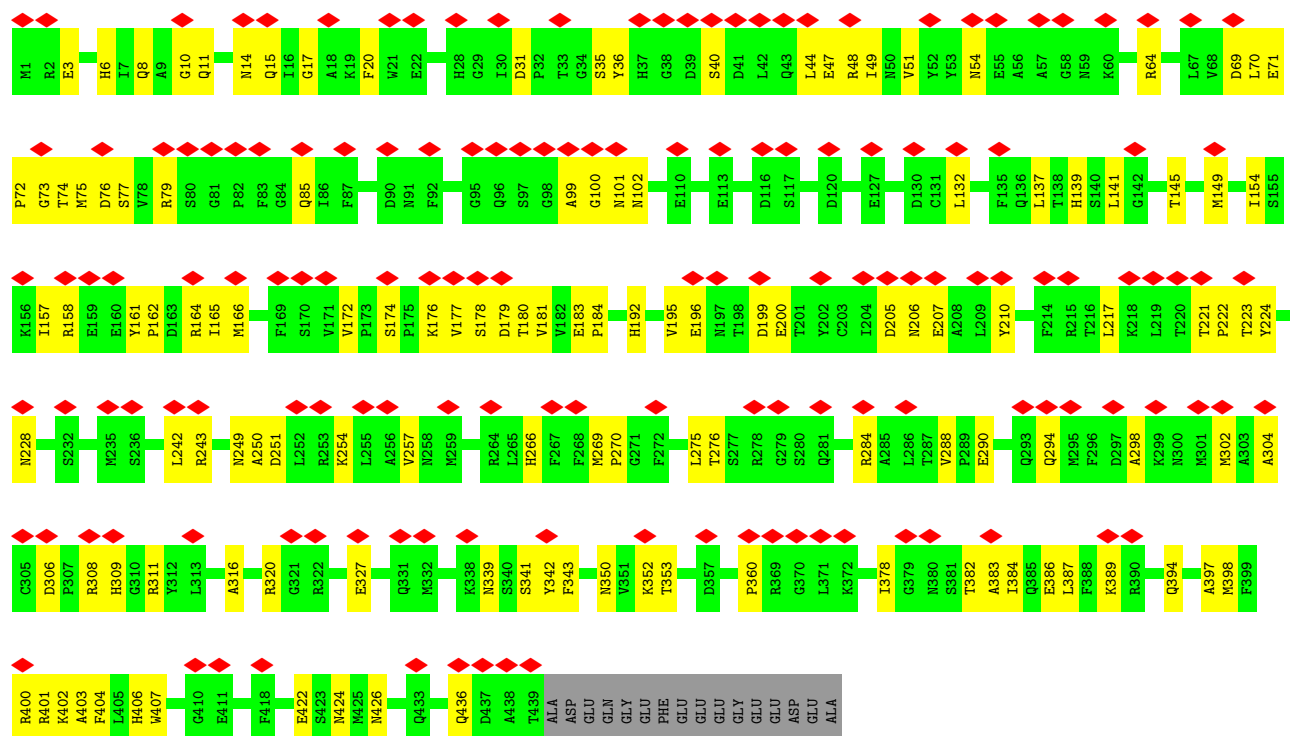


• Molecule 2: Tubulin beta chain

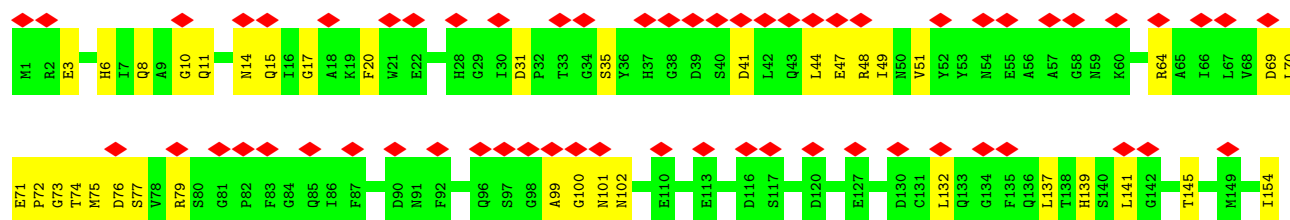


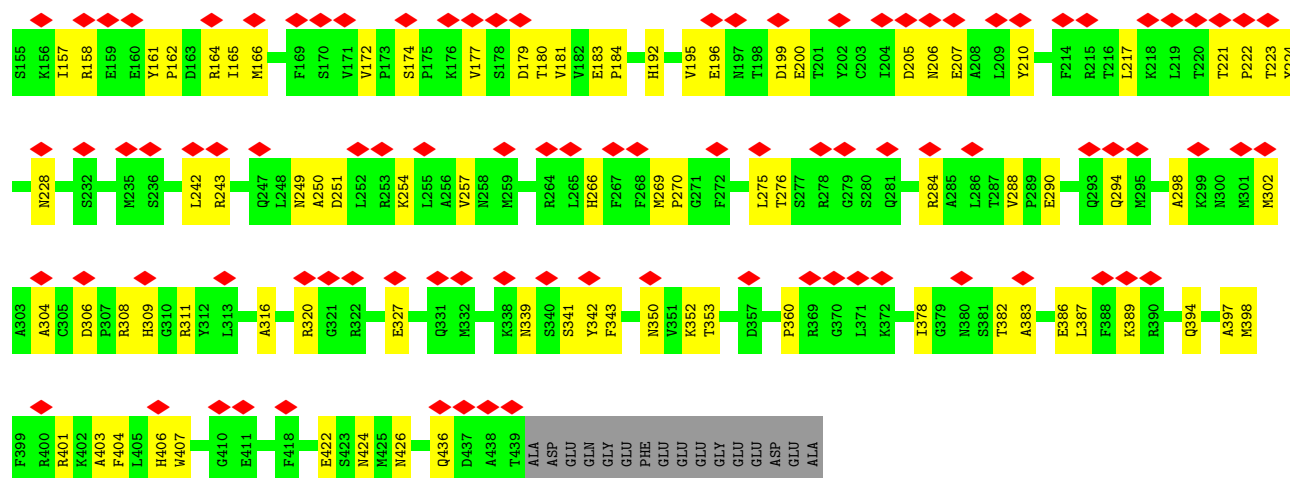


• Molecule 2: Tubulin beta chain

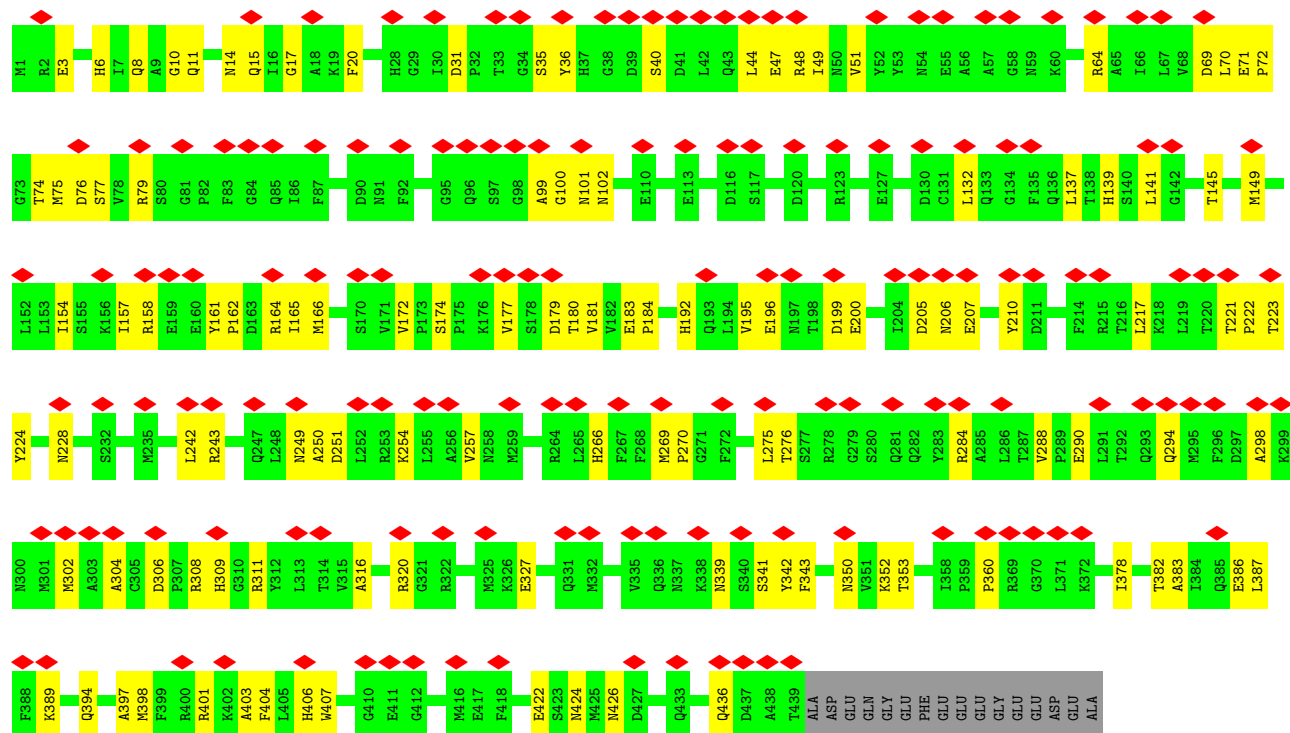


• Molecule 2: Tubulin beta chain

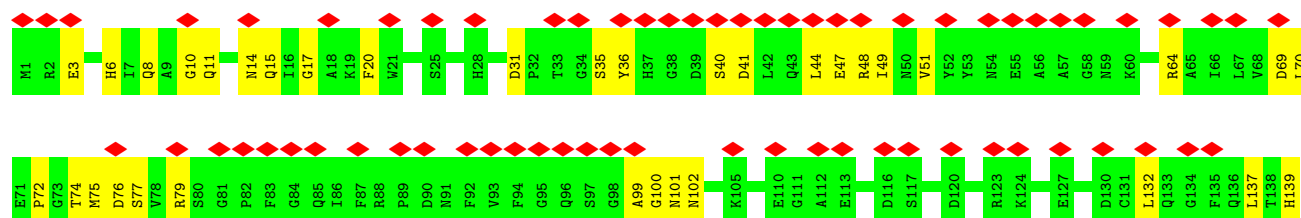




• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain

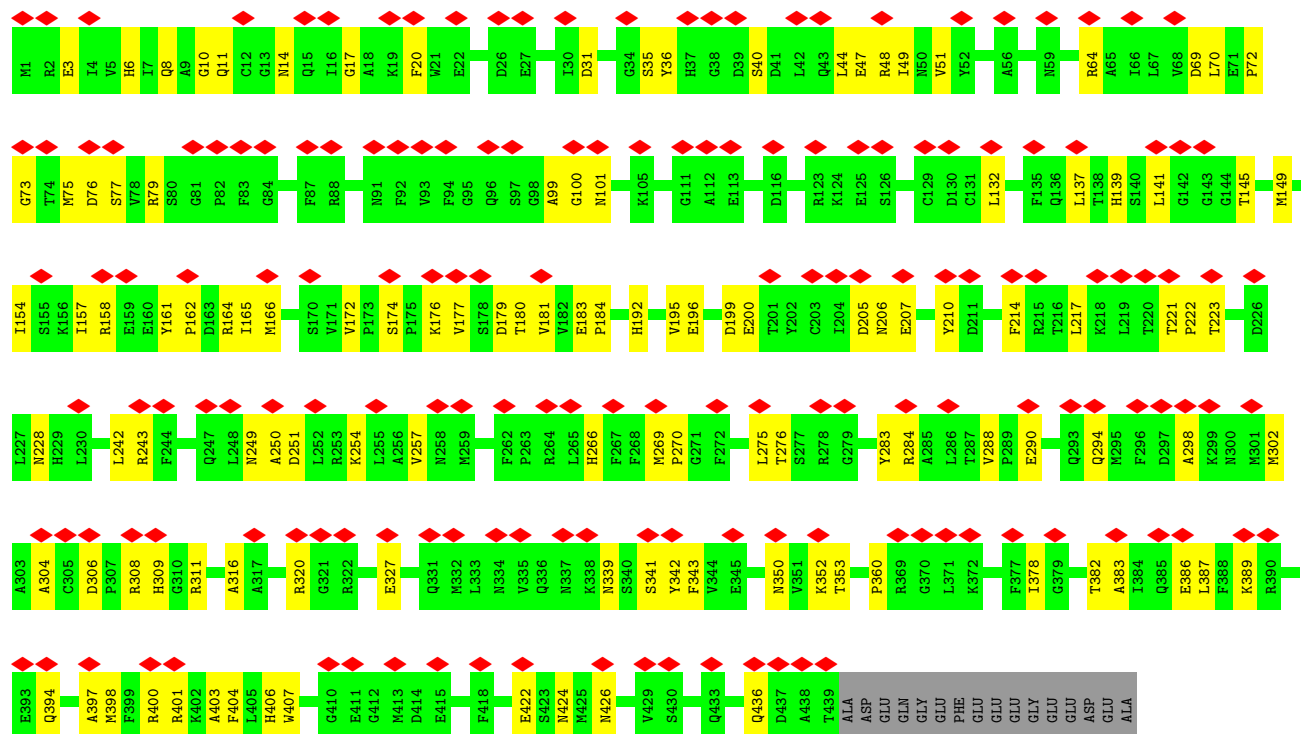






• Molecule 2: Tubulin beta chain

Chain 4Z: 



## 4 Experimental information

| Property                           | Value                                             | Source    |
|------------------------------------|---------------------------------------------------|-----------|
| EM reconstruction method           | HELICAL                                           | Depositor |
| Imposed symmetry                   | HELICAL, twist=-27.7°, rise=9.3 Å, axial sym=C1   | Depositor |
| Number of segments used            | 18432                                             | Depositor |
| Resolution determination method    | FSC 0.143 CUT-OFF                                 | Depositor |
| CTF correction method              | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 | Depositor |
| Microscope                         | FEI TITAN KRIOS                                   | Depositor |
| Voltage (kV)                       | 300                                               | Depositor |
| Electron dose ( $e^-/\text{Å}^2$ ) | 25                                                | Depositor |
| Minimum defocus (nm)               | 1422.3                                            | Depositor |
| Maximum defocus (nm)               | 2706.1                                            | Depositor |
| Magnification                      | 23364                                             | Depositor |
| Image detector                     | GATAN K2 SUMMIT (4k x 4k)                         | Depositor |
| Maximum map value                  | 14.128                                            | Depositor |
| Minimum map value                  | -8.846                                            | Depositor |
| Average map value                  | -0.000                                            | Depositor |
| Map value standard deviation       | 0.928                                             | Depositor |
| Recommended contour level          | 4                                                 | Depositor |
| Map size (Å)                       | 548.91003, 548.91003, 548.91003                   | wwPDB     |
| Map dimensions                     | 513, 513, 513                                     | wwPDB     |
| Map angles (°)                     | 90.0, 90.0, 90.0                                  | wwPDB     |
| Pixel spacing (Å)                  | 1.07, 1.07, 1.07                                  | 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, MG, GDP

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 1A    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1B    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1C    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1D    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1E    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1F    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1G    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1I    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1J    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1K    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1L    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1M    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 1N    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2A    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2B    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2C    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2D    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2E    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2F    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2G    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2I    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2J    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2K    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2L    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2M    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 2N    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3A    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3B    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3C    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3D    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3E    | 0.27         | 0/3492      | 0.48        | 0/4741      |
| 1   | 3F    | 0.27         | 0/3492      | 0.48        | 0/4741      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | 3G    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3I    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3J    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3K    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3L    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3M    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 3N    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4A    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4B    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4C    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4D    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4E    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4F    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4G    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4I    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4J    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4K    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4L    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4M    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 1   | 4N    | 0.27         | 0/3492  | 0.48        | 0/4741  |
| 2   | 1H    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1O    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1P    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1Q    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1R    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1S    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1T    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1U    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1V    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1W    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1X    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1Y    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 1Z    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2H    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2O    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2P    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2Q    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2R    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2S    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2T    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2U    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2V    | 0.28         | 0/3443  | 0.49        | 0/4666  |
| 2   | 2W    | 0.28         | 0/3443  | 0.49        | 0/4666  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 2   | 2X    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 2Y    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 2Z    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3H    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3O    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3P    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3Q    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3R    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3S    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3T    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3U    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3V    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3W    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3X    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3Y    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 3Z    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4H    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4O    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4P    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4Q    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4R    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4S    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4T    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4U    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4V    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4W    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4X    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4Y    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| 2   | 4Z    | 0.28         | 0/3443   | 0.49        | 0/4666   |
| All | All   | 0.28         | 0/360620 | 0.48        | 0/489164 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1A    | 3415  | 0        | 3313     | 270     | 0            |
| 1   | 1B    | 3415  | 0        | 3311     | 344     | 0            |
| 1   | 1C    | 3415  | 0        | 3311     | 403     | 0            |
| 1   | 1D    | 3415  | 0        | 3310     | 434     | 0            |
| 1   | 1E    | 3415  | 0        | 3310     | 449     | 0            |
| 1   | 1F    | 3415  | 0        | 3312     | 432     | 0            |
| 1   | 1G    | 3415  | 0        | 3313     | 403     | 0            |
| 1   | 1I    | 3415  | 0        | 3313     | 339     | 0            |
| 1   | 1J    | 3415  | 0        | 3313     | 282     | 0            |
| 1   | 1K    | 3415  | 0        | 3313     | 244     | 0            |
| 1   | 1L    | 3415  | 0        | 3313     | 239     | 0            |
| 1   | 1M    | 3415  | 0        | 3313     | 251     | 0            |
| 1   | 1N    | 3415  | 0        | 3313     | 223     | 0            |
| 1   | 2A    | 3415  | 0        | 3313     | 127     | 0            |
| 1   | 2B    | 3415  | 0        | 3313     | 107     | 0            |
| 1   | 2C    | 3415  | 0        | 3313     | 99      | 0            |
| 1   | 2D    | 3415  | 0        | 3313     | 107     | 0            |
| 1   | 2E    | 3415  | 0        | 3313     | 123     | 0            |
| 1   | 2F    | 3415  | 0        | 3313     | 141     | 0            |
| 1   | 2G    | 3415  | 0        | 3313     | 159     | 0            |
| 1   | 2I    | 3415  | 0        | 3313     | 176     | 0            |
| 1   | 2J    | 3415  | 0        | 3313     | 194     | 0            |
| 1   | 2K    | 3415  | 0        | 3312     | 195     | 0            |
| 1   | 2L    | 3415  | 0        | 3312     | 199     | 0            |
| 1   | 2M    | 3415  | 0        | 3312     | 179     | 0            |
| 1   | 2N    | 3415  | 0        | 3313     | 143     | 0            |
| 1   | 3A    | 3415  | 0        | 3312     | 205     | 0            |
| 1   | 3B    | 3415  | 0        | 3312     | 212     | 0            |
| 1   | 3C    | 3415  | 0        | 3312     | 222     | 0            |
| 1   | 3D    | 3415  | 0        | 3312     | 225     | 0            |
| 1   | 3E    | 3415  | 0        | 3313     | 241     | 0            |
| 1   | 3F    | 3415  | 0        | 3313     | 249     | 0            |
| 1   | 3G    | 3415  | 0        | 3313     | 242     | 0            |
| 1   | 3I    | 3415  | 0        | 3313     | 236     | 0            |
| 1   | 3J    | 3415  | 0        | 3313     | 236     | 0            |
| 1   | 3K    | 3415  | 0        | 3313     | 225     | 0            |
| 1   | 3L    | 3415  | 0        | 3313     | 217     | 0            |
| 1   | 3M    | 3415  | 0        | 3313     | 198     | 0            |
| 1   | 3N    | 3415  | 0        | 3313     | 199     | 0            |
| 1   | 4A    | 3415  | 0        | 3313     | 63      | 0            |
| 1   | 4B    | 3415  | 0        | 3313     | 60      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 4C    | 3415  | 0        | 3313     | 62      | 0            |
| 1   | 4D    | 3415  | 0        | 3313     | 63      | 0            |
| 1   | 4E    | 3415  | 0        | 3313     | 61      | 0            |
| 1   | 4F    | 3415  | 0        | 3313     | 63      | 0            |
| 1   | 4G    | 3415  | 0        | 3313     | 63      | 0            |
| 1   | 4I    | 3415  | 0        | 3313     | 61      | 0            |
| 1   | 4J    | 3415  | 0        | 3313     | 62      | 0            |
| 1   | 4K    | 3415  | 0        | 3313     | 61      | 0            |
| 1   | 4L    | 3415  | 0        | 3313     | 62      | 0            |
| 1   | 4M    | 3415  | 0        | 3313     | 57      | 0            |
| 1   | 4N    | 3415  | 0        | 3313     | 55      | 0            |
| 2   | 1H    | 3368  | 0        | 3246     | 122     | 0            |
| 2   | 1O    | 3368  | 0        | 3246     | 106     | 0            |
| 2   | 1P    | 3368  | 0        | 3246     | 101     | 0            |
| 2   | 1Q    | 3368  | 0        | 3246     | 107     | 0            |
| 2   | 1R    | 3368  | 0        | 3246     | 122     | 0            |
| 2   | 1S    | 3368  | 0        | 3246     | 141     | 0            |
| 2   | 1T    | 3368  | 0        | 3246     | 160     | 0            |
| 2   | 1U    | 3368  | 0        | 3246     | 177     | 0            |
| 2   | 1V    | 3368  | 0        | 3246     | 193     | 0            |
| 2   | 1W    | 3368  | 0        | 3245     | 193     | 0            |
| 2   | 1X    | 3368  | 0        | 3245     | 196     | 0            |
| 2   | 1Y    | 3368  | 0        | 3245     | 180     | 0            |
| 2   | 1Z    | 3368  | 0        | 3246     | 143     | 0            |
| 2   | 2H    | 3368  | 0        | 3246     | 198     | 0            |
| 2   | 2O    | 3368  | 0        | 3246     | 207     | 0            |
| 2   | 2P    | 3368  | 0        | 3246     | 218     | 0            |
| 2   | 2Q    | 3368  | 0        | 3246     | 220     | 0            |
| 2   | 2R    | 3368  | 0        | 3246     | 235     | 0            |
| 2   | 2S    | 3368  | 0        | 3246     | 243     | 0            |
| 2   | 2T    | 3368  | 0        | 3246     | 234     | 0            |
| 2   | 2U    | 3368  | 0        | 3246     | 232     | 0            |
| 2   | 2V    | 3368  | 0        | 3246     | 230     | 0            |
| 2   | 2W    | 3368  | 0        | 3246     | 219     | 0            |
| 2   | 2X    | 3368  | 0        | 3246     | 212     | 0            |
| 2   | 2Y    | 3368  | 0        | 3246     | 197     | 0            |
| 2   | 2Z    | 3368  | 0        | 3246     | 198     | 0            |
| 2   | 3H    | 3368  | 0        | 3246     | 60      | 0            |
| 2   | 3O    | 3368  | 0        | 3246     | 60      | 0            |
| 2   | 3P    | 3368  | 0        | 3246     | 63      | 0            |
| 2   | 3Q    | 3368  | 0        | 3246     | 62      | 0            |
| 2   | 3R    | 3368  | 0        | 3246     | 59      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 3S    | 3368  | 0        | 3246     | 63      | 0            |
| 2   | 3T    | 3368  | 0        | 3246     | 62      | 0            |
| 2   | 3U    | 3368  | 0        | 3246     | 61      | 0            |
| 2   | 3V    | 3368  | 0        | 3246     | 61      | 0            |
| 2   | 3W    | 3368  | 0        | 3246     | 60      | 0            |
| 2   | 3X    | 3368  | 0        | 3246     | 61      | 0            |
| 2   | 3Y    | 3368  | 0        | 3246     | 62      | 0            |
| 2   | 3Z    | 3368  | 0        | 3246     | 59      | 0            |
| 2   | 4H    | 3368  | 0        | 3246     | 262     | 0            |
| 2   | 4O    | 3368  | 0        | 3246     | 338     | 0            |
| 2   | 4P    | 3368  | 0        | 3246     | 398     | 0            |
| 2   | 4Q    | 3368  | 0        | 3245     | 427     | 0            |
| 2   | 4R    | 3368  | 0        | 3245     | 443     | 0            |
| 2   | 4S    | 3368  | 0        | 3246     | 428     | 0            |
| 2   | 4T    | 3368  | 0        | 3246     | 396     | 0            |
| 2   | 4U    | 3368  | 0        | 3246     | 337     | 0            |
| 2   | 4V    | 3368  | 0        | 3246     | 276     | 0            |
| 2   | 4W    | 3368  | 0        | 3246     | 241     | 0            |
| 2   | 4X    | 3368  | 0        | 3246     | 236     | 0            |
| 2   | 4Y    | 3368  | 0        | 3246     | 251     | 0            |
| 2   | 4Z    | 3368  | 0        | 3246     | 222     | 0            |
| 3   | 1A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1B    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1D    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1E    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1F    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1G    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1I    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1J    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1K    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1L    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1M    | 32    | 0        | 12       | 2       | 0            |
| 3   | 1N    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2B    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2D    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2E    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2F    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2G    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2I    | 32    | 0        | 12       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 2J    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2K    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2L    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2M    | 32    | 0        | 12       | 2       | 0            |
| 3   | 2N    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3B    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3D    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3E    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3F    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3G    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3I    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3J    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3K    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3L    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3M    | 32    | 0        | 12       | 2       | 0            |
| 3   | 3N    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4A    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4B    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4C    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4D    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4E    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4F    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4G    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4I    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4J    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4K    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4L    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4M    | 32    | 0        | 12       | 2       | 0            |
| 3   | 4N    | 32    | 0        | 12       | 2       | 0            |
| 4   | 1A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1B    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1D    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1F    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1G    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1I    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1J    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1K    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1L    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | 1M    | 1     | 0        | 0        | 0       | 0            |
| 4   | 1N    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2B    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2D    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2F    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2G    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2I    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2J    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2K    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2L    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2M    | 1     | 0        | 0        | 0       | 0            |
| 4   | 2N    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3B    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3D    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3F    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3G    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3I    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3J    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3K    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3L    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3M    | 1     | 0        | 0        | 0       | 0            |
| 4   | 3N    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4A    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4B    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4C    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4D    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4E    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4F    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4G    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4I    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4J    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4K    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4L    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4M    | 1     | 0        | 0        | 0       | 0            |
| 4   | 4N    | 1     | 0        | 0        | 0       | 0            |
| 5   | 1H    | 28    | 0        | 12       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 1O    | 28    | 0        | 12       | 4       | 0            |
| 5   | 1P    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1Q    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1R    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1S    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1T    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1U    | 28    | 0        | 12       | 3       | 0            |
| 5   | 1V    | 28    | 0        | 12       | 4       | 0            |
| 5   | 1W    | 28    | 0        | 12       | 4       | 0            |
| 5   | 1X    | 28    | 0        | 12       | 5       | 0            |
| 5   | 1Y    | 28    | 0        | 12       | 5       | 0            |
| 5   | 1Z    | 28    | 0        | 12       | 6       | 0            |
| 5   | 2H    | 28    | 0        | 12       | 7       | 0            |
| 5   | 2O    | 28    | 0        | 12       | 7       | 0            |
| 5   | 2P    | 28    | 0        | 12       | 7       | 0            |
| 5   | 2Q    | 28    | 0        | 12       | 7       | 0            |
| 5   | 2R    | 28    | 0        | 12       | 7       | 0            |
| 5   | 2S    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2T    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2U    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2V    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2W    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2X    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2Y    | 28    | 0        | 12       | 8       | 0            |
| 5   | 2Z    | 28    | 0        | 12       | 7       | 0            |
| 5   | 3H    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3O    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3P    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3Q    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3R    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3S    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3T    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3U    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3V    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3W    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3X    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3Y    | 28    | 0        | 12       | 3       | 0            |
| 5   | 3Z    | 28    | 0        | 12       | 3       | 0            |
| 5   | 4H    | 28    | 0        | 12       | 8       | 0            |
| 5   | 4O    | 28    | 0        | 12       | 9       | 0            |
| 5   | 4P    | 28    | 0        | 12       | 9       | 0            |
| 5   | 4Q    | 28    | 0        | 12       | 10      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5   | 4R    | 28     | 0        | 12       | 9       | 0            |
| 5   | 4S    | 28     | 0        | 12       | 7       | 0            |
| 5   | 4T    | 28     | 0        | 12       | 7       | 0            |
| 5   | 4U    | 28     | 0        | 12       | 7       | 0            |
| 5   | 4V    | 28     | 0        | 12       | 7       | 0            |
| 5   | 4W    | 28     | 0        | 12       | 6       | 0            |
| 5   | 4X    | 28     | 0        | 12       | 6       | 0            |
| 5   | 4Y    | 28     | 0        | 12       | 6       | 0            |
| 5   | 4Z    | 28     | 0        | 12       | 8       | 0            |
| All | All   | 355888 | 0        | 342293   | 12808   | 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 18.

All (12808) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1I:262:TYR:HA  | 2:4U:406:HIS:CD2  | 1.37                     | 1.60              |
| 1:1F:262:TYR:HA  | 2:4S:406:HIS:CD2  | 1.37                     | 1.57              |
| 1:1G:262:TYR:HA  | 2:4T:406:HIS:CD2  | 1.34                     | 1.56              |
| 1:1F:245:ASP:CG  | 2:4S:77:SER:HB3   | 1.30                     | 1.56              |
| 1:1J:262:TYR:HA  | 2:4V:406:HIS:CD2  | 1.45                     | 1.51              |
| 1:1G:245:ASP:CG  | 2:4T:77:SER:HB3   | 1.30                     | 1.50              |
| 2:2V:406:HIS:CD2 | 1:3J:263:PRO:HD3  | 1.44                     | 1.50              |
| 1:1A:249:ASN:N   | 2:4H:11:GLN:HE22  | 1.03                     | 1.50              |
| 2:2W:406:HIS:CD2 | 1:3K:263:PRO:HD3  | 1.44                     | 1.49              |
| 1:1G:249:ASN:N   | 2:4T:11:GLN:HE22  | 1.06                     | 1.48              |
| 1:1G:260:VAL:O   | 2:4T:407:TRP:CD1  | 1.67                     | 1.48              |
| 1:1E:262:TYR:HA  | 2:4R:406:HIS:CD2  | 1.47                     | 1.48              |
| 1:1I:245:ASP:CG  | 2:4U:77:SER:HB3   | 1.37                     | 1.48              |
| 1:1D:332:ILE:CG2 | 2:4Q:177:VAL:HG23 | 1.43                     | 1.48              |
| 1:1E:260:VAL:HB  | 2:4R:407:TRP:NE1  | 1.26                     | 1.47              |
| 2:2X:406:HIS:CD2 | 1:3L:263:PRO:HD3  | 1.48                     | 1.47              |
| 2:2U:406:HIS:CD2 | 1:3I:263:PRO:HD3  | 1.47                     | 1.47              |
| 1:1E:245:ASP:CG  | 2:4R:77:SER:HB3   | 1.36                     | 1.47              |
| 1:1F:249:ASN:H   | 2:4S:11:GLN:NE2   | 0.98                     | 1.47              |
| 2:1V:181:VAL:N   | 1:2J:258:ASN:HD22 | 1.02                     | 1.46              |
| 1:1I:262:TYR:CA  | 2:4U:406:HIS:NE2  | 1.76                     | 1.46              |
| 2:1W:100:GLY:HA3 | 1:2K:253:THR:CG2  | 1.44                     | 1.45              |
| 2:1X:100:GLY:HA3 | 1:2L:253:THR:CG2  | 1.46                     | 1.45              |
| 1:1F:262:TYR:CA  | 2:4S:406:HIS:CD2  | 2.00                     | 1.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:262:TYR:CA   | 2:4T:406:HIS:NE2  | 1.79                     | 1.45              |
| 1:1J:262:TYR:CA   | 2:4V:406:HIS:NE2  | 1.78                     | 1.44              |
| 2:2S:11:GLN:NE2   | 1:3F:249:ASN:H    | 1.13                     | 1.44              |
| 2:2T:406:HIS:CD2  | 1:3G:263:PRO:HD3  | 1.53                     | 1.44              |
| 1:1K:262:TYR:HA   | 2:4W:406:HIS:CD2  | 1.52                     | 1.44              |
| 1:1D:348:PRO:HG3  | 2:4Q:394:GLN:CA   | 1.47                     | 1.43              |
| 1:1D:249:ASN:N    | 2:4Q:11:GLN:NE2   | 1.64                     | 1.43              |
| 1:1K:262:TYR:CA   | 2:4W:406:HIS:NE2  | 1.81                     | 1.43              |
| 2:1V:181:VAL:H    | 1:2J:258:ASN:ND2  | 1.04                     | 1.43              |
| 1:1E:262:TYR:C    | 2:4R:406:HIS:NE2  | 1.77                     | 1.42              |
| 2:2T:11:GLN:HE22  | 1:3G:249:ASN:N    | 1.14                     | 1.42              |
| 1:1C:332:ILE:CG2  | 2:4P:177:VAL:HG23 | 1.46                     | 1.42              |
| 1:1E:348:PRO:HG3  | 2:4R:394:GLN:CA   | 1.49                     | 1.42              |
| 1:1G:249:ASN:H    | 2:4T:11:GLN:NE2   | 1.09                     | 1.42              |
| 1:1E:332:ILE:CG2  | 2:4R:177:VAL:HG23 | 1.49                     | 1.42              |
| 1:1N:249:ASN:H    | 2:4Z:11:GLN:NE2   | 1.15                     | 1.42              |
| 1:1F:260:VAL:O    | 2:4S:407:TRP:CD1  | 1.71                     | 1.42              |
| 2:2U:11:GLN:HE22  | 1:3I:249:ASN:N    | 1.18                     | 1.42              |
| 1:1B:249:ASN:N    | 2:4O:11:GLN:HE22  | 0.96                     | 1.42              |
| 1:1F:249:ASN:N    | 2:4S:11:GLN:HE22  | 0.98                     | 1.42              |
| 1:1C:435:VAL:HA   | 2:4P:401:ARG:NH2  | 1.30                     | 1.41              |
| 2:2R:11:GLN:NE2   | 1:3E:249:ASN:H    | 1.17                     | 1.41              |
| 1:1C:249:ASN:N    | 2:4P:11:GLN:HE22  | 0.92                     | 1.41              |
| 1:1D:348:PRO:CB   | 2:4Q:394:GLN:HG2  | 1.49                     | 1.41              |
| 1:1N:249:ASN:N    | 2:4Z:11:GLN:HE22  | 1.11                     | 1.41              |
| 1:1D:262:TYR:C    | 2:4Q:406:HIS:NE2  | 1.78                     | 1.41              |
| 1:1D:346:TRP:CB   | 2:4Q:397:ALA:O    | 1.67                     | 1.41              |
| 1:1E:260:VAL:CB   | 2:4R:407:TRP:HE1  | 1.32                     | 1.41              |
| 1:1L:262:TYR:HA   | 2:4X:406:HIS:CD2  | 1.56                     | 1.41              |
| 1:1D:245:ASP:CG   | 2:4Q:77:SER:HB3   | 1.46                     | 1.40              |
| 1:1M:262:TYR:CA   | 2:4Y:406:HIS:NE2  | 1.84                     | 1.40              |
| 1:1A:249:ASN:H    | 2:4H:11:GLN:NE2   | 1.03                     | 1.40              |
| 1:1D:435:VAL:HA   | 2:4Q:401:ARG:NH2  | 1.35                     | 1.40              |
| 1:1L:262:TYR:CA   | 2:4X:406:HIS:NE2  | 1.84                     | 1.40              |
| 2:1V:181:VAL:CG2  | 1:2J:258:ASN:O    | 1.68                     | 1.40              |
| 2:2Y:406:HIS:CD2  | 1:3M:263:PRO:HD3  | 1.55                     | 1.40              |
| 1:1B:249:ASN:H    | 2:4O:11:GLN:NE2   | 0.93                     | 1.40              |
| 1:1D:260:VAL:HB   | 2:4Q:407:TRP:NE1  | 1.32                     | 1.40              |
| 1:1D:248:LEU:HD13 | 5:4Q:501:GDP:C8   | 1.54                     | 1.39              |
| 1:1I:249:ASN:N    | 2:4U:11:GLN:HE22  | 1.15                     | 1.39              |
| 1:1J:245:ASP:CG   | 2:4V:77:SER:HB3   | 1.46                     | 1.39              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1V:100:GLY:HA3  | 1:2J:253:THR:CG2  | 1.51                     | 1.39              |
| 1:1M:262:TYR:HA   | 2:4Y:406:HIS:CD2  | 1.56                     | 1.39              |
| 1:1C:348:PRO:CB   | 2:4P:394:GLN:HG2  | 1.52                     | 1.39              |
| 1:1G:262:TYR:CA   | 2:4T:406:HIS:CD2  | 2.03                     | 1.39              |
| 1:1E:249:ASN:N    | 2:4R:11:GLN:NE2   | 1.64                     | 1.39              |
| 2:2U:11:GLN:NE2   | 1:3I:249:ASN:H    | 1.16                     | 1.39              |
| 2:2R:11:GLN:HE22  | 1:3E:249:ASN:N    | 1.20                     | 1.38              |
| 1:1F:260:VAL:HB   | 2:4S:407:TRP:NE1  | 1.32                     | 1.38              |
| 1:1M:249:ASN:N    | 2:4Y:11:GLN:HE22  | 1.17                     | 1.38              |
| 1:1C:248:LEU:HD13 | 5:4P:501:GDP:C8   | 1.55                     | 1.37              |
| 2:2S:11:GLN:HE22  | 1:3F:249:ASN:N    | 1.15                     | 1.37              |
| 1:1D:260:VAL:CB   | 2:4Q:407:TRP:HE1  | 1.36                     | 1.37              |
| 2:2V:11:GLN:NE2   | 1:3J:249:ASN:H    | 1.23                     | 1.37              |
| 2:2T:11:GLN:NE2   | 1:3G:249:ASN:H    | 1.13                     | 1.37              |
| 1:1F:262:TYR:CA   | 2:4S:406:HIS:NE2  | 1.87                     | 1.37              |
| 1:1I:249:ASN:H    | 2:4U:11:GLN:NE2   | 1.20                     | 1.37              |
| 1:1E:262:TYR:CA   | 2:4R:406:HIS:CD2  | 2.05                     | 1.36              |
| 1:1J:249:ASN:N    | 2:4V:11:GLN:HE22  | 1.23                     | 1.36              |
| 1:1D:262:TYR:HA   | 2:4Q:406:HIS:CD2  | 1.59                     | 1.36              |
| 1:1C:249:ASN:H    | 2:4P:11:GLN:NE2   | 0.88                     | 1.36              |
| 1:1E:353:VAL:CB   | 2:4R:179:ASP:OD1  | 1.74                     | 1.36              |
| 1:1E:346:TRP:CB   | 2:4R:397:ALA:O    | 1.73                     | 1.36              |
| 1:1M:249:ASN:H    | 2:4Y:11:GLN:NE2   | 1.23                     | 1.36              |
| 2:1V:214:PHE:CB   | 1:2J:326:LYS:HE2  | 1.53                     | 1.36              |
| 2:2Q:401:ARG:NH2  | 1:3D:435:VAL:HA   | 1.40                     | 1.35              |
| 2:1W:181:VAL:CG2  | 1:2K:258:ASN:O    | 1.70                     | 1.35              |
| 1:1B:329:ASN:ND2  | 2:4O:207:GLU:OE1  | 1.57                     | 1.35              |
| 1:1C:262:TYR:C    | 2:4P:406:HIS:NE2  | 1.83                     | 1.35              |
| 1:1B:435:VAL:HA   | 2:4O:401:ARG:NH2  | 1.40                     | 1.35              |
| 2:1Y:100:GLY:HA3  | 1:2M:253:THR:CG2  | 1.55                     | 1.35              |
| 1:1C:348:PRO:HG3  | 2:4P:394:GLN:CA   | 1.57                     | 1.34              |
| 2:2H:207:GLU:OE1  | 1:3A:329:ASN:ND2  | 1.58                     | 1.34              |
| 2:2O:401:ARG:NH2  | 1:3B:435:VAL:HA   | 1.40                     | 1.34              |
| 2:2Z:406:HIS:CD2  | 1:3N:263:PRO:HD3  | 1.61                     | 1.34              |
| 1:1E:348:PRO:CB   | 2:4R:394:GLN:HG2  | 1.57                     | 1.34              |
| 2:1U:181:VAL:N    | 1:2I:258:ASN:HD22 | 1.21                     | 1.34              |
| 2:2S:406:HIS:CD2  | 1:3F:263:PRO:HD3  | 1.60                     | 1.34              |
| 1:1C:346:TRP:CB   | 2:4P:397:ALA:O    | 1.74                     | 1.34              |
| 1:1F:260:VAL:CB   | 2:4S:407:TRP:HE1  | 1.39                     | 1.34              |
| 1:1F:262:TYR:C    | 2:4S:406:HIS:NE2  | 1.83                     | 1.34              |
| 2:2P:401:ARG:NH2  | 1:3C:435:VAL:HA   | 1.38                     | 1.34              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:346:TRP:O    | 2:4T:398:MET:CG   | 1.75                     | 1.33              |
| 1:1C:258:ASN:ND2  | 2:4P:180:THR:HG23 | 1.38                     | 1.33              |
| 1:1E:248:LEU:HD13 | 5:4R:501:GDP:C8   | 1.62                     | 1.33              |
| 2:1W:214:PHE:CB   | 1:2K:326:LYS:HE2  | 1.56                     | 1.33              |
| 1:1I:262:TYR:N    | 2:4U:406:HIS:NE2  | 1.75                     | 1.33              |
| 1:1K:245:ASP:CG   | 2:4W:77:SER:HB3   | 1.53                     | 1.33              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:CG   | 1.75                     | 1.33              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:HG2  | 1.17                     | 1.33              |
| 2:1U:181:VAL:H    | 1:2I:258:ASN:ND2  | 1.19                     | 1.33              |
| 2:1U:214:PHE:CB   | 1:2I:326:LYS:HE2  | 1.59                     | 1.33              |
| 2:2V:11:GLN:HE22  | 1:3J:249:ASN:N    | 1.24                     | 1.33              |
| 1:1E:329:ASN:ND2  | 2:4R:207:GLU:OE1  | 1.57                     | 1.32              |
| 1:1G:262:TYR:N    | 2:4T:406:HIS:NE2  | 1.77                     | 1.32              |
| 2:2Q:11:GLN:NE2   | 1:3D:249:ASN:H    | 1.23                     | 1.32              |
| 2:2R:401:ARG:NH2  | 1:3E:435:VAL:HA   | 1.45                     | 1.32              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:CG   | 1.78                     | 1.32              |
| 1:1L:249:ASN:N    | 2:4X:11:GLN:HE22  | 1.25                     | 1.32              |
| 1:1C:353:VAL:HB   | 2:4P:179:ASP:OD1  | 1.15                     | 1.31              |
| 1:1F:353:VAL:CB   | 2:4S:179:ASP:OD1  | 1.78                     | 1.31              |
| 1:1B:258:ASN:ND2  | 2:4O:180:THR:HG23 | 1.40                     | 1.31              |
| 1:1E:260:VAL:O    | 2:4R:407:TRP:CD1  | 1.82                     | 1.31              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:HG2  | 1.23                     | 1.31              |
| 2:2R:207:GLU:OE1  | 1:3E:329:ASN:ND2  | 1.63                     | 1.31              |
| 1:1M:245:ASP:OD1  | 2:4Y:77:SER:HB3   | 1.26                     | 1.31              |
| 1:1N:245:ASP:OD1  | 2:4Z:77:SER:HB3   | 1.27                     | 1.31              |
| 2:1U:181:VAL:CG2  | 1:2I:258:ASN:O    | 1.77                     | 1.31              |
| 1:1A:263:PRO:HD3  | 2:4H:406:HIS:CD2  | 1.66                     | 1.31              |
| 2:1X:224:TYR:CD2  | 1:2L:247:ALA:O    | 1.83                     | 1.31              |
| 2:1Y:179:ASP:OD2  | 1:2M:248:LEU:HD21 | 1.23                     | 1.31              |
| 1:1I:353:VAL:HB   | 2:4U:179:ASP:OD1  | 1.25                     | 1.30              |
| 1:1L:260:VAL:O    | 2:4X:407:TRP:NE1  | 1.58                     | 1.30              |
| 2:1W:224:TYR:CD2  | 1:2K:247:ALA:O    | 1.83                     | 1.30              |
| 2:2Q:11:GLN:HE22  | 1:3D:249:ASN:N    | 1.27                     | 1.30              |
| 1:1B:332:ILE:CG2  | 2:4O:177:VAL:HG23 | 1.59                     | 1.30              |
| 1:1K:249:ASN:N    | 2:4W:11:GLN:HE22  | 1.27                     | 1.30              |
| 1:1D:258:ASN:ND2  | 2:4Q:180:THR:HG23 | 1.43                     | 1.29              |
| 1:1F:348:PRO:HG3  | 2:4S:394:GLN:CA   | 1.61                     | 1.29              |
| 1:1D:435:VAL:C    | 2:4Q:401:ARG:HH22 | 1.40                     | 1.29              |
| 2:1Y:181:VAL:HG21 | 1:2M:258:ASN:O    | 1.27                     | 1.29              |
| 1:1F:437:VAL:O    | 2:4S:401:ARG:NH1  | 1.64                     | 1.29              |
| 1:1F:332:ILE:CG2  | 2:4S:177:VAL:HG23 | 1.63                     | 1.29              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:262:TYR:CA   | 2:4U:406:HIS:CD2  | 2.12                     | 1.29              |
| 2:1S:181:VAL:HG21 | 1:2F:258:ASN:O    | 1.32                     | 1.29              |
| 2:1V:404:PHE:CE1  | 1:2J:260:VAL:O    | 1.85                     | 1.29              |
| 1:1D:353:VAL:CB   | 2:4Q:179:ASP:OD1  | 1.80                     | 1.28              |
| 1:1J:249:ASN:H    | 2:4V:11:GLN:NE2   | 1.29                     | 1.28              |
| 1:1L:245:ASP:CG   | 2:4X:77:SER:HB3   | 1.58                     | 1.28              |
| 2:1U:100:GLY:HA3  | 1:2I:253:THR:CG2  | 1.64                     | 1.28              |
| 2:2W:11:GLN:NE2   | 1:3K:249:ASN:H    | 1.30                     | 1.28              |
| 1:1G:437:VAL:O    | 2:4T:401:ARG:NH1  | 1.64                     | 1.28              |
| 2:2R:406:HIS:CD2  | 1:3E:263:PRO:HD3  | 1.66                     | 1.28              |
| 1:1B:348:PRO:CB   | 2:4O:394:GLN:HG2  | 1.64                     | 1.28              |
| 1:1D:262:TYR:CA   | 2:4Q:406:HIS:CD2  | 2.17                     | 1.28              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:CB   | 2.12                     | 1.28              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:HG2  | 1.15                     | 1.28              |
| 2:1X:179:ASP:OD2  | 1:2L:248:LEU:HD21 | 1.30                     | 1.28              |
| 2:2H:401:ARG:NH2  | 1:3A:435:VAL:HA   | 1.45                     | 1.28              |
| 1:1B:262:TYR:C    | 2:4O:406:HIS:NE2  | 1.91                     | 1.28              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:HG2  | 1.17                     | 1.28              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:CG   | 1.81                     | 1.28              |
| 2:1T:181:VAL:HG21 | 1:2G:258:ASN:O    | 1.10                     | 1.28              |
| 2:2H:406:HIS:CD2  | 1:3A:263:PRO:HD3  | 1.67                     | 1.28              |
| 1:1A:245:ASP:OD1  | 2:4H:77:SER:HB3   | 1.34                     | 1.27              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:CG   | 1.80                     | 1.27              |
| 1:1J:262:TYR:N    | 2:4V:406:HIS:NE2  | 1.79                     | 1.27              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:CG   | 1.81                     | 1.27              |
| 2:1X:181:VAL:CG2  | 1:2L:258:ASN:O    | 1.81                     | 1.27              |
| 2:2P:11:GLN:NE2   | 1:3C:249:ASN:H    | 1.30                     | 1.27              |
| 1:1E:435:VAL:C    | 2:4R:401:ARG:HH22 | 1.42                     | 1.27              |
| 2:1Z:179:ASP:OD2  | 1:2N:248:LEU:HD21 | 1.32                     | 1.27              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:HG2  | 1.15                     | 1.27              |
| 1:1C:260:VAL:HB   | 2:4P:407:TRP:NE1  | 1.49                     | 1.27              |
| 1:1B:248:LEU:HD13 | 5:4O:501:GDP:C8   | 1.67                     | 1.27              |
| 2:1W:404:PHE:CE1  | 1:2K:260:VAL:O    | 1.87                     | 1.27              |
| 1:1C:245:ASP:CG   | 2:4P:77:SER:HB3   | 1.58                     | 1.26              |
| 1:1F:2:ARG:CD     | 2:4S:72:PRO:HD2   | 1.64                     | 1.26              |
| 1:1G:262:TYR:C    | 2:4T:406:HIS:NE2  | 1.93                     | 1.26              |
| 1:1L:249:ASN:H    | 2:4X:11:GLN:NE2   | 1.31                     | 1.26              |
| 1:1A:258:ASN:ND2  | 2:4H:180:THR:HG23 | 1.51                     | 1.26              |
| 1:1F:254:GLU:HA   | 2:4S:100:GLY:C    | 1.60                     | 1.26              |
| 1:1B:263:PRO:HD3  | 2:4O:406:HIS:CD2  | 1.68                     | 1.26              |
| 1:1C:262:TYR:HA   | 2:4P:406:HIS:CD2  | 1.70                     | 1.26              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:1Z:181:VAL:H    | 1:2N:258:ASN:ND2 | 1.32                     | 1.26              |
| 1:1G:260:VAL:HB   | 2:4T:407:TRP:NE1 | 1.47                     | 1.26              |
| 2:2Z:207:GLU:OE1  | 1:3N:329:ASN:ND2 | 1.66                     | 1.26              |
| 1:1E:435:VAL:HA   | 2:4R:401:ARG:NH2 | 1.50                     | 1.26              |
| 1:1E:254:GLU:HA   | 2:4R:100:GLY:C   | 1.58                     | 1.25              |
| 1:1G:260:VAL:O    | 2:4T:407:TRP:NE1 | 1.69                     | 1.25              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:CG  | 1.83                     | 1.25              |
| 1:1M:245:ASP:CG   | 2:4Y:77:SER:HB3  | 1.57                     | 1.25              |
| 1:1M:260:VAL:O    | 2:4Y:407:TRP:NE1 | 1.67                     | 1.25              |
| 2:2T:180:THR:HG23 | 1:3G:258:ASN:ND2 | 1.50                     | 1.25              |
| 1:1J:245:ASP:OD1  | 2:4V:77:SER:HB3  | 1.35                     | 1.25              |
| 2:2U:180:THR:HG23 | 1:3I:258:ASN:ND2 | 1.50                     | 1.25              |
| 1:1K:249:ASN:H    | 2:4W:11:GLN:NE2  | 1.33                     | 1.25              |
| 2:1X:181:VAL:HG21 | 1:2L:258:ASN:O   | 1.09                     | 1.25              |
| 2:1Y:401:ARG:HB3  | 1:2M:262:TYR:OH  | 1.33                     | 1.25              |
| 1:1B:353:VAL:HB   | 2:4O:179:ASP:OD1 | 1.35                     | 1.24              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:HB3 | 1.66                     | 1.24              |
| 2:1X:401:ARG:HB3  | 1:2L:262:TYR:OH  | 1.31                     | 1.24              |
| 1:1L:245:ASP:OD1  | 2:4X:77:SER:HB3  | 1.31                     | 1.24              |
| 2:2P:11:GLN:HE22  | 1:3C:249:ASN:N   | 1.35                     | 1.24              |
| 1:1E:2:ARG:CD     | 2:4R:72:PRO:HD2  | 1.67                     | 1.24              |
| 2:1W:100:GLY:CA   | 1:2K:253:THR:CG2 | 2.14                     | 1.24              |
| 2:2Q:406:HIS:CD2  | 1:3D:263:PRO:HD3 | 1.71                     | 1.24              |
| 2:2Z:401:ARG:NH2  | 1:3N:435:VAL:HA  | 1.51                     | 1.24              |
| 1:1D:435:VAL:CA   | 2:4Q:401:ARG:NH2 | 1.99                     | 1.24              |
| 1:1F:262:TYR:OH   | 2:4S:401:ARG:O   | 1.52                     | 1.24              |
| 2:2P:406:HIS:CD2  | 1:3C:263:PRO:HD3 | 1.72                     | 1.23              |
| 1:1D:254:GLU:HA   | 2:4Q:100:GLY:O   | 1.38                     | 1.23              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:CB  | 2.15                     | 1.23              |
| 1:1I:437:VAL:O    | 2:4U:401:ARG:NH1 | 1.71                     | 1.23              |
| 2:2O:406:HIS:CD2  | 1:3B:263:PRO:HD3 | 1.71                     | 1.23              |
| 2:2S:180:THR:HG23 | 1:3F:258:ASN:ND2 | 1.51                     | 1.23              |
| 1:1D:332:ILE:CG2  | 2:4Q:177:VAL:CG2 | 2.15                     | 1.23              |
| 1:1G:2:ARG:CD     | 2:4T:72:PRO:HD2  | 1.69                     | 1.23              |
| 2:1Z:207:GLU:OE1  | 1:2N:329:ASN:ND2 | 1.67                     | 1.23              |
| 2:2Y:100:GLY:HA3  | 1:3M:253:THR:CG2 | 1.68                     | 1.23              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:HB3 | 1.68                     | 1.23              |
| 1:1I:245:ASP:OD1  | 2:4U:77:SER:HB3  | 1.36                     | 1.23              |
| 2:2V:180:THR:HG23 | 1:3J:258:ASN:ND2 | 1.52                     | 1.23              |
| 1:1G:245:ASP:OD1  | 2:4T:77:SER:HB3  | 1.38                     | 1.23              |
| 1:1G:260:VAL:HB   | 2:4T:407:TRP:CE2 | 1.74                     | 1.23              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1X:214:PHE:CB   | 1:2L:326:LYS:HE2  | 1.66                     | 1.23              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:CB   | 2.17                     | 1.22              |
| 1:1F:329:ASN:ND2  | 2:4S:207:GLU:OE1  | 1.72                     | 1.22              |
| 1:1B:262:TYR:OH   | 2:4O:401:ARG:O    | 1.53                     | 1.22              |
| 1:1C:260:VAL:CB   | 2:4P:407:TRP:HE1  | 1.52                     | 1.22              |
| 1:1E:254:GLU:HA   | 2:4R:100:GLY:O    | 1.34                     | 1.22              |
| 1:1E:262:TYR:CA   | 2:4R:406:HIS:NE2  | 1.97                     | 1.22              |
| 1:1K:245:ASP:OD1  | 2:4W:77:SER:HB3   | 1.34                     | 1.22              |
| 2:1Y:224:TYR:CD2  | 1:2M:247:ALA:O    | 1.92                     | 1.22              |
| 2:2R:180:THR:HG23 | 1:3E:258:ASN:ND2  | 1.54                     | 1.22              |
| 1:1E:332:ILE:CG2  | 2:4R:177:VAL:CG2  | 2.16                     | 1.22              |
| 1:1F:260:VAL:HB   | 2:4S:407:TRP:CE2  | 1.74                     | 1.22              |
| 1:1J:349:THR:O    | 2:4V:181:VAL:HA   | 1.40                     | 1.22              |
| 2:1V:100:GLY:CA   | 1:2J:253:THR:CG2  | 2.16                     | 1.22              |
| 2:2W:11:GLN:HE22  | 1:3K:249:ASN:N    | 1.33                     | 1.22              |
| 1:1B:263:PRO:HD3  | 2:4O:406:HIS:CG   | 1.73                     | 1.21              |
| 1:1C:263:PRO:HD3  | 2:4P:406:HIS:CG   | 1.74                     | 1.21              |
| 1:1C:435:VAL:CA   | 2:4P:401:ARG:NH2  | 2.01                     | 1.21              |
| 1:1E:245:ASP:CG   | 2:4R:77:SER:CB    | 2.13                     | 1.21              |
| 2:2S:207:GLU:OE1  | 1:3F:329:ASN:ND2  | 1.73                     | 1.21              |
| 1:1N:263:PRO:HD3  | 2:4Z:406:HIS:CD2  | 1.73                     | 1.21              |
| 2:2S:401:ARG:NH2  | 1:3F:435:VAL:HA   | 1.52                     | 1.21              |
| 1:1E:258:ASN:ND2  | 2:4R:180:THR:HG23 | 1.54                     | 1.21              |
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:HB3  | 1.70                     | 1.21              |
| 2:1T:181:VAL:H    | 1:2G:258:ASN:ND2  | 1.36                     | 1.21              |
| 2:2X:100:GLY:HA3  | 1:3L:253:THR:CG2  | 1.70                     | 1.21              |
| 1:1E:437:VAL:O    | 2:4R:401:ARG:NH1  | 1.73                     | 1.21              |
| 1:1K:262:TYR:N    | 2:4W:406:HIS:NE2  | 1.88                     | 1.21              |
| 2:1V:224:TYR:CD2  | 1:2J:247:ALA:O    | 1.93                     | 1.21              |
| 2:1W:401:ARG:HB3  | 1:2K:262:TYR:OH   | 1.40                     | 1.21              |
| 2:2O:11:GLN:NE2   | 1:3B:249:ASN:H    | 1.37                     | 1.21              |
| 1:1D:348:PRO:HG3  | 2:4Q:394:GLN:CB   | 1.68                     | 1.21              |
| 2:1V:221:THR:HA   | 1:2J:324:VAL:CG1  | 1.69                     | 1.21              |
| 1:1A:263:PRO:HD3  | 2:4H:406:HIS:CG   | 1.74                     | 1.20              |
| 1:1D:254:GLU:HA   | 2:4Q:100:GLY:C    | 1.66                     | 1.20              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:CA   | 1.71                     | 1.20              |
| 1:1L:349:THR:O    | 2:4X:181:VAL:HA   | 1.41                     | 1.20              |
| 1:1N:262:TYR:CA   | 2:4Z:406:HIS:NE2  | 2.04                     | 1.20              |
| 2:1V:224:TYR:HD2  | 1:2J:247:ALA:O    | 1.24                     | 1.20              |
| 2:1W:179:ASP:O    | 1:2K:352:LYS:CD   | 1.88                     | 1.20              |
| 1:1D:263:PRO:HD3  | 2:4Q:406:HIS:CG   | 1.75                     | 1.20              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:346:TRP:O    | 2:4R:398:MET:CG   | 1.89                     | 1.20              |
| 1:1F:245:ASP:CG   | 2:4S:77:SER:CB    | 2.12                     | 1.20              |
| 1:1F:262:TYR:N    | 2:4S:406:HIS:NE2  | 1.88                     | 1.20              |
| 1:1G:349:THR:CG2  | 2:4T:184:PRO:HD3  | 1.71                     | 1.20              |
| 1:1J:353:VAL:HB   | 2:4V:179:ASP:OD1  | 1.41                     | 1.20              |
| 2:2X:11:GLN:NE2   | 1:3L:249:ASN:H    | 1.37                     | 1.20              |
| 1:1B:262:TYR:HA   | 2:4O:406:HIS:CD2  | 1.77                     | 1.20              |
| 1:1F:346:TRP:CB   | 2:4S:397:ALA:O    | 1.90                     | 1.20              |
| 1:1L:260:VAL:O    | 2:4X:407:TRP:CD1  | 1.93                     | 1.20              |
| 1:1G:353:VAL:HB   | 2:4T:179:ASP:OD1  | 1.08                     | 1.20              |
| 2:1T:214:PHE:CB   | 1:2G:326:LYS:HE2  | 1.72                     | 1.20              |
| 2:1X:179:ASP:O    | 1:2L:352:LYS:CD   | 1.89                     | 1.20              |
| 2:2Z:100:GLY:HA3  | 1:3N:253:THR:CG2  | 1.70                     | 1.20              |
| 1:1K:349:THR:O    | 2:4W:181:VAL:HA   | 1.38                     | 1.20              |
| 1:1N:263:PRO:HD3  | 2:4Z:406:HIS:CG   | 1.76                     | 1.19              |
| 2:1U:404:PHE:CE1  | 1:2I:260:VAL:O    | 1.94                     | 1.19              |
| 1:1C:263:PRO:HD3  | 2:4P:406:HIS:CD2  | 1.78                     | 1.19              |
| 1:1E:348:PRO:HG3  | 2:4R:394:GLN:CB   | 1.71                     | 1.19              |
| 1:1J:248:LEU:HA   | 2:4V:11:GLN:NE2   | 1.58                     | 1.19              |
| 2:1U:221:THR:HA   | 1:2I:324:VAL:CG1  | 1.71                     | 1.19              |
| 2:1W:181:VAL:HB   | 1:2K:258:ASN:HA   | 1.19                     | 1.19              |
| 2:1X:100:GLY:CA   | 1:2L:253:THR:CG2  | 2.21                     | 1.19              |
| 2:2Z:214:PHE:HB2  | 1:3N:326:LYS:HE2  | 1.21                     | 1.19              |
| 1:1D:248:LEU:CD1  | 5:4Q:501:GDP:H8   | 1.54                     | 1.19              |
| 1:1E:263:PRO:HD3  | 2:4R:406:HIS:CG   | 1.77                     | 1.19              |
| 1:1I:349:THR:CG2  | 2:4U:184:PRO:HD3  | 1.70                     | 1.19              |
| 1:1B:346:TRP:CB   | 2:4O:397:ALA:O    | 1.91                     | 1.19              |
| 1:1F:248:LEU:HD13 | 5:4S:501:GDP:C8   | 1.76                     | 1.19              |
| 1:1G:353:VAL:CB   | 2:4T:179:ASP:OD1  | 1.90                     | 1.19              |
| 2:2W:180:THR:HG23 | 1:3K:258:ASN:ND2  | 1.56                     | 1.19              |
| 1:1B:245:ASP:CG   | 2:4O:77:SER:HB3   | 1.69                     | 1.18              |
| 1:1C:348:PRO:HG3  | 2:4P:394:GLN:CB   | 1.70                     | 1.18              |
| 1:1C:435:VAL:C    | 2:4P:401:ARG:HH22 | 1.51                     | 1.18              |
| 2:2H:100:GLY:HA3  | 1:3A:253:THR:CG2  | 1.73                     | 1.18              |
| 2:2Y:401:ARG:NH2  | 1:3M:435:VAL:HA   | 1.57                     | 1.18              |
| 1:1D:260:VAL:O    | 2:4Q:407:TRP:CD1  | 1.97                     | 1.18              |
| 1:1M:260:VAL:O    | 2:4Y:407:TRP:CD1  | 1.96                     | 1.18              |
| 2:2Q:180:THR:HG23 | 1:3D:258:ASN:ND2  | 1.58                     | 1.18              |
| 2:2X:11:GLN:HE22  | 1:3L:249:ASN:N    | 1.40                     | 1.18              |
| 1:1F:249:ASN:H    | 2:4S:11:GLN:CD    | 1.50                     | 1.18              |
| 2:1W:404:PHE:CE1  | 1:2K:260:VAL:C    | 2.20                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:254:GLU:HA   | 2:4S:100:GLY:O    | 1.40                     | 1.18              |
| 1:1F:351:PHE:O    | 2:4S:180:THR:C    | 1.87                     | 1.18              |
| 1:1G:260:VAL:CB   | 2:4T:407:TRP:HE1  | 1.56                     | 1.18              |
| 2:1V:404:PHE:CE1  | 1:2J:260:VAL:C    | 2.20                     | 1.18              |
| 2:2Y:207:GLU:OE1  | 1:3M:329:ASN:ND2  | 1.74                     | 1.18              |
| 1:1A:262:TYR:C    | 2:4H:406:HIS:NE2  | 2.02                     | 1.18              |
| 1:1E:351:PHE:O    | 2:4R:180:THR:C    | 1.86                     | 1.18              |
| 1:1G:245:ASP:CG   | 2:4T:77:SER:CB    | 2.17                     | 1.18              |
| 2:2H:100:GLY:HA3  | 1:3A:253:THR:HG22 | 1.20                     | 1.18              |
| 2:2T:77:SER:HB3   | 1:3G:245:ASP:OD1  | 1.44                     | 1.18              |
| 1:1C:332:ILE:CG2  | 2:4P:177:VAL:CG2  | 2.21                     | 1.17              |
| 1:1D:262:TYR:CA   | 2:4Q:406:HIS:NE2  | 2.07                     | 1.17              |
| 1:1F:348:PRO:CB   | 2:4S:394:GLN:HG2  | 1.73                     | 1.17              |
| 1:1A:329:ASN:ND2  | 2:4H:207:GLU:OE1  | 1.75                     | 1.17              |
| 1:1B:245:ASP:OD1  | 2:4O:77:SER:HB3   | 1.41                     | 1.17              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:HA   | 1.17                     | 1.17              |
| 1:1F:263:PRO:HD3  | 2:4S:406:HIS:CG   | 1.79                     | 1.17              |
| 1:1N:262:TYR:HA   | 2:4Z:406:HIS:CD2  | 1.79                     | 1.17              |
| 1:1E:346:TRP:HB2  | 2:4R:398:MET:HA   | 1.27                     | 1.17              |
| 2:2T:100:GLY:HA3  | 1:3G:253:THR:HG22 | 1.19                     | 1.17              |
| 2:2U:77:SER:HB3   | 1:3I:245:ASP:OD1  | 1.44                     | 1.17              |
| 2:2H:11:GLN:NE2   | 1:3A:249:ASN:H    | 1.41                     | 1.16              |
| 2:2O:11:GLN:HE22  | 1:3B:249:ASN:N    | 1.42                     | 1.16              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:CA   | 1.74                     | 1.16              |
| 1:1G:254:GLU:HA   | 2:4T:100:GLY:C    | 1.71                     | 1.16              |
| 2:1T:181:VAL:N    | 1:2G:258:ASN:HD22 | 1.44                     | 1.16              |
| 2:1V:214:PHE:CG   | 1:2J:326:LYS:HE2  | 1.80                     | 1.16              |
| 1:1C:248:LEU:CD1  | 5:4P:501:GDP:H8   | 1.55                     | 1.16              |
| 1:1F:245:ASP:OD1  | 2:4S:77:SER:HB3   | 1.41                     | 1.16              |
| 1:1J:349:THR:CG2  | 2:4V:184:PRO:HD3  | 1.76                     | 1.16              |
| 2:2W:100:GLY:HA3  | 1:3K:253:THR:CG2  | 1.75                     | 1.16              |
| 2:2Z:207:GLU:CD   | 1:3N:329:ASN:HD21 | 1.53                     | 1.16              |
| 1:1C:348:PRO:HB2  | 2:4P:394:GLN:HG2  | 1.23                     | 1.16              |
| 1:1C:348:PRO:HG2  | 2:4P:394:GLN:HB3  | 1.16                     | 1.16              |
| 1:1D:245:ASP:CG   | 2:4Q:77:SER:CB    | 2.19                     | 1.16              |
| 1:1K:2:ARG:HD3    | 2:4W:72:PRO:HD2   | 1.16                     | 1.15              |
| 2:1W:101:ASN:HB2  | 1:2K:254:GLU:HG2  | 1.17                     | 1.15              |
| 2:2Y:11:GLN:NE2   | 1:3M:249:ASN:H    | 1.42                     | 1.15              |
| 1:1C:258:ASN:HD21 | 2:4P:180:THR:CG2  | 1.59                     | 1.15              |
| 1:1D:353:VAL:HB   | 2:4Q:179:ASP:OD1  | 1.00                     | 1.15              |
| 1:1I:248:LEU:HA   | 2:4U:11:GLN:NE2   | 1.59                     | 1.15              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1L:2:ARG:HD3    | 2:4X:72:PRO:HD2   | 1.21                     | 1.15              |
| 2:1W:179:ASP:OD2  | 1:2K:248:LEU:HD21 | 1.43                     | 1.15              |
| 2:2T:401:ARG:NH2  | 1:3G:435:VAL:HA   | 1.59                     | 1.15              |
| 2:2X:180:THR:HG23 | 1:3L:258:ASN:ND2  | 1.59                     | 1.15              |
| 2:2Y:401:ARG:HH22 | 1:3M:435:VAL:HA   | 1.00                     | 1.15              |
| 1:1D:245:ASP:OD1  | 2:4Q:77:SER:HB3   | 1.47                     | 1.15              |
| 1:1E:245:ASP:OD1  | 2:4R:77:SER:HB3   | 1.45                     | 1.15              |
| 2:1Y:207:GLU:CD   | 1:2M:329:ASN:HD21 | 1.54                     | 1.15              |
| 2:2Z:11:GLN:NE2   | 1:3N:249:ASN:H    | 1.42                     | 1.15              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:HG2  | 1.34                     | 1.15              |
| 1:1I:346:TRP:HB2  | 2:4U:398:MET:HA   | 1.29                     | 1.15              |
| 2:1W:404:PHE:CD1  | 1:2K:260:VAL:O    | 1.99                     | 1.15              |
| 2:1X:179:ASP:O    | 1:2L:352:LYS:HD2  | 1.43                     | 1.15              |
| 1:1E:254:GLU:N    | 2:4R:100:GLY:HA2  | 1.61                     | 1.15              |
| 2:1T:181:VAL:CG2  | 1:2G:258:ASN:O    | 1.95                     | 1.15              |
| 1:1A:262:TYR:HA   | 2:4H:406:HIS:CD2  | 1.80                     | 1.14              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:HB3  | 1.76                     | 1.14              |
| 1:1N:346:TRP:O    | 2:4Z:398:MET:HG2  | 1.43                     | 1.14              |
| 2:1H:207:GLU:OE1  | 1:2A:329:ASN:ND2  | 1.80                     | 1.14              |
| 2:1W:214:PHE:CG   | 1:2K:326:LYS:HE2  | 1.82                     | 1.14              |
| 2:2T:214:PHE:HB2  | 1:3G:326:LYS:HE2  | 1.26                     | 1.14              |
| 1:1B:348:PRO:HG3  | 2:4O:394:GLN:CA   | 1.75                     | 1.14              |
| 1:1G:248:LEU:C    | 2:4T:11:GLN:HE22  | 1.55                     | 1.14              |
| 1:1K:248:LEU:HA   | 2:4W:11:GLN:NE2   | 1.62                     | 1.14              |
| 2:1Z:100:GLY:HA3  | 1:2N:253:THR:CG2  | 1.78                     | 1.14              |
| 2:2P:401:ARG:O    | 1:3C:262:TYR:OH   | 1.65                     | 1.14              |
| 1:1I:260:VAL:HB   | 2:4U:407:TRP:CE2  | 1.81                     | 1.14              |
| 2:1X:404:PHE:CE1  | 1:2L:260:VAL:O    | 1.99                     | 1.14              |
| 2:2Z:179:ASP:O    | 1:3N:352:LYS:HD2  | 1.46                     | 1.14              |
| 1:1C:353:VAL:CB   | 2:4P:179:ASP:OD1  | 1.94                     | 1.14              |
| 1:1D:2:ARG:CD     | 2:4Q:72:PRO:HD2   | 1.77                     | 1.14              |
| 1:1F:332:ILE:CG2  | 2:4S:177:VAL:CG2  | 2.25                     | 1.14              |
| 2:1W:221:THR:HA   | 1:2K:324:VAL:CG1  | 1.77                     | 1.14              |
| 2:2H:179:ASP:O    | 1:3A:352:LYS:HD2  | 1.45                     | 1.14              |
| 2:2P:180:THR:CG2  | 1:3C:258:ASN:HD21 | 1.61                     | 1.14              |
| 5:2Q:501:GDP:C8   | 1:3D:248:LEU:HD13 | 1.83                     | 1.14              |
| 2:2X:401:ARG:HH22 | 1:3L:435:VAL:HA   | 1.08                     | 1.14              |
| 1:1A:332:ILE:CG2  | 2:4H:177:VAL:HG23 | 1.78                     | 1.14              |
| 1:1F:260:VAL:CB   | 2:4S:407:TRP:NE1  | 2.04                     | 1.14              |
| 2:1Y:179:ASP:O    | 1:2M:352:LYS:HD2  | 1.45                     | 1.14              |
| 1:1F:348:PRO:HG3  | 2:4S:394:GLN:CB   | 1.78                     | 1.13              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:437:VAL:O    | 2:4V:401:ARG:NH1  | 1.81                     | 1.13              |
| 2:2O:179:ASP:O    | 1:3B:352:LYS:HD2  | 1.47                     | 1.13              |
| 1:1A:435:VAL:HA   | 2:4H:401:ARG:NH2  | 1.61                     | 1.13              |
| 1:1E:348:PRO:HB2  | 2:4R:394:GLN:HG2  | 1.20                     | 1.13              |
| 1:1F:349:THR:HG21 | 2:4S:184:PRO:HD3  | 1.25                     | 1.13              |
| 2:1V:181:VAL:HG23 | 1:2J:258:ASN:HB3  | 1.29                     | 1.13              |
| 2:1X:404:PHE:CE1  | 1:2L:260:VAL:C    | 2.27                     | 1.13              |
| 2:1Y:401:ARG:HH22 | 1:2M:435:VAL:HA   | 1.10                     | 1.13              |
| 2:2H:214:PHE:HB2  | 1:3A:326:LYS:HE2  | 1.30                     | 1.13              |
| 1:1F:353:VAL:HB   | 2:4S:179:ASP:OD1  | 0.95                     | 1.13              |
| 2:1X:207:GLU:CD   | 1:2L:329:ASN:HD21 | 1.56                     | 1.13              |
| 2:2H:180:THR:CG2  | 1:3A:258:ASN:HD21 | 1.61                     | 1.13              |
| 2:2P:180:THR:HG23 | 1:3C:258:ASN:ND2  | 1.61                     | 1.13              |
| 2:2X:401:ARG:NH2  | 1:3L:435:VAL:HA   | 1.63                     | 1.13              |
| 2:2Y:11:GLN:HE22  | 1:3M:249:ASN:N    | 1.46                     | 1.13              |
| 1:1C:262:TYR:CA   | 2:4P:406:HIS:CD2  | 2.31                     | 1.13              |
| 1:1F:254:GLU:N    | 2:4S:100:GLY:HA2  | 1.62                     | 1.13              |
| 1:1L:262:TYR:N    | 2:4X:406:HIS:NE2  | 1.96                     | 1.13              |
| 2:1W:100:GLY:HA2  | 1:2K:253:THR:CB   | 1.79                     | 1.13              |
| 2:1Z:207:GLU:CD   | 1:2N:329:ASN:HD21 | 1.55                     | 1.13              |
| 5:2R:501:GDP:C8   | 1:3E:248:LEU:HD13 | 1.83                     | 1.13              |
| 2:2V:404:PHE:CD1  | 1:3J:261:PRO:HA   | 1.84                     | 1.13              |
| 1:1C:245:ASP:OD1  | 2:4P:77:SER:HB3   | 1.45                     | 1.12              |
| 1:1E:2:ARG:HD3    | 2:4R:72:PRO:HD2   | 1.15                     | 1.12              |
| 1:1E:435:VAL:CA   | 2:4R:401:ARG:NH2  | 2.10                     | 1.13              |
| 1:1F:435:VAL:C    | 2:4S:401:ARG:HH22 | 1.57                     | 1.13              |
| 1:1F:248:LEU:C    | 2:4S:11:GLN:HE22  | 1.57                     | 1.12              |
| 2:1V:179:ASP:O    | 1:2J:352:LYS:CD   | 1.97                     | 1.12              |
| 2:1V:214:PHE:HB2  | 1:2J:326:LYS:HE2  | 1.13                     | 1.13              |
| 2:2O:180:THR:CG2  | 1:3B:258:ASN:HD21 | 1.61                     | 1.12              |
| 2:2Q:401:ARG:O    | 1:3D:262:TYR:OH   | 1.65                     | 1.12              |
| 2:2V:406:HIS:CD2  | 1:3J:263:PRO:CD   | 2.30                     | 1.12              |
| 2:2Z:180:THR:CG2  | 1:3N:258:ASN:HD21 | 1.62                     | 1.13              |
| 1:1A:262:TYR:CA   | 2:4H:406:HIS:NE2  | 2.12                     | 1.12              |
| 1:1D:254:GLU:HG2  | 2:4Q:101:ASN:N    | 1.65                     | 1.12              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:HG2  | 1.49                     | 1.12              |
| 1:1G:263:PRO:HD3  | 2:4T:406:HIS:CG   | 1.83                     | 1.12              |
| 1:1I:262:TYR:C    | 2:4U:406:HIS:NE2  | 2.05                     | 1.12              |
| 1:1K:349:THR:OG1  | 2:4W:181:VAL:O    | 1.65                     | 1.12              |
| 1:1M:349:THR:O    | 2:4Y:181:VAL:HA   | 1.47                     | 1.12              |
| 2:1T:100:GLY:HA3  | 1:2G:253:THR:CG2  | 1.80                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1X:181:VAL:HB   | 1:2L:258:ASN:HA   | 1.15                     | 1.12              |
| 2:1X:221:THR:HA   | 1:2L:324:VAL:HG11 | 1.17                     | 1.12              |
| 1:1B:348:PRO:HG3  | 2:4O:394:GLN:CB   | 1.77                     | 1.12              |
| 2:1W:179:ASP:O    | 1:2K:352:LYS:HD2  | 1.48                     | 1.12              |
| 2:2S:100:GLY:HA3  | 1:3F:253:THR:HG22 | 1.24                     | 1.12              |
| 2:2T:207:GLU:OE1  | 1:3G:329:ASN:ND2  | 1.82                     | 1.12              |
| 2:2Y:180:THR:HG23 | 1:3M:258:ASN:ND2  | 1.62                     | 1.12              |
| 2:2Z:180:THR:HG23 | 1:3N:258:ASN:ND2  | 1.64                     | 1.12              |
| 1:1E:254:GLU:HG2  | 2:4R:101:ASN:N    | 1.63                     | 1.12              |
| 1:1E:348:PRO:HB2  | 2:4R:394:GLN:CG   | 1.79                     | 1.12              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:CA   | 1.80                     | 1.12              |
| 2:1W:224:TYR:HD2  | 1:2K:247:ALA:O    | 1.18                     | 1.12              |
| 2:2H:11:GLN:HE22  | 1:3A:249:ASN:N    | 1.46                     | 1.12              |
| 2:2V:221:THR:OG1  | 1:3J:324:VAL:HG21 | 1.47                     | 1.12              |
| 2:2W:222:PRO:HG2  | 1:3K:326:LYS:HB2  | 1.28                     | 1.12              |
| 1:1C:249:ASN:H    | 2:4P:11:GLN:CD    | 1.58                     | 1.12              |
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:CB   | 2.27                     | 1.12              |
| 2:1X:404:PHE:CD1  | 1:2L:260:VAL:O    | 2.03                     | 1.12              |
| 2:2Y:180:THR:CG2  | 1:3M:258:ASN:HD21 | 1.63                     | 1.12              |
| 2:2Y:207:GLU:CD   | 1:3M:329:ASN:HD21 | 1.57                     | 1.12              |
| 1:1J:349:THR:OG1  | 2:4V:181:VAL:O    | 1.66                     | 1.11              |
| 2:1Y:179:ASP:O    | 1:2M:352:LYS:CD   | 1.98                     | 1.11              |
| 5:2S:501:GDP:C8   | 1:3F:248:LEU:HD13 | 1.85                     | 1.11              |
| 2:2U:221:THR:OG1  | 1:3I:324:VAL:HG21 | 1.48                     | 1.11              |
| 2:2Y:179:ASP:O    | 1:3M:352:LYS:HD2  | 1.48                     | 1.11              |
| 1:1D:348:PRO:HB2  | 2:4Q:394:GLN:CG   | 1.78                     | 1.11              |
| 2:1Y:181:VAL:HG23 | 1:2M:258:ASN:HB3  | 1.14                     | 1.11              |
| 2:2O:180:THR:HG23 | 1:3B:258:ASN:ND2  | 1.63                     | 1.11              |
| 2:2U:404:PHE:CD1  | 1:3I:261:PRO:HA   | 1.86                     | 1.11              |
| 2:2U:406:HIS:CD2  | 1:3I:263:PRO:CD   | 2.31                     | 1.11              |
| 2:2W:406:HIS:CD2  | 1:3K:263:PRO:CD   | 2.32                     | 1.11              |
| 2:2Z:100:GLY:HA3  | 1:3N:253:THR:HG22 | 1.14                     | 1.11              |
| 1:1A:332:ILE:HG22 | 2:4H:177:VAL:HG23 | 1.32                     | 1.11              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:CG   | 1.98                     | 1.11              |
| 1:1E:260:VAL:HB   | 2:4R:407:TRP:CE2  | 1.84                     | 1.11              |
| 1:1F:348:PRO:HG3  | 2:4S:394:GLN:HA   | 1.32                     | 1.11              |
| 1:1G:348:PRO:CG   | 2:4T:394:GLN:HB3  | 1.80                     | 1.11              |
| 1:1I:2:ARG:CD     | 2:4U:72:PRO:HD2   | 1.79                     | 1.11              |
| 2:1U:100:GLY:CA   | 1:2I:253:THR:CG2  | 2.27                     | 1.11              |
| 2:1Y:100:GLY:HA3  | 1:2M:253:THR:HG21 | 1.20                     | 1.11              |
| 2:2O:100:GLY:HA3  | 1:3B:253:THR:CG2  | 1.79                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:77:SER:HB3   | 1:3F:245:ASP:OD1  | 1.50                     | 1.11              |
| 2:2U:401:ARG:NH2  | 1:3I:435:VAL:HA   | 1.64                     | 1.11              |
| 1:1F:249:ASN:N    | 2:4S:11:GLN:NE2   | 1.68                     | 1.11              |
| 1:1F:348:PRO:HG2  | 2:4S:394:GLN:HB3  | 1.25                     | 1.11              |
| 1:1J:262:TYR:CA   | 2:4V:406:HIS:CD2  | 2.24                     | 1.11              |
| 2:1V:100:GLY:HA2  | 1:2J:253:THR:HB   | 1.20                     | 1.11              |
| 2:1Y:181:VAL:CG2  | 1:2M:258:ASN:O    | 1.98                     | 1.11              |
| 2:2O:100:GLY:HA3  | 1:3B:253:THR:HG22 | 1.25                     | 1.11              |
| 2:2X:394:GLN:HG2  | 1:3L:348:PRO:CG   | 1.81                     | 1.11              |
| 1:1I:349:THR:O    | 2:4U:181:VAL:HA   | 1.48                     | 1.11              |
| 2:1U:404:PHE:CE1  | 1:2I:260:VAL:C    | 2.29                     | 1.11              |
| 2:1V:404:PHE:CD1  | 1:2J:260:VAL:O    | 2.04                     | 1.11              |
| 2:1W:181:VAL:HG21 | 1:2K:258:ASN:O    | 0.94                     | 1.11              |
| 2:2Y:394:GLN:HG2  | 1:3M:348:PRO:CG   | 1.81                     | 1.11              |
| 1:1A:248:LEU:HD13 | 5:4H:501:GDP:C8   | 1.85                     | 1.10              |
| 1:1C:346:TRP:HB2  | 2:4P:397:ALA:O    | 1.50                     | 1.10              |
| 1:1D:346:TRP:HB2  | 2:4Q:397:ALA:O    | 1.50                     | 1.10              |
| 1:1E:248:LEU:CD1  | 5:4R:501:GDP:H8   | 1.62                     | 1.10              |
| 2:1U:221:THR:CA   | 1:2I:324:VAL:HG11 | 1.81                     | 1.10              |
| 1:1F:346:TRP:CH2  | 2:4S:403:ALA:HB1  | 1.86                     | 1.10              |
| 1:1F:349:THR:CG2  | 2:4S:184:PRO:HD3  | 1.80                     | 1.10              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:CA   | 1.80                     | 1.10              |
| 1:1L:349:THR:HG21 | 2:4X:184:PRO:HD3  | 1.22                     | 1.10              |
| 2:1R:221:THR:HA   | 1:2E:324:VAL:HG11 | 1.29                     | 1.10              |
| 2:1S:221:THR:HA   | 1:2F:324:VAL:HG11 | 1.10                     | 1.10              |
| 2:2U:100:GLY:HA3  | 1:3I:253:THR:HG22 | 1.13                     | 1.10              |
| 2:2Z:11:GLN:HE22  | 1:3N:249:ASN:N    | 1.47                     | 1.10              |
| 1:1B:263:PRO:CD   | 2:4O:406:HIS:CD2  | 2.35                     | 1.10              |
| 1:1B:348:PRO:CG   | 2:4O:394:GLN:CB   | 2.29                     | 1.10              |
| 1:1G:261:PRO:HA   | 2:4T:404:PHE:HA   | 1.25                     | 1.10              |
| 1:1M:346:TRP:HB2  | 2:4Y:398:MET:HA   | 1.33                     | 1.10              |
| 2:1R:214:PHE:HB2  | 1:2E:326:LYS:HE2  | 1.29                     | 1.10              |
| 2:1W:214:PHE:HB2  | 1:2K:326:LYS:HE2  | 1.22                     | 1.10              |
| 2:1Z:181:VAL:N    | 1:2N:258:ASN:ND2  | 1.97                     | 1.10              |
| 2:2S:214:PHE:HB2  | 1:3F:326:LYS:HE2  | 1.34                     | 1.10              |
| 1:1C:262:TYR:CA   | 2:4P:406:HIS:NE2  | 2.14                     | 1.10              |
| 1:1C:332:ILE:HG21 | 2:4P:177:VAL:CG2  | 1.81                     | 1.10              |
| 1:1I:260:VAL:HB   | 2:4U:407:TRP:NE1  | 1.67                     | 1.10              |
| 1:1M:349:THR:HG21 | 2:4Y:184:PRO:HD3  | 1.31                     | 1.10              |
| 1:1N:258:ASN:ND2  | 2:4Z:180:THR:HG23 | 1.67                     | 1.10              |
| 2:2Y:214:PHE:HB2  | 1:3M:326:LYS:HE2  | 1.14                     | 1.10              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1N:261:PRO:HA   | 2:4Z:404:PHE:CD1  | 1.87                     | 1.10              |
| 2:2H:180:THR:HG23 | 1:3A:258:ASN:ND2  | 1.64                     | 1.10              |
| 2:2V:222:PRO:HG2  | 1:3J:326:LYS:HB2  | 1.24                     | 1.10              |
| 2:2X:207:GLU:OE1  | 1:3L:329:ASN:ND2  | 1.83                     | 1.10              |
| 2:2Z:401:ARG:HH22 | 1:3N:435:VAL:HA   | 0.95                     | 1.10              |
| 1:1E:260:VAL:CB   | 2:4R:407:TRP:NE1  | 2.01                     | 1.09              |
| 2:1H:401:ARG:HH22 | 1:2A:435:VAL:HA   | 1.10                     | 1.09              |
| 2:1S:214:PHE:HB2  | 1:2F:326:LYS:HE2  | 1.18                     | 1.09              |
| 2:1U:100:GLY:HA3  | 1:2I:253:THR:HG21 | 1.26                     | 1.09              |
| 2:1U:181:VAL:HG21 | 1:2I:258:ASN:O    | 0.94                     | 1.09              |
| 2:1X:100:GLY:HA2  | 1:2L:253:THR:CB   | 1.81                     | 1.09              |
| 5:2P:501:GDP:C8   | 1:3C:248:LEU:HD13 | 1.85                     | 1.09              |
| 2:2Q:180:THR:CG2  | 1:3D:258:ASN:HD21 | 1.63                     | 1.09              |
| 1:1B:262:TYR:CA   | 2:4O:406:HIS:NE2  | 2.15                     | 1.09              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:HA   | 1.16                     | 1.09              |
| 1:1G:346:TRP:HB2  | 2:4T:398:MET:HA   | 1.24                     | 1.09              |
| 2:2R:401:ARG:O    | 1:3E:262:TYR:OH   | 1.69                     | 1.09              |
| 2:2U:214:PHE:HB2  | 1:3I:326:LYS:HE2  | 1.17                     | 1.09              |
| 1:1D:348:PRO:CB   | 2:4Q:394:GLN:CG   | 2.31                     | 1.09              |
| 1:1E:346:TRP:CA   | 2:4R:397:ALA:O    | 1.99                     | 1.09              |
| 1:1M:262:TYR:HA   | 2:4Y:406:HIS:NE2  | 1.57                     | 1.09              |
| 1:1M:263:PRO:HD3  | 2:4Y:406:HIS:CG   | 1.85                     | 1.09              |
| 2:1Y:214:PHE:CB   | 1:2M:326:LYS:HE2  | 1.81                     | 1.09              |
| 2:1Z:179:ASP:O    | 1:2N:352:LYS:HD2  | 1.51                     | 1.09              |
| 2:2X:180:THR:CG2  | 1:3L:258:ASN:HD21 | 1.65                     | 1.09              |
| 1:1E:348:PRO:HG3  | 2:4R:394:GLN:HA   | 1.16                     | 1.09              |
| 1:1G:332:ILE:CG2  | 2:4T:177:VAL:HG23 | 1.81                     | 1.09              |
| 2:1V:214:PHE:CG   | 1:2J:326:LYS:CE   | 2.34                     | 1.09              |
| 2:2T:406:HIS:CD2  | 1:3G:263:PRO:CD   | 2.34                     | 1.09              |
| 2:2X:179:ASP:O    | 1:3L:352:LYS:HD2  | 1.53                     | 1.09              |
| 1:1B:258:ASN:HD21 | 2:4O:180:THR:CG2  | 1.63                     | 1.09              |
| 1:1B:435:VAL:CA   | 2:4O:401:ARG:NH2  | 2.15                     | 1.09              |
| 1:1C:333:ALA:HB1  | 2:4P:176:LYS:HE2  | 1.31                     | 1.09              |
| 1:1D:2:ARG:HD3    | 2:4Q:72:PRO:HD2   | 1.28                     | 1.09              |
| 1:1F:346:TRP:HB2  | 2:4S:398:MET:HA   | 1.23                     | 1.09              |
| 1:1G:249:ASN:N    | 2:4T:11:GLN:NE2   | 1.77                     | 1.09              |
| 1:1I:245:ASP:CG   | 2:4U:77:SER:CB    | 2.25                     | 1.09              |
| 1:1I:332:ILE:HG22 | 2:4U:177:VAL:HG23 | 1.31                     | 1.09              |
| 2:1T:221:THR:HA   | 1:2G:324:VAL:CG1  | 1.81                     | 1.09              |
| 2:1W:181:VAL:HG23 | 1:2K:258:ASN:HB3  | 1.15                     | 1.09              |
| 2:2O:401:ARG:O    | 1:3B:262:TYR:OH   | 1.71                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:77:SER:HB3   | 1:3J:245:ASP:OD1  | 1.49                     | 1.09              |
| 2:2V:100:GLY:HA3  | 1:3J:253:THR:CG2  | 1.81                     | 1.09              |
| 2:2W:214:PHE:HB2  | 1:3K:326:LYS:CE   | 1.82                     | 1.09              |
| 1:1A:245:ASP:CG   | 2:4H:77:SER:HB3   | 1.76                     | 1.08              |
| 1:1B:348:PRO:HG3  | 2:4O:394:GLN:HA   | 1.32                     | 1.08              |
| 1:1I:248:LEU:C    | 2:4U:11:GLN:HE22  | 1.58                     | 1.08              |
| 2:2Q:100:GLY:HA3  | 1:3D:253:THR:HG22 | 1.29                     | 1.08              |
| 2:2R:100:GLY:HA3  | 1:3E:253:THR:HG22 | 1.28                     | 1.08              |
| 2:2R:180:THR:CG2  | 1:3E:258:ASN:HD21 | 1.65                     | 1.08              |
| 2:2W:404:PHE:CD1  | 1:3K:261:PRO:HA   | 1.88                     | 1.08              |
| 1:1C:348:PRO:HG3  | 2:4P:394:GLN:HA   | 1.15                     | 1.08              |
| 1:1D:258:ASN:HD21 | 2:4Q:180:THR:CG2  | 1.66                     | 1.08              |
| 1:1D:351:PHE:O    | 2:4Q:180:THR:C    | 1.94                     | 1.08              |
| 1:1G:332:ILE:HG22 | 2:4T:177:VAL:HG23 | 1.19                     | 1.08              |
| 1:1G:346:TRP:CZ3  | 2:4T:403:ALA:HB1  | 1.87                     | 1.08              |
| 1:1I:346:TRP:CZ3  | 2:4U:403:ALA:HB1  | 1.87                     | 1.08              |
| 1:1N:258:ASN:HD21 | 2:4Z:180:THR:HG23 | 1.03                     | 1.08              |
| 1:1N:346:TRP:O    | 2:4Z:398:MET:CG   | 2.01                     | 1.08              |
| 2:1R:181:VAL:HG21 | 1:2E:258:ASN:O    | 1.54                     | 1.08              |
| 2:1Y:181:VAL:HB   | 1:2M:258:ASN:HA   | 1.21                     | 1.08              |
| 2:2U:222:PRO:HG2  | 1:3I:326:LYS:HB2  | 1.26                     | 1.08              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:HA   | 1.29                     | 1.08              |
| 1:1D:348:PRO:HB2  | 2:4Q:394:GLN:HG2  | 1.15                     | 1.08              |
| 1:1F:258:ASN:ND2  | 2:4S:180:THR:HG23 | 1.68                     | 1.08              |
| 1:1F:332:ILE:HG22 | 2:4S:177:VAL:HG23 | 1.09                     | 1.08              |
| 1:1I:263:PRO:HD3  | 2:4U:406:HIS:CG   | 1.89                     | 1.08              |
| 2:1V:181:VAL:HB   | 1:2J:258:ASN:HA   | 1.32                     | 1.08              |
| 5:2T:501:GDP:C8   | 1:3G:248:LEU:HD13 | 1.89                     | 1.08              |
| 2:2V:401:ARG:NH2  | 1:3J:435:VAL:HA   | 1.67                     | 1.08              |
| 2:2W:394:GLN:HG2  | 1:3K:348:PRO:CG   | 1.82                     | 1.08              |
| 2:2X:406:HIS:CD2  | 1:3L:263:PRO:CD   | 2.36                     | 1.08              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:CA   | 2.02                     | 1.08              |
| 1:1F:346:TRP:CZ3  | 2:4S:403:ALA:CB   | 2.37                     | 1.08              |
| 1:1G:248:LEU:HA   | 2:4T:11:GLN:NE2   | 1.66                     | 1.08              |
| 1:1G:349:THR:HG21 | 2:4T:184:PRO:HD3  | 1.11                     | 1.08              |
| 1:1K:353:VAL:HB   | 2:4W:179:ASP:OD1  | 1.51                     | 1.08              |
| 2:2S:180:THR:CG2  | 1:3F:258:ASN:HD21 | 1.66                     | 1.08              |
| 2:2T:221:THR:OG1  | 1:3G:324:VAL:HG21 | 1.54                     | 1.08              |
| 2:2W:401:ARG:NH2  | 1:3K:435:VAL:HA   | 1.67                     | 1.08              |
| 1:1A:348:PRO:CB   | 2:4H:394:GLN:HG2  | 1.83                     | 1.07              |
| 1:1B:332:ILE:HG22 | 2:4O:177:VAL:HG23 | 1.21                     | 1.07              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:314:ALA:HB1  | 2:4P:181:VAL:HG21 | 1.34                     | 1.07              |
| 1:1D:254:GLU:N    | 2:4Q:100:GLY:HA2  | 1.68                     | 1.07              |
| 1:1D:437:VAL:O    | 2:4Q:401:ARG:NH1  | 1.86                     | 1.07              |
| 2:1X:224:TYR:HD2  | 1:2L:247:ALA:O    | 1.23                     | 1.07              |
| 2:1Y:181:VAL:CG2  | 1:2M:258:ASN:HB3  | 1.84                     | 1.07              |
| 2:1Z:100:GLY:HA2  | 1:2N:253:THR:HB   | 1.26                     | 1.07              |
| 2:2P:179:ASP:O    | 1:3C:352:LYS:HD2  | 1.52                     | 1.07              |
| 2:2V:214:PHE:HB2  | 1:3J:326:LYS:CE   | 1.82                     | 1.07              |
| 1:1B:332:ILE:CG2  | 2:4O:177:VAL:CG2  | 2.32                     | 1.07              |
| 2:1T:214:PHE:HB2  | 1:2G:326:LYS:HE2  | 1.10                     | 1.07              |
| 2:1W:214:PHE:CG   | 1:2K:326:LYS:CE   | 2.36                     | 1.07              |
| 2:2W:221:THR:OG1  | 1:3K:324:VAL:HG21 | 1.50                     | 1.07              |
| 1:1G:351:PHE:O    | 2:4T:180:THR:C    | 1.97                     | 1.07              |
| 1:1J:2:ARG:HD3    | 2:4V:72:PRO:HD2   | 1.07                     | 1.07              |
| 2:1V:101:ASN:HB2  | 1:2J:254:GLU:HG2  | 1.34                     | 1.07              |
| 2:1Y:221:THR:HA   | 1:2M:324:VAL:HG11 | 1.33                     | 1.07              |
| 2:2H:394:GLN:HG2  | 1:3A:348:PRO:CG   | 1.85                     | 1.07              |
| 2:2T:180:THR:CG2  | 1:3G:258:ASN:HD21 | 1.68                     | 1.07              |
| 1:1B:348:PRO:HG2  | 2:4O:394:GLN:HB3  | 1.32                     | 1.07              |
| 1:1D:348:PRO:HG3  | 2:4Q:394:GLN:HA   | 1.10                     | 1.07              |
| 1:1E:353:VAL:HB   | 2:4R:179:ASP:OD1  | 0.92                     | 1.07              |
| 1:1F:351:PHE:O    | 2:4S:180:THR:CA   | 2.03                     | 1.07              |
| 1:1K:349:THR:CG2  | 2:4W:184:PRO:HD3  | 1.83                     | 1.07              |
| 1:1L:248:LEU:HA   | 2:4X:11:GLN:NE2   | 1.70                     | 1.07              |
| 2:1H:181:VAL:H    | 1:2A:258:ASN:ND2  | 1.51                     | 1.07              |
| 2:1S:181:VAL:H    | 1:2F:258:ASN:ND2  | 1.53                     | 1.07              |
| 2:1V:100:GLY:HA3  | 1:2J:253:THR:HG21 | 1.09                     | 1.07              |
| 2:2U:207:GLU:OE1  | 1:3I:329:ASN:ND2  | 1.88                     | 1.07              |
| 2:2V:394:GLN:HG2  | 1:3J:348:PRO:CG   | 1.84                     | 1.07              |
| 2:2X:222:PRO:HG2  | 1:3L:326:LYS:HB2  | 1.36                     | 1.07              |
| 2:2Z:394:GLN:HG2  | 1:3N:348:PRO:CG   | 1.83                     | 1.07              |
| 1:1G:346:TRP:CZ3  | 2:4T:403:ALA:CB   | 2.37                     | 1.07              |
| 2:1U:100:GLY:HA2  | 1:2I:253:THR:HB   | 1.37                     | 1.07              |
| 2:1U:214:PHE:HB2  | 1:2I:326:LYS:HE2  | 1.08                     | 1.07              |
| 1:1C:254:GLU:HA   | 2:4P:100:GLY:O    | 1.53                     | 1.06              |
| 1:1E:348:PRO:HG2  | 2:4R:394:GLN:HB3  | 1.12                     | 1.06              |
| 2:1W:222:PRO:O    | 1:2K:325:PRO:HD2  | 1.54                     | 1.06              |
| 2:1Z:181:VAL:N    | 1:2N:258:ASN:HD22 | 1.52                     | 1.06              |
| 2:2V:404:PHE:CE2  | 1:3J:261:PRO:HB3  | 1.90                     | 1.06              |
| 1:1A:253:THR:HG22 | 2:4H:100:GLY:HA3  | 1.37                     | 1.06              |
| 1:1B:248:LEU:CD1  | 5:4O:501:GDP:H8   | 1.67                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:263:PRO:CD   | 2:4P:406:HIS:CD2  | 2.37                     | 1.06              |
| 1:1D:2:ARG:CG     | 2:4Q:72:PRO:HD2   | 1.85                     | 1.06              |
| 1:1D:332:ILE:HG21 | 2:4Q:177:VAL:CG2  | 1.82                     | 1.06              |
| 1:1F:346:TRP:CA   | 2:4S:397:ALA:O    | 2.03                     | 1.06              |
| 2:2P:100:GLY:HA3  | 1:3C:253:THR:CG2  | 1.85                     | 1.06              |
| 2:2U:406:HIS:CG   | 1:3I:263:PRO:HD3  | 1.90                     | 1.06              |
| 2:2V:180:THR:CG2  | 1:3J:258:ASN:HD21 | 1.68                     | 1.06              |
| 2:2W:180:THR:CG2  | 1:3K:258:ASN:HD21 | 1.67                     | 1.06              |
| 1:1B:253:THR:HG22 | 2:4O:100:GLY:HA3  | 1.36                     | 1.06              |
| 1:1D:263:PRO:HD3  | 2:4Q:406:HIS:CD2  | 1.90                     | 1.06              |
| 1:1E:262:TYR:N    | 2:4R:406:HIS:NE2  | 2.04                     | 1.06              |
| 1:1F:435:VAL:HA   | 2:4S:401:ARG:NH2  | 1.71                     | 1.06              |
| 2:1T:221:THR:CA   | 1:2G:324:VAL:HG11 | 1.84                     | 1.06              |
| 2:1U:214:PHE:CG   | 1:2I:326:LYS:HE2  | 1.89                     | 1.06              |
| 2:1W:181:VAL:HG21 | 1:2K:258:ASN:C    | 1.79                     | 1.06              |
| 2:1Z:401:ARG:HH22 | 1:2N:435:VAL:HA   | 0.92                     | 1.06              |
| 1:1D:346:TRP:HB2  | 2:4Q:398:MET:HA   | 1.32                     | 1.06              |
| 1:1F:348:PRO:HB2  | 2:4S:394:GLN:HG2  | 1.35                     | 1.06              |
| 1:1G:346:TRP:CH2  | 2:4T:403:ALA:HB1  | 1.90                     | 1.06              |
| 1:1K:349:THR:HG21 | 2:4W:184:PRO:HD3  | 1.13                     | 1.06              |
| 1:1L:349:THR:OG1  | 2:4X:181:VAL:O    | 1.72                     | 1.06              |
| 1:1M:2:ARG:HD3    | 2:4Y:72:PRO:HD2   | 1.24                     | 1.06              |
| 2:1W:207:GLU:CD   | 1:2K:329:ASN:HD21 | 1.64                     | 1.06              |
| 2:1X:181:VAL:CG2  | 1:2L:258:ASN:HB3  | 1.86                     | 1.06              |
| 5:2O:501:GDP:C8   | 1:3B:248:LEU:HD13 | 1.88                     | 1.06              |
| 2:2P:100:GLY:HA3  | 1:3C:253:THR:HG22 | 1.29                     | 1.06              |
| 2:2P:401:ARG:HH22 | 1:3C:435:VAL:CA   | 1.68                     | 1.06              |
| 1:1F:254:GLU:HG2  | 2:4S:101:ASN:N    | 1.71                     | 1.06              |
| 2:1U:224:TYR:HD2  | 1:2I:247:ALA:O    | 1.37                     | 1.06              |
| 2:1X:214:PHE:HB2  | 1:2L:326:LYS:HE2  | 1.33                     | 1.06              |
| 2:2O:214:PHE:HB2  | 1:3B:326:LYS:HE2  | 1.37                     | 1.06              |
| 2:2V:404:PHE:CG   | 1:3J:261:PRO:HA   | 1.89                     | 1.06              |
| 1:1A:348:PRO:HG3  | 2:4H:394:GLN:CB   | 1.86                     | 1.05              |
| 1:1B:314:ALA:HB1  | 2:4O:181:VAL:HG21 | 1.34                     | 1.05              |
| 1:1D:346:TRP:HB3  | 2:4Q:397:ALA:O    | 1.54                     | 1.05              |
| 1:1G:254:GLU:HA   | 2:4T:100:GLY:O    | 1.54                     | 1.05              |
| 1:1G:329:ASN:ND2  | 2:4T:207:GLU:OE1  | 1.88                     | 1.05              |
| 1:1L:353:VAL:HB   | 2:4X:179:ASP:OD1  | 1.56                     | 1.05              |
| 1:1N:262:TYR:C    | 2:4Z:406:HIS:NE2  | 2.12                     | 1.05              |
| 2:1H:101:ASN:HB2  | 1:2A:254:GLU:HG2  | 1.37                     | 1.05              |
| 2:2T:406:HIS:CG   | 1:3G:263:PRO:HD3  | 1.90                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2X:214:PHE:CB   | 1:3L:326:LYS:HE2  | 1.84                     | 1.05              |
| 1:1A:353:VAL:HB   | 2:4H:179:ASP:OD1  | 1.54                     | 1.05              |
| 1:1C:245:ASP:CG   | 2:4P:77:SER:CB    | 2.28                     | 1.05              |
| 1:1C:254:GLU:HA   | 2:4P:100:GLY:C    | 1.81                     | 1.05              |
| 1:1F:248:LEU:HD13 | 5:4S:501:GDP:H8   | 1.07                     | 1.05              |
| 1:1J:261:PRO:C    | 2:4V:406:HIS:NE2  | 2.13                     | 1.05              |
| 1:1J:349:THR:HG21 | 2:4V:184:PRO:HD3  | 1.06                     | 1.05              |
| 1:1N:326:LYS:HB2  | 2:4Z:222:PRO:HG2  | 1.35                     | 1.05              |
| 2:1Z:179:ASP:OD2  | 1:2N:248:LEU:CD2  | 2.04                     | 1.05              |
| 2:2T:222:PRO:HG2  | 1:3G:326:LYS:HB2  | 1.33                     | 1.05              |
| 2:2T:404:PHE:CD1  | 1:3G:261:PRO:HA   | 1.92                     | 1.05              |
| 2:2U:404:PHE:CG   | 1:3I:261:PRO:HA   | 1.90                     | 1.05              |
| 2:2X:207:GLU:CD   | 1:3L:329:ASN:HD21 | 1.64                     | 1.05              |
| 1:1B:260:VAL:HB   | 2:4O:407:TRP:NE1  | 1.70                     | 1.05              |
| 1:1E:258:ASN:HD21 | 2:4R:180:THR:HG23 | 1.06                     | 1.05              |
| 1:1L:262:TYR:HA   | 2:4X:406:HIS:NE2  | 1.56                     | 1.05              |
| 2:2U:180:THR:CG2  | 1:3I:258:ASN:HD21 | 1.68                     | 1.05              |
| 2:2U:214:PHE:HB2  | 1:3I:326:LYS:CE   | 1.85                     | 1.05              |
| 2:2U:404:PHE:CE2  | 1:3I:261:PRO:HB3  | 1.92                     | 1.05              |
| 1:1D:332:ILE:HG22 | 2:4Q:177:VAL:HG23 | 1.05                     | 1.05              |
| 1:1G:349:THR:HG21 | 2:4T:184:PRO:CD   | 1.86                     | 1.05              |
| 1:1I:257:THR:HG21 | 2:4U:102:ASN:HB2  | 1.39                     | 1.05              |
| 1:1M:262:TYR:N    | 2:4Y:406:HIS:NE2  | 2.03                     | 1.05              |
| 2:1V:100:GLY:HA2  | 1:2J:253:THR:CB   | 1.86                     | 1.05              |
| 2:1V:181:VAL:HG21 | 1:2J:258:ASN:O    | 0.88                     | 1.05              |
| 2:2Q:179:ASP:O    | 1:3D:352:LYS:HD2  | 1.57                     | 1.05              |
| 2:2V:394:GLN:HG2  | 1:3J:348:PRO:HG3  | 1.39                     | 1.05              |
| 2:2W:207:GLU:OE1  | 1:3K:329:ASN:ND2  | 1.89                     | 1.05              |
| 2:2W:394:GLN:HG2  | 1:3K:348:PRO:HG3  | 1.36                     | 1.05              |
| 1:1E:346:TRP:CH2  | 2:4R:403:ALA:HB1  | 1.91                     | 1.05              |
| 1:1G:254:GLU:N    | 2:4T:100:GLY:HA2  | 1.72                     | 1.05              |
| 1:1G:262:TYR:OH   | 2:4T:401:ARG:O    | 1.72                     | 1.05              |
| 2:1W:100:GLY:HA2  | 1:2K:253:THR:HB   | 1.08                     | 1.05              |
| 2:2U:394:GLN:HG2  | 1:3I:348:PRO:CG   | 1.87                     | 1.05              |
| 2:2W:404:PHE:CE2  | 1:3K:261:PRO:HB3  | 1.92                     | 1.05              |
| 2:2X:100:GLY:HA3  | 1:3L:253:THR:HG22 | 1.05                     | 1.05              |
| 1:1C:332:ILE:HG22 | 2:4P:177:VAL:HG23 | 1.12                     | 1.04              |
| 1:1F:260:VAL:O    | 2:4S:407:TRP:NE1  | 1.87                     | 1.04              |
| 1:1G:260:VAL:CB   | 2:4T:407:TRP:NE1  | 2.16                     | 1.04              |
| 1:1I:346:TRP:CE3  | 2:4U:403:ALA:CB   | 2.40                     | 1.04              |
| 2:1V:401:ARG:HB3  | 1:2J:262:TYR:OH   | 1.57                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1X:181:VAL:HG23 | 1:2L:258:ASN:HB3  | 1.09                     | 1.04              |
| 2:1Z:101:ASN:HB2  | 1:2N:254:GLU:HG2  | 1.11                     | 1.04              |
| 2:1Z:401:ARG:NH2  | 1:2N:435:VAL:HA   | 1.72                     | 1.04              |
| 2:2W:404:PHE:CG   | 1:3K:261:PRO:HA   | 1.91                     | 1.04              |
| 2:2X:214:PHE:HB2  | 1:3L:326:LYS:CE   | 1.85                     | 1.04              |
| 1:1C:260:VAL:O    | 2:4P:407:TRP:CD1  | 2.10                     | 1.04              |
| 1:1F:346:TRP:HA   | 2:4S:397:ALA:O    | 1.58                     | 1.04              |
| 1:1G:249:ASN:H    | 2:4T:11:GLN:CD    | 1.65                     | 1.04              |
| 1:1J:346:TRP:HB2  | 2:4V:398:MET:HA   | 1.35                     | 1.04              |
| 1:1M:353:VAL:HB   | 2:4Y:179:ASP:OD1  | 1.54                     | 1.04              |
| 2:1V:221:THR:CA   | 1:2J:324:VAL:HG11 | 1.86                     | 1.04              |
| 2:2S:406:HIS:CD2  | 1:3F:263:PRO:CD   | 2.39                     | 1.04              |
| 2:2V:207:GLU:OE1  | 1:3J:329:ASN:ND2  | 1.91                     | 1.04              |
| 2:2Y:214:PHE:CB   | 1:3M:326:LYS:HE2  | 1.86                     | 1.04              |
| 1:1B:348:PRO:CG   | 2:4O:394:GLN:HB3  | 1.87                     | 1.04              |
| 1:1I:349:THR:HG21 | 2:4U:184:PRO:HD3  | 1.05                     | 1.04              |
| 1:1N:245:ASP:CG   | 2:4Z:77:SER:HB3   | 1.80                     | 1.04              |
| 2:1V:222:PRO:O    | 1:2J:325:PRO:HD2  | 1.55                     | 1.04              |
| 2:1X:181:VAL:HB   | 1:2L:258:ASN:CA   | 1.87                     | 1.04              |
| 2:1Y:100:GLY:CA   | 1:2M:253:THR:CG2  | 2.35                     | 1.04              |
| 2:2X:221:THR:OG1  | 1:3L:324:VAL:HG21 | 1.57                     | 1.04              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:CG   | 2.05                     | 1.04              |
| 2:1Z:101:ASN:HB2  | 1:2N:254:GLU:CG   | 1.87                     | 1.04              |
| 2:2O:394:GLN:HG2  | 1:3B:348:PRO:CG   | 1.87                     | 1.04              |
| 2:2W:100:GLY:HA3  | 1:3K:253:THR:HG22 | 1.05                     | 1.04              |
| 2:2W:214:PHE:CB   | 1:3K:326:LYS:HE2  | 1.86                     | 1.04              |
| 1:1A:263:PRO:CD   | 2:4H:406:HIS:CD2  | 2.39                     | 1.04              |
| 1:1A:346:TRP:O    | 2:4H:398:MET:CG   | 2.06                     | 1.04              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:CA   | 1.87                     | 1.04              |
| 1:1J:248:LEU:C    | 2:4V:11:GLN:HE22  | 1.65                     | 1.04              |
| 2:2O:401:ARG:HH22 | 1:3B:435:VAL:CA   | 1.68                     | 1.04              |
| 1:1B:332:ILE:HG21 | 2:4O:177:VAL:CG2  | 1.88                     | 1.03              |
| 1:1B:333:ALA:HB1  | 2:4O:176:LYS:HE2  | 1.33                     | 1.03              |
| 1:1C:346:TRP:HB3  | 2:4P:397:ALA:O    | 1.58                     | 1.03              |
| 1:1I:349:THR:HG21 | 2:4U:184:PRO:CD   | 1.87                     | 1.03              |
| 1:1K:437:VAL:O    | 2:4W:401:ARG:NH1  | 1.90                     | 1.03              |
| 2:1U:214:PHE:CG   | 1:2I:326:LYS:CE   | 2.41                     | 1.03              |
| 2:2V:214:PHE:HB2  | 1:3J:326:LYS:HE2  | 1.09                     | 1.03              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:CA   | 2.05                     | 1.03              |
| 1:1M:262:TYR:C    | 2:4Y:406:HIS:NE2  | 2.15                     | 1.03              |
| 2:2Y:100:GLY:HA3  | 1:3M:253:THR:HG22 | 1.09                     | 1.03              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:100:GLY:HA2  | 1:3N:253:THR:HB   | 1.40                     | 1.03              |
| 1:1C:348:PRO:CB   | 2:4P:394:GLN:CG   | 2.35                     | 1.03              |
| 1:1L:263:PRO:HD3  | 2:4X:406:HIS:CG   | 1.93                     | 1.03              |
| 2:1H:179:ASP:OD2  | 1:2A:248:LEU:HD21 | 1.57                     | 1.03              |
| 2:1X:182:VAL:HG21 | 1:2L:257:THR:CG2  | 1.89                     | 1.03              |
| 2:1Y:100:GLY:CA   | 1:2M:253:THR:HB   | 1.86                     | 1.03              |
| 2:2U:100:GLY:HA3  | 1:3I:253:THR:CG2  | 1.87                     | 1.03              |
| 2:2X:394:GLN:HG2  | 1:3L:348:PRO:HG3  | 1.38                     | 1.03              |
| 1:1A:262:TYR:OH   | 2:4H:401:ARG:O    | 1.77                     | 1.03              |
| 1:1C:348:PRO:HB2  | 2:4P:394:GLN:CG   | 1.87                     | 1.03              |
| 1:1D:346:TRP:CA   | 2:4Q:397:ALA:O    | 2.06                     | 1.03              |
| 1:1I:353:VAL:CB   | 2:4U:179:ASP:OD1  | 2.06                     | 1.03              |
| 1:1K:261:PRO:C    | 2:4W:406:HIS:NE2  | 2.17                     | 1.03              |
| 5:2H:501:GDP:C8   | 1:3A:248:LEU:HD13 | 1.93                     | 1.03              |
| 2:2W:77:SER:HB3   | 1:3K:245:ASP:OD1  | 1.58                     | 1.03              |
| 1:1D:253:THR:C    | 2:4Q:100:GLY:CA   | 2.32                     | 1.03              |
| 1:1D:333:ALA:HB1  | 2:4Q:176:LYS:HE2  | 1.39                     | 1.03              |
| 1:1E:324:VAL:HG13 | 2:4R:222:PRO:O    | 1.59                     | 1.03              |
| 1:1G:248:LEU:HD13 | 5:4T:501:GDP:C8   | 1.94                     | 1.03              |
| 2:1S:214:PHE:CB   | 1:2F:326:LYS:HE2  | 1.88                     | 1.03              |
| 2:1X:401:ARG:HH22 | 1:2L:435:VAL:HA   | 1.18                     | 1.03              |
| 2:1Y:100:GLY:HA2  | 1:2M:253:THR:HB   | 1.07                     | 1.03              |
| 2:2R:177:VAL:HG23 | 1:3E:332:ILE:CG2  | 1.88                     | 1.03              |
| 2:2R:214:PHE:HB2  | 1:3E:326:LYS:HE2  | 1.40                     | 1.03              |
| 2:2V:406:HIS:CG   | 1:3J:263:PRO:HD3  | 1.94                     | 1.03              |
| 2:2X:214:PHE:HB2  | 1:3L:326:LYS:HE2  | 1.07                     | 1.03              |
| 2:2Y:406:HIS:CD2  | 1:3M:263:PRO:CD   | 2.42                     | 1.03              |
| 1:1D:314:ALA:HB1  | 2:4Q:181:VAL:HG21 | 1.39                     | 1.02              |
| 1:1E:348:PRO:CB   | 2:4R:394:GLN:CG   | 2.35                     | 1.02              |
| 1:1J:346:TRP:CZ3  | 2:4V:403:ALA:HB1  | 1.93                     | 1.02              |
| 1:1N:324:VAL:HG21 | 2:4Z:221:THR:OG1  | 1.59                     | 1.02              |
| 2:1Q:214:PHE:HB2  | 1:2D:326:LYS:HE2  | 1.40                     | 1.02              |
| 2:1X:100:GLY:HA3  | 1:2L:253:THR:HG21 | 1.05                     | 1.02              |
| 2:2T:404:PHE:CG   | 1:3G:261:PRO:HA   | 1.93                     | 1.02              |
| 5:2U:501:GDP:C8   | 1:3I:248:LEU:HD13 | 1.93                     | 1.02              |
| 1:1A:346:TRP:O    | 2:4H:398:MET:HG2  | 1.59                     | 1.02              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:CA   | 2.07                     | 1.02              |
| 1:1F:2:ARG:HD3    | 2:4S:72:PRO:HD2   | 1.03                     | 1.02              |
| 1:1J:262:TYR:C    | 2:4V:406:HIS:NE2  | 2.16                     | 1.02              |
| 2:1U:224:TYR:CD2  | 1:2I:247:ALA:O    | 2.10                     | 1.02              |
| 2:1Y:224:TYR:HD2  | 1:2M:247:ALA:O    | 1.35                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Q:401:ARG:HH22 | 1:3D:435:VAL:CA   | 1.71                     | 1.02              |
| 2:2T:394:GLN:HG2  | 1:3G:348:PRO:CG   | 1.89                     | 1.02              |
| 2:2W:401:ARG:HH22 | 1:3K:435:VAL:HA   | 1.16                     | 1.02              |
| 1:1D:348:PRO:HG2  | 2:4Q:394:GLN:HB3  | 1.08                     | 1.02              |
| 1:1F:258:ASN:HD21 | 2:4S:180:THR:HG23 | 1.21                     | 1.02              |
| 1:1G:351:PHE:O    | 2:4T:180:THR:CA   | 2.06                     | 1.02              |
| 1:1I:349:THR:OG1  | 2:4U:181:VAL:O    | 1.76                     | 1.02              |
| 1:1J:260:VAL:HB   | 2:4V:407:TRP:CE2  | 1.94                     | 1.02              |
| 2:1T:404:PHE:CE1  | 1:2G:260:VAL:O    | 2.11                     | 1.02              |
| 2:1X:101:ASN:HB2  | 1:2L:254:GLU:HG2  | 1.04                     | 1.02              |
| 2:2H:100:GLY:HA2  | 1:3A:253:THR:HB   | 1.42                     | 1.02              |
| 2:2V:100:GLY:HA3  | 1:3J:253:THR:HG22 | 1.08                     | 1.02              |
| 2:2W:404:PHE:N    | 1:3K:261:PRO:O    | 1.92                     | 1.02              |
| 2:2X:221:THR:HA   | 1:3L:324:VAL:HG11 | 1.42                     | 1.02              |
| 1:1B:348:PRO:HB2  | 2:4O:394:GLN:HG2  | 1.41                     | 1.02              |
| 1:1D:324:VAL:HG13 | 2:4Q:222:PRO:O    | 1.58                     | 1.02              |
| 1:1M:332:ILE:HG22 | 2:4Y:177:VAL:HG23 | 1.38                     | 1.02              |
| 2:1X:100:GLY:CA   | 1:2L:253:THR:HB   | 1.88                     | 1.02              |
| 2:1X:214:PHE:CG   | 1:2L:326:LYS:HE2  | 1.94                     | 1.02              |
| 2:2Q:177:VAL:HG23 | 1:3D:332:ILE:CG2  | 1.90                     | 1.02              |
| 1:1E:2:ARG:CG     | 2:4R:72:PRO:HD2   | 1.89                     | 1.02              |
| 1:1G:248:LEU:HD13 | 5:4T:501:GDP:H8   | 1.25                     | 1.02              |
| 1:1I:261:PRO:C    | 2:4U:406:HIS:NE2  | 2.17                     | 1.02              |
| 2:2H:401:ARG:HH22 | 1:3A:435:VAL:CA   | 1.71                     | 1.02              |
| 2:2X:404:PHE:CG   | 1:3L:261:PRO:HA   | 1.95                     | 1.02              |
| 1:1B:346:TRP:HB2  | 2:4O:398:MET:HA   | 1.41                     | 1.01              |
| 1:1C:2:ARG:CD     | 2:4P:72:PRO:HD2   | 1.90                     | 1.01              |
| 1:1C:346:TRP:HB2  | 2:4P:398:MET:HA   | 1.38                     | 1.01              |
| 2:2P:394:GLN:HG2  | 1:3C:348:PRO:CG   | 1.89                     | 1.01              |
| 2:2Q:100:GLY:HA3  | 1:3D:253:THR:CG2  | 1.90                     | 1.01              |
| 2:2R:77:SER:HB3   | 1:3E:245:ASP:OD1  | 1.59                     | 1.01              |
| 1:1B:346:TRP:O    | 2:4O:398:MET:CG   | 2.08                     | 1.01              |
| 1:1E:253:THR:C    | 2:4R:100:GLY:CA   | 2.33                     | 1.01              |
| 1:1E:349:THR:OG1  | 2:4R:184:PRO:CD   | 2.09                     | 1.01              |
| 1:1L:346:TRP:HB2  | 2:4X:398:MET:HA   | 1.39                     | 1.01              |
| 1:1N:262:TYR:HA   | 2:4Z:406:HIS:NE2  | 1.71                     | 1.01              |
| 2:1Y:181:VAL:HB   | 1:2M:258:ASN:CA   | 1.90                     | 1.01              |
| 2:1Z:100:GLY:CA   | 1:2N:253:THR:HB   | 1.89                     | 1.01              |
| 2:2W:179:ASP:O    | 1:3K:352:LYS:HD2  | 1.58                     | 1.01              |
| 2:2W:214:PHE:HB2  | 1:3K:326:LYS:HE2  | 1.06                     | 1.01              |
| 1:1B:261:PRO:HA   | 2:4O:404:PHE:CG   | 1.96                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:332:ILE:HG22 | 2:4R:177:VAL:HG23 | 1.04                     | 1.01              |
| 1:1E:346:TRP:CZ3  | 2:4R:403:ALA:CB   | 2.44                     | 1.01              |
| 1:1E:351:PHE:O    | 2:4R:180:THR:CA   | 2.07                     | 1.01              |
| 1:1F:348:PRO:HB2  | 2:4S:394:GLN:CG   | 1.91                     | 1.01              |
| 1:1N:346:TRP:HB2  | 2:4Z:398:MET:HA   | 1.43                     | 1.01              |
| 2:1V:179:ASP:O    | 1:2J:352:LYS:HD2  | 1.57                     | 1.01              |
| 2:1V:221:THR:OG1  | 1:2J:324:VAL:HG22 | 1.60                     | 1.01              |
| 2:2V:404:PHE:N    | 1:3J:261:PRO:O    | 1.93                     | 1.01              |
| 2:2X:404:PHE:N    | 1:3L:261:PRO:O    | 1.92                     | 1.01              |
| 2:2Y:100:GLY:HA2  | 1:3M:253:THR:HB   | 1.42                     | 1.01              |
| 1:1A:314:ALA:HB1  | 2:4H:181:VAL:HG21 | 1.39                     | 1.01              |
| 1:1B:260:VAL:CB   | 2:4O:407:TRP:HE1  | 1.73                     | 1.01              |
| 1:1C:258:ASN:ND2  | 2:4P:180:THR:CG2  | 2.20                     | 1.01              |
| 1:1D:258:ASN:ND2  | 2:4Q:180:THR:CG2  | 2.23                     | 1.01              |
| 1:1J:263:PRO:HD3  | 2:4V:406:HIS:CG   | 1.94                     | 1.01              |
| 2:1V:181:VAL:N    | 1:2J:258:ASN:ND2  | 1.73                     | 1.01              |
| 2:1V:181:VAL:HG21 | 1:2J:258:ASN:C    | 1.83                     | 1.01              |
| 2:2S:406:HIS:CG   | 1:3F:263:PRO:HD3  | 1.94                     | 1.01              |
| 2:2Y:394:GLN:HG2  | 1:3M:348:PRO:HG3  | 1.42                     | 1.01              |
| 1:1D:263:PRO:CD   | 2:4Q:406:HIS:CD2  | 2.44                     | 1.01              |
| 1:1E:435:VAL:C    | 2:4R:401:ARG:NH2  | 2.16                     | 1.01              |
| 1:1G:346:TRP:CE3  | 2:4T:403:ALA:CB   | 2.44                     | 1.01              |
| 1:1I:248:LEU:CA   | 2:4U:11:GLN:NE2   | 2.23                     | 1.01              |
| 1:1J:245:ASP:CG   | 2:4V:77:SER:CB    | 2.34                     | 1.01              |
| 1:1N:326:LYS:CB   | 2:4Z:222:PRO:HG2  | 1.89                     | 1.01              |
| 2:1V:179:ASP:OD2  | 1:2J:248:LEU:HD21 | 1.60                     | 1.01              |
| 2:1W:221:THR:HA   | 1:2K:324:VAL:HG11 | 1.01                     | 1.01              |
| 2:1X:100:GLY:HA2  | 1:2L:253:THR:HB   | 1.03                     | 1.01              |
| 2:1Y:404:PHE:CD1  | 1:2M:260:VAL:O    | 2.14                     | 1.01              |
| 2:2T:214:PHE:HB2  | 1:3G:326:LYS:CE   | 1.91                     | 1.01              |
| 1:1C:2:ARG:CG     | 2:4P:72:PRO:HD2   | 1.90                     | 1.00              |
| 1:1E:329:ASN:HB2  | 2:4R:210:TYR:CE2  | 1.95                     | 1.00              |
| 1:1G:332:ILE:CG2  | 2:4T:177:VAL:CG2  | 2.38                     | 1.00              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:CB   | 1.90                     | 1.00              |
| 1:1J:332:ILE:HG22 | 2:4V:177:VAL:HG23 | 1.42                     | 1.00              |
| 2:1U:221:THR:OG1  | 1:2I:324:VAL:HG22 | 1.61                     | 1.00              |
| 2:2Q:394:GLN:HG2  | 1:3D:348:PRO:CG   | 1.91                     | 1.00              |
| 2:2R:406:HIS:CD2  | 1:3E:263:PRO:CD   | 2.45                     | 1.00              |
| 2:2S:401:ARG:O    | 1:3F:262:TYR:OH   | 1.77                     | 1.00              |
| 2:2Y:214:PHE:HB2  | 1:3M:326:LYS:CE   | 1.91                     | 1.00              |
| 1:1J:2:ARG:CD     | 2:4V:72:PRO:HD2   | 1.91                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:346:TRP:CE3  | 2:4V:403:ALA:CB   | 2.43                     | 1.00              |
| 1:1K:346:TRP:HB2  | 2:4W:398:MET:HA   | 1.39                     | 1.00              |
| 1:1L:349:THR:CG2  | 2:4X:184:PRO:HD3  | 1.92                     | 1.00              |
| 2:2P:214:PHE:HB2  | 1:3C:326:LYS:HE2  | 1.42                     | 1.00              |
| 2:2R:394:GLN:HG2  | 1:3E:348:PRO:CG   | 1.92                     | 1.00              |
| 2:2S:210:TYR:HD2  | 1:3F:329:ASN:HD22 | 1.08                     | 1.00              |
| 2:2Y:404:PHE:N    | 1:3M:261:PRO:O    | 1.93                     | 1.00              |
| 1:1A:261:PRO:HA   | 2:4H:404:PHE:CD1  | 1.95                     | 1.00              |
| 1:1A:434:GLU:O    | 2:4H:401:ARG:NH2  | 1.94                     | 1.00              |
| 1:1B:434:GLU:O    | 2:4O:401:ARG:NH2  | 1.95                     | 1.00              |
| 1:1C:435:VAL:CA   | 2:4P:401:ARG:HH22 | 1.68                     | 1.00              |
| 1:1E:346:TRP:HB3  | 2:4R:397:ALA:O    | 1.59                     | 1.00              |
| 1:1E:349:THR:HG21 | 2:4R:184:PRO:HD3  | 1.42                     | 1.00              |
| 1:1F:329:ASN:HB2  | 2:4S:210:TYR:CE2  | 1.95                     | 1.00              |
| 1:1G:257:THR:HG21 | 2:4T:102:ASN:HB2  | 1.41                     | 1.00              |
| 2:2S:177:VAL:HG23 | 1:3F:332:ILE:CG2  | 1.90                     | 1.00              |
| 2:2Z:404:PHE:N    | 1:3N:261:PRO:O    | 1.94                     | 1.00              |
| 2:1X:181:VAL:HG21 | 1:2L:258:ASN:C    | 1.86                     | 1.00              |
| 2:1Y:101:ASN:HB2  | 1:2M:254:GLU:CG   | 1.91                     | 1.00              |
| 2:2S:394:GLN:HG2  | 1:3F:348:PRO:CG   | 1.91                     | 1.00              |
| 1:1D:260:VAL:CG1  | 2:4Q:407:TRP:HE1  | 1.75                     | 1.00              |
| 1:1D:435:VAL:C    | 2:4Q:401:ARG:NH2  | 2.17                     | 1.00              |
| 1:1F:349:THR:HG21 | 2:4S:184:PRO:CD   | 1.91                     | 1.00              |
| 2:1Y:100:GLY:HA2  | 1:2M:253:THR:CB   | 1.91                     | 1.00              |
| 2:1Y:404:PHE:CE1  | 1:2M:260:VAL:C    | 2.40                     | 1.00              |
| 2:2X:404:PHE:CD1  | 1:3L:261:PRO:HA   | 1.96                     | 1.00              |
| 1:1B:262:TYR:CA   | 2:4O:406:HIS:CD2  | 2.45                     | 1.00              |
| 2:2P:71:GLU:HB2   | 1:3C:2:ARG:HD3    | 1.42                     | 1.00              |
| 2:2Z:214:PHE:CB   | 1:3N:326:LYS:HE2  | 1.92                     | 1.00              |
| 1:1K:263:PRO:HD3  | 2:4W:406:HIS:CG   | 1.96                     | 1.00              |
| 1:1M:248:LEU:HA   | 2:4Y:11:GLN:NE2   | 1.77                     | 1.00              |
| 2:1Y:101:ASN:CB   | 1:2M:254:GLU:HG2  | 1.92                     | 1.00              |
| 2:2R:207:GLU:CD   | 1:3E:329:ASN:HD21 | 1.68                     | 1.00              |
| 1:1A:346:TRP:HB2  | 2:4H:398:MET:HA   | 1.43                     | 0.99              |
| 1:1C:2:ARG:HD3    | 2:4P:72:PRO:HD2   | 1.40                     | 0.99              |
| 1:1E:249:ASN:N    | 2:4R:11:GLN:CD    | 2.20                     | 0.99              |
| 1:1N:332:ILE:HG22 | 2:4Z:177:VAL:HG23 | 1.42                     | 0.99              |
| 2:1X:221:THR:HA   | 1:2L:324:VAL:CG1  | 1.91                     | 0.99              |
| 2:2O:71:GLU:HB2   | 1:3B:2:ARG:HD3    | 1.42                     | 0.99              |
| 2:2S:222:PRO:HG2  | 1:3F:326:LYS:HB2  | 1.43                     | 0.99              |
| 1:1G:2:ARG:HD3    | 2:4T:72:PRO:CD    | 1.91                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:260:VAL:HB   | 2:4U:407:TRP:CZ2  | 1.96                     | 0.99              |
| 1:1I:346:TRP:CZ3  | 2:4U:403:ALA:CB   | 2.45                     | 0.99              |
| 2:2P:401:ARG:HH22 | 1:3C:435:VAL:HA   | 0.96                     | 0.99              |
| 2:1H:100:GLY:HA3  | 1:2A:253:THR:CG2  | 1.92                     | 0.99              |
| 2:1X:222:PRO:O    | 1:2L:325:PRO:HD2  | 1.61                     | 0.99              |
| 1:1E:326:LYS:HE2  | 2:4R:210:TYR:O    | 1.62                     | 0.99              |
| 1:1I:254:GLU:HA   | 2:4U:100:GLY:C    | 1.86                     | 0.99              |
| 2:2H:401:ARG:O    | 1:3A:262:TYR:OH   | 1.79                     | 0.99              |
| 1:1C:262:TYR:HA   | 2:4P:406:HIS:HD2  | 1.21                     | 0.99              |
| 1:1F:326:LYS:HA   | 2:4S:210:TYR:CE1  | 1.97                     | 0.99              |
| 2:2V:214:PHE:CB   | 1:3J:326:LYS:HE2  | 1.92                     | 0.99              |
| 5:2Z:501:GDP:C8   | 1:3N:248:LEU:HD13 | 1.96                     | 0.99              |
| 1:1I:261:PRO:HA   | 2:4U:404:PHE:HA   | 1.41                     | 0.99              |
| 2:2H:401:ARG:HH22 | 1:3A:435:VAL:HA   | 0.91                     | 0.99              |
| 2:2T:406:HIS:NE2  | 1:3G:262:TYR:C    | 2.20                     | 0.99              |
| 1:1A:324:VAL:HG21 | 2:4H:221:THR:OG1  | 1.62                     | 0.99              |
| 1:1D:329:ASN:HB2  | 2:4Q:210:TYR:CE2  | 1.98                     | 0.99              |
| 1:1E:346:TRP:HA   | 2:4R:397:ALA:C    | 1.88                     | 0.99              |
| 2:2Q:214:PHE:HB2  | 1:3D:326:LYS:HE2  | 1.43                     | 0.99              |
| 2:2S:404:PHE:CG   | 1:3F:261:PRO:HA   | 1.98                     | 0.99              |
| 2:2V:210:TYR:HD2  | 1:3J:329:ASN:HD22 | 1.00                     | 0.99              |
| 1:1G:248:LEU:CA   | 2:4T:11:GLN:NE2   | 2.24                     | 0.99              |
| 2:2H:404:PHE:N    | 1:3A:261:PRO:O    | 1.96                     | 0.99              |
| 1:1I:249:ASN:N    | 2:4U:11:GLN:NE2   | 1.88                     | 0.99              |
| 1:1J:257:THR:HG21 | 2:4V:102:ASN:HB2  | 1.44                     | 0.99              |
| 1:1C:260:VAL:HB   | 2:4P:407:TRP:HE1  | 1.05                     | 0.99              |
| 1:1D:258:ASN:HD21 | 2:4Q:180:THR:HG23 | 0.91                     | 0.99              |
| 1:1G:346:TRP:CB   | 2:4T:397:ALA:O    | 2.11                     | 0.99              |
| 1:1G:348:PRO:HG2  | 2:4T:394:GLN:HB3  | 1.43                     | 0.99              |
| 2:1W:100:GLY:HA3  | 1:2K:253:THR:HG21 | 1.01                     | 0.99              |
| 2:1Y:179:ASP:OD2  | 1:2M:248:LEU:CD2  | 2.10                     | 0.99              |
| 2:2S:406:HIS:NE2  | 1:3F:262:TYR:C    | 2.21                     | 0.99              |
| 2:2T:100:GLY:HA3  | 1:3G:253:THR:CG2  | 1.92                     | 0.99              |
| 1:1C:254:GLU:HG2  | 2:4P:101:ASN:N    | 1.76                     | 0.98              |
| 1:1G:348:PRO:CB   | 2:4T:394:GLN:HG2  | 1.92                     | 0.98              |
| 1:1J:260:VAL:HB   | 2:4V:407:TRP:CZ2  | 1.96                     | 0.98              |
| 2:2R:179:ASP:O    | 1:3E:352:LYS:HD2  | 1.62                     | 0.98              |
| 2:2S:77:SER:HB3   | 1:3F:245:ASP:CG   | 1.88                     | 0.98              |
| 2:2T:404:PHE:CE2  | 1:3G:261:PRO:HB3  | 1.97                     | 0.98              |
| 1:1D:351:PHE:HB2  | 2:4Q:178:SER:OG   | 1.63                     | 0.98              |
| 1:1G:329:ASN:HB2  | 2:4T:210:TYR:CE2  | 1.98                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:406:HIS:CD2  | 1:2I:263:PRO:HD3  | 1.97                     | 0.98              |
| 2:1Y:182:VAL:HG21 | 1:2M:257:THR:CG2  | 1.93                     | 0.98              |
| 2:2R:100:GLY:HA3  | 1:3E:253:THR:CG2  | 1.93                     | 0.98              |
| 2:2U:394:GLN:HG2  | 1:3I:348:PRO:HG3  | 1.45                     | 0.98              |
| 2:2U:401:ARG:NH2  | 1:3I:434:GLU:O    | 1.96                     | 0.98              |
| 1:1B:248:LEU:HD13 | 5:4O:501:GDP:H8   | 1.20                     | 0.98              |
| 1:1B:248:LEU:CD1  | 5:4O:501:GDP:C8   | 2.45                     | 0.98              |
| 1:1F:262:TYR:C    | 2:4S:406:HIS:CE1  | 2.42                     | 0.98              |
| 1:1I:348:PRO:CG   | 2:4U:394:GLN:HB3  | 1.93                     | 0.98              |
| 2:2R:394:GLN:HG2  | 1:3E:348:PRO:CB   | 1.93                     | 0.98              |
| 2:2S:221:THR:OG1  | 1:3F:324:VAL:HG21 | 1.62                     | 0.98              |
| 5:2V:501:GDP:C8   | 1:3J:248:LEU:HD13 | 1.97                     | 0.98              |
| 2:1U:404:PHE:CD1  | 1:2I:260:VAL:O    | 2.16                     | 0.98              |
| 1:1F:346:TRP:HA   | 2:4S:397:ALA:C    | 1.89                     | 0.98              |
| 1:1J:349:THR:HG21 | 2:4V:184:PRO:CD   | 1.94                     | 0.98              |
| 1:1L:437:VAL:O    | 2:4X:401:ARG:NH1  | 1.95                     | 0.98              |
| 2:1X:224:TYR:CE2  | 1:2L:247:ALA:O    | 2.17                     | 0.98              |
| 1:1B:435:VAL:C    | 2:4O:401:ARG:HH22 | 1.72                     | 0.98              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:CG   | 2.42                     | 0.98              |
| 1:1D:325:PRO:O    | 2:4Q:210:TYR:CZ   | 2.16                     | 0.98              |
| 2:2S:100:GLY:HA3  | 1:3F:253:THR:CG2  | 1.94                     | 0.98              |
| 2:2W:207:GLU:CD   | 1:3K:329:ASN:HD21 | 1.71                     | 0.98              |
| 1:1B:260:VAL:HB   | 2:4O:407:TRP:HE1  | 1.24                     | 0.98              |
| 2:2X:404:PHE:CE2  | 1:3L:261:PRO:HB3  | 1.97                     | 0.98              |
| 1:1E:346:TRP:HB2  | 2:4R:397:ALA:O    | 1.62                     | 0.98              |
| 2:1T:406:HIS:CD2  | 1:2G:263:PRO:HD3  | 1.99                     | 0.98              |
| 2:1V:100:GLY:HA3  | 1:2J:253:THR:HG22 | 1.44                     | 0.98              |
| 2:1Y:214:PHE:HB2  | 1:2M:326:LYS:HE2  | 1.44                     | 0.98              |
| 2:2U:222:PRO:HG2  | 1:3I:326:LYS:CB   | 1.94                     | 0.98              |
| 2:2W:210:TYR:HD2  | 1:3K:329:ASN:HD22 | 1.08                     | 0.98              |
| 1:1C:248:LEU:CD1  | 5:4P:501:GDP:C8   | 2.38                     | 0.98              |
| 1:1G:262:TYR:C    | 2:4T:406:HIS:CE1  | 2.40                     | 0.98              |
| 1:1L:329:ASN:HD22 | 2:4X:210:TYR:HD2  | 1.10                     | 0.98              |
| 2:1W:181:VAL:CB   | 1:2K:258:ASN:O    | 2.12                     | 0.98              |
| 2:1Y:207:GLU:OE1  | 1:2M:329:ASN:ND2  | 1.96                     | 0.98              |
| 2:2R:401:ARG:HH22 | 1:3E:435:VAL:CA   | 1.77                     | 0.98              |
| 2:2U:404:PHE:N    | 1:3I:261:PRO:O    | 1.95                     | 0.98              |
| 5:2Y:501:GDP:C8   | 1:3M:248:LEU:HD13 | 1.99                     | 0.98              |
| 1:1F:260:VAL:O    | 2:4S:407:TRP:HD1  | 1.34                     | 0.98              |
| 1:1G:346:TRP:HA   | 2:4T:397:ALA:O    | 1.61                     | 0.98              |
| 1:1G:349:THR:O    | 2:4T:181:VAL:HA   | 1.62                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:329:ASN:HD22 | 2:4Y:210:TYR:HD2  | 1.02                     | 0.98              |
| 2:1U:222:PRO:O    | 1:2I:325:PRO:HD2  | 1.64                     | 0.98              |
| 2:2P:177:VAL:HG23 | 1:3C:332:ILE:CG2  | 1.94                     | 0.98              |
| 1:1F:346:TRP:CZ3  | 2:4S:403:ALA:HB1  | 1.95                     | 0.97              |
| 1:1I:2:ARG:HD3    | 2:4U:72:PRO:CD    | 1.94                     | 0.97              |
| 2:2S:394:GLN:HG2  | 1:3F:348:PRO:CB   | 1.94                     | 0.97              |
| 2:2V:179:ASP:O    | 1:3J:352:LYS:HD2  | 1.63                     | 0.97              |
| 1:1D:262:TYR:C    | 2:4Q:406:HIS:CD2  | 2.39                     | 0.97              |
| 1:1F:329:ASN:HB2  | 2:4S:210:TYR:HE2  | 1.28                     | 0.97              |
| 1:1G:2:ARG:HD3    | 2:4T:72:PRO:HD2   | 0.97                     | 0.97              |
| 1:1I:2:ARG:HD3    | 2:4U:72:PRO:HD2   | 1.00                     | 0.97              |
| 2:1W:100:GLY:HA3  | 1:2K:253:THR:HG22 | 1.46                     | 0.97              |
| 2:1X:181:VAL:CB   | 1:2L:258:ASN:O    | 2.12                     | 0.97              |
| 2:1Y:404:PHE:CE1  | 1:2M:260:VAL:O    | 2.16                     | 0.97              |
| 1:1I:262:TYR:C    | 2:4U:406:HIS:CE1  | 2.43                     | 0.97              |
| 2:1W:401:ARG:HH22 | 1:2K:435:VAL:HA   | 1.28                     | 0.97              |
| 2:2T:210:TYR:HD2  | 1:3G:329:ASN:HD22 | 1.00                     | 0.97              |
| 2:2T:404:PHE:N    | 1:3G:261:PRO:O    | 1.96                     | 0.97              |
| 2:2Z:401:ARG:HH22 | 1:3N:435:VAL:CA   | 1.76                     | 0.97              |
| 1:1E:314:ALA:HB1  | 2:4R:181:VAL:HG21 | 1.46                     | 0.97              |
| 2:1H:100:GLY:HA2  | 1:2A:253:THR:HB   | 1.46                     | 0.97              |
| 1:1E:332:ILE:HG21 | 2:4R:177:VAL:CG2  | 1.90                     | 0.97              |
| 1:1K:262:TYR:C    | 2:4W:406:HIS:NE2  | 2.23                     | 0.97              |
| 2:2T:177:VAL:HG23 | 1:3G:332:ILE:CG2  | 1.94                     | 0.97              |
| 2:2Z:406:HIS:CD2  | 1:3N:263:PRO:CD   | 2.46                     | 0.97              |
| 1:1E:326:LYS:HA   | 2:4R:210:TYR:CE1  | 2.00                     | 0.97              |
| 1:1G:329:ASN:HB2  | 2:4T:210:TYR:HE2  | 1.30                     | 0.97              |
| 2:1Y:224:TYR:CE2  | 1:2M:247:ALA:O    | 2.17                     | 0.97              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:HG2  | 1.63                     | 0.97              |
| 1:1J:248:LEU:CA   | 2:4V:11:GLN:NE2   | 2.27                     | 0.97              |
| 1:1M:437:VAL:O    | 2:4Y:401:ARG:NH1  | 1.96                     | 0.97              |
| 2:1X:214:PHE:CG   | 1:2L:326:LYS:CE   | 2.48                     | 0.97              |
| 2:1Y:101:ASN:HB2  | 1:2M:254:GLU:HG2  | 0.98                     | 0.97              |
| 2:2V:401:ARG:NH2  | 1:3J:434:GLU:O    | 1.97                     | 0.97              |
| 2:2Y:221:THR:OG1  | 1:3M:324:VAL:HG21 | 1.65                     | 0.97              |
| 1:1A:258:ASN:HD21 | 2:4H:180:THR:CG2  | 1.77                     | 0.97              |
| 1:1D:326:LYS:HE2  | 2:4Q:210:TYR:O    | 1.65                     | 0.97              |
| 2:1U:179:ASP:O    | 1:2I:352:LYS:CD   | 2.13                     | 0.97              |
| 1:1A:245:ASP:OD1  | 2:4H:77:SER:CB    | 2.12                     | 0.97              |
| 1:1C:261:PRO:O    | 2:4P:404:PHE:N    | 1.97                     | 0.97              |
| 1:1E:349:THR:CG2  | 2:4R:184:PRO:HD3  | 1.94                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:248:LEU:C    | 2:4W:11:GLN:HE22  | 1.72                     | 0.97              |
| 2:1U:100:GLY:HA3  | 1:2I:253:THR:HG22 | 1.45                     | 0.97              |
| 2:2W:221:THR:HA   | 1:3K:324:VAL:HG11 | 1.44                     | 0.97              |
| 1:1C:253:THR:HG22 | 2:4P:100:GLY:HA3  | 1.45                     | 0.97              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:CG   | 1.99                     | 0.97              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:CA   | 2.39                     | 0.97              |
| 2:1X:182:VAL:CG2  | 1:2L:257:THR:HG22 | 1.95                     | 0.97              |
| 1:1B:245:ASP:OD1  | 2:4O:77:SER:CB    | 2.13                     | 0.96              |
| 1:1F:248:LEU:HA   | 2:4S:11:GLN:NE2   | 1.80                     | 0.96              |
| 2:1V:406:HIS:CD2  | 1:2J:263:PRO:HD3  | 1.99                     | 0.96              |
| 2:2O:401:ARG:HH22 | 1:3B:435:VAL:HA   | 0.91                     | 0.96              |
| 2:2Q:394:GLN:HG2  | 1:3D:348:PRO:CB   | 1.95                     | 0.96              |
| 2:2U:210:TYR:HD2  | 1:3I:329:ASN:HD22 | 0.97                     | 0.96              |
| 2:2Y:404:PHE:CG   | 1:3M:261:PRO:HA   | 2.00                     | 0.96              |
| 1:1E:346:TRP:HA   | 2:4R:397:ALA:O    | 1.63                     | 0.96              |
| 1:1K:332:ILE:HG22 | 2:4W:177:VAL:HG23 | 1.47                     | 0.96              |
| 1:1B:435:VAL:CA   | 2:4O:401:ARG:HH22 | 1.75                     | 0.96              |
| 1:1D:253:THR:C    | 2:4Q:100:GLY:HA2  | 1.90                     | 0.96              |
| 1:1D:260:VAL:HB   | 2:4Q:407:TRP:CE2  | 2.00                     | 0.96              |
| 1:1F:248:LEU:CD1  | 5:4S:501:GDP:H8   | 1.77                     | 0.96              |
| 2:1Q:221:THR:HA   | 1:2D:324:VAL:HG11 | 1.45                     | 0.96              |
| 2:1W:181:VAL:HB   | 1:2K:258:ASN:CA   | 1.94                     | 0.96              |
| 2:2T:77:SER:HB3   | 1:3G:245:ASP:CG   | 1.90                     | 0.96              |
| 2:2T:401:ARG:NH2  | 1:3G:434:GLU:O    | 1.98                     | 0.96              |
| 2:2U:406:HIS:NE2  | 1:3I:262:TYR:C    | 2.23                     | 0.96              |
| 2:2W:100:GLY:CA   | 1:3K:253:THR:HG22 | 1.95                     | 0.96              |
| 1:1F:349:THR:OG1  | 2:4S:184:PRO:CD   | 2.14                     | 0.96              |
| 1:1G:348:PRO:CG   | 2:4T:394:GLN:CB   | 2.43                     | 0.96              |
| 2:1T:100:GLY:CA   | 1:2G:253:THR:CG2  | 2.42                     | 0.96              |
| 2:1X:100:GLY:CA   | 1:2L:253:THR:CB   | 2.42                     | 0.96              |
| 2:2R:179:ASP:OD1  | 1:3E:353:VAL:HB   | 1.65                     | 0.96              |
| 2:2R:404:PHE:N    | 1:3E:261:PRO:O    | 1.98                     | 0.96              |
| 2:2S:404:PHE:CD1  | 1:3F:261:PRO:HA   | 2.01                     | 0.96              |
| 1:1D:346:TRP:CD1  | 2:4Q:401:ARG:HG3  | 2.01                     | 0.96              |
| 1:1L:332:ILE:HG22 | 2:4X:177:VAL:HG23 | 1.46                     | 0.96              |
| 1:1N:245:ASP:OD1  | 2:4Z:77:SER:CB    | 2.12                     | 0.96              |
| 1:1B:346:TRP:HB2  | 2:4O:397:ALA:O    | 1.62                     | 0.96              |
| 1:1B:353:VAL:CB   | 2:4O:179:ASP:OD1  | 2.12                     | 0.96              |
| 1:1E:332:ILE:HB   | 2:4R:177:VAL:HG21 | 1.45                     | 0.96              |
| 2:1U:221:THR:OG1  | 1:2I:324:VAL:CG2  | 2.14                     | 0.96              |
| 2:1Z:401:ARG:HB3  | 1:2N:262:TYR:OH   | 1.64                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:207:GLU:CD   | 1:3F:329:ASN:HD21 | 1.74                     | 0.96              |
| 2:2U:406:HIS:NE2  | 1:3I:263:PRO:N    | 2.14                     | 0.96              |
| 1:1D:260:VAL:CB   | 2:4Q:407:TRP:NE1  | 2.08                     | 0.96              |
| 1:1E:325:PRO:O    | 2:4R:210:TYR:CZ   | 2.19                     | 0.96              |
| 2:1Z:71:GLU:HB2   | 1:2N:2:ARG:HD3    | 1.46                     | 0.96              |
| 1:1A:258:ASN:HD21 | 2:4H:180:THR:HG23 | 0.82                     | 0.96              |
| 1:1F:260:VAL:HG12 | 2:4S:406:HIS:HE1  | 1.27                     | 0.96              |
| 2:1T:404:PHE:CE1  | 1:2G:260:VAL:C    | 2.44                     | 0.96              |
| 2:2V:406:HIS:NE2  | 1:3J:263:PRO:N    | 2.14                     | 0.96              |
| 5:2W:501:GDP:C8   | 1:3K:248:LEU:HD13 | 1.99                     | 0.96              |
| 1:1C:260:VAL:CG1  | 2:4P:407:TRP:HE1  | 1.79                     | 0.96              |
| 2:1W:182:VAL:HG21 | 1:2K:257:THR:CG2  | 1.95                     | 0.96              |
| 2:2O:100:GLY:HA2  | 1:3B:253:THR:HB   | 1.46                     | 0.96              |
| 2:2V:222:PRO:HG2  | 1:3J:326:LYS:CB   | 1.96                     | 0.96              |
| 5:2X:501:GDP:C8   | 1:3L:248:LEU:HD13 | 2.00                     | 0.96              |
| 2:2Y:222:PRO:HG2  | 1:3M:326:LYS:HB2  | 1.47                     | 0.96              |
| 1:1B:245:ASP:CG   | 2:4O:77:SER:CB    | 2.38                     | 0.96              |
| 1:1C:245:ASP:OD1  | 2:4P:77:SER:CB    | 2.13                     | 0.96              |
| 1:1E:260:VAL:CG1  | 2:4R:407:TRP:HE1  | 1.79                     | 0.96              |
| 2:1O:207:GLU:OE1  | 1:2B:329:ASN:ND2  | 1.99                     | 0.96              |
| 2:1S:100:GLY:HA3  | 1:2F:253:THR:CG2  | 1.96                     | 0.96              |
| 2:1S:221:THR:CA   | 1:2F:324:VAL:HG11 | 1.95                     | 0.96              |
| 2:2H:71:GLU:HB2   | 1:3A:2:ARG:HD3    | 1.46                     | 0.96              |
| 2:2S:404:PHE:N    | 1:3F:261:PRO:O    | 1.97                     | 0.96              |
| 2:2X:100:GLY:HA2  | 1:3L:253:THR:HB   | 1.48                     | 0.96              |
| 1:1E:260:VAL:HG12 | 2:4R:406:HIS:CE1  | 2.01                     | 0.95              |
| 2:2T:176:LYS:HE2  | 1:3G:333:ALA:HB1  | 1.48                     | 0.95              |
| 1:1A:261:PRO:HA   | 2:4H:404:PHE:CG   | 2.00                     | 0.95              |
| 1:1A:326:LYS:HB2  | 2:4H:222:PRO:HG2  | 1.46                     | 0.95              |
| 1:1F:332:ILE:HB   | 2:4S:177:VAL:HG21 | 1.47                     | 0.95              |
| 1:1G:346:TRP:CE3  | 2:4T:403:ALA:HB3  | 2.00                     | 0.95              |
| 1:1J:261:PRO:O    | 2:4V:406:HIS:CD2  | 2.18                     | 0.95              |
| 1:1C:253:THR:C    | 2:4P:100:GLY:CA   | 2.39                     | 0.95              |
| 1:1D:349:THR:OG1  | 2:4Q:184:PRO:CD   | 2.13                     | 0.95              |
| 1:1K:262:TYR:CA   | 2:4W:406:HIS:CD2  | 2.34                     | 0.95              |
| 1:1N:263:PRO:CD   | 2:4Z:406:HIS:CD2  | 2.49                     | 0.95              |
| 2:2Y:221:THR:HA   | 1:3M:324:VAL:HG11 | 1.45                     | 0.95              |
| 1:1B:261:PRO:O    | 2:4O:404:PHE:N    | 1.98                     | 0.95              |
| 1:1C:434:GLU:O    | 2:4P:401:ARG:NH2  | 1.99                     | 0.95              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:CA   | 2.42                     | 0.95              |
| 2:1V:100:GLY:CA   | 1:2J:253:THR:HG21 | 1.88                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1V:180:THR:HA   | 1:2J:258:ASN:ND2  | 1.81                     | 0.95              |
| 1:1D:249:ASN:N    | 2:4Q:11:GLN:CD    | 2.23                     | 0.95              |
| 1:1M:349:THR:OG1  | 2:4Y:181:VAL:O    | 1.84                     | 0.95              |
| 1:1N:325:PRO:HD2  | 2:4Z:223:THR:HA   | 1.46                     | 0.95              |
| 2:1U:178:SER:HB3  | 1:2I:349:THR:HB   | 1.48                     | 0.95              |
| 2:2P:404:PHE:N    | 1:3C:261:PRO:O    | 1.98                     | 0.95              |
| 2:2Q:176:LYS:HE2  | 1:3D:333:ALA:HB1  | 1.49                     | 0.95              |
| 2:2R:77:SER:HB3   | 1:3E:245:ASP:CG   | 1.92                     | 0.95              |
| 2:2T:181:VAL:HG21 | 1:3G:314:ALA:HB1  | 1.47                     | 0.95              |
| 2:2W:406:HIS:CG   | 1:3K:263:PRO:HD3  | 2.02                     | 0.95              |
| 1:1A:326:LYS:HE2  | 2:4H:214:PHE:HB2  | 1.48                     | 0.95              |
| 1:1N:329:ASN:ND2  | 2:4Z:207:GLU:OE1  | 1.98                     | 0.95              |
| 2:1O:401:ARG:HH22 | 1:2B:435:VAL:HA   | 1.32                     | 0.95              |
| 2:1Z:101:ASN:CB   | 1:2N:254:GLU:HG2  | 1.95                     | 0.95              |
| 2:2Q:406:HIS:CD2  | 1:3D:263:PRO:CD   | 2.49                     | 0.95              |
| 1:1A:346:TRP:CB   | 2:4H:397:ALA:O    | 2.15                     | 0.95              |
| 1:1D:245:ASP:OD1  | 2:4Q:77:SER:CB    | 2.12                     | 0.95              |
| 1:1L:262:TYR:C    | 2:4X:406:HIS:NE2  | 2.22                     | 0.95              |
| 2:2H:180:THR:HG23 | 1:3A:258:ASN:HD21 | 0.78                     | 0.95              |
| 2:2O:404:PHE:N    | 1:3B:261:PRO:O    | 1.97                     | 0.95              |
| 2:2W:221:THR:OG1  | 1:3K:324:VAL:CG2  | 2.14                     | 0.95              |
| 1:1A:333:ALA:HB1  | 2:4H:176:LYS:HE2  | 1.45                     | 0.95              |
| 2:2S:176:LYS:HE2  | 1:3F:333:ALA:HB1  | 1.47                     | 0.95              |
| 2:2V:401:ARG:HH22 | 1:3J:435:VAL:HA   | 1.22                     | 0.95              |
| 2:2X:404:PHE:CE1  | 1:3L:260:VAL:C    | 2.44                     | 0.95              |
| 1:1D:326:LYS:HA   | 2:4Q:210:TYR:CD1  | 2.02                     | 0.95              |
| 1:1E:254:GLU:CA   | 2:4R:100:GLY:C    | 2.39                     | 0.95              |
| 1:1J:249:ASN:N    | 2:4V:11:GLN:NE2   | 1.98                     | 0.95              |
| 2:1T:100:GLY:HA3  | 1:2G:253:THR:HG21 | 1.48                     | 0.95              |
| 1:1C:437:VAL:O    | 2:4P:401:ARG:NH1  | 2.00                     | 0.95              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:HA   | 1.97                     | 0.95              |
| 1:1N:314:ALA:HB1  | 2:4Z:181:VAL:HG21 | 1.49                     | 0.95              |
| 1:1N:326:LYS:HE2  | 2:4Z:214:PHE:HB2  | 1.48                     | 0.95              |
| 1:1C:333:ALA:CB   | 2:4P:176:LYS:HE2  | 1.97                     | 0.94              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:HA   | 1.95                     | 0.94              |
| 1:1E:351:PHE:HB2  | 2:4R:178:SER:OG   | 1.66                     | 0.94              |
| 1:1F:2:ARG:HD3    | 2:4S:72:PRO:CD    | 1.94                     | 0.94              |
| 1:1N:434:GLU:O    | 2:4Z:401:ARG:NH2  | 1.99                     | 0.94              |
| 2:2Q:404:PHE:N    | 1:3D:261:PRO:O    | 1.99                     | 0.94              |
| 2:2S:214:PHE:HB2  | 1:3F:326:LYS:CE   | 1.97                     | 0.94              |
| 2:2X:100:GLY:CA   | 1:3L:253:THR:HG22 | 1.96                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:324:VAL:HG13 | 2:4P:222:PRO:O    | 1.67                     | 0.94              |
| 1:1E:253:THR:C    | 2:4R:100:GLY:HA2  | 1.92                     | 0.94              |
| 1:1E:324:VAL:CG1  | 2:4R:222:PRO:O    | 2.15                     | 0.94              |
| 1:1G:260:VAL:HG12 | 2:4T:406:HIS:HE1  | 1.32                     | 0.94              |
| 1:1G:262:TYR:HA   | 2:4T:406:HIS:HD2  | 1.13                     | 0.94              |
| 1:1J:248:LEU:CA   | 2:4V:11:GLN:HE22  | 1.81                     | 0.94              |
| 2:1O:181:VAL:H    | 1:2B:258:ASN:ND2  | 1.65                     | 0.94              |
| 2:1X:401:ARG:CB   | 1:2L:262:TYR:OH   | 2.13                     | 0.94              |
| 2:2O:180:THR:HG23 | 1:3B:258:ASN:HD21 | 0.78                     | 0.94              |
| 2:2S:181:VAL:HG21 | 1:3F:314:ALA:HB1  | 1.49                     | 0.94              |
| 2:2T:222:PRO:HG2  | 1:3G:326:LYS:CB   | 1.97                     | 0.94              |
| 2:2Z:214:PHE:HB2  | 1:3N:326:LYS:CE   | 1.97                     | 0.94              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:CA   | 2.15                     | 0.94              |
| 1:1K:260:VAL:HB   | 2:4W:407:TRP:CZ2  | 2.02                     | 0.94              |
| 2:2S:401:ARG:HH22 | 1:3F:435:VAL:HA   | 1.18                     | 0.94              |
| 1:1A:329:ASN:HD22 | 2:4H:210:TYR:HD2  | 1.03                     | 0.94              |
| 1:1G:245:ASP:OD2  | 2:4T:77:SER:CB    | 2.14                     | 0.94              |
| 1:1I:248:LEU:CA   | 2:4U:11:GLN:HE22  | 1.80                     | 0.94              |
| 1:1K:262:TYR:HA   | 2:4W:406:HIS:NE2  | 1.58                     | 0.94              |
| 2:1W:181:VAL:CG2  | 1:2K:258:ASN:HB3  | 1.96                     | 0.94              |
| 1:1B:348:PRO:CG   | 2:4O:394:GLN:CG   | 2.44                     | 0.94              |
| 1:1C:258:ASN:HD21 | 2:4P:180:THR:HG23 | 0.78                     | 0.94              |
| 1:1C:329:ASN:HB2  | 2:4P:210:TYR:CE2  | 2.02                     | 0.94              |
| 1:1E:258:ASN:HD21 | 2:4R:180:THR:CG2  | 1.80                     | 0.94              |
| 1:1F:260:VAL:HG12 | 2:4S:406:HIS:CE1  | 2.02                     | 0.94              |
| 1:1M:245:ASP:OD1  | 2:4Y:77:SER:CB    | 2.16                     | 0.94              |
| 2:1H:207:GLU:CD   | 1:2A:329:ASN:HD21 | 1.75                     | 0.94              |
| 2:1W:394:GLN:HG2  | 1:2K:348:PRO:CG   | 1.97                     | 0.94              |
| 2:1X:181:VAL:HG23 | 1:2L:258:ASN:CB   | 1.95                     | 0.94              |
| 2:2R:406:HIS:NE2  | 1:3E:262:TYR:C    | 2.26                     | 0.94              |
| 1:1F:435:VAL:CA   | 2:4S:401:ARG:NH2  | 2.30                     | 0.94              |
| 2:1W:181:VAL:HG23 | 1:2K:258:ASN:CB   | 1.97                     | 0.94              |
| 2:1W:221:THR:OG1  | 1:2K:324:VAL:HG22 | 1.68                     | 0.94              |
| 2:1Y:100:GLY:CA   | 1:2M:253:THR:CB   | 2.46                     | 0.94              |
| 2:2T:179:ASP:O    | 1:3G:352:LYS:HD2  | 1.68                     | 0.94              |
| 2:2U:181:VAL:HG21 | 1:3I:314:ALA:HB1  | 1.47                     | 0.94              |
| 2:2V:221:THR:OG1  | 1:3J:324:VAL:CG2  | 2.15                     | 0.94              |
| 1:1B:348:PRO:CG   | 2:4O:394:GLN:HG2  | 1.96                     | 0.94              |
| 1:1C:2:ARG:HD3    | 2:4P:71:GLU:HB2   | 1.48                     | 0.94              |
| 1:1E:346:TRP:CD1  | 2:4R:401:ARG:HG3  | 2.01                     | 0.94              |
| 2:1U:181:VAL:N    | 1:2I:258:ASN:ND2  | 1.91                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1W:401:ARG:HB3  | 1:2K:262:TYR:HH   | 1.24                     | 0.94              |
| 2:2Q:179:ASP:OD1  | 1:3D:353:VAL:HB   | 1.66                     | 0.94              |
| 2:2S:179:ASP:O    | 1:3F:352:LYS:HD2  | 1.66                     | 0.94              |
| 1:1C:254:GLU:N    | 2:4P:100:GLY:HA2  | 1.82                     | 0.94              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:HA   | 1.46                     | 0.94              |
| 1:1D:2:ARG:NH2    | 2:4Q:73:GLY:HA3   | 1.83                     | 0.94              |
| 1:1D:260:VAL:O    | 2:4Q:407:TRP:HD1  | 1.45                     | 0.94              |
| 1:1F:347:CYS:HA   | 2:4S:398:MET:HG2  | 1.50                     | 0.94              |
| 1:1G:260:VAL:HB   | 2:4T:407:TRP:CZ2  | 2.03                     | 0.94              |
| 1:1I:351:PHE:O    | 2:4U:180:THR:CA   | 2.15                     | 0.94              |
| 1:1J:257:THR:HB   | 2:4V:100:GLY:O    | 1.68                     | 0.94              |
| 1:1M:349:THR:CG2  | 2:4Y:184:PRO:HD3  | 1.98                     | 0.94              |
| 2:1S:181:VAL:CG2  | 1:2F:258:ASN:O    | 2.16                     | 0.94              |
| 2:2U:179:ASP:O    | 1:3I:352:LYS:HD2  | 1.67                     | 0.94              |
| 2:2W:101:ASN:O    | 1:3K:257:THR:HG21 | 1.65                     | 0.94              |
| 2:2W:404:PHE:CE1  | 1:3K:260:VAL:C    | 2.46                     | 0.94              |
| 2:2X:101:ASN:O    | 1:3L:257:THR:HG21 | 1.68                     | 0.94              |
| 1:1B:263:PRO:N    | 2:4O:406:HIS:NE2  | 2.14                     | 0.94              |
| 1:1C:253:THR:C    | 2:4P:100:GLY:HA2  | 1.93                     | 0.94              |
| 1:1E:326:LYS:HA   | 2:4R:210:TYR:CD1  | 2.03                     | 0.94              |
| 1:1G:258:ASN:ND2  | 2:4T:180:THR:HG23 | 1.82                     | 0.94              |
| 2:2Q:71:GLU:HB2   | 1:3D:2:ARG:HD3    | 1.46                     | 0.94              |
| 2:2R:404:PHE:CG   | 1:3E:261:PRO:HA   | 2.03                     | 0.94              |
| 2:2V:101:ASN:O    | 1:3J:257:THR:HG21 | 1.66                     | 0.94              |
| 1:1K:346:TRP:CE3  | 2:4W:403:ALA:CB   | 2.51                     | 0.94              |
| 1:1L:261:PRO:C    | 2:4X:406:HIS:NE2  | 2.26                     | 0.94              |
| 2:1T:100:GLY:HA3  | 1:2G:253:THR:HG22 | 1.49                     | 0.94              |
| 2:1V:180:THR:CA   | 1:2J:258:ASN:HD21 | 1.80                     | 0.94              |
| 2:2R:406:HIS:CG   | 1:3E:263:PRO:HD3  | 2.02                     | 0.94              |
| 2:2Y:401:ARG:HH22 | 1:3M:435:VAL:CA   | 1.81                     | 0.94              |
| 1:1A:348:PRO:CG   | 2:4H:394:GLN:CB   | 2.46                     | 0.93              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:HG2  | 1.98                     | 0.93              |
| 1:1C:351:PHE:O    | 2:4P:180:THR:C    | 2.10                     | 0.93              |
| 1:1E:346:TRP:HD1  | 2:4R:401:ARG:HG3  | 1.32                     | 0.93              |
| 1:1G:260:VAL:C    | 2:4T:407:TRP:HE1  | 1.76                     | 0.93              |
| 1:1G:261:PRO:HA   | 2:4T:404:PHE:CA   | 1.97                     | 0.93              |
| 1:1I:257:THR:HB   | 2:4U:100:GLY:O    | 1.68                     | 0.93              |
| 2:1V:207:GLU:CD   | 1:2J:329:ASN:HD21 | 1.75                     | 0.93              |
| 2:2V:207:GLU:CD   | 1:3J:329:ASN:HD21 | 1.76                     | 0.93              |
| 1:1G:326:LYS:HA   | 2:4T:210:TYR:CE1  | 2.02                     | 0.93              |
| 2:2R:176:LYS:HE2  | 1:3E:333:ALA:HB1  | 1.47                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Y:404:PHE:CE1  | 1:3M:260:VAL:C    | 2.45                     | 0.93              |
| 1:1A:332:ILE:CG2  | 2:4H:177:VAL:CG2  | 2.46                     | 0.93              |
| 1:1B:2:ARG:HD3    | 2:4O:72:PRO:HD2   | 1.49                     | 0.93              |
| 1:1B:260:VAL:O    | 2:4O:407:TRP:CD1  | 2.21                     | 0.93              |
| 1:1F:257:THR:HG21 | 2:4S:102:ASN:HB2  | 1.50                     | 0.93              |
| 1:1I:346:TRP:CE3  | 2:4U:403:ALA:HB3  | 2.03                     | 0.93              |
| 1:1N:253:THR:HG22 | 2:4Z:100:GLY:HA3  | 1.48                     | 0.93              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:CB   | 1.97                     | 0.93              |
| 1:1B:249:ASN:H    | 2:4O:11:GLN:CD    | 1.77                     | 0.93              |
| 1:1C:263:PRO:N    | 2:4P:406:HIS:NE2  | 2.16                     | 0.93              |
| 1:1G:349:THR:CG2  | 2:4T:184:PRO:CD   | 2.45                     | 0.93              |
| 1:1M:245:ASP:CG   | 2:4Y:77:SER:CB    | 2.41                     | 0.93              |
| 2:1H:179:ASP:O    | 1:2A:352:LYS:HD2  | 1.69                     | 0.93              |
| 2:1R:181:VAL:H    | 1:2E:258:ASN:HD22 | 1.00                     | 0.93              |
| 2:2H:207:GLU:CD   | 1:3A:329:ASN:ND2  | 2.27                     | 0.93              |
| 2:2P:176:LYS:HE2  | 1:3C:333:ALA:HB1  | 1.50                     | 0.93              |
| 2:2T:394:GLN:HG2  | 1:3G:348:PRO:CB   | 1.98                     | 0.93              |
| 1:1A:348:PRO:HG3  | 2:4H:394:GLN:CA   | 1.98                     | 0.93              |
| 1:1D:346:TRP:CH2  | 2:4Q:403:ALA:HB1  | 2.04                     | 0.93              |
| 1:1E:263:PRO:HD3  | 2:4R:406:HIS:CD2  | 2.03                     | 0.93              |
| 1:1F:324:VAL:HG13 | 2:4S:222:PRO:O    | 1.69                     | 0.93              |
| 1:1I:346:TRP:CH2  | 2:4U:403:ALA:HB1  | 2.02                     | 0.93              |
| 2:1T:221:THR:OG1  | 1:2G:324:VAL:CG2  | 2.17                     | 0.93              |
| 2:1U:181:VAL:HB   | 1:2I:258:ASN:HA   | 1.51                     | 0.93              |
| 2:1W:182:VAL:CG2  | 1:2K:257:THR:HG22 | 1.98                     | 0.93              |
| 2:1X:101:ASN:HB2  | 1:2L:254:GLU:CG   | 1.98                     | 0.93              |
| 2:2P:180:THR:HG23 | 1:3C:258:ASN:HD21 | 0.76                     | 0.93              |
| 2:2X:77:SER:HB3   | 1:3L:245:ASP:OD1  | 1.68                     | 0.93              |
| 1:1G:346:TRP:CA   | 2:4T:397:ALA:O    | 2.16                     | 0.93              |
| 2:2U:176:LYS:HE2  | 1:3I:333:ALA:HB1  | 1.50                     | 0.93              |
| 1:1A:348:PRO:CG   | 2:4H:394:GLN:HB3  | 1.99                     | 0.93              |
| 1:1F:326:LYS:HE2  | 2:4S:210:TYR:O    | 1.69                     | 0.93              |
| 1:1K:346:TRP:CZ3  | 2:4W:403:ALA:HB1  | 2.02                     | 0.93              |
| 2:1S:181:VAL:N    | 1:2F:258:ASN:HD22 | 1.65                     | 0.93              |
| 2:1S:406:HIS:CD2  | 1:2F:263:PRO:HD3  | 2.04                     | 0.93              |
| 2:1U:181:VAL:HG23 | 1:2I:258:ASN:HB3  | 1.49                     | 0.93              |
| 1:1C:435:VAL:HA   | 2:4P:401:ARG:HH21 | 1.10                     | 0.93              |
| 1:1E:260:VAL:O    | 2:4R:407:TRP:HD1  | 1.35                     | 0.93              |
| 1:1F:248:LEU:CA   | 2:4S:11:GLN:NE2   | 2.32                     | 0.93              |
| 1:1N:332:ILE:CG2  | 2:4Z:177:VAL:HG23 | 1.98                     | 0.93              |
| 2:2Q:77:SER:HB3   | 1:3D:245:ASP:OD1  | 1.69                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2U:214:PHE:CB   | 1:3I:326:LYS:HE2  | 1.99                     | 0.93              |
| 1:1A:326:LYS:CB   | 2:4H:222:PRO:HG2  | 1.98                     | 0.93              |
| 1:1C:2:ARG:NH2    | 2:4P:73:GLY:HA3   | 1.83                     | 0.93              |
| 1:1F:253:THR:C    | 2:4S:100:GLY:CA   | 2.41                     | 0.93              |
| 2:1X:394:GLN:HG2  | 1:2L:348:PRO:CG   | 1.99                     | 0.93              |
| 2:2T:406:HIS:NE2  | 1:3G:263:PRO:N    | 2.17                     | 0.93              |
| 2:2X:180:THR:HG23 | 1:3L:258:ASN:HD21 | 0.78                     | 0.93              |
| 2:2Y:180:THR:HG23 | 1:3M:258:ASN:HD21 | 0.79                     | 0.93              |
| 1:1B:348:PRO:CB   | 2:4O:394:GLN:CG   | 2.47                     | 0.92              |
| 1:1D:263:PRO:CD   | 2:4Q:406:HIS:CG   | 2.51                     | 0.92              |
| 1:1J:260:VAL:HB   | 2:4V:407:TRP:NE1  | 1.84                     | 0.92              |
| 1:1K:245:ASP:CG   | 2:4W:77:SER:CB    | 2.41                     | 0.92              |
| 2:2H:214:PHE:CB   | 1:3A:326:LYS:HE2  | 1.98                     | 0.92              |
| 2:2T:401:ARG:HH22 | 1:3G:435:VAL:HA   | 1.23                     | 0.92              |
| 2:2V:221:THR:HA   | 1:3J:324:VAL:HG11 | 1.51                     | 0.92              |
| 1:1D:263:PRO:N    | 2:4Q:406:HIS:CD2  | 2.37                     | 0.92              |
| 1:1E:263:PRO:CD   | 2:4R:406:HIS:CG   | 2.52                     | 0.92              |
| 2:1V:221:THR:OG1  | 1:2J:324:VAL:CG2  | 2.17                     | 0.92              |
| 2:2R:221:THR:OG1  | 1:3E:324:VAL:HG21 | 1.70                     | 0.92              |
| 2:2Y:404:PHE:CE2  | 1:3M:261:PRO:HB3  | 2.05                     | 0.92              |
| 1:1F:348:PRO:CB   | 2:4S:394:GLN:CG   | 2.46                     | 0.92              |
| 1:1F:435:VAL:HA   | 2:4S:401:ARG:HH21 | 1.26                     | 0.92              |
| 2:2P:394:GLN:HG2  | 1:3C:348:PRO:CB   | 1.99                     | 0.92              |
| 1:1E:353:VAL:HG23 | 2:4R:179:ASP:HA   | 1.52                     | 0.92              |
| 1:1F:349:THR:CB   | 2:4S:184:PRO:HD3  | 1.98                     | 0.92              |
| 2:2W:401:ARG:NH2  | 1:3K:434:GLU:O    | 2.03                     | 0.92              |
| 1:1F:435:VAL:C    | 2:4S:401:ARG:NH2  | 2.26                     | 0.92              |
| 1:1L:248:LEU:C    | 2:4X:11:GLN:HE22  | 1.76                     | 0.92              |
| 1:1M:326:LYS:CB   | 2:4Y:222:PRO:HG2  | 2.00                     | 0.92              |
| 2:1P:214:PHE:HB2  | 1:2C:326:LYS:HE2  | 1.48                     | 0.92              |
| 2:2O:100:GLY:CA   | 1:3B:253:THR:HB   | 1.99                     | 0.92              |
| 1:1D:2:ARG:HD3    | 2:4Q:71:GLU:HB2   | 1.49                     | 0.92              |
| 1:1F:2:ARG:CG     | 2:4S:72:PRO:HD2   | 1.99                     | 0.92              |
| 1:1F:346:TRP:HB2  | 2:4S:398:MET:CA   | 2.00                     | 0.92              |
| 1:1I:261:PRO:O    | 2:4U:406:HIS:CD2  | 2.21                     | 0.92              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:HG3  | 1.70                     | 0.92              |
| 1:1G:245:ASP:OD1  | 2:4T:77:SER:CB    | 2.15                     | 0.92              |
| 1:1K:261:PRO:O    | 2:4W:406:HIS:CD2  | 2.22                     | 0.92              |
| 1:1M:248:LEU:C    | 2:4Y:11:GLN:HE22  | 1.76                     | 0.92              |
| 2:1P:11:GLN:HE22  | 1:2C:249:ASN:H    | 1.18                     | 0.92              |
| 2:2T:207:GLU:CD   | 1:3G:329:ASN:HD21 | 1.77                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2W:406:HIS:NE2  | 1:3K:263:PRO:N    | 2.17                     | 0.92              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:HA   | 1.70                     | 0.92              |
| 2:1R:181:VAL:H    | 1:2E:258:ASN:ND2  | 1.66                     | 0.92              |
| 2:2H:406:HIS:CD2  | 1:3A:263:PRO:CD   | 2.50                     | 0.92              |
| 5:2Q:501:GDP:H8   | 1:3D:248:LEU:CD1  | 1.83                     | 0.92              |
| 2:2S:401:ARG:NH2  | 1:3F:434:GLU:O    | 2.03                     | 0.92              |
| 2:2S:401:ARG:HH22 | 1:3F:435:VAL:CA   | 1.82                     | 0.92              |
| 2:2Z:401:ARG:O    | 1:3N:262:TYR:OH   | 1.88                     | 0.92              |
| 1:1B:324:VAL:HG21 | 2:4O:221:THR:OG1  | 1.70                     | 0.92              |
| 1:1E:333:ALA:HB1  | 2:4R:176:LYS:HE2  | 1.52                     | 0.92              |
| 1:1M:329:ASN:HB2  | 2:4Y:210:TYR:CE2  | 2.05                     | 0.92              |
| 2:2S:179:ASP:OD1  | 1:3F:353:VAL:HB   | 1.69                     | 0.92              |
| 2:2U:101:ASN:O    | 1:3I:257:THR:HG21 | 1.70                     | 0.92              |
| 2:2Z:180:THR:HG23 | 1:3N:258:ASN:HD21 | 0.79                     | 0.92              |
| 1:1B:258:ASN:ND2  | 2:4O:180:THR:CG2  | 2.25                     | 0.92              |
| 1:1E:349:THR:CB   | 2:4R:184:PRO:HD3  | 1.99                     | 0.92              |
| 1:1F:346:TRP:CE3  | 2:4S:403:ALA:HB3  | 2.05                     | 0.92              |
| 1:1I:329:ASN:HB2  | 2:4U:210:TYR:CE2  | 2.04                     | 0.92              |
| 2:1T:221:THR:HA   | 1:2G:324:VAL:HG11 | 0.94                     | 0.92              |
| 2:1U:100:GLY:HA2  | 1:2I:253:THR:CB   | 2.00                     | 0.92              |
| 2:1U:101:ASN:HB2  | 1:2I:254:GLU:HG2  | 1.52                     | 0.92              |
| 2:1W:406:HIS:CD2  | 1:2K:263:PRO:HD3  | 2.04                     | 0.92              |
| 2:1X:401:ARG:HB3  | 1:2L:262:TYR:HH   | 1.25                     | 0.92              |
| 1:1E:262:TYR:C    | 2:4R:406:HIS:CD2  | 2.37                     | 0.91              |
| 1:1F:245:ASP:OD2  | 2:4S:77:SER:CB    | 2.16                     | 0.91              |
| 1:1I:332:ILE:CG2  | 2:4U:177:VAL:HG23 | 1.98                     | 0.91              |
| 1:1K:257:THR:HB   | 2:4W:100:GLY:O    | 1.70                     | 0.91              |
| 1:1L:245:ASP:CG   | 2:4X:77:SER:CB    | 2.44                     | 0.91              |
| 2:2S:404:PHE:CE2  | 1:3F:261:PRO:HB3  | 2.05                     | 0.91              |
| 2:2V:100:GLY:CA   | 1:3J:253:THR:HG22 | 1.99                     | 0.91              |
| 1:1A:261:PRO:HB3  | 2:4H:404:PHE:CE2  | 2.06                     | 0.91              |
| 2:2O:406:HIS:CD2  | 1:3B:263:PRO:CD   | 2.52                     | 0.91              |
| 2:2P:397:ALA:O    | 1:3C:346:TRP:HB2  | 1.69                     | 0.91              |
| 2:2W:180:THR:HG23 | 1:3K:258:ASN:HD21 | 0.76                     | 0.91              |
| 2:2Z:394:GLN:HG2  | 1:3N:348:PRO:HG3  | 1.48                     | 0.91              |
| 1:1D:353:VAL:HG23 | 2:4Q:179:ASP:HA   | 1.52                     | 0.91              |
| 1:1E:329:ASN:HB2  | 2:4R:210:TYR:HE2  | 1.33                     | 0.91              |
| 1:1G:260:VAL:O    | 2:4T:407:TRP:HD1  | 1.42                     | 0.91              |
| 1:1G:261:PRO:C    | 2:4T:406:HIS:NE2  | 2.29                     | 0.91              |
| 2:1H:401:ARG:NH2  | 1:2A:435:VAL:HA   | 1.86                     | 0.91              |
| 2:1W:100:GLY:CA   | 1:2K:253:THR:HG21 | 1.87                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1X:100:GLY:HA3  | 1:2L:253:THR:HG22 | 1.51                     | 0.91              |
| 2:2O:177:VAL:HG23 | 1:3B:332:ILE:CG2  | 2.00                     | 0.91              |
| 2:2Z:404:PHE:CG   | 1:3N:261:PRO:HA   | 2.04                     | 0.91              |
| 1:1B:346:TRP:HB3  | 2:4O:397:ALA:O    | 1.70                     | 0.91              |
| 1:1E:262:TYR:C    | 2:4R:406:HIS:CE1  | 2.47                     | 0.91              |
| 1:1E:435:VAL:O    | 2:4R:401:ARG:NH2  | 2.04                     | 0.91              |
| 1:1I:245:ASP:OD1  | 2:4U:77:SER:CB    | 2.19                     | 0.91              |
| 2:2R:210:TYR:HD2  | 1:3E:329:ASN:HD22 | 1.18                     | 0.91              |
| 2:2T:401:ARG:O    | 1:3G:262:TYR:OH   | 1.86                     | 0.91              |
| 2:2X:221:THR:OG1  | 1:3L:324:VAL:CG2  | 2.17                     | 0.91              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:CG   | 2.47                     | 0.91              |
| 1:1E:245:ASP:OD1  | 2:4R:77:SER:CB    | 2.12                     | 0.91              |
| 1:1I:245:ASP:OD2  | 2:4U:77:SER:CB    | 2.18                     | 0.91              |
| 1:1I:260:VAL:CB   | 2:4U:407:TRP:NE1  | 2.34                     | 0.91              |
| 1:1J:262:TYR:C    | 2:4V:406:HIS:CE1  | 2.48                     | 0.91              |
| 1:1N:329:ASN:ND2  | 2:4Z:210:TYR:HD2  | 1.68                     | 0.91              |
| 2:1S:221:THR:HA   | 1:2F:324:VAL:CG1  | 1.99                     | 0.91              |
| 2:1T:214:PHE:CG   | 1:2G:326:LYS:HE2  | 2.05                     | 0.91              |
| 2:1Y:181:VAL:HG11 | 1:2M:258:ASN:O    | 1.71                     | 0.91              |
| 1:1B:435:VAL:HA   | 2:4O:401:ARG:HH21 | 1.29                     | 0.91              |
| 1:1C:263:PRO:CD   | 2:4P:406:HIS:CG   | 2.53                     | 0.91              |
| 1:1F:254:GLU:CA   | 2:4S:100:GLY:C    | 2.43                     | 0.91              |
| 1:1N:353:VAL:HB   | 2:4Z:179:ASP:OD1  | 1.71                     | 0.91              |
| 2:1T:178:SER:HB3  | 1:2G:349:THR:HB   | 1.51                     | 0.91              |
| 2:1V:404:PHE:CE2  | 1:2J:261:PRO:HA   | 2.04                     | 0.91              |
| 2:1Y:207:GLU:CD   | 1:2M:329:ASN:ND2  | 2.27                     | 0.91              |
| 2:2Q:180:THR:HG23 | 1:3D:258:ASN:HD21 | 0.74                     | 0.91              |
| 2:2U:177:VAL:HG23 | 1:3I:332:ILE:CG2  | 2.00                     | 0.91              |
| 1:1D:324:VAL:CG1  | 2:4Q:222:PRO:O    | 2.18                     | 0.91              |
| 2:1H:181:VAL:H    | 1:2A:258:ASN:HD22 | 1.13                     | 0.91              |
| 2:1O:181:VAL:H    | 1:2B:258:ASN:HD22 | 1.19                     | 0.91              |
| 2:1Y:401:ARG:CB   | 1:2M:262:TYR:OH   | 2.18                     | 0.91              |
| 2:2P:406:HIS:CD2  | 1:3C:263:PRO:CD   | 2.52                     | 0.91              |
| 1:1E:263:PRO:CD   | 2:4R:406:HIS:CD2  | 2.54                     | 0.91              |
| 1:1K:260:VAL:HB   | 2:4W:407:TRP:CE2  | 2.05                     | 0.91              |
| 2:1V:394:GLN:HG2  | 1:2J:348:PRO:CG   | 2.01                     | 0.91              |
| 2:2H:179:ASP:OD2  | 1:3A:248:LEU:HD21 | 1.71                     | 0.91              |
| 2:2U:207:GLU:CD   | 1:3I:329:ASN:HD21 | 1.78                     | 0.91              |
| 1:1C:261:PRO:C    | 2:4P:404:PHE:H    | 1.78                     | 0.91              |
| 1:1E:346:TRP:HB2  | 2:4R:398:MET:CA   | 1.99                     | 0.91              |
| 1:1I:329:ASN:ND2  | 2:4U:207:GLU:OE1  | 2.03                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1O:214:PHE:HB2  | 1:2B:326:LYS:HE2  | 1.53                     | 0.91              |
| 2:1U:180:THR:HA   | 1:2I:258:ASN:ND2  | 1.85                     | 0.91              |
| 2:2Q:394:GLN:HA   | 1:3D:348:PRO:HG3  | 1.52                     | 0.91              |
| 2:2U:401:ARG:HH22 | 1:3I:435:VAL:HA   | 1.24                     | 0.91              |
| 1:1A:263:PRO:N    | 2:4H:406:HIS:NE2  | 2.19                     | 0.91              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:HA   | 1.52                     | 0.91              |
| 1:1M:257:THR:HB   | 2:4Y:100:GLY:O    | 1.71                     | 0.91              |
| 2:1W:401:ARG:CB   | 1:2K:262:TYR:OH   | 2.18                     | 0.91              |
| 2:2R:222:PRO:HG2  | 1:3E:326:LYS:HB2  | 1.53                     | 0.91              |
| 1:1E:435:VAL:HA   | 2:4R:401:ARG:HH21 | 1.10                     | 0.90              |
| 1:1I:348:PRO:HG3  | 2:4U:394:GLN:CA   | 2.00                     | 0.90              |
| 1:1K:248:LEU:CA   | 2:4W:11:GLN:NE2   | 2.34                     | 0.90              |
| 1:1K:329:ASN:HD22 | 2:4W:210:TYR:HD2  | 1.17                     | 0.90              |
| 2:2Q:397:ALA:O    | 1:3D:346:TRP:HB2  | 1.70                     | 0.90              |
| 1:1A:2:ARG:HD3    | 2:4H:72:PRO:HD2   | 1.53                     | 0.90              |
| 1:1D:314:ALA:HB2  | 2:4Q:181:VAL:HG11 | 1.52                     | 0.90              |
| 1:1G:435:VAL:C    | 2:4T:401:ARG:HH22 | 1.77                     | 0.90              |
| 2:2U:77:SER:CB    | 1:3I:245:ASP:OD1  | 2.19                     | 0.90              |
| 2:2Z:221:THR:OG1  | 1:3N:324:VAL:HG21 | 1.71                     | 0.90              |
| 2:1U:179:ASP:O    | 1:2I:352:LYS:HD2  | 1.71                     | 0.90              |
| 1:1B:261:PRO:HA   | 2:4O:404:PHE:CD1  | 2.07                     | 0.90              |
| 1:1C:325:PRO:O    | 2:4P:210:TYR:CZ   | 2.24                     | 0.90              |
| 1:1D:254:GLU:CA   | 2:4Q:100:GLY:C    | 2.45                     | 0.90              |
| 1:1D:346:TRP:HA   | 2:4Q:397:ALA:C    | 1.96                     | 0.90              |
| 1:1E:353:VAL:HB   | 2:4R:179:ASP:CG   | 1.96                     | 0.90              |
| 1:1I:351:PHE:O    | 2:4U:180:THR:C    | 2.13                     | 0.90              |
| 1:1L:257:THR:HB   | 2:4X:100:GLY:O    | 1.71                     | 0.90              |
| 1:1M:325:PRO:HD2  | 2:4Y:223:THR:HA   | 1.53                     | 0.90              |
| 2:1Q:181:VAL:HG21 | 1:2D:258:ASN:O    | 1.71                     | 0.90              |
| 2:2H:100:GLY:CA   | 1:3A:253:THR:HB   | 1.99                     | 0.90              |
| 2:2Z:221:THR:HA   | 1:3N:324:VAL:HG11 | 1.53                     | 0.90              |
| 1:1B:262:TYR:HA   | 2:4O:406:HIS:HD2  | 1.37                     | 0.90              |
| 2:1Y:182:VAL:CG2  | 1:2M:257:THR:HG22 | 2.02                     | 0.90              |
| 5:2R:501:GDP:H8   | 1:3E:248:LEU:CD1  | 1.83                     | 0.90              |
| 1:1B:332:ILE:HG21 | 2:4O:177:VAL:HG23 | 1.48                     | 0.90              |
| 1:1D:324:VAL:HG13 | 2:4Q:222:PRO:C    | 1.95                     | 0.90              |
| 1:1D:351:PHE:O    | 2:4Q:180:THR:CA   | 2.18                     | 0.90              |
| 1:1M:257:THR:CB   | 2:4Y:100:GLY:O    | 2.20                     | 0.90              |
| 2:1U:181:VAL:HG21 | 1:2I:258:ASN:C    | 1.96                     | 0.90              |
| 2:1Y:401:ARG:HB3  | 1:2M:262:TYR:HH   | 1.21                     | 0.90              |
| 1:1F:324:VAL:CG1  | 2:4S:222:PRO:O    | 2.20                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:2P:501:GDP:H8   | 1:3C:248:LEU:CD1  | 1.84                     | 0.90              |
| 2:2V:404:PHE:CE1  | 1:3J:260:VAL:C    | 2.50                     | 0.90              |
| 2:2V:406:HIS:NE2  | 1:3J:262:TYR:C    | 2.29                     | 0.90              |
| 2:2Z:71:GLU:HB2   | 1:3N:2:ARG:HD3    | 1.53                     | 0.90              |
| 2:2Z:404:PHE:CE1  | 1:3N:260:VAL:C    | 2.49                     | 0.90              |
| 1:1E:346:TRP:CH2  | 2:4R:403:ALA:CB   | 2.55                     | 0.90              |
| 2:1W:221:THR:CA   | 1:2K:324:VAL:HG11 | 1.98                     | 0.90              |
| 2:2R:71:GLU:HB2   | 1:3E:2:ARG:HD3    | 1.52                     | 0.90              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:CA   | 2.20                     | 0.90              |
| 1:1E:258:ASN:ND2  | 2:4R:180:THR:CG2  | 2.35                     | 0.90              |
| 1:1G:254:GLU:HG2  | 2:4T:101:ASN:N    | 1.87                     | 0.90              |
| 1:1I:262:TYR:HA   | 2:4U:406:HIS:HD2  | 1.30                     | 0.90              |
| 1:1M:258:ASN:HD21 | 2:4Y:180:THR:HG23 | 1.37                     | 0.90              |
| 2:1W:224:TYR:HE2  | 1:2K:248:LEU:HB2  | 1.37                     | 0.90              |
| 2:2Y:404:PHE:CD1  | 1:3M:261:PRO:HA   | 2.06                     | 0.90              |
| 1:1D:262:TYR:N    | 2:4Q:406:HIS:NE2  | 2.20                     | 0.90              |
| 1:1F:435:VAL:O    | 2:4S:401:ARG:NH2  | 2.05                     | 0.90              |
| 1:1N:248:LEU:HD13 | 5:4Z:501:GDP:C8   | 2.07                     | 0.90              |
| 2:1H:180:THR:HG23 | 1:2A:258:ASN:HD21 | 1.37                     | 0.90              |
| 2:1V:394:GLN:HG2  | 1:2J:348:PRO:HG3  | 1.53                     | 0.90              |
| 2:1Z:180:THR:HG23 | 1:2N:258:ASN:HD21 | 1.36                     | 0.90              |
| 2:2P:100:GLY:CA   | 1:3C:253:THR:HB   | 2.02                     | 0.90              |
| 2:2V:181:VAL:HG21 | 1:3J:314:ALA:HB1  | 1.51                     | 0.90              |
| 1:1B:329:ASN:HB2  | 2:4O:210:TYR:CE2  | 2.07                     | 0.89              |
| 1:1C:352:LYS:HD2  | 2:4P:179:ASP:O    | 1.72                     | 0.89              |
| 1:1G:257:THR:CG2  | 2:4T:102:ASN:HB2  | 2.01                     | 0.89              |
| 1:1I:329:ASN:HB2  | 2:4U:210:TYR:HE2  | 1.37                     | 0.89              |
| 1:1I:349:THR:CG2  | 2:4U:184:PRO:CD   | 2.48                     | 0.89              |
| 2:1V:100:GLY:CA   | 1:2J:253:THR:HG22 | 1.98                     | 0.89              |
| 2:2X:210:TYR:HD2  | 1:3L:329:ASN:HD22 | 1.19                     | 0.89              |
| 1:1D:351:PHE:O    | 2:4Q:180:THR:N    | 2.05                     | 0.89              |
| 1:1F:346:TRP:CE3  | 2:4S:403:ALA:CB   | 2.54                     | 0.89              |
| 2:2T:77:SER:CB    | 1:3G:245:ASP:OD1  | 2.19                     | 0.89              |
| 2:2U:394:GLN:CG   | 1:3I:348:PRO:CG   | 2.50                     | 0.89              |
| 2:2Y:100:GLY:CA   | 1:3M:253:THR:HG22 | 2.00                     | 0.89              |
| 1:1C:263:PRO:N    | 2:4P:406:HIS:CD2  | 2.39                     | 0.89              |
| 1:1D:261:PRO:O    | 2:4Q:404:PHE:N    | 2.06                     | 0.89              |
| 1:1E:351:PHE:O    | 2:4R:180:THR:N    | 2.04                     | 0.89              |
| 1:1F:314:ALA:HB1  | 2:4S:181:VAL:HG21 | 1.55                     | 0.89              |
| 2:1W:224:TYR:CE2  | 1:2K:247:ALA:O    | 2.26                     | 0.89              |
| 2:2U:77:SER:HB3   | 1:3I:245:ASP:CG   | 1.96                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2X:100:GLY:CA   | 1:3L:253:THR:CG2  | 2.48                     | 0.89              |
| 2:2Y:100:GLY:CA   | 1:3M:253:THR:CG2  | 2.49                     | 0.89              |
| 1:1B:352:LYS:HD2  | 2:4O:179:ASP:O    | 1.72                     | 0.89              |
| 2:1T:100:GLY:HA2  | 1:2G:253:THR:HB   | 1.54                     | 0.89              |
| 2:1X:207:GLU:OE2  | 1:2L:329:ASN:ND2  | 2.06                     | 0.89              |
| 2:2P:401:ARG:NH2  | 1:3C:435:VAL:CA   | 2.30                     | 0.89              |
| 5:2S:501:GDP:H8   | 1:3F:248:LEU:CD1  | 1.85                     | 0.89              |
| 2:2V:394:GLN:CG   | 1:3J:348:PRO:CG   | 2.51                     | 0.89              |
| 1:1C:262:TYR:C    | 2:4P:406:HIS:CD2  | 2.50                     | 0.89              |
| 1:1I:254:GLU:N    | 2:4U:100:GLY:HA2  | 1.87                     | 0.89              |
| 1:1K:248:LEU:CA   | 2:4W:11:GLN:HE22  | 1.86                     | 0.89              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:CG   | 2.07                     | 0.89              |
| 1:1F:352:LYS:HD3  | 2:4S:101:ASN:ND2  | 1.86                     | 0.89              |
| 1:1G:352:LYS:HD3  | 2:4T:101:ASN:ND2  | 1.88                     | 0.89              |
| 1:1N:2:ARG:HD3    | 2:4Z:72:PRO:HD2   | 1.53                     | 0.89              |
| 2:1T:221:THR:OG1  | 1:2G:324:VAL:HG22 | 1.71                     | 0.89              |
| 2:1U:214:PHE:CD1  | 1:2I:326:LYS:HE3  | 2.08                     | 0.89              |
| 2:1U:394:GLN:HG2  | 1:2I:348:PRO:HG3  | 1.53                     | 0.89              |
| 2:2P:100:GLY:HA2  | 1:3C:253:THR:HB   | 1.53                     | 0.89              |
| 1:1D:332:ILE:HB   | 2:4Q:177:VAL:HG21 | 1.53                     | 0.89              |
| 1:1K:257:THR:HG21 | 2:4W:102:ASN:HB2  | 1.53                     | 0.89              |
| 2:1X:207:GLU:CD   | 1:2L:329:ASN:ND2  | 2.30                     | 0.89              |
| 2:2W:222:PRO:HG2  | 1:3K:326:LYS:CB   | 2.03                     | 0.89              |
| 1:1D:434:GLU:O    | 2:4Q:401:ARG:NH2  | 2.06                     | 0.89              |
| 1:1I:254:GLU:HA   | 2:4U:100:GLY:O    | 1.72                     | 0.89              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:CB   | 2.20                     | 0.89              |
| 2:1Q:181:VAL:H    | 1:2D:258:ASN:HD22 | 1.13                     | 0.89              |
| 2:1Y:181:VAL:CB   | 1:2M:258:ASN:O    | 2.21                     | 0.89              |
| 2:2U:221:THR:OG1  | 1:3I:324:VAL:CG2  | 2.20                     | 0.89              |
| 2:2Y:101:ASN:O    | 1:3M:257:THR:HG21 | 1.73                     | 0.89              |
| 1:1B:2:ARG:CG     | 2:4O:72:PRO:HD2   | 2.03                     | 0.89              |
| 1:1D:261:PRO:C    | 2:4Q:404:PHE:H    | 1.81                     | 0.89              |
| 1:1I:260:VAL:CB   | 2:4U:407:TRP:CZ2  | 2.56                     | 0.89              |
| 2:2S:177:VAL:HG23 | 1:3F:332:ILE:HG22 | 1.53                     | 0.89              |
| 2:2T:394:GLN:HG2  | 1:3G:348:PRO:HG3  | 1.52                     | 0.89              |
| 2:2V:176:LYS:HE2  | 1:3J:333:ALA:HB1  | 1.52                     | 0.89              |
| 2:2Z:100:GLY:CA   | 1:3N:253:THR:HB   | 2.02                     | 0.89              |
| 1:1B:346:TRP:O    | 2:4O:398:MET:HG2  | 1.71                     | 0.88              |
| 1:1D:346:TRP:CZ3  | 2:4Q:403:ALA:CB   | 2.56                     | 0.88              |
| 2:1V:221:THR:CB   | 1:2J:324:VAL:HG21 | 2.03                     | 0.88              |
| 2:1Z:181:VAL:HG21 | 1:2N:258:ASN:O    | 1.73                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:351:PHE:HB2  | 2:4P:178:SER:OG   | 1.72                     | 0.88              |
| 1:1I:346:TRP:HA   | 2:4U:397:ALA:O    | 1.72                     | 0.88              |
| 2:1O:11:GLN:HE22  | 1:2B:249:ASN:H    | 1.16                     | 0.88              |
| 2:1V:180:THR:CA   | 1:2J:258:ASN:ND2  | 2.36                     | 0.88              |
| 2:1V:221:THR:HA   | 1:2J:324:VAL:HG11 | 0.90                     | 0.88              |
| 2:1Y:222:PRO:O    | 1:2M:325:PRO:HD2  | 1.74                     | 0.88              |
| 2:2R:181:VAL:HG21 | 1:3E:314:ALA:HB1  | 1.55                     | 0.88              |
| 1:1B:254:GLU:HA   | 2:4O:100:GLY:C    | 1.99                     | 0.88              |
| 1:1B:329:ASN:HD22 | 2:4O:210:TYR:HD2  | 1.21                     | 0.88              |
| 1:1E:324:VAL:HG13 | 2:4R:222:PRO:C    | 1.98                     | 0.88              |
| 1:1F:346:TRP:HB3  | 2:4S:397:ALA:O    | 1.72                     | 0.88              |
| 1:1G:258:ASN:HD21 | 2:4T:180:THR:HG23 | 1.35                     | 0.88              |
| 1:1J:353:VAL:CB   | 2:4V:179:ASP:OD1  | 2.21                     | 0.88              |
| 2:1P:181:VAL:H    | 1:2C:258:ASN:HD22 | 1.19                     | 0.88              |
| 2:1V:181:VAL:CB   | 1:2J:258:ASN:O    | 2.20                     | 0.88              |
| 2:1X:101:ASN:CB   | 1:2L:254:GLU:HG2  | 1.99                     | 0.88              |
| 2:2O:397:ALA:O    | 1:3B:346:TRP:HB2  | 1.71                     | 0.88              |
| 1:1D:346:TRP:HD1  | 2:4Q:401:ARG:HG3  | 1.36                     | 0.88              |
| 1:1G:257:THR:HB   | 2:4T:100:GLY:O    | 1.72                     | 0.88              |
| 2:1H:214:PHE:HB2  | 1:2A:326:LYS:HE2  | 1.55                     | 0.88              |
| 2:1W:404:PHE:CE2  | 1:2K:261:PRO:HA   | 2.08                     | 0.88              |
| 2:2O:176:LYS:HE2  | 1:3B:333:ALA:HB1  | 1.52                     | 0.88              |
| 2:2O:179:ASP:OD2  | 1:3B:248:LEU:HD21 | 1.73                     | 0.88              |
| 2:2P:394:GLN:HA   | 1:3C:348:PRO:HG3  | 1.54                     | 0.88              |
| 2:2R:401:ARG:HH22 | 1:3E:435:VAL:HA   | 1.11                     | 0.88              |
| 1:1A:348:PRO:HG2  | 2:4H:394:GLN:HB3  | 1.52                     | 0.88              |
| 1:1B:333:ALA:CB   | 2:4O:176:LYS:HE2  | 2.03                     | 0.88              |
| 1:1E:347:CYS:HA   | 2:4R:398:MET:HG2  | 1.55                     | 0.88              |
| 1:1F:346:TRP:CH2  | 2:4S:403:ALA:CB   | 2.56                     | 0.88              |
| 1:1I:348:PRO:HG3  | 2:4U:394:GLN:CB   | 2.02                     | 0.88              |
| 1:1L:260:VAL:C    | 2:4X:407:TRP:HE1  | 1.79                     | 0.88              |
| 2:1W:11:GLN:HE22  | 1:2K:249:ASN:HB2  | 1.34                     | 0.88              |
| 2:2Z:176:LYS:HE2  | 1:3N:333:ALA:HB1  | 1.56                     | 0.88              |
| 1:1D:353:VAL:HB   | 2:4Q:179:ASP:CG   | 1.98                     | 0.88              |
| 1:1E:260:VAL:HG12 | 2:4R:406:HIS:HE1  | 1.33                     | 0.88              |
| 2:2Q:404:PHE:CG   | 1:3D:261:PRO:HA   | 2.07                     | 0.88              |
| 5:2Q:501:GDP:C8   | 1:3D:248:LEU:CD1  | 2.57                     | 0.88              |
| 1:1C:346:TRP:CA   | 2:4P:397:ALA:O    | 2.21                     | 0.88              |
| 1:1E:2:ARG:NH2    | 2:4R:73:GLY:HA3   | 1.88                     | 0.88              |
| 1:1E:314:ALA:HB2  | 2:4R:181:VAL:HG11 | 1.56                     | 0.88              |
| 1:1F:245:ASP:OD1  | 2:4S:77:SER:CB    | 2.13                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:262:TYR:OH   | 2:4U:401:ARG:O    | 1.91                     | 0.88              |
| 1:1J:349:THR:O    | 2:4V:181:VAL:CA   | 2.22                     | 0.88              |
| 2:2R:394:GLN:HA   | 1:3E:348:PRO:HG3  | 1.56                     | 0.88              |
| 1:1A:326:LYS:CE   | 2:4H:214:PHE:HB2  | 2.03                     | 0.88              |
| 1:1D:333:ALA:CB   | 2:4Q:176:LYS:HE2  | 2.03                     | 0.88              |
| 1:1G:347:CYS:HA   | 2:4T:398:MET:HG2  | 1.54                     | 0.88              |
| 1:1J:346:TRP:CZ3  | 2:4V:403:ALA:CB   | 2.56                     | 0.88              |
| 2:1W:100:GLY:CA   | 1:2K:253:THR:CB   | 2.45                     | 0.88              |
| 2:2H:176:LYS:HE2  | 1:3A:333:ALA:HB1  | 1.54                     | 0.88              |
| 1:1A:332:ILE:HG21 | 2:4H:177:VAL:CG2  | 2.03                     | 0.88              |
| 1:1D:346:TRP:HB2  | 2:4Q:398:MET:CA   | 2.04                     | 0.88              |
| 1:1I:332:ILE:CG2  | 2:4U:177:VAL:CG2  | 2.52                     | 0.88              |
| 2:1T:224:TYR:HD2  | 1:2G:247:ALA:O    | 1.56                     | 0.88              |
| 2:1X:179:ASP:OD2  | 1:2L:248:LEU:CD2  | 2.21                     | 0.88              |
| 2:2U:223:THR:HA   | 1:3I:325:PRO:HD2  | 1.56                     | 0.88              |
| 2:2Z:222:PRO:HG2  | 1:3N:326:LYS:HB2  | 1.54                     | 0.88              |
| 1:1C:249:ASN:N    | 2:4P:11:GLN:NE2   | 1.69                     | 0.88              |
| 1:1D:263:PRO:N    | 2:4Q:406:HIS:NE2  | 2.22                     | 0.88              |
| 1:1K:2:ARG:CD     | 2:4W:72:PRO:HD2   | 2.01                     | 0.88              |
| 1:1K:349:THR:O    | 2:4W:181:VAL:CA   | 2.22                     | 0.88              |
| 2:1H:181:VAL:N    | 1:2A:258:ASN:ND2  | 2.21                     | 0.88              |
| 2:1T:214:PHE:CG   | 1:2G:326:LYS:CE   | 2.57                     | 0.88              |
| 2:1V:224:TYR:HE2  | 1:2J:248:LEU:HB2  | 1.37                     | 0.88              |
| 2:2R:214:PHE:HB2  | 1:3E:326:LYS:CE   | 2.03                     | 0.88              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:HG3  | 1.71                     | 0.87              |
| 1:1I:249:ASN:H    | 2:4U:11:GLN:CD    | 1.82                     | 0.87              |
| 1:1M:348:PRO:CG   | 2:4Y:394:GLN:HB3  | 2.04                     | 0.87              |
| 2:1V:221:THR:HB   | 1:2J:324:VAL:HG21 | 1.53                     | 0.87              |
| 2:2H:214:PHE:HB2  | 1:3A:326:LYS:CE   | 2.03                     | 0.87              |
| 2:2H:394:GLN:HG2  | 1:3A:348:PRO:HG3  | 1.55                     | 0.87              |
| 2:2H:404:PHE:CG   | 1:3A:261:PRO:HA   | 2.08                     | 0.87              |
| 1:1A:248:LEU:CD1  | 5:4H:501:GDP:H8   | 1.86                     | 0.87              |
| 1:1B:253:THR:C    | 2:4O:100:GLY:HA2  | 1.99                     | 0.87              |
| 1:1C:346:TRP:CD1  | 2:4P:401:ARG:HG3  | 2.09                     | 0.87              |
| 1:1D:326:LYS:HA   | 2:4Q:210:TYR:CE1  | 2.10                     | 0.87              |
| 1:1G:346:TRP:HA   | 2:4T:397:ALA:C    | 1.99                     | 0.87              |
| 1:1I:245:ASP:OD2  | 2:4U:77:SER:HB3   | 1.74                     | 0.87              |
| 1:1I:257:THR:CG2  | 2:4U:102:ASN:HB2  | 2.02                     | 0.87              |
| 2:2P:179:ASP:OD1  | 1:3C:353:VAL:HB   | 1.72                     | 0.87              |
| 2:2Q:406:HIS:NE2  | 1:3D:262:TYR:C    | 2.33                     | 0.87              |
| 2:2U:394:GLN:HG2  | 1:3I:348:PRO:CB   | 2.03                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:260:VAL:O    | 2:4H:407:TRP:CD1  | 2.27                     | 0.87              |
| 1:1A:348:PRO:CG   | 2:4H:394:GLN:HG2  | 2.04                     | 0.87              |
| 1:1F:263:PRO:CD   | 2:4S:406:HIS:CG   | 2.57                     | 0.87              |
| 1:1K:262:TYR:C    | 2:4W:406:HIS:CE1  | 2.53                     | 0.87              |
| 1:1M:348:PRO:HG3  | 2:4Y:394:GLN:CB   | 2.04                     | 0.87              |
| 2:1V:401:ARG:HH22 | 1:2J:435:VAL:HA   | 1.39                     | 0.87              |
| 2:1Y:179:ASP:CG   | 1:2M:248:LEU:HD21 | 1.98                     | 0.87              |
| 2:2Q:77:SER:HB3   | 1:3D:245:ASP:CG   | 1.99                     | 0.87              |
| 2:2T:394:GLN:CG   | 1:3G:348:PRO:CG   | 2.51                     | 0.87              |
| 2:2X:406:HIS:NE2  | 1:3L:263:PRO:N    | 2.22                     | 0.87              |
| 2:2Z:179:ASP:OD2  | 1:3N:248:LEU:HD21 | 1.74                     | 0.87              |
| 1:1A:348:PRO:HG3  | 2:4H:394:GLN:HA   | 1.56                     | 0.87              |
| 1:1B:254:GLU:HA   | 2:4O:100:GLY:O    | 1.74                     | 0.87              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:CA   | 2.48                     | 0.87              |
| 1:1D:2:ARG:NH1    | 2:4Q:71:GLU:HG3   | 1.88                     | 0.87              |
| 1:1N:257:THR:CB   | 2:4Z:100:GLY:O    | 2.23                     | 0.87              |
| 2:2S:222:PRO:HG2  | 1:3F:326:LYS:CB   | 2.04                     | 0.87              |
| 5:2S:501:GDP:C8   | 1:3F:248:LEU:CD1  | 2.57                     | 0.87              |
| 2:2T:177:VAL:HG23 | 1:3G:332:ILE:HG22 | 1.55                     | 0.87              |
| 2:2V:394:GLN:CG   | 1:3J:348:PRO:HG3  | 2.04                     | 0.87              |
| 2:2Y:176:LYS:HE2  | 1:3M:333:ALA:HB1  | 1.56                     | 0.87              |
| 2:2Y:404:PHE:CD1  | 1:3M:260:VAL:O    | 2.27                     | 0.87              |
| 1:1D:261:PRO:CA   | 2:4Q:404:PHE:HA   | 2.03                     | 0.87              |
| 1:1E:260:VAL:O    | 2:4R:407:TRP:NE1  | 2.06                     | 0.87              |
| 1:1E:348:PRO:HB3  | 2:4R:394:GLN:HG2  | 1.57                     | 0.87              |
| 2:2O:394:GLN:HG2  | 1:3B:348:PRO:CB   | 2.04                     | 0.87              |
| 2:2Q:397:ALA:O    | 1:3D:346:TRP:CB   | 2.23                     | 0.87              |
| 1:1E:254:GLU:N    | 2:4R:100:GLY:CA   | 2.37                     | 0.87              |
| 1:1J:245:ASP:OD1  | 2:4V:77:SER:CB    | 2.22                     | 0.87              |
| 1:1N:260:VAL:O    | 2:4Z:407:TRP:CD1  | 2.27                     | 0.87              |
| 2:1R:406:HIS:CD2  | 1:2E:263:PRO:HD3  | 2.09                     | 0.87              |
| 2:1W:214:PHE:CG   | 1:2K:326:LYS:HE3  | 2.09                     | 0.87              |
| 1:1A:329:ASN:HB2  | 2:4H:210:TYR:CE2  | 2.10                     | 0.87              |
| 1:1B:2:ARG:CD     | 2:4O:72:PRO:HD2   | 2.04                     | 0.87              |
| 1:1C:324:VAL:HG13 | 2:4P:222:PRO:C    | 1.99                     | 0.87              |
| 1:1E:2:ARG:HD3    | 2:4R:72:PRO:CD    | 2.02                     | 0.87              |
| 1:1E:332:ILE:HB   | 2:4R:177:VAL:CG2  | 2.04                     | 0.87              |
| 2:1H:11:GLN:HE22  | 1:2A:249:ASN:H    | 1.22                     | 0.87              |
| 2:1Z:214:PHE:HB2  | 1:2N:326:LYS:HE2  | 1.55                     | 0.87              |
| 2:2H:101:ASN:HB2  | 1:3A:254:GLU:HG2  | 1.55                     | 0.87              |
| 5:2P:501:GDP:C8   | 1:3C:248:LEU:CD1  | 2.57                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:406:HIS:NE2  | 1:3F:263:PRO:N    | 2.21                     | 0.87              |
| 2:2W:100:GLY:HA2  | 1:3K:253:THR:HB   | 1.56                     | 0.87              |
| 2:2X:401:ARG:HH22 | 1:3L:435:VAL:CA   | 1.86                     | 0.87              |
| 1:1M:262:TYR:C    | 2:4Y:406:HIS:CE1  | 2.53                     | 0.87              |
| 1:1N:261:PRO:HB3  | 2:4Z:404:PHE:CE2  | 2.08                     | 0.87              |
| 2:1V:214:PHE:CG   | 1:2J:326:LYS:HE3  | 2.07                     | 0.87              |
| 5:2O:501:GDP:C8   | 1:3B:248:LEU:CD1  | 2.58                     | 0.87              |
| 2:2W:394:GLN:CG   | 1:3K:348:PRO:CG   | 2.52                     | 0.87              |
| 2:2O:101:ASN:HB2  | 1:3B:254:GLU:HG2  | 1.57                     | 0.87              |
| 2:2U:394:GLN:CG   | 1:3I:348:PRO:HG3  | 2.05                     | 0.87              |
| 1:1E:349:THR:HG21 | 2:4R:184:PRO:CD   | 2.03                     | 0.86              |
| 1:1F:257:THR:CG2  | 2:4S:102:ASN:HB2  | 2.05                     | 0.86              |
| 1:1J:348:PRO:CG   | 2:4V:394:GLN:HB3  | 2.05                     | 0.86              |
| 2:2O:214:PHE:CB   | 1:3B:326:LYS:HE2  | 2.05                     | 0.86              |
| 2:2Z:101:ASN:HB2  | 1:3N:254:GLU:HG2  | 1.57                     | 0.86              |
| 5:2O:501:GDP:H8   | 1:3B:248:LEU:CD1  | 1.88                     | 0.86              |
| 5:2T:501:GDP:H8   | 1:3G:248:LEU:CD1  | 1.89                     | 0.86              |
| 1:1E:253:THR:C    | 2:4R:100:GLY:HA3  | 1.99                     | 0.86              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:HA   | 1.73                     | 0.86              |
| 1:1L:257:THR:CB   | 2:4X:100:GLY:O    | 2.23                     | 0.86              |
| 2:1Y:181:VAL:HG23 | 1:2M:258:ASN:CB   | 2.02                     | 0.86              |
| 2:1Y:182:VAL:HG21 | 1:2M:257:THR:HG22 | 1.56                     | 0.86              |
| 2:2R:397:ALA:O    | 1:3E:346:TRP:HB2  | 1.74                     | 0.86              |
| 2:2V:100:GLY:O    | 1:3J:257:THR:OG1  | 1.92                     | 0.86              |
| 1:1A:245:ASP:CG   | 2:4H:77:SER:CB    | 2.47                     | 0.86              |
| 1:1F:346:TRP:CB   | 2:4S:398:MET:HA   | 2.05                     | 0.86              |
| 1:1G:248:LEU:CA   | 2:4T:11:GLN:HE22  | 1.87                     | 0.86              |
| 1:1K:349:THR:HG21 | 2:4W:184:PRO:CD   | 2.02                     | 0.86              |
| 1:1M:2:ARG:CD     | 2:4Y:72:PRO:HD2   | 2.06                     | 0.86              |
| 1:1N:263:PRO:N    | 2:4Z:406:HIS:CE1  | 2.43                     | 0.86              |
| 2:1V:214:PHE:CD1  | 1:2J:326:LYS:HE3  | 2.09                     | 0.86              |
| 2:2R:397:ALA:O    | 1:3E:346:TRP:CB   | 2.23                     | 0.86              |
| 2:2X:404:PHE:CD1  | 1:3L:260:VAL:O    | 2.28                     | 0.86              |
| 1:1N:348:PRO:CB   | 2:4Z:394:GLN:HG2  | 2.05                     | 0.86              |
| 2:2Q:406:HIS:CG   | 1:3D:263:PRO:HD3  | 2.11                     | 0.86              |
| 2:2S:394:GLN:CG   | 1:3F:348:PRO:CG   | 2.53                     | 0.86              |
| 2:2V:77:SER:CB    | 1:3J:245:ASP:OD1  | 2.22                     | 0.86              |
| 1:1C:258:ASN:OD1  | 2:4P:101:ASN:ND2  | 2.08                     | 0.86              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:CB   | 2.23                     | 0.86              |
| 1:1G:349:THR:CB   | 2:4T:184:PRO:HD3  | 2.05                     | 0.86              |
| 1:1G:349:THR:OG1  | 2:4T:181:VAL:O    | 1.92                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:248:LEU:HD13 | 5:4U:501:GDP:C8   | 2.11                     | 0.86              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:HA   | 1.75                     | 0.86              |
| 1:1J:329:ASN:HB2  | 2:4V:210:TYR:CE2  | 2.09                     | 0.86              |
| 2:2R:404:PHE:CD1  | 1:3E:261:PRO:HA   | 2.10                     | 0.86              |
| 2:2W:181:VAL:HG21 | 1:3K:314:ALA:HB1  | 1.57                     | 0.86              |
| 1:1B:261:PRO:HB3  | 2:4O:404:PHE:CE2  | 2.10                     | 0.86              |
| 1:1D:262:TYR:HA   | 2:4Q:406:HIS:HD2  | 1.07                     | 0.86              |
| 1:1E:329:ASN:CG   | 2:4R:207:GLU:OE1  | 2.19                     | 0.86              |
| 1:1F:120:ASP:OD2  | 1:1F:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:HG3  | 1.72                     | 0.86              |
| 2:1R:214:PHE:CB   | 1:2E:326:LYS:HE2  | 2.05                     | 0.86              |
| 2:1X:11:GLN:HE22  | 1:2L:249:ASN:HB2  | 1.40                     | 0.86              |
| 1:2F:120:ASP:OD2  | 1:2F:124:LYS:NZ   | 2.09                     | 0.86              |
| 2:2O:404:PHE:CG   | 1:3B:261:PRO:HA   | 2.10                     | 0.86              |
| 2:2T:401:ARG:HH22 | 1:3G:435:VAL:CA   | 1.88                     | 0.86              |
| 1:3F:120:ASP:OD2  | 1:3F:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1D:120:ASP:OD2  | 1:1D:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1D:260:VAL:HG12 | 2:4Q:406:HIS:CE1  | 2.09                     | 0.86              |
| 2:1U:100:GLY:CA   | 1:2I:253:THR:HG21 | 2.00                     | 0.86              |
| 5:2R:501:GDP:C8   | 1:3E:248:LEU:CD1  | 2.56                     | 0.86              |
| 5:2T:501:GDP:C8   | 1:3G:248:LEU:CD1  | 2.58                     | 0.86              |
| 1:3I:120:ASP:OD2  | 1:3I:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:4F:120:ASP:OD2  | 1:4F:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:4I:120:ASP:OD2  | 1:4I:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1C:326:LYS:HA   | 2:4P:210:TYR:CD1  | 2.10                     | 0.86              |
| 1:1D:435:VAL:HA   | 2:4Q:401:ARG:HH21 | 1.04                     | 0.86              |
| 1:1E:332:ILE:CB   | 2:4R:177:VAL:CG2  | 2.54                     | 0.86              |
| 1:1I:120:ASP:OD2  | 1:1I:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1N:261:PRO:CA   | 2:4Z:404:PHE:CD1  | 2.59                     | 0.86              |
| 1:1N:435:VAL:HA   | 2:4Z:401:ARG:NH2  | 1.89                     | 0.86              |
| 2:1Q:181:VAL:H    | 1:2D:258:ASN:ND2  | 1.73                     | 0.86              |
| 2:1U:221:THR:HB   | 1:2I:324:VAL:HG21 | 1.58                     | 0.86              |
| 1:2D:120:ASP:OD2  | 1:2D:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:2I:120:ASP:OD2  | 1:2I:124:LYS:NZ   | 2.09                     | 0.86              |
| 2:2P:404:PHE:CG   | 1:3C:261:PRO:HA   | 2.10                     | 0.86              |
| 2:2Q:177:VAL:HG23 | 1:3D:332:ILE:HG21 | 1.57                     | 0.86              |
| 2:2W:100:GLY:CA   | 1:3K:253:THR:CG2  | 2.51                     | 0.86              |
| 2:2W:176:LYS:HE2  | 1:3K:333:ALA:HB1  | 1.54                     | 0.86              |
| 2:2Z:100:GLY:CA   | 1:3N:253:THR:CG2  | 2.53                     | 0.86              |
| 1:3D:120:ASP:OD2  | 1:3D:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1C:326:LYS:HE2  | 2:4P:210:TYR:O    | 1.76                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:262:TYR:C    | 2:4S:406:HIS:CD2  | 2.45                     | 0.86              |
| 1:1F:332:ILE:HG21 | 2:4S:177:VAL:CG2  | 2.05                     | 0.86              |
| 1:1F:346:TRP:CD1  | 2:4S:401:ARG:HG3  | 2.11                     | 0.86              |
| 1:1G:260:VAL:CB   | 2:4T:407:TRP:CZ2  | 2.59                     | 0.86              |
| 2:1P:221:THR:HA   | 1:2C:324:VAL:HG11 | 1.58                     | 0.86              |
| 2:1U:404:PHE:CE2  | 1:2I:261:PRO:HA   | 2.11                     | 0.86              |
| 2:1V:178:SER:HB3  | 1:2J:349:THR:HB   | 1.55                     | 0.86              |
| 2:1X:207:GLU:OE1  | 1:2L:329:ASN:ND2  | 2.08                     | 0.86              |
| 5:2H:501:GDP:C8   | 1:3A:248:LEU:CD1  | 2.59                     | 0.86              |
| 2:2X:176:LYS:HE2  | 1:3L:333:ALA:HB1  | 1.55                     | 0.86              |
| 2:2Y:221:THR:OG1  | 1:3M:324:VAL:CG2  | 2.23                     | 0.86              |
| 1:4C:120:ASP:OD2  | 1:4C:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:4D:120:ASP:OD2  | 1:4D:124:LYS:NZ   | 2.09                     | 0.86              |
| 1:1D:258:ASN:OD1  | 2:4Q:101:ASN:ND2  | 2.09                     | 0.85              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:HG2  | 1.72                     | 0.85              |
| 1:2C:120:ASP:OD2  | 1:2C:124:LYS:NZ   | 2.09                     | 0.85              |
| 2:2R:177:VAL:HG23 | 1:3E:332:ILE:HG22 | 1.55                     | 0.85              |
| 2:2U:100:GLY:O    | 1:3I:257:THR:OG1  | 1.93                     | 0.85              |
| 2:2W:394:GLN:CG   | 1:3K:348:PRO:HG3  | 2.05                     | 0.85              |
| 2:2Z:404:PHE:CE2  | 1:3N:261:PRO:HB3  | 2.11                     | 0.85              |
| 1:3A:120:ASP:OD2  | 1:3A:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1A:120:ASP:OD2  | 1:1A:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1F:349:THR:CG2  | 2:4S:184:PRO:CD   | 2.49                     | 0.85              |
| 2:1Q:11:GLN:HE22  | 1:2D:249:ASN:H    | 1.24                     | 0.85              |
| 2:1X:181:VAL:HG11 | 1:2L:258:ASN:O    | 1.76                     | 0.85              |
| 2:2X:224:TYR:HE2  | 1:3L:248:LEU:HB2  | 1.41                     | 0.85              |
| 2:2Z:404:PHE:CD1  | 1:3N:260:VAL:O    | 2.30                     | 0.85              |
| 1:3C:120:ASP:OD2  | 1:3C:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4A:120:ASP:OD2  | 1:4A:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1A:348:PRO:CG   | 2:4H:394:GLN:CG   | 2.55                     | 0.85              |
| 1:1C:120:ASP:OD2  | 1:1C:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1E:120:ASP:OD2  | 1:1E:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1F:253:THR:C    | 2:4S:100:GLY:HA2  | 1.99                     | 0.85              |
| 1:1J:254:GLU:HA   | 2:4V:100:GLY:C    | 2.01                     | 0.85              |
| 1:1N:257:THR:OG1  | 2:4Z:100:GLY:O    | 1.94                     | 0.85              |
| 2:1X:406:HIS:CD2  | 1:2L:263:PRO:HD3  | 2.10                     | 0.85              |
| 2:1Y:181:VAL:HG21 | 1:2M:258:ASN:C    | 2.00                     | 0.85              |
| 1:2A:120:ASP:OD2  | 1:2A:124:LYS:NZ   | 2.09                     | 0.85              |
| 2:2H:177:VAL:HG23 | 1:3A:332:ILE:CG2  | 2.05                     | 0.85              |
| 2:2T:394:GLN:CB   | 1:3G:348:PRO:HG3  | 2.06                     | 0.85              |
| 1:1A:262:TYR:CA   | 2:4H:406:HIS:CD2  | 2.56                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:258:ASN:HD21 | 2:4O:180:THR:HG23 | 0.73                     | 0.85              |
| 1:1F:346:TRP:HD1  | 2:4S:401:ARG:HG3  | 1.39                     | 0.85              |
| 1:1G:346:TRP:CB   | 2:4T:398:MET:HA   | 2.06                     | 0.85              |
| 1:1J:120:ASP:OD2  | 1:1J:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1L:286:LEU:O    | 1:1L:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:1L:325:PRO:HD2  | 2:4X:223:THR:HA   | 1.59                     | 0.85              |
| 2:1H:181:VAL:N    | 1:2A:258:ASN:HD22 | 1.72                     | 0.85              |
| 2:1W:100:GLY:CA   | 1:2K:253:THR:HG22 | 2.03                     | 0.85              |
| 2:1Z:224:TYR:CD2  | 1:2N:247:ALA:O    | 2.30                     | 0.85              |
| 1:2L:286:LEU:O    | 1:2L:373:ARG:NH1  | 2.10                     | 0.85              |
| 2:2Q:401:ARG:HH22 | 1:3D:435:VAL:HA   | 1.03                     | 0.85              |
| 2:2X:394:GLN:CG   | 1:3L:348:PRO:CG   | 2.54                     | 0.85              |
| 1:3E:120:ASP:OD2  | 1:3E:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:3K:120:ASP:OD2  | 1:3K:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1G:435:VAL:HA   | 2:4T:401:ARG:NH2  | 1.92                     | 0.85              |
| 1:1L:262:TYR:C    | 2:4X:406:HIS:CE1  | 2.55                     | 0.85              |
| 1:1M:120:ASP:OD2  | 1:1M:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1N:120:ASP:OD2  | 1:1N:124:LYS:NZ   | 2.09                     | 0.85              |
| 2:1U:221:THR:CB   | 1:2I:324:VAL:HG21 | 2.06                     | 0.85              |
| 2:1Y:394:GLN:HG2  | 1:2M:348:PRO:CG   | 2.06                     | 0.85              |
| 1:2E:120:ASP:OD2  | 1:2E:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:2K:120:ASP:OD2  | 1:2K:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:2M:120:ASP:OD2  | 1:2M:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:3J:120:ASP:OD2  | 1:3J:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:3L:286:LEU:O    | 1:3L:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:3M:120:ASP:OD2  | 1:3M:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4E:120:ASP:OD2  | 1:4E:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4K:120:ASP:OD2  | 1:4K:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4L:286:LEU:O    | 1:4L:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:4M:120:ASP:OD2  | 1:4M:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1D:352:LYS:HA   | 2:4Q:179:ASP:O    | 1.75                     | 0.85              |
| 1:1F:351:PHE:O    | 2:4S:180:THR:N    | 2.09                     | 0.85              |
| 1:1G:348:PRO:HB2  | 2:4T:394:GLN:HG2  | 1.55                     | 0.85              |
| 1:1J:261:PRO:HA   | 2:4V:404:PHE:HA   | 1.58                     | 0.85              |
| 1:1K:120:ASP:OD2  | 1:1K:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1N:261:PRO:HA   | 2:4Z:404:PHE:CG   | 2.11                     | 0.85              |
| 2:1O:100:GLY:HA3  | 1:2B:253:THR:CG2  | 2.05                     | 0.85              |
| 1:2N:120:ASP:OD2  | 1:2N:124:LYS:NZ   | 2.09                     | 0.85              |
| 2:2T:101:ASN:O    | 1:3G:257:THR:HG21 | 1.76                     | 0.85              |
| 1:3N:120:ASP:OD2  | 1:3N:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4J:120:ASP:OD2  | 1:4J:124:LYS:NZ   | 2.09                     | 0.85              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:4N:120:ASP:OD2 | 1:4N:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1A:263:PRO:N   | 2:4H:406:HIS:CE1  | 2.45                     | 0.85              |
| 1:1B:2:ARG:HD3   | 2:4O:71:GLU:HB2   | 1.59                     | 0.85              |
| 1:1M:263:PRO:HD3 | 2:4Y:406:HIS:CD2  | 2.10                     | 0.85              |
| 1:2J:120:ASP:OD2 | 1:2J:124:LYS:NZ   | 2.09                     | 0.85              |
| 5:2U:501:GDP:C8  | 1:3I:248:LEU:CD1  | 2.59                     | 0.85              |
| 1:1B:120:ASP:OD2 | 1:1B:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1F:325:PRO:CB  | 2:4S:224:TYR:CE1  | 2.60                     | 0.85              |
| 1:1L:2:ARG:CD    | 2:4X:72:PRO:HD2   | 2.06                     | 0.85              |
| 1:1N:260:VAL:O   | 2:4Z:407:TRP:NE1  | 2.08                     | 0.85              |
| 2:2P:77:SER:HB3  | 1:3C:245:ASP:OD1  | 1.77                     | 0.85              |
| 2:2R:404:PHE:CE2 | 1:3E:261:PRO:HB3  | 2.12                     | 0.85              |
| 2:2T:179:ASP:OD1 | 1:3G:353:VAL:HB   | 1.76                     | 0.85              |
| 1:1A:435:VAL:CA  | 2:4H:401:ARG:NH2  | 2.40                     | 0.85              |
| 1:1B:2:ARG:NH2   | 2:4O:73:GLY:HA3   | 1.91                     | 0.85              |
| 1:1B:261:PRO:HA  | 2:4O:404:PHE:CA   | 2.07                     | 0.85              |
| 1:1I:346:TRP:O   | 2:4U:398:MET:CB   | 2.24                     | 0.85              |
| 1:1L:120:ASP:OD2 | 1:1L:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1M:286:LEU:O   | 1:1M:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:2B:120:ASP:OD2 | 1:2B:124:LYS:NZ   | 2.09                     | 0.85              |
| 2:2H:221:THR:OG1 | 1:3A:324:VAL:HG21 | 1.77                     | 0.85              |
| 2:2R:401:ARG:NH2 | 1:3E:434:GLU:O    | 2.10                     | 0.85              |
| 2:2S:394:GLN:HG2 | 1:3F:348:PRO:HG3  | 1.58                     | 0.85              |
| 1:3B:120:ASP:OD2 | 1:3B:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:3M:286:LEU:O   | 1:3M:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:1A:248:LEU:CD1 | 5:4H:501:GDP:C8   | 2.60                     | 0.85              |
| 1:1A:286:LEU:O   | 1:1A:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:1B:326:LYS:HE2 | 2:4O:214:PHE:HB2  | 1.58                     | 0.85              |
| 1:1D:261:PRO:CA  | 2:4Q:404:PHE:H    | 1.88                     | 0.85              |
| 1:1E:346:TRP:CZ3 | 2:4R:403:ALA:HB1  | 2.09                     | 0.85              |
| 2:1V:11:GLN:HE22 | 1:2J:249:ASN:HB2  | 1.38                     | 0.85              |
| 1:2A:286:LEU:O   | 1:2A:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:2L:120:ASP:OD2 | 1:2L:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:2M:286:LEU:O   | 1:2M:373:ARG:NH1  | 2.10                     | 0.85              |
| 2:2Q:221:THR:OG1 | 1:3D:324:VAL:HG21 | 1.76                     | 0.85              |
| 2:2R:394:GLN:CG  | 1:3E:348:PRO:CG   | 2.55                     | 0.85              |
| 1:3A:286:LEU:O   | 1:3A:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:3L:120:ASP:OD2 | 1:3L:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4A:286:LEU:O   | 1:4A:373:ARG:NH1  | 2.10                     | 0.85              |
| 1:4B:120:ASP:OD2 | 1:4B:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:4I:286:LEU:O   | 1:4I:373:ARG:NH1  | 2.10                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4L:120:ASP:OD2  | 1:4L:124:LYS:NZ   | 2.09                     | 0.85              |
| 1:1B:260:VAL:CG1  | 2:4O:407:TRP:HE1  | 1.90                     | 0.84              |
| 1:1B:326:LYS:CE   | 2:4O:214:PHE:HB2  | 2.07                     | 0.84              |
| 1:1C:351:PHE:O    | 2:4P:180:THR:N    | 2.10                     | 0.84              |
| 1:1C:352:LYS:HA   | 2:4P:179:ASP:O    | 1.76                     | 0.84              |
| 1:1D:349:THR:HG21 | 2:4Q:184:PRO:HD3  | 1.57                     | 0.84              |
| 1:1E:325:PRO:CB   | 2:4R:224:TYR:CE1  | 2.60                     | 0.84              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:N    | 2.09                     | 0.84              |
| 1:1F:349:THR:CG2  | 2:4S:184:PRO:CG   | 2.55                     | 0.84              |
| 1:1G:257:THR:HG21 | 2:4T:102:ASN:CB   | 2.07                     | 0.84              |
| 1:1G:260:VAL:CA   | 2:4T:407:TRP:HE1  | 1.89                     | 0.84              |
| 1:1I:326:LYS:HA   | 2:4U:210:TYR:CE1  | 2.11                     | 0.84              |
| 1:1J:286:LEU:O    | 1:1J:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1J:329:ASN:HD22 | 2:4V:210:TYR:HD2  | 1.24                     | 0.84              |
| 1:1L:249:ASN:N    | 2:4X:11:GLN:NE2   | 2.03                     | 0.84              |
| 1:1L:329:ASN:HB2  | 2:4X:210:TYR:CE2  | 2.11                     | 0.84              |
| 1:1N:329:ASN:HB2  | 2:4Z:210:TYR:CE2  | 2.11                     | 0.84              |
| 2:1S:100:GLY:HA3  | 1:2F:253:THR:HG22 | 1.56                     | 0.84              |
| 1:2I:286:LEU:O    | 1:2I:373:ARG:NH1  | 2.10                     | 0.84              |
| 2:2S:77:SER:CB    | 1:3F:245:ASP:OD1  | 2.24                     | 0.84              |
| 2:2U:401:ARG:O    | 1:3I:262:TYR:OH   | 1.95                     | 0.84              |
| 2:2V:177:VAL:HG23 | 1:3J:332:ILE:CG2  | 2.06                     | 0.84              |
| 2:2V:180:THR:HG23 | 1:3J:258:ASN:HD21 | 0.74                     | 0.84              |
| 1:3I:286:LEU:O    | 1:3I:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:4M:286:LEU:O    | 1:4M:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1A:261:PRO:O    | 2:4H:404:PHE:N    | 2.09                     | 0.84              |
| 1:1A:325:PRO:HD2  | 2:4H:223:THR:HA   | 1.59                     | 0.84              |
| 1:1E:248:LEU:HD13 | 5:4R:501:GDP:H8   | 0.94                     | 0.84              |
| 1:1G:346:TRP:HB2  | 2:4T:398:MET:CA   | 2.06                     | 0.84              |
| 1:1I:286:LEU:O    | 1:1I:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1N:329:ASN:HD22 | 2:4Z:210:TYR:HD2  | 0.86                     | 0.84              |
| 2:1U:401:ARG:HB3  | 1:2I:262:TYR:OH   | 1.78                     | 0.84              |
| 2:1W:394:GLN:HG2  | 1:2K:348:PRO:HG3  | 1.58                     | 0.84              |
| 1:2J:286:LEU:O    | 1:2J:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:2N:286:LEU:O    | 1:2N:373:ARG:NH1  | 2.10                     | 0.84              |
| 2:2Q:407:TRP:HE1  | 1:3D:260:VAL:HB   | 1.42                     | 0.84              |
| 2:2S:394:GLN:CB   | 1:3F:348:PRO:HG3  | 2.07                     | 0.84              |
| 2:2X:406:HIS:CG   | 1:3L:263:PRO:HD3  | 2.11                     | 0.84              |
| 1:3J:286:LEU:O    | 1:3J:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:4N:286:LEU:O    | 1:4N:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1C:349:THR:OG1  | 2:4P:184:PRO:CD   | 2.25                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:120:ASP:OD2  | 1:1G:124:LYS:NZ   | 2.09                     | 0.84              |
| 1:1L:260:VAL:HB   | 2:4X:407:TRP:CZ2  | 2.12                     | 0.84              |
| 2:2V:404:PHE:CE1  | 1:3J:261:PRO:N    | 2.45                     | 0.84              |
| 2:2X:401:ARG:NH2  | 1:3L:434:GLU:O    | 2.10                     | 0.84              |
| 5:2Z:501:GDP:C8   | 1:3N:248:LEU:CD1  | 2.60                     | 0.84              |
| 1:4J:286:LEU:O    | 1:4J:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:4K:286:LEU:O    | 1:4K:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1E:245:ASP:OD2  | 2:4R:77:SER:CB    | 2.24                     | 0.84              |
| 1:1E:352:LYS:HD3  | 2:4R:101:ASN:ND2  | 1.93                     | 0.84              |
| 1:1F:326:LYS:HA   | 2:4S:210:TYR:CD1  | 2.11                     | 0.84              |
| 1:1N:286:LEU:O    | 1:1N:373:ARG:NH1  | 2.10                     | 0.84              |
| 2:1P:181:VAL:H    | 1:2C:258:ASN:ND2  | 1.73                     | 0.84              |
| 2:1S:221:THR:OG1  | 1:2F:324:VAL:CG2  | 2.25                     | 0.84              |
| 2:1U:179:ASP:OD2  | 1:2I:248:LEU:HD21 | 1.77                     | 0.84              |
| 1:2K:286:LEU:O    | 1:2K:373:ARG:NH1  | 2.10                     | 0.84              |
| 2:2Q:100:GLY:CA   | 1:3D:253:THR:HB   | 2.07                     | 0.84              |
| 2:2U:404:PHE:CD1  | 1:3I:261:PRO:CA   | 2.60                     | 0.84              |
| 1:3N:286:LEU:O    | 1:3N:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1E:346:TRP:CA   | 2:4R:397:ALA:C    | 2.48                     | 0.84              |
| 1:1F:260:VAL:CG1  | 2:4S:407:TRP:HE1  | 1.89                     | 0.84              |
| 1:1G:332:ILE:HB   | 2:4T:177:VAL:HG21 | 1.56                     | 0.84              |
| 1:1L:346:TRP:CZ3  | 2:4X:403:ALA:HB1  | 2.12                     | 0.84              |
| 2:1S:222:PRO:HG2  | 1:2F:326:LYS:HB2  | 1.59                     | 0.84              |
| 2:1T:222:PRO:O    | 1:2G:325:PRO:HD2  | 1.78                     | 0.84              |
| 2:1Y:214:PHE:CG   | 1:2M:326:LYS:HE2  | 2.11                     | 0.84              |
| 2:1Z:179:ASP:O    | 1:2N:352:LYS:CD   | 2.25                     | 0.84              |
| 2:1Z:179:ASP:CG   | 1:2N:248:LEU:HD21 | 2.02                     | 0.84              |
| 2:1Z:181:VAL:HG23 | 1:2N:258:ASN:HB3  | 1.56                     | 0.84              |
| 2:2T:214:PHE:CB   | 1:3G:326:LYS:HE2  | 2.06                     | 0.84              |
| 5:2X:501:GDP:C8   | 1:3L:248:LEU:CD1  | 2.60                     | 0.84              |
| 2:2Y:77:SER:HB3   | 1:3M:245:ASP:OD1  | 1.77                     | 0.84              |
| 1:3G:120:ASP:OD2  | 1:3G:124:LYS:NZ   | 2.09                     | 0.84              |
| 1:3K:286:LEU:O    | 1:3K:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1B:263:PRO:CD   | 2:4O:406:HIS:CG   | 2.57                     | 0.84              |
| 1:1D:262:TYR:C    | 2:4Q:406:HIS:CE1  | 2.55                     | 0.84              |
| 1:1E:263:PRO:N    | 2:4R:406:HIS:CD2  | 2.44                     | 0.84              |
| 1:1E:352:LYS:HA   | 2:4R:179:ASP:O    | 1.78                     | 0.84              |
| 1:1G:260:VAL:HG12 | 2:4T:406:HIS:CE1  | 2.12                     | 0.84              |
| 1:1K:286:LEU:O    | 1:1K:373:ARG:NH1  | 2.10                     | 0.84              |
| 1:1L:326:LYS:CB   | 2:4X:222:PRO:HG2  | 2.07                     | 0.84              |
| 2:1H:179:ASP:OD2  | 1:2A:248:LEU:CD2  | 2.25                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Y:100:GLY:HA3  | 1:2M:253:THR:HG22 | 1.58                     | 0.84              |
| 2:1Z:180:THR:CG2  | 1:2N:258:ASN:HD21 | 1.91                     | 0.84              |
| 1:2G:120:ASP:OD2  | 1:2G:124:LYS:NZ   | 2.09                     | 0.84              |
| 2:2H:404:PHE:CE1  | 1:3A:260:VAL:C    | 2.54                     | 0.84              |
| 2:2O:177:VAL:HG23 | 1:3B:332:ILE:HG21 | 1.57                     | 0.84              |
| 2:2P:177:VAL:HG23 | 1:3C:332:ILE:HG21 | 1.56                     | 0.84              |
| 2:2S:401:ARG:NH2  | 1:3F:435:VAL:CA   | 2.39                     | 0.84              |
| 1:4G:120:ASP:OD2  | 1:4G:124:LYS:NZ   | 2.09                     | 0.84              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:HG2  | 2.08                     | 0.84              |
| 1:1E:2:ARG:NH1    | 2:4R:71:GLU:HG3   | 1.92                     | 0.84              |
| 1:1M:261:PRO:HA   | 2:4Y:404:PHE:CD1  | 2.12                     | 0.84              |
| 2:1U:180:THR:HA   | 1:2I:258:ASN:HD21 | 1.38                     | 0.84              |
| 2:2U:404:PHE:CE1  | 1:3I:260:VAL:C    | 2.56                     | 0.84              |
| 2:2W:404:PHE:CE1  | 1:3K:261:PRO:N    | 2.46                     | 0.84              |
| 1:1D:348:PRO:HB3  | 2:4Q:394:GLN:HG2  | 1.56                     | 0.84              |
| 1:1E:349:THR:OG1  | 2:4R:184:PRO:HD3  | 1.77                     | 0.84              |
| 1:1F:325:PRO:O    | 2:4S:210:TYR:CZ   | 2.30                     | 0.84              |
| 1:1I:248:LEU:HD13 | 5:4U:501:GDP:H8   | 1.43                     | 0.84              |
| 1:1K:257:THR:CB   | 2:4W:100:GLY:O    | 2.25                     | 0.84              |
| 1:1L:248:LEU:CA   | 2:4X:11:GLN:NE2   | 2.41                     | 0.84              |
| 2:2H:397:ALA:O    | 1:3A:346:TRP:HB2  | 1.77                     | 0.84              |
| 2:2V:223:THR:HA   | 1:3J:325:PRO:HD2  | 1.59                     | 0.84              |
| 5:2V:501:GDP:C8   | 1:3J:248:LEU:CD1  | 2.60                     | 0.84              |
| 2:2W:404:PHE:CD1  | 1:3K:260:VAL:O    | 2.31                     | 0.84              |
| 5:2W:501:GDP:C8   | 1:3K:248:LEU:CD1  | 2.60                     | 0.84              |
| 2:2Y:224:TYR:HE2  | 1:3M:248:LEU:HB2  | 1.42                     | 0.84              |
| 1:1B:253:THR:CG2  | 2:4O:100:GLY:HA3  | 2.07                     | 0.84              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:HG3  | 1.75                     | 0.84              |
| 1:1M:258:ASN:ND2  | 2:4Y:180:THR:HG23 | 1.92                     | 0.84              |
| 1:1N:326:LYS:CE   | 2:4Z:214:PHE:HB2  | 2.07                     | 0.84              |
| 2:1W:221:THR:HB   | 1:2K:324:VAL:HG21 | 1.59                     | 0.84              |
| 1:1C:314:ALA:HB2  | 2:4P:181:VAL:HG11 | 1.57                     | 0.84              |
| 1:1D:346:TRP:CA   | 2:4Q:397:ALA:C    | 2.50                     | 0.84              |
| 1:1E:248:LEU:C    | 2:4R:11:GLN:NE2   | 2.36                     | 0.84              |
| 1:1M:332:ILE:CG2  | 2:4Y:177:VAL:HG23 | 2.07                     | 0.84              |
| 2:1T:394:GLN:HG2  | 1:2G:348:PRO:HG3  | 1.59                     | 0.84              |
| 2:1Y:207:GLU:OE2  | 1:2M:329:ASN:ND2  | 2.09                     | 0.84              |
| 2:2P:397:ALA:O    | 1:3C:346:TRP:CB   | 2.26                     | 0.84              |
| 2:2Y:401:ARG:O    | 1:3M:262:TYR:OH   | 1.95                     | 0.84              |
| 1:1D:261:PRO:HB3  | 2:4Q:404:PHE:CD2  | 2.13                     | 0.83              |
| 1:1D:435:VAL:CA   | 2:4Q:401:ARG:HH22 | 1.74                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1F:325:PRO:O   | 2:4S:210:TYR:OH   | 1.96                     | 0.83              |
| 1:1F:332:ILE:HB  | 2:4S:177:VAL:CG2  | 2.08                     | 0.83              |
| 1:1G:348:PRO:HB2 | 2:4T:394:GLN:CG   | 2.08                     | 0.83              |
| 1:1K:329:ASN:HB2 | 2:4W:210:TYR:CE2  | 2.12                     | 0.83              |
| 1:1L:245:ASP:OD1 | 2:4X:77:SER:CB    | 2.21                     | 0.83              |
| 1:1L:261:PRO:O   | 2:4X:406:HIS:CD2  | 2.31                     | 0.83              |
| 1:1L:346:TRP:CE3 | 2:4X:403:ALA:CB   | 2.61                     | 0.83              |
| 2:1T:178:SER:CB  | 1:2G:349:THR:HB   | 2.07                     | 0.83              |
| 5:2Y:501:GDP:C8  | 1:3M:248:LEU:CD1  | 2.60                     | 0.83              |
| 1:1D:346:TRP:HA  | 2:4Q:397:ALA:O    | 1.76                     | 0.83              |
| 2:1O:101:ASN:HB2 | 1:2B:254:GLU:HG2  | 1.60                     | 0.83              |
| 2:1T:224:TYR:CD2 | 1:2G:247:ALA:O    | 2.31                     | 0.83              |
| 2:1U:180:THR:CA  | 1:2I:258:ASN:HD21 | 1.91                     | 0.83              |
| 2:1U:214:PHE:HB2 | 1:2I:326:LYS:CE   | 2.02                     | 0.83              |
| 2:1W:221:THR:OG1 | 1:2K:324:VAL:CG2  | 2.26                     | 0.83              |
| 2:1X:100:GLY:CA  | 1:2L:253:THR:HG21 | 1.95                     | 0.83              |
| 2:2Q:100:GLY:HA2 | 1:3D:253:THR:HB   | 1.60                     | 0.83              |
| 1:1B:326:LYS:CB  | 2:4O:222:PRO:HG2  | 2.07                     | 0.83              |
| 1:1C:261:PRO:HB3 | 2:4P:404:PHE:CD2  | 2.13                     | 0.83              |
| 1:1C:286:LEU:O   | 1:1C:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1E:349:THR:CG2 | 2:4R:184:PRO:CG   | 2.56                     | 0.83              |
| 1:1F:260:VAL:CA  | 2:4S:407:TRP:HE1  | 1.89                     | 0.83              |
| 1:1F:286:LEU:O   | 1:1F:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1G:245:ASP:OD2 | 2:4T:77:SER:HB3   | 1.75                     | 0.83              |
| 1:1J:245:ASP:OD2 | 2:4V:77:SER:CB    | 2.26                     | 0.83              |
| 1:1J:346:TRP:CE3 | 2:4V:403:ALA:HB3  | 2.12                     | 0.83              |
| 2:1S:178:SER:CB  | 1:2F:349:THR:HB   | 2.09                     | 0.83              |
| 1:2F:286:LEU:O   | 1:2F:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:3C:286:LEU:O   | 1:3C:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:3F:286:LEU:O   | 1:3F:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1A:260:VAL:HB  | 2:4H:407:TRP:NE1  | 1.93                     | 0.83              |
| 1:1E:325:PRO:O   | 2:4R:210:TYR:OH   | 1.95                     | 0.83              |
| 1:1F:263:PRO:HD3 | 2:4S:406:HIS:CD2  | 2.14                     | 0.83              |
| 2:1W:207:GLU:OE2 | 1:2K:329:ASN:ND2  | 2.12                     | 0.83              |
| 1:2C:286:LEU:O   | 1:2C:373:ARG:NH1  | 2.10                     | 0.83              |
| 2:2Y:71:GLU:HB2  | 1:3M:2:ARG:HD3    | 1.59                     | 0.83              |
| 1:4C:286:LEU:O   | 1:4C:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:4F:286:LEU:O   | 1:4F:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1B:286:LEU:O   | 1:1B:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1B:348:PRO:HB2 | 2:4O:394:GLN:CG   | 2.04                     | 0.83              |
| 1:1J:2:ARG:HD3   | 2:4V:72:PRO:CD    | 2.01                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:221:THR:HA   | 1:2I:324:VAL:HG11 | 0.87                     | 0.83              |
| 2:2Q:222:PRO:HG2  | 1:3D:326:LYS:HB2  | 1.61                     | 0.83              |
| 2:2S:397:ALA:O    | 1:3F:346:TRP:CB   | 2.26                     | 0.83              |
| 1:1F:254:GLU:N    | 2:4S:100:GLY:CA   | 2.41                     | 0.83              |
| 1:1J:351:PHE:O    | 2:4V:180:THR:CA   | 2.26                     | 0.83              |
| 2:1Q:406:HIS:CD2  | 1:2D:263:PRO:HD3  | 2.14                     | 0.83              |
| 2:2S:71:GLU:HB2   | 1:3F:2:ARG:HD3    | 1.60                     | 0.83              |
| 2:2T:394:GLN:CG   | 1:3G:348:PRO:HG3  | 2.09                     | 0.83              |
| 2:2W:100:GLY:O    | 1:3K:257:THR:OG1  | 1.95                     | 0.83              |
| 2:2W:401:ARG:HH22 | 1:3K:435:VAL:CA   | 1.91                     | 0.83              |
| 2:2X:222:PRO:O    | 1:3L:325:PRO:HD2  | 1.79                     | 0.83              |
| 2:2Y:100:GLY:CA   | 1:3M:253:THR:HB   | 2.07                     | 0.83              |
| 1:1A:258:ASN:ND2  | 2:4H:180:THR:CG2  | 2.40                     | 0.83              |
| 1:1D:348:PRO:HG2  | 2:4Q:394:GLN:CB   | 1.89                     | 0.83              |
| 1:1G:261:PRO:O    | 2:4T:406:HIS:CD2  | 2.32                     | 0.83              |
| 1:1J:260:VAL:CB   | 2:4V:407:TRP:CZ2  | 2.60                     | 0.83              |
| 2:1V:181:VAL:HG23 | 1:2J:258:ASN:CB   | 2.07                     | 0.83              |
| 2:2O:214:PHE:HB2  | 1:3B:326:LYS:CE   | 2.07                     | 0.83              |
| 1:3B:286:LEU:O    | 1:3B:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:HG2  | 1.75                     | 0.83              |
| 1:1D:261:PRO:CA   | 2:4Q:404:PHE:CA   | 2.56                     | 0.83              |
| 1:1D:286:LEU:O    | 1:1D:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:N    | 2.11                     | 0.83              |
| 2:1V:180:THR:C    | 1:2J:258:ASN:ND2  | 2.35                     | 0.83              |
| 2:1W:221:THR:CB   | 1:2K:324:VAL:HG21 | 2.08                     | 0.83              |
| 1:2B:286:LEU:O    | 1:2B:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:4G:286:LEU:O    | 1:4G:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1A:261:PRO:CA   | 2:4H:404:PHE:CD1  | 2.61                     | 0.83              |
| 1:1C:248:LEU:HD13 | 5:4P:501:GDP:H8   | 1.01                     | 0.83              |
| 1:1D:349:THR:CB   | 2:4Q:184:PRO:HD3  | 2.09                     | 0.83              |
| 1:1F:245:ASP:OD2  | 2:4S:77:SER:HB2   | 1.79                     | 0.83              |
| 1:2G:286:LEU:O    | 1:2G:373:ARG:NH1  | 2.10                     | 0.83              |
| 2:2H:177:VAL:HG23 | 1:3A:332:ILE:HG21 | 1.59                     | 0.83              |
| 1:4B:286:LEU:O    | 1:4B:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1G:349:THR:OG1  | 2:4T:184:PRO:CD   | 2.26                     | 0.83              |
| 1:2D:286:LEU:O    | 1:2D:373:ARG:NH1  | 2.10                     | 0.83              |
| 2:2W:406:HIS:NE2  | 1:3K:262:TYR:C    | 2.37                     | 0.83              |
| 2:2Y:179:ASP:OD2  | 1:3M:248:LEU:HD21 | 1.79                     | 0.83              |
| 2:2Y:394:GLN:CG   | 1:3M:348:PRO:CG   | 2.56                     | 0.83              |
| 1:3D:286:LEU:O    | 1:3D:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:3G:286:LEU:O    | 1:3G:373:ARG:NH1  | 2.10                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4E:286:LEU:O    | 1:4E:373:ARG:NH1  | 2.10                     | 0.83              |
| 1:1E:349:THR:CG2  | 2:4R:184:PRO:HG3  | 2.08                     | 0.82              |
| 1:1G:286:LEU:O    | 1:1G:373:ARG:NH1  | 2.10                     | 0.82              |
| 2:2Q:214:PHE:HB2  | 1:3D:326:LYS:CE   | 2.07                     | 0.82              |
| 2:2R:177:VAL:HG23 | 1:3E:332:ILE:HG21 | 1.60                     | 0.82              |
| 2:2V:404:PHE:CD1  | 1:3J:261:PRO:CA   | 2.60                     | 0.82              |
| 1:4D:286:LEU:O    | 1:4D:373:ARG:NH1  | 2.10                     | 0.82              |
| 2:1V:181:VAL:CG2  | 1:2J:258:ASN:C    | 2.48                     | 0.82              |
| 2:1V:224:TYR:CE2  | 1:2J:248:LEU:HB2  | 2.14                     | 0.82              |
| 2:1Z:249:ASN:O    | 2:1Z:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:2E:286:LEU:O    | 1:2E:373:ARG:NH1  | 2.10                     | 0.82              |
| 2:2U:221:THR:HA   | 1:3I:324:VAL:HG11 | 1.61                     | 0.82              |
| 1:3E:286:LEU:O    | 1:3E:373:ARG:NH1  | 2.10                     | 0.82              |
| 2:3Z:249:ASN:O    | 2:3Z:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1D:253:THR:HG22 | 2:4Q:100:GLY:HA3  | 1.59                     | 0.82              |
| 1:1D:254:GLU:HB3  | 2:4Q:101:ASN:HB2  | 1.59                     | 0.82              |
| 1:1N:245:ASP:CG   | 2:4Z:77:SER:CB    | 2.53                     | 0.82              |
| 2:1O:249:ASN:O    | 2:1O:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2O:394:GLN:HA   | 1:3B:348:PRO:HG3  | 1.60                     | 0.82              |
| 2:2Q:401:ARG:NH2  | 1:3D:435:VAL:CA   | 2.31                     | 0.82              |
| 2:2T:223:THR:HA   | 1:3G:325:PRO:HD2  | 1.59                     | 0.82              |
| 2:2W:224:TYR:HE2  | 1:3K:248:LEU:HB2  | 1.43                     | 0.82              |
| 2:2Z:249:ASN:O    | 2:2Z:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2Z:404:PHE:CD1  | 1:3N:261:PRO:HA   | 2.13                     | 0.82              |
| 2:4Z:249:ASN:O    | 2:4Z:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1A:329:ASN:HD21 | 2:4H:207:GLU:CD   | 1.86                     | 0.82              |
| 1:1B:437:VAL:O    | 2:4O:401:ARG:NH1  | 2.12                     | 0.82              |
| 1:1D:248:LEU:CD1  | 5:4Q:501:GDP:C8   | 2.40                     | 0.82              |
| 1:1D:332:ILE:CB   | 2:4Q:177:VAL:CG2  | 2.57                     | 0.82              |
| 1:1E:286:LEU:O    | 1:1E:373:ARG:NH1  | 2.10                     | 0.82              |
| 1:1F:349:THR:O    | 2:4S:181:VAL:HA   | 1.79                     | 0.82              |
| 1:1J:348:PRO:HD2  | 2:4V:398:MET:SD   | 2.20                     | 0.82              |
| 1:1L:260:VAL:HB   | 2:4X:407:TRP:CE2  | 2.14                     | 0.82              |
| 1:1M:261:PRO:C    | 2:4Y:406:HIS:NE2  | 2.37                     | 0.82              |
| 2:1R:222:PRO:HG2  | 1:2E:326:LYS:HB2  | 1.60                     | 0.82              |
| 2:2S:406:HIS:CD2  | 1:3F:262:TYR:HA   | 2.14                     | 0.82              |
| 2:3O:249:ASN:O    | 2:3O:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1B:253:THR:C    | 2:4O:100:GLY:CA   | 2.52                     | 0.82              |
| 1:1B:263:PRO:N    | 2:4O:406:HIS:CE1  | 2.47                     | 0.82              |
| 1:1B:326:LYS:HB2  | 2:4O:222:PRO:HG2  | 1.61                     | 0.82              |
| 1:1E:434:GLU:O    | 2:4R:401:ARG:NH2  | 2.13                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1N:348:PRO:CG   | 2:4Z:394:GLN:HB3  | 2.09                     | 0.82              |
| 2:1W:249:ASN:O    | 2:1W:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2O:249:ASN:O    | 2:2O:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2O:394:GLN:HG2  | 1:3B:348:PRO:HG3  | 1.61                     | 0.82              |
| 2:2Q:394:GLN:CG   | 1:3D:348:PRO:CG   | 2.57                     | 0.82              |
| 2:2U:394:GLN:CB   | 1:3I:348:PRO:HG3  | 2.09                     | 0.82              |
| 2:2U:401:ARG:HH22 | 1:3I:435:VAL:CA   | 1.91                     | 0.82              |
| 2:2X:249:ASN:O    | 2:2X:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2Z:101:ASN:O    | 1:3N:257:THR:HG21 | 1.79                     | 0.82              |
| 2:2Z:177:VAL:HG23 | 1:3N:332:ILE:CG2  | 2.10                     | 0.82              |
| 2:4O:249:ASN:O    | 2:4O:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:4X:249:ASN:O    | 2:4X:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1B:258:ASN:OD1  | 2:4O:101:ASN:ND2  | 2.12                     | 0.82              |
| 1:1D:253:THR:C    | 2:4Q:100:GLY:HA3  | 2.03                     | 0.82              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:CA   | 2.54                     | 0.82              |
| 1:1M:329:ASN:ND2  | 2:4Y:207:GLU:OE1  | 2.12                     | 0.82              |
| 2:2R:180:THR:HG23 | 1:3E:258:ASN:HD21 | 0.73                     | 0.82              |
| 2:2T:406:HIS:NE2  | 1:3G:262:TYR:CA   | 2.42                     | 0.82              |
| 2:2U:100:GLY:CA   | 1:3I:253:THR:HG22 | 2.05                     | 0.82              |
| 2:2V:394:GLN:HG2  | 1:3J:348:PRO:CB   | 2.08                     | 0.82              |
| 2:3W:249:ASN:O    | 2:3W:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:3X:249:ASN:O    | 2:3X:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:H    | 1.92                     | 0.82              |
| 1:1F:257:THR:HG21 | 2:4S:102:ASN:CB   | 2.08                     | 0.82              |
| 1:1L:349:THR:O    | 2:4X:181:VAL:CA   | 2.27                     | 0.82              |
| 2:1H:100:GLY:CA   | 1:2A:253:THR:HB   | 2.10                     | 0.82              |
| 2:1R:100:GLY:HA3  | 1:2E:253:THR:CG2  | 2.08                     | 0.82              |
| 2:1U:100:GLY:CA   | 1:2I:253:THR:HG22 | 2.00                     | 0.82              |
| 2:1U:224:TYR:HE2  | 1:2I:248:LEU:HB2  | 1.44                     | 0.82              |
| 2:1U:394:GLN:HG2  | 1:2I:348:PRO:CG   | 2.09                     | 0.82              |
| 2:1U:404:PHE:CZ   | 1:2I:261:PRO:HA   | 2.14                     | 0.82              |
| 2:1X:224:TYR:HE2  | 1:2L:248:LEU:HB2  | 1.43                     | 0.82              |
| 2:1X:249:ASN:O    | 2:1X:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2P:176:LYS:HE2  | 1:3C:333:ALA:CB   | 2.10                     | 0.82              |
| 5:2U:501:GDP:H8   | 1:3I:248:LEU:CD1  | 1.93                     | 0.82              |
| 2:2W:249:ASN:O    | 2:2W:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1E:263:PRO:HD3  | 2:4R:406:HIS:CB   | 2.09                     | 0.82              |
| 1:1J:257:THR:CG2  | 2:4V:102:ASN:HB2  | 2.09                     | 0.82              |
| 1:1J:349:THR:CG2  | 2:4V:184:PRO:CD   | 2.56                     | 0.82              |
| 1:1K:245:ASP:OD1  | 2:4W:77:SER:CB    | 2.23                     | 0.82              |
| 2:1V:214:PHE:HB2  | 1:2J:326:LYS:CE   | 2.04                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2H:394:GLN:HG2  | 1:3A:348:PRO:CB   | 2.09                     | 0.82              |
| 2:4V:249:ASN:O    | 2:4V:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:4W:249:ASN:O    | 2:4W:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1D:261:PRO:CA   | 2:4Q:404:PHE:N    | 2.42                     | 0.82              |
| 1:1I:258:ASN:ND2  | 2:4U:180:THR:HG23 | 1.95                     | 0.82              |
| 2:1W:224:TYR:CE2  | 1:2K:248:LEU:HB2  | 2.13                     | 0.82              |
| 2:1Y:249:ASN:O    | 2:1Y:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:2P:407:TRP:HE1  | 1:3C:260:VAL:HB   | 1.45                     | 0.82              |
| 2:2U:210:TYR:HD2  | 1:3I:329:ASN:ND2  | 1.78                     | 0.82              |
| 2:2U:249:ASN:O    | 2:2U:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:3U:249:ASN:O    | 2:3U:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:1H:71:GLU:HB2   | 1:2A:2:ARG:HD3    | 1.61                     | 0.82              |
| 2:1Q:249:ASN:O    | 2:1Q:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:1U:249:ASN:O    | 2:1U:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:1Z:181:VAL:H    | 1:2N:258:ASN:HD22 | 1.03                     | 0.82              |
| 2:1Z:214:PHE:CB   | 1:2N:326:LYS:HE2  | 2.09                     | 0.82              |
| 2:2V:249:ASN:O    | 2:2V:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:3V:249:ASN:O    | 2:3V:254:LYS:NZ   | 2.13                     | 0.82              |
| 2:4U:249:ASN:O    | 2:4U:254:LYS:NZ   | 2.13                     | 0.82              |
| 1:1B:346:TRP:O    | 2:4O:398:MET:HG3  | 1.79                     | 0.81              |
| 1:1F:262:TYR:HA   | 2:4S:406:HIS:HD2  | 1.01                     | 0.81              |
| 1:1F:353:VAL:HG23 | 2:4S:179:ASP:HA   | 1.62                     | 0.81              |
| 1:1I:349:THR:O    | 2:4U:181:VAL:CA   | 2.27                     | 0.81              |
| 1:1M:348:PRO:HG3  | 2:4Y:394:GLN:HB3  | 1.60                     | 0.81              |
| 2:1V:249:ASN:O    | 2:1V:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:1X:182:VAL:HG21 | 1:2L:257:THR:HG22 | 1.56                     | 0.81              |
| 2:2P:221:THR:OG1  | 1:3C:324:VAL:HG21 | 1.80                     | 0.81              |
| 2:2Q:249:ASN:O    | 2:2Q:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:3Q:249:ASN:O    | 2:3Q:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:3Y:249:ASN:O    | 2:3Y:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1C:435:VAL:C    | 2:4P:401:ARG:NH2  | 2.30                     | 0.81              |
| 1:1D:348:PRO:HB2  | 2:4Q:394:GLN:CD   | 2.04                     | 0.81              |
| 2:1T:404:PHE:CD1  | 1:2G:260:VAL:O    | 2.33                     | 0.81              |
| 2:1W:404:PHE:CD2  | 1:2K:261:PRO:HA   | 2.15                     | 0.81              |
| 2:2O:176:LYS:HE2  | 1:3B:333:ALA:CB   | 2.10                     | 0.81              |
| 2:2R:407:TRP:HE1  | 1:3E:260:VAL:HB   | 1.43                     | 0.81              |
| 2:2Y:249:ASN:O    | 2:2Y:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2Z:394:GLN:CG   | 1:3N:348:PRO:CG   | 2.58                     | 0.81              |
| 2:4Q:249:ASN:O    | 2:4Q:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1C:348:PRO:HB3  | 2:4P:394:GLN:HG2  | 1.61                     | 0.81              |
| 1:1E:346:TRP:CB   | 2:4R:398:MET:HA   | 2.10                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:329:ASN:ND2  | 2:4V:207:GLU:OE1  | 2.13                     | 0.81              |
| 1:1L:248:LEU:CA   | 2:4X:11:GLN:HE22  | 1.93                     | 0.81              |
| 2:1H:101:ASN:HB2  | 1:2A:254:GLU:CG   | 2.09                     | 0.81              |
| 2:1S:249:ASN:O    | 2:1S:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2H:404:PHE:CD1  | 1:3A:260:VAL:O    | 2.33                     | 0.81              |
| 2:2P:179:ASP:OD2  | 1:3C:248:LEU:HD21 | 1.79                     | 0.81              |
| 2:2P:249:ASN:O    | 2:2P:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2R:177:VAL:CG2  | 1:3E:332:ILE:HG21 | 2.11                     | 0.81              |
| 2:2S:249:ASN:O    | 2:2S:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2S:397:ALA:O    | 1:3F:346:TRP:HB2  | 1.81                     | 0.81              |
| 2:2T:406:HIS:CD2  | 1:3G:262:TYR:HA   | 2.14                     | 0.81              |
| 2:2U:180:THR:CG2  | 1:3I:258:ASN:ND2  | 2.36                     | 0.81              |
| 2:2U:404:PHE:CE1  | 1:3I:261:PRO:N    | 2.48                     | 0.81              |
| 2:2V:100:GLY:CA   | 1:3J:253:THR:CG2  | 2.57                     | 0.81              |
| 2:2V:401:ARG:HH22 | 1:3J:435:VAL:CA   | 1.92                     | 0.81              |
| 2:2Y:406:HIS:NE2  | 1:3M:263:PRO:N    | 2.27                     | 0.81              |
| 2:3S:249:ASN:O    | 2:3S:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4H:249:ASN:O    | 2:4H:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4P:249:ASN:O    | 2:4P:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4Y:249:ASN:O    | 2:4Y:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1D:349:THR:OG1  | 2:4Q:184:PRO:HD3  | 1.78                     | 0.81              |
| 1:1F:257:THR:HB   | 2:4S:100:GLY:O    | 1.81                     | 0.81              |
| 1:1I:348:PRO:CB   | 2:4U:394:GLN:HG2  | 2.11                     | 0.81              |
| 2:1P:249:ASN:O    | 2:1P:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:1W:179:ASP:O    | 1:2K:352:LYS:HD3  | 1.80                     | 0.81              |
| 2:2H:222:PRO:HG2  | 1:3A:326:LYS:HB2  | 1.62                     | 0.81              |
| 2:2H:249:ASN:O    | 2:2H:254:LYS:NZ   | 2.13                     | 0.81              |
| 5:2H:501:GDP:H8   | 1:3A:248:LEU:CD1  | 1.92                     | 0.81              |
| 2:2R:406:HIS:NE2  | 1:3E:263:PRO:N    | 2.27                     | 0.81              |
| 2:3P:249:ASN:O    | 2:3P:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1C:324:VAL:HG21 | 2:4P:221:THR:OG1  | 1.81                     | 0.81              |
| 1:1E:325:PRO:HG2  | 2:4R:224:TYR:CD1  | 2.16                     | 0.81              |
| 1:1I:260:VAL:CB   | 2:4U:407:TRP:HE1  | 1.76                     | 0.81              |
| 1:1J:257:THR:CB   | 2:4V:100:GLY:O    | 2.28                     | 0.81              |
| 1:1N:349:THR:O    | 2:4Z:181:VAL:HA   | 1.79                     | 0.81              |
| 2:1H:100:GLY:HA3  | 1:2A:253:THR:HG22 | 1.63                     | 0.81              |
| 2:1H:249:ASN:O    | 2:1H:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:1R:100:GLY:HA3  | 1:2E:253:THR:HG22 | 1.63                     | 0.81              |
| 2:1T:214:PHE:CD1  | 1:2G:326:LYS:HE3  | 2.15                     | 0.81              |
| 2:2H:100:GLY:CA   | 1:3A:253:THR:CG2  | 2.58                     | 0.81              |
| 2:2P:214:PHE:HB2  | 1:3C:326:LYS:CE   | 2.09                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3H:249:ASN:O    | 2:3H:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4S:249:ASN:O    | 2:4S:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4T:249:ASN:O    | 2:4T:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1D:260:VAL:CG1  | 2:4Q:407:TRP:NE1  | 2.41                     | 0.81              |
| 1:1D:349:THR:CG2  | 2:4Q:184:PRO:HD3  | 2.10                     | 0.81              |
| 1:1E:2:ARG:HD3    | 2:4R:71:GLU:HB2   | 1.60                     | 0.81              |
| 2:1O:180:THR:HG23 | 1:2B:258:ASN:HD21 | 1.42                     | 0.81              |
| 2:2Q:210:TYR:HD2  | 1:3D:329:ASN:HD22 | 1.28                     | 0.81              |
| 2:2T:249:ASN:O    | 2:2T:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2Z:179:ASP:O    | 1:3N:352:LYS:CD   | 2.28                     | 0.81              |
| 1:1A:435:VAL:HA   | 2:4H:401:ARG:HH22 | 1.46                     | 0.81              |
| 1:1E:260:VAL:CG1  | 2:4R:407:TRP:NE1  | 2.40                     | 0.81              |
| 1:1G:245:ASP:OD2  | 2:4T:77:SER:HB2   | 1.80                     | 0.81              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:HG3  | 1.78                     | 0.81              |
| 2:1X:180:THR:CG2  | 1:2L:258:ASN:HD21 | 1.93                     | 0.81              |
| 2:1X:181:VAL:CG1  | 1:2L:258:ASN:O    | 2.28                     | 0.81              |
| 2:2X:394:GLN:CG   | 1:3L:348:PRO:HG3  | 2.10                     | 0.81              |
| 2:3T:249:ASN:O    | 2:3T:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1B:254:GLU:HG2  | 2:4O:101:ASN:N    | 1.96                     | 0.81              |
| 1:1C:248:LEU:C    | 2:4P:11:GLN:HE22  | 1.87                     | 0.81              |
| 1:1C:348:PRO:HG2  | 2:4P:394:GLN:CB   | 1.92                     | 0.81              |
| 1:1E:352:LYS:CE   | 2:4R:101:ASN:ND2  | 2.44                     | 0.81              |
| 1:1F:253:THR:C    | 2:4S:100:GLY:HA3  | 2.05                     | 0.81              |
| 1:1L:257:THR:HG21 | 2:4X:102:ASN:HB2  | 1.61                     | 0.81              |
| 2:1T:100:GLY:CA   | 1:2G:253:THR:HG22 | 2.08                     | 0.81              |
| 2:1T:222:PRO:HG2  | 1:2G:326:LYS:HB2  | 1.63                     | 0.81              |
| 2:1T:249:ASN:O    | 2:1T:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:4R:249:ASN:O    | 2:4R:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1B:329:ASN:ND2  | 2:4O:207:GLU:CD   | 2.39                     | 0.81              |
| 1:1C:260:VAL:O    | 2:4P:407:TRP:HD1  | 1.60                     | 0.81              |
| 1:1G:261:PRO:CA   | 2:4T:404:PHE:HA   | 2.07                     | 0.81              |
| 1:1I:260:VAL:HG12 | 2:4U:406:HIS:HE1  | 1.44                     | 0.81              |
| 2:1P:406:HIS:CD2  | 1:2C:263:PRO:HD3  | 2.16                     | 0.81              |
| 2:1T:181:VAL:N    | 1:2G:258:ASN:ND2  | 2.12                     | 0.81              |
| 2:1V:179:ASP:O    | 1:2J:352:LYS:HD3  | 1.81                     | 0.81              |
| 2:2Q:181:VAL:HG21 | 1:3D:314:ALA:HB1  | 1.61                     | 0.81              |
| 2:2R:249:ASN:O    | 2:2R:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2R:394:GLN:CB   | 1:3E:348:PRO:HG3  | 2.11                     | 0.81              |
| 2:2S:177:VAL:CG2  | 1:3F:332:ILE:HG21 | 2.10                     | 0.81              |
| 2:2U:177:VAL:HG23 | 1:3I:332:ILE:HG22 | 1.61                     | 0.81              |
| 2:2Y:222:PRO:O    | 1:3M:325:PRO:HD2  | 1.79                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3R:249:ASN:O    | 2:3R:254:LYS:NZ   | 2.13                     | 0.81              |
| 1:1G:348:PRO:HD2  | 2:4T:398:MET:HG3  | 1.62                     | 0.81              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:CA   | 2.28                     | 0.81              |
| 1:1M:260:VAL:C    | 2:4Y:407:TRP:HE1  | 1.88                     | 0.81              |
| 2:1R:249:ASN:O    | 2:1R:254:LYS:NZ   | 2.13                     | 0.81              |
| 2:2S:394:GLN:HA   | 1:3F:348:PRO:HG3  | 1.63                     | 0.81              |
| 2:2Y:179:ASP:O    | 1:3M:352:LYS:CD   | 2.27                     | 0.81              |
| 2:1O:179:ASP:OD2  | 1:2B:248:LEU:HD21 | 1.80                     | 0.80              |
| 2:1S:404:PHE:CE1  | 1:2F:260:VAL:O    | 2.33                     | 0.80              |
| 2:1V:182:VAL:HG21 | 1:2J:257:THR:CG2  | 2.10                     | 0.80              |
| 1:1F:263:PRO:HD3  | 2:4S:406:HIS:CB   | 2.11                     | 0.80              |
| 1:1F:351:PHE:HB2  | 2:4S:178:SER:OG   | 1.79                     | 0.80              |
| 1:1N:263:PRO:N    | 2:4Z:406:HIS:NE2  | 2.29                     | 0.80              |
| 2:2O:221:THR:OG1  | 1:3B:324:VAL:HG21 | 1.80                     | 0.80              |
| 1:1I:348:PRO:HD2  | 2:4U:398:MET:CG   | 2.09                     | 0.80              |
| 2:1O:406:HIS:CD2  | 1:2B:263:PRO:HD3  | 2.16                     | 0.80              |
| 2:1W:214:PHE:HB2  | 1:2K:326:LYS:CE   | 2.10                     | 0.80              |
| 2:2R:401:ARG:NH2  | 1:3E:435:VAL:CA   | 2.34                     | 0.80              |
| 1:1L:348:PRO:CG   | 2:4X:394:GLN:HB3  | 2.11                     | 0.80              |
| 2:1U:207:GLU:CD   | 1:2I:329:ASN:HD21 | 1.88                     | 0.80              |
| 2:1V:181:VAL:HB   | 1:2J:258:ASN:CA   | 2.09                     | 0.80              |
| 2:2H:221:THR:HA   | 1:3A:324:VAL:HG11 | 1.62                     | 0.80              |
| 1:1C:324:VAL:CG1  | 2:4P:222:PRO:O    | 2.29                     | 0.80              |
| 1:1D:254:GLU:N    | 2:4Q:100:GLY:CA   | 2.43                     | 0.80              |
| 1:1D:329:ASN:HB2  | 2:4Q:210:TYR:HE2  | 1.42                     | 0.80              |
| 1:1E:248:LEU:HA   | 2:4R:11:GLN:NE2   | 1.96                     | 0.80              |
| 1:1I:352:LYS:HD3  | 2:4U:101:ASN:ND2  | 1.97                     | 0.80              |
| 1:1J:329:ASN:HB2  | 2:4V:210:TYR:HE2  | 1.45                     | 0.80              |
| 2:1Y:221:THR:HA   | 1:2M:324:VAL:CG1  | 2.10                     | 0.80              |
| 2:2Q:176:LYS:HE2  | 1:3D:333:ALA:CB   | 2.12                     | 0.80              |
| 2:2Q:177:VAL:HG23 | 1:3D:332:ILE:HG22 | 1.62                     | 0.80              |
| 2:2W:177:VAL:HG23 | 1:3K:332:ILE:CG2  | 2.11                     | 0.80              |
| 1:1B:261:PRO:C    | 2:4O:404:PHE:H    | 1.88                     | 0.80              |
| 1:1C:2:ARG:NH1    | 2:4P:71:GLU:HG3   | 1.95                     | 0.80              |
| 1:1E:248:LEU:CA   | 2:4R:11:GLN:NE2   | 2.45                     | 0.80              |
| 1:1E:258:ASN:OD1  | 2:4R:101:ASN:ND2  | 2.14                     | 0.80              |
| 1:1J:348:PRO:HG3  | 2:4V:394:GLN:CB   | 2.12                     | 0.80              |
| 2:1S:100:GLY:CA   | 1:2F:253:THR:CG2  | 2.60                     | 0.80              |
| 2:1Z:181:VAL:CG2  | 1:2N:258:ASN:HB3  | 2.11                     | 0.80              |
| 2:2O:101:ASN:HB2  | 1:3B:254:GLU:CG   | 2.12                     | 0.80              |
| 2:2O:179:ASP:OD1  | 1:3B:353:VAL:HB   | 1.81                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2T:221:THR:OG1  | 1:3G:324:VAL:CG2  | 2.28                     | 0.80              |
| 2:2X:181:VAL:HG21 | 1:3L:314:ALA:HB1  | 1.64                     | 0.80              |
| 2:2Z:77:SER:HB3   | 1:3N:245:ASP:OD1  | 1.81                     | 0.80              |
| 1:1D:332:ILE:HB   | 2:4Q:177:VAL:CG2  | 2.10                     | 0.80              |
| 1:1G:348:PRO:HD2  | 2:4T:398:MET:CG   | 2.12                     | 0.80              |
| 1:1G:435:VAL:O    | 2:4T:401:ARG:NH2  | 2.14                     | 0.80              |
| 1:1J:346:TRP:CH2  | 2:4V:403:ALA:HB1  | 2.17                     | 0.80              |
| 1:1M:329:ASN:ND2  | 2:4Y:210:TYR:HD2  | 1.77                     | 0.80              |
| 2:1V:182:VAL:CG2  | 1:2J:257:THR:HG22 | 2.11                     | 0.80              |
| 2:2S:214:PHE:CB   | 1:3F:326:LYS:HE2  | 2.12                     | 0.80              |
| 2:2Y:101:ASN:HB2  | 1:3M:254:GLU:HG2  | 1.61                     | 0.80              |
| 2:2Y:210:TYR:HD2  | 1:3M:329:ASN:HD22 | 1.29                     | 0.80              |
| 2:2Z:177:VAL:HG23 | 1:3N:332:ILE:HG21 | 1.63                     | 0.80              |
| 1:1B:263:PRO:N    | 2:4O:406:HIS:CD2  | 2.50                     | 0.80              |
| 1:1D:346:TRP:CH2  | 2:4Q:403:ALA:CB   | 2.64                     | 0.80              |
| 1:1F:346:TRP:CZ3  | 2:4S:403:ALA:HB3  | 2.17                     | 0.80              |
| 1:1G:260:VAL:CB   | 2:4T:407:TRP:CE2  | 2.58                     | 0.80              |
| 1:1I:258:ASN:HD21 | 2:4U:180:THR:HG23 | 1.46                     | 0.80              |
| 1:1I:348:PRO:HG3  | 2:4U:394:GLN:HB3  | 1.61                     | 0.80              |
| 2:1T:180:THR:HA   | 1:2G:258:ASN:ND2  | 1.97                     | 0.80              |
| 2:1X:221:THR:OG1  | 1:2L:324:VAL:HG22 | 1.81                     | 0.80              |
| 2:1Y:180:THR:CG2  | 1:2M:258:ASN:HD21 | 1.95                     | 0.80              |
| 2:2H:394:GLN:CG   | 1:3A:348:PRO:CG   | 2.59                     | 0.80              |
| 1:1D:314:ALA:CB   | 2:4Q:181:VAL:HG11 | 2.12                     | 0.80              |
| 1:1E:348:PRO:HB2  | 2:4R:394:GLN:CD   | 2.06                     | 0.80              |
| 1:1E:349:THR:CG2  | 2:4R:184:PRO:CD   | 2.59                     | 0.80              |
| 1:1G:263:PRO:CD   | 2:4T:406:HIS:CG   | 2.65                     | 0.80              |
| 2:1V:404:PHE:CD2  | 1:2J:261:PRO:HA   | 2.17                     | 0.80              |
| 1:2C:280:LYS:NZ   | 1:2D:90:GLU:OE2   | 2.14                     | 0.80              |
| 2:2H:100:GLY:CA   | 1:3A:253:THR:CB   | 2.60                     | 0.80              |
| 2:2T:177:VAL:CG2  | 1:3G:332:ILE:HG21 | 2.12                     | 0.80              |
| 2:2X:404:PHE:CE1  | 1:3L:261:PRO:N    | 2.50                     | 0.80              |
| 2:2Z:224:TYR:HE2  | 1:3N:248:LEU:HB2  | 1.46                     | 0.80              |
| 1:1C:280:LYS:NZ   | 1:1D:90:GLU:OE2   | 2.14                     | 0.80              |
| 1:1C:353:VAL:HG23 | 2:4P:179:ASP:HA   | 1.63                     | 0.80              |
| 1:1G:248:LEU:CD1  | 5:4T:501:GDP:H8   | 1.95                     | 0.80              |
| 2:1U:214:PHE:CG   | 1:2I:326:LYS:HE3  | 2.15                     | 0.80              |
| 2:2H:179:ASP:O    | 1:3A:352:LYS:CD   | 2.30                     | 0.80              |
| 2:2T:404:PHE:CD1  | 1:3G:261:PRO:CA   | 2.64                     | 0.80              |
| 1:3C:280:LYS:NZ   | 1:3D:90:GLU:OE2   | 2.14                     | 0.80              |
| 1:1E:257:THR:HG21 | 2:4R:102:ASN:CA   | 2.12                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:346:TRP:HZ3  | 2:4W:404:PHE:CE2  | 2.00                     | 0.79              |
| 1:1K:348:PRO:CG   | 2:4W:394:GLN:HB3  | 2.11                     | 0.79              |
| 1:1M:249:ASN:N    | 2:4Y:11:GLN:NE2   | 1.97                     | 0.79              |
| 1:1M:326:LYS:HB2  | 2:4Y:222:PRO:HG2  | 1.62                     | 0.79              |
| 2:1H:406:HIS:CD2  | 1:2A:263:PRO:HD3  | 2.17                     | 0.79              |
| 2:1R:221:THR:CA   | 1:2E:324:VAL:HG11 | 2.10                     | 0.79              |
| 2:1Z:100:GLY:HA3  | 1:2N:253:THR:HG22 | 1.61                     | 0.79              |
| 2:2P:406:HIS:NE2  | 1:3C:262:TYR:C    | 2.40                     | 0.79              |
| 2:2U:406:HIS:NE2  | 1:3I:262:TYR:CA   | 2.45                     | 0.79              |
| 2:2V:77:SER:HB3   | 1:3J:245:ASP:CG   | 2.06                     | 0.79              |
| 2:2X:222:PRO:HG2  | 1:3L:326:LYS:CB   | 2.12                     | 0.79              |
| 2:2Y:100:GLY:HA2  | 1:3M:253:THR:CB   | 2.12                     | 0.79              |
| 2:2Z:221:THR:OG1  | 1:3N:324:VAL:CG2  | 2.30                     | 0.79              |
| 1:1C:263:PRO:N    | 2:4P:406:HIS:CE1  | 2.50                     | 0.79              |
| 1:1E:346:TRP:CE3  | 2:4R:403:ALA:HB3  | 2.18                     | 0.79              |
| 1:1G:329:ASN:CB   | 2:4T:210:TYR:CE2  | 2.65                     | 0.79              |
| 1:1J:262:TYR:HA   | 2:4V:406:HIS:HD2  | 1.46                     | 0.79              |
| 1:1J:332:ILE:CG2  | 2:4V:177:VAL:HG23 | 2.11                     | 0.79              |
| 1:1B:261:PRO:HB3  | 2:4O:404:PHE:CD2  | 2.17                     | 0.79              |
| 1:1C:253:THR:CG2  | 2:4P:100:GLY:HA3  | 2.11                     | 0.79              |
| 1:1G:324:VAL:CG1  | 2:4T:222:PRO:O    | 2.31                     | 0.79              |
| 1:1K:325:PRO:HD2  | 2:4W:223:THR:HA   | 1.65                     | 0.79              |
| 2:1U:100:GLY:HA2  | 1:2I:253:THR:CG2  | 2.11                     | 0.79              |
| 2:1W:182:VAL:HG22 | 1:2K:257:THR:HG22 | 1.62                     | 0.79              |
| 2:1Y:181:VAL:CG1  | 1:2M:258:ASN:O    | 2.29                     | 0.79              |
| 1:2A:280:LYS:NZ   | 1:2B:90:GLU:OE2   | 2.14                     | 0.79              |
| 2:2S:101:ASN:O    | 1:3F:257:THR:HG21 | 1.83                     | 0.79              |
| 2:2S:406:HIS:NE2  | 1:3F:262:TYR:CA   | 2.45                     | 0.79              |
| 2:2V:210:TYR:HD2  | 1:3J:329:ASN:ND2  | 1.80                     | 0.79              |
| 2:2W:221:THR:CA   | 1:3K:324:VAL:HG11 | 2.13                     | 0.79              |
| 1:3A:280:LYS:NZ   | 1:3B:90:GLU:OE2   | 2.14                     | 0.79              |
| 1:1B:352:LYS:HA   | 2:4O:179:ASP:O    | 1.82                     | 0.79              |
| 1:1C:346:TRP:HB2  | 2:4P:398:MET:CA   | 2.12                     | 0.79              |
| 1:1F:324:VAL:HG13 | 2:4S:222:PRO:C    | 2.07                     | 0.79              |
| 1:1J:348:PRO:HD2  | 2:4V:398:MET:CG   | 2.13                     | 0.79              |
| 1:1K:249:ASN:N    | 2:4W:11:GLN:NE2   | 2.03                     | 0.79              |
| 2:1Y:214:PHE:CG   | 1:2M:326:LYS:CE   | 2.66                     | 0.79              |
| 2:1Z:100:GLY:CA   | 1:2N:253:THR:CB   | 2.60                     | 0.79              |
| 2:1Z:406:HIS:CD2  | 1:2N:263:PRO:HD3  | 2.18                     | 0.79              |
| 2:2H:404:PHE:CE2  | 1:3A:261:PRO:HB3  | 2.17                     | 0.79              |
| 2:2P:101:ASN:HB2  | 1:3C:254:GLU:HG2  | 1.64                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:280:LYS:NZ   | 1:1B:90:GLU:OE2   | 2.14                     | 0.79              |
| 1:1F:348:PRO:HD2  | 2:4S:398:MET:HG3  | 1.63                     | 0.79              |
| 1:1I:348:PRO:HD2  | 2:4U:398:MET:SD   | 2.21                     | 0.79              |
| 2:1V:180:THR:HA   | 1:2J:258:ASN:HD21 | 1.36                     | 0.79              |
| 2:1Z:207:GLU:CD   | 1:2N:329:ASN:ND2  | 2.26                     | 0.79              |
| 2:2H:176:LYS:HE2  | 1:3A:333:ALA:CB   | 2.11                     | 0.79              |
| 2:2P:214:PHE:CB   | 1:3C:326:LYS:HE2  | 2.11                     | 0.79              |
| 1:1C:348:PRO:HB2  | 2:4P:394:GLN:CD   | 2.07                     | 0.79              |
| 1:1F:329:ASN:CB   | 2:4S:210:TYR:CE2  | 2.65                     | 0.79              |
| 1:1F:349:THR:OG1  | 2:4S:184:PRO:HD2  | 1.81                     | 0.79              |
| 1:1G:326:LYS:HE2  | 2:4T:210:TYR:O    | 1.82                     | 0.79              |
| 1:1K:260:VAL:HB   | 2:4W:407:TRP:NE1  | 1.97                     | 0.79              |
| 2:1S:178:SER:HB3  | 1:2F:349:THR:HB   | 1.62                     | 0.79              |
| 2:1U:404:PHE:CZ   | 1:2I:261:PRO:CA   | 2.66                     | 0.79              |
| 2:2P:394:GLN:CG   | 1:3C:348:PRO:CG   | 2.59                     | 0.79              |
| 2:2V:224:TYR:HE2  | 1:3J:248:LEU:HB2  | 1.48                     | 0.79              |
| 2:2W:77:SER:CB    | 1:3K:245:ASP:OD1  | 2.29                     | 0.79              |
| 1:1A:260:VAL:HB   | 2:4H:407:TRP:HE1  | 1.48                     | 0.79              |
| 1:1D:352:LYS:HD2  | 2:4Q:179:ASP:O    | 1.83                     | 0.79              |
| 1:1G:253:THR:C    | 2:4T:100:GLY:CA   | 2.56                     | 0.79              |
| 1:1N:332:ILE:CG2  | 2:4Z:177:VAL:CG2  | 2.61                     | 0.79              |
| 2:1S:404:PHE:CE1  | 1:2F:260:VAL:C    | 2.61                     | 0.79              |
| 2:2Q:177:VAL:CG2  | 1:3D:332:ILE:HG21 | 2.13                     | 0.79              |
| 2:2Q:404:PHE:CE2  | 1:3D:261:PRO:HB3  | 2.18                     | 0.79              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:CG   | 2.59                     | 0.79              |
| 1:1I:257:THR:CB   | 2:4U:100:GLY:O    | 2.31                     | 0.79              |
| 2:1Z:394:GLN:HG2  | 1:2N:348:PRO:CG   | 2.13                     | 0.79              |
| 2:2O:77:SER:HB3   | 1:3B:245:ASP:OD1  | 1.82                     | 0.79              |
| 2:2Q:394:GLN:HG2  | 1:3D:348:PRO:HG3  | 1.65                     | 0.79              |
| 2:2V:100:GLY:HA2  | 1:3J:253:THR:HB   | 1.63                     | 0.79              |
| 2:2W:222:PRO:O    | 1:3K:325:PRO:HD2  | 1.82                     | 0.79              |
| 2:2Y:177:VAL:HG23 | 1:3M:332:ILE:CG2  | 2.13                     | 0.79              |
| 1:1C:260:VAL:HB   | 2:4P:407:TRP:CE2  | 2.17                     | 0.79              |
| 1:1E:245:ASP:OD2  | 2:4R:77:SER:HB2   | 1.83                     | 0.79              |
| 1:1E:332:ILE:CB   | 2:4R:177:VAL:HG23 | 2.12                     | 0.79              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:HA   | 1.82                     | 0.79              |
| 2:1T:404:PHE:CZ   | 1:2G:261:PRO:HA   | 2.17                     | 0.79              |
| 2:2O:404:PHE:CE1  | 1:3B:260:VAL:C    | 2.60                     | 0.79              |
| 2:2P:222:PRO:HG2  | 1:3C:326:LYS:HB2  | 1.65                     | 0.79              |
| 2:2Z:100:GLY:CA   | 1:3N:253:THR:CB   | 2.60                     | 0.79              |
| 1:1C:260:VAL:CB   | 2:4P:407:TRP:NE1  | 2.24                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:349:THR:CG2  | 2:4Q:184:PRO:HG3  | 2.13                     | 0.79              |
| 2:1X:214:PHE:CG   | 1:2L:326:LYS:HE3  | 2.18                     | 0.79              |
| 2:2R:394:GLN:HG2  | 1:3E:348:PRO:HG3  | 1.63                     | 0.79              |
| 2:2Z:222:PRO:O    | 1:3N:325:PRO:HD2  | 1.83                     | 0.79              |
| 1:1A:435:VAL:CA   | 2:4H:401:ARG:HH22 | 1.95                     | 0.78              |
| 1:1B:324:VAL:HG13 | 2:4O:222:PRO:C    | 2.09                     | 0.78              |
| 1:1B:324:VAL:HG13 | 2:4O:222:PRO:O    | 1.83                     | 0.78              |
| 1:1F:332:ILE:CB   | 2:4S:177:VAL:CG2  | 2.61                     | 0.78              |
| 1:1I:348:PRO:HG2  | 2:4U:394:GLN:HB3  | 1.63                     | 0.78              |
| 1:1K:2:ARG:HD3    | 2:4W:72:PRO:CD    | 2.07                     | 0.78              |
| 1:1K:249:ASN:H    | 2:4W:11:GLN:HE22  | 0.83                     | 0.78              |
| 2:1H:181:VAL:HG21 | 1:2A:258:ASN:O    | 1.82                     | 0.78              |
| 2:1P:181:VAL:HG21 | 1:2C:258:ASN:O    | 1.81                     | 0.78              |
| 2:1X:394:GLN:HG2  | 1:2L:348:PRO:HG2  | 1.62                     | 0.78              |
| 2:2Y:100:GLY:CA   | 1:3M:253:THR:CB   | 2.61                     | 0.78              |
| 1:1B:329:ASN:CG   | 2:4O:207:GLU:OE1  | 2.26                     | 0.78              |
| 1:1C:261:PRO:HB3  | 2:4P:404:PHE:CE2  | 2.18                     | 0.78              |
| 1:1D:260:VAL:HG12 | 2:4Q:406:HIS:HE1  | 1.47                     | 0.78              |
| 1:1K:346:TRP:CZ3  | 2:4W:403:ALA:CB   | 2.66                     | 0.78              |
| 1:1M:248:LEU:CA   | 2:4Y:11:GLN:NE2   | 2.47                     | 0.78              |
| 1:1M:260:VAL:HB   | 2:4Y:407:TRP:CE2  | 2.18                     | 0.78              |
| 2:1O:100:GLY:HA3  | 1:2B:253:THR:HG22 | 1.66                     | 0.78              |
| 2:1W:207:GLU:CD   | 1:2K:329:ASN:ND2  | 2.40                     | 0.78              |
| 2:2P:394:GLN:HG2  | 1:3C:348:PRO:HG3  | 1.65                     | 0.78              |
| 2:1P:100:GLY:HA3  | 1:2C:253:THR:CG2  | 2.13                     | 0.78              |
| 2:1T:179:ASP:O    | 1:2G:352:LYS:CD   | 2.31                     | 0.78              |
| 2:2H:101:ASN:HB2  | 1:3A:254:GLU:CG   | 2.14                     | 0.78              |
| 2:2P:406:HIS:CG   | 1:3C:263:PRO:HD3  | 2.18                     | 0.78              |
| 2:2V:401:ARG:O    | 1:3J:262:TYR:OH   | 2.01                     | 0.78              |
| 2:2Z:406:HIS:NE2  | 1:3N:263:PRO:N    | 2.31                     | 0.78              |
| 1:1A:260:VAL:CB   | 2:4H:407:TRP:HE1  | 1.96                     | 0.78              |
| 1:1E:257:THR:HG21 | 2:4R:102:ASN:HB2  | 1.66                     | 0.78              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:CG   | 2.19                     | 0.78              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:N    | 2.46                     | 0.78              |
| 1:1E:261:PRO:HB3  | 2:4R:404:PHE:CD2  | 2.18                     | 0.78              |
| 1:1F:263:PRO:CD   | 2:4S:406:HIS:CD2  | 2.66                     | 0.78              |
| 1:1G:435:VAL:HA   | 2:4T:401:ARG:HH21 | 1.47                     | 0.78              |
| 1:1J:348:PRO:HG3  | 2:4V:394:GLN:HB3  | 1.66                     | 0.78              |
| 1:1K:326:LYS:CB   | 2:4W:222:PRO:HG2  | 2.13                     | 0.78              |
| 1:1K:348:PRO:HD2  | 2:4W:398:MET:SD   | 2.24                     | 0.78              |
| 1:1M:332:ILE:CG2  | 2:4Y:177:VAL:CG2  | 2.61                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1W:181:VAL:CB   | 1:2K:258:ASN:HA   | 2.08                     | 0.78              |
| 2:2O:394:GLN:CG   | 1:3B:348:PRO:CG   | 2.60                     | 0.78              |
| 2:2Q:406:HIS:NE2  | 1:3D:263:PRO:N    | 2.32                     | 0.78              |
| 2:2V:404:PHE:CD1  | 1:3J:260:VAL:O    | 2.36                     | 0.78              |
| 2:2X:100:GLY:CA   | 1:3L:253:THR:HB   | 2.13                     | 0.78              |
| 2:2X:177:VAL:HG23 | 1:3L:332:ILE:CG2  | 2.13                     | 0.78              |
| 1:1D:348:PRO:CG   | 2:4Q:394:GLN:HA   | 2.04                     | 0.78              |
| 1:1E:254:GLU:HB3  | 2:4R:101:ASN:HB2  | 1.64                     | 0.78              |
| 1:1F:260:VAL:HB   | 2:4S:407:TRP:CZ2  | 2.18                     | 0.78              |
| 1:1G:260:VAL:HG11 | 2:4T:407:TRP:CZ2  | 2.18                     | 0.78              |
| 1:1I:257:THR:HG21 | 2:4U:102:ASN:CB   | 2.12                     | 0.78              |
| 1:1N:325:PRO:CD   | 2:4Z:223:THR:HA   | 2.14                     | 0.78              |
| 2:1W:181:VAL:CG2  | 1:2K:258:ASN:C    | 2.44                     | 0.78              |
| 2:1X:394:GLN:HG2  | 1:2L:348:PRO:HG3  | 1.66                     | 0.78              |
| 2:2O:222:PRO:HG2  | 1:3B:326:LYS:HB2  | 1.66                     | 0.78              |
| 2:2P:77:SER:HB3   | 1:3C:245:ASP:CG   | 2.09                     | 0.78              |
| 2:2Q:404:PHE:CD1  | 1:3D:261:PRO:HA   | 2.19                     | 0.78              |
| 1:4I:280:LYS:NZ   | 1:4J:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:1G:351:PHE:O    | 2:4T:180:THR:N    | 2.17                     | 0.78              |
| 1:1I:346:TRP:CB   | 2:4U:398:MET:HA   | 2.12                     | 0.78              |
| 1:1I:347:CYS:HA   | 2:4U:398:MET:HG2  | 1.65                     | 0.78              |
| 1:1L:348:PRO:HG3  | 2:4X:394:GLN:CB   | 2.14                     | 0.78              |
| 2:1W:180:THR:CG2  | 1:2K:258:ASN:HD21 | 1.96                     | 0.78              |
| 1:2I:280:LYS:NZ   | 1:2J:90:GLU:OE2   | 2.14                     | 0.78              |
| 2:2R:222:PRO:HG2  | 1:3E:326:LYS:CB   | 2.13                     | 0.78              |
| 2:2T:77:SER:CB    | 1:3G:245:ASP:CG   | 2.57                     | 0.78              |
| 2:2T:397:ALA:O    | 1:3G:346:TRP:CB   | 2.32                     | 0.78              |
| 1:1E:254:GLU:HG2  | 2:4R:101:ASN:H    | 1.48                     | 0.78              |
| 2:1Y:406:HIS:CD2  | 1:2M:263:PRO:HD3  | 2.17                     | 0.78              |
| 2:2R:406:HIS:CD2  | 1:3E:262:TYR:HA   | 2.19                     | 0.78              |
| 2:2T:100:GLY:O    | 1:3G:257:THR:OG1  | 2.00                     | 0.78              |
| 2:2Y:177:VAL:HG23 | 1:3M:332:ILE:HG21 | 1.66                     | 0.78              |
| 1:3I:280:LYS:NZ   | 1:3J:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:4K:280:LYS:NZ   | 1:4L:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:1A:348:PRO:HB2  | 2:4H:394:GLN:HG2  | 1.65                     | 0.78              |
| 1:1D:263:PRO:N    | 2:4Q:406:HIS:CE1  | 2.52                     | 0.78              |
| 1:1D:325:PRO:HG2  | 2:4Q:224:TYR:CD1  | 2.19                     | 0.78              |
| 1:1M:353:VAL:CB   | 2:4Y:179:ASP:OD1  | 2.32                     | 0.78              |
| 2:1O:100:GLY:HA2  | 1:2B:253:THR:HB   | 1.64                     | 0.78              |
| 2:1U:180:THR:CA   | 1:2I:258:ASN:ND2  | 2.46                     | 0.78              |
| 2:2R:100:GLY:CA   | 1:3E:253:THR:HB   | 2.14                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2W:394:GLN:HG2  | 1:3K:348:PRO:CB   | 2.13                     | 0.78              |
| 1:1A:352:LYS:HD2  | 2:4H:179:ASP:O    | 1.83                     | 0.78              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:CD1  | 2.19                     | 0.78              |
| 1:1E:346:TRP:CZ3  | 2:4R:403:ALA:HB3  | 2.18                     | 0.78              |
| 1:1E:349:THR:OG1  | 2:4R:184:PRO:HD2  | 1.83                     | 0.78              |
| 1:1F:260:VAL:CB   | 2:4S:407:TRP:CE2  | 2.57                     | 0.78              |
| 1:1F:348:PRO:HB3  | 2:4S:394:GLN:HG2  | 1.64                     | 0.78              |
| 1:1I:280:LYS:NZ   | 1:1J:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:HA   | 1.84                     | 0.78              |
| 2:1O:221:THR:HA   | 1:2B:324:VAL:HG11 | 1.65                     | 0.78              |
| 2:1X:179:ASP:CG   | 1:2L:248:LEU:HD21 | 2.09                     | 0.78              |
| 1:2K:280:LYS:NZ   | 1:2L:90:GLU:OE2   | 2.14                     | 0.78              |
| 2:2U:223:THR:HA   | 1:3I:325:PRO:CD   | 2.13                     | 0.78              |
| 2:2Z:394:GLN:HG2  | 1:3N:348:PRO:CB   | 2.13                     | 0.78              |
| 1:4F:280:LYS:NZ   | 1:4G:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:1A:257:THR:OG1  | 2:4H:100:GLY:O    | 2.01                     | 0.78              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:CD1  | 2.67                     | 0.78              |
| 1:1B:351:PHE:O    | 2:4O:180:THR:N    | 2.17                     | 0.78              |
| 1:1F:325:PRO:HB3  | 2:4S:224:TYR:CZ   | 2.19                     | 0.78              |
| 1:1F:346:TRP:O    | 2:4S:398:MET:N    | 2.17                     | 0.78              |
| 1:1F:353:VAL:HB   | 2:4S:179:ASP:CG   | 2.04                     | 0.78              |
| 1:1J:245:ASP:OD2  | 2:4V:77:SER:HB3   | 1.79                     | 0.78              |
| 1:1L:346:TRP:HZ3  | 2:4X:404:PHE:CE2  | 2.02                     | 0.78              |
| 2:1X:178:SER:OG   | 1:2L:351:PHE:O    | 2.02                     | 0.78              |
| 2:1Z:181:VAL:HG11 | 1:2N:258:ASN:O    | 1.83                     | 0.78              |
| 2:2O:397:ALA:O    | 1:3B:346:TRP:CB   | 2.31                     | 0.78              |
| 2:2R:77:SER:CB    | 1:3E:245:ASP:OD1  | 2.31                     | 0.78              |
| 1:3K:280:LYS:NZ   | 1:3L:90:GLU:OE2   | 2.14                     | 0.78              |
| 1:1D:332:ILE:CB   | 2:4Q:177:VAL:HG23 | 2.13                     | 0.77              |
| 1:1K:280:LYS:NZ   | 1:1L:90:GLU:OE2   | 2.14                     | 0.77              |
| 2:1W:214:PHE:CD1  | 1:2K:326:LYS:HE3  | 2.19                     | 0.77              |
| 2:1W:394:GLN:HG2  | 1:2K:348:PRO:HG2  | 1.65                     | 0.77              |
| 2:1Z:181:VAL:HB   | 1:2N:258:ASN:HA   | 1.66                     | 0.77              |
| 2:1Z:221:THR:HA   | 1:2N:324:VAL:HG11 | 1.65                     | 0.77              |
| 1:2F:280:LYS:NZ   | 1:2G:90:GLU:OE2   | 2.14                     | 0.77              |
| 2:2R:394:GLN:CA   | 1:3E:348:PRO:HG3  | 2.13                     | 0.77              |
| 2:2V:223:THR:HA   | 1:3J:325:PRO:CD   | 2.14                     | 0.77              |
| 2:2X:221:THR:CA   | 1:3L:324:VAL:HG11 | 2.14                     | 0.77              |
| 5:2Z:501:GDP:H8   | 1:3N:248:LEU:CD1  | 1.95                     | 0.77              |
| 1:1F:349:THR:OG1  | 2:4S:184:PRO:HD3  | 1.83                     | 0.77              |
| 2:2Y:401:ARG:NH2  | 1:3M:434:GLU:O    | 2.18                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3F:280:LYS:NZ   | 1:3G:90:GLU:OE2   | 2.14                     | 0.77              |
| 1:1A:346:TRP:O    | 2:4H:398:MET:HG3  | 1.84                     | 0.77              |
| 1:1B:254:GLU:N    | 2:4O:100:GLY:HA2  | 1.98                     | 0.77              |
| 1:1C:351:PHE:O    | 2:4P:180:THR:CA   | 2.31                     | 0.77              |
| 1:1D:2:ARG:CD     | 2:4Q:71:GLU:HB2   | 2.14                     | 0.77              |
| 1:1E:314:ALA:CB   | 2:4R:181:VAL:HG11 | 2.15                     | 0.77              |
| 1:1E:345:ASP:O    | 2:4R:397:ALA:HB1  | 1.84                     | 0.77              |
| 1:1F:325:PRO:HB2  | 2:4S:224:TYR:CE1  | 2.20                     | 0.77              |
| 1:1K:346:TRP:CZ3  | 2:4W:404:PHE:CE2  | 2.72                     | 0.77              |
| 1:1L:348:PRO:HG3  | 2:4X:394:GLN:HB3  | 1.66                     | 0.77              |
| 1:1M:263:PRO:N    | 2:4Y:406:HIS:CE1  | 2.53                     | 0.77              |
| 2:1T:179:ASP:O    | 1:2G:352:LYS:HD2  | 1.85                     | 0.77              |
| 2:1X:182:VAL:HG22 | 1:2L:257:THR:HG22 | 1.65                     | 0.77              |
| 2:2R:100:GLY:HA2  | 1:3E:253:THR:HB   | 1.67                     | 0.77              |
| 2:2S:180:THR:HG23 | 1:3F:258:ASN:HD21 | 0.72                     | 0.77              |
| 2:2S:394:GLN:CG   | 1:3F:348:PRO:HG3  | 2.14                     | 0.77              |
| 2:2T:404:PHE:CE1  | 1:3G:260:VAL:C    | 2.62                     | 0.77              |
| 2:2X:100:GLY:HA2  | 1:3L:253:THR:CB   | 2.14                     | 0.77              |
| 2:2X:179:ASP:O    | 1:3L:352:LYS:CD   | 2.30                     | 0.77              |
| 1:1F:254:GLU:HG2  | 2:4S:100:GLY:C    | 2.10                     | 0.77              |
| 1:1F:280:LYS:NZ   | 1:1G:90:GLU:OE2   | 2.14                     | 0.77              |
| 1:1G:325:PRO:CB   | 2:4T:224:TYR:CE1  | 2.67                     | 0.77              |
| 1:1J:248:LEU:HD12 | 2:4V:11:GLN:CD    | 2.08                     | 0.77              |
| 2:2U:406:HIS:CD2  | 1:3I:262:TYR:HA   | 2.20                     | 0.77              |
| 1:1F:352:LYS:CE   | 2:4S:101:ASN:ND2  | 2.48                     | 0.77              |
| 2:1O:181:VAL:HG21 | 1:2B:258:ASN:O    | 1.85                     | 0.77              |
| 2:2Q:401:ARG:NH2  | 1:3D:434:GLU:O    | 2.17                     | 0.77              |
| 1:1D:326:LYS:HG2  | 2:4Q:210:TYR:HB3  | 1.66                     | 0.77              |
| 1:1E:2:ARG:HG3    | 2:4R:72:PRO:CG    | 2.14                     | 0.77              |
| 1:1E:349:THR:HG23 | 2:4R:184:PRO:HG3  | 1.67                     | 0.77              |
| 1:1F:249:ASN:N    | 2:4S:11:GLN:CD    | 2.24                     | 0.77              |
| 1:1G:314:ALA:HB1  | 2:4T:181:VAL:HG21 | 1.65                     | 0.77              |
| 1:1L:346:TRP:CZ3  | 2:4X:404:PHE:CE2  | 2.73                     | 0.77              |
| 2:1Q:100:GLY:HA3  | 1:2D:253:THR:CG2  | 2.14                     | 0.77              |
| 2:2O:100:GLY:CA   | 1:3B:253:THR:CB   | 2.61                     | 0.77              |
| 2:2S:223:THR:HA   | 1:3F:325:PRO:HD2  | 1.67                     | 0.77              |
| 2:2W:180:THR:CG2  | 1:3K:258:ASN:ND2  | 2.37                     | 0.77              |
| 2:2W:404:PHE:CD1  | 1:3K:261:PRO:CA   | 2.65                     | 0.77              |
| 1:1A:253:THR:C    | 2:4H:100:GLY:HA2  | 2.09                     | 0.77              |
| 1:1E:262:TYR:HA   | 2:4R:406:HIS:HD2  | 0.99                     | 0.77              |
| 1:1G:349:THR:CG2  | 2:4T:184:PRO:CG   | 2.61                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:346:TRP:CB   | 2:4U:397:ALA:O    | 2.32                     | 0.77              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:CB   | 2.33                     | 0.77              |
| 1:1L:258:ASN:HD21 | 2:4X:180:THR:HG23 | 1.48                     | 0.77              |
| 2:2T:71:GLU:HB2   | 1:3G:2:ARG:HD3    | 1.67                     | 0.77              |
| 2:2Z:397:ALA:O    | 1:3N:346:TRP:HB2  | 1.84                     | 0.77              |
| 1:1B:261:PRO:HA   | 2:4O:404:PHE:HA   | 1.65                     | 0.77              |
| 1:1C:260:VAL:C    | 2:4P:404:PHE:CD1  | 2.63                     | 0.77              |
| 1:1E:263:PRO:N    | 2:4R:406:HIS:NE2  | 2.32                     | 0.77              |
| 1:1F:260:VAL:C    | 2:4S:407:TRP:HE1  | 1.92                     | 0.77              |
| 1:1F:346:TRP:HB2  | 2:4S:397:ALA:O    | 1.82                     | 0.77              |
| 1:1N:262:TYR:OH   | 2:4Z:401:ARG:O    | 2.03                     | 0.77              |
| 2:1Y:71:GLU:HB2   | 1:2M:2:ARG:HD3    | 1.67                     | 0.77              |
| 2:1Y:394:GLN:HG2  | 1:2M:348:PRO:HG2  | 1.67                     | 0.77              |
| 2:2H:77:SER:HB3   | 1:3A:245:ASP:OD1  | 1.84                     | 0.77              |
| 2:2S:77:SER:CB    | 1:3F:245:ASP:CG   | 2.57                     | 0.77              |
| 2:2W:223:THR:HA   | 1:3K:325:PRO:HD2  | 1.66                     | 0.77              |
| 5:2Y:501:GDP:H8   | 1:3M:248:LEU:CD1  | 1.98                     | 0.77              |
| 1:1A:329:ASN:ND2  | 2:4H:210:TYR:HD2  | 1.82                     | 0.77              |
| 1:1A:353:VAL:CB   | 2:4H:179:ASP:OD1  | 2.31                     | 0.77              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:H    | 1.97                     | 0.77              |
| 1:1C:353:VAL:HB   | 2:4P:179:ASP:CG   | 2.10                     | 0.77              |
| 1:1D:262:TYR:CE1  | 2:4Q:402:LYS:O    | 2.38                     | 0.77              |
| 1:1G:2:ARG:CG     | 2:4T:72:PRO:HD2   | 2.14                     | 0.77              |
| 1:1G:348:PRO:CB   | 2:4T:394:GLN:CG   | 2.62                     | 0.77              |
| 1:1M:324:VAL:HG21 | 2:4Y:221:THR:OG1  | 1.85                     | 0.77              |
| 2:1T:180:THR:HA   | 1:2G:258:ASN:HD21 | 1.50                     | 0.77              |
| 2:1Y:181:VAL:CG2  | 1:2M:258:ASN:CB   | 2.62                     | 0.77              |
| 2:2Q:214:PHE:CB   | 1:3D:326:LYS:HE2  | 2.15                     | 0.77              |
| 2:2U:177:VAL:CG2  | 1:3I:332:ILE:HG21 | 2.15                     | 0.77              |
| 5:2V:501:GDP:H8   | 1:3J:248:LEU:CD1  | 1.97                     | 0.77              |
| 1:1D:263:PRO:HD3  | 2:4Q:406:HIS:CB   | 2.14                     | 0.77              |
| 1:1F:258:ASN:HD21 | 2:4S:180:THR:CG2  | 1.98                     | 0.77              |
| 1:1I:329:ASN:CB   | 2:4U:210:TYR:CE2  | 2.67                     | 0.77              |
| 1:1N:333:ALA:HB1  | 2:4Z:176:LYS:HE2  | 1.64                     | 0.77              |
| 2:2O:404:PHE:CE2  | 1:3B:261:PRO:HB3  | 2.20                     | 0.77              |
| 2:2R:394:GLN:CB   | 1:3E:348:PRO:CG   | 2.64                     | 0.77              |
| 1:1E:263:PRO:N    | 2:4R:406:HIS:CE1  | 2.53                     | 0.76              |
| 1:1E:326:LYS:HG2  | 2:4R:210:TYR:CB   | 2.15                     | 0.76              |
| 1:1I:260:VAL:CG1  | 2:4U:407:TRP:CZ2  | 2.68                     | 0.76              |
| 1:1K:248:LEU:HD12 | 2:4W:11:GLN:CD    | 2.09                     | 0.76              |
| 2:2P:101:ASN:HB2  | 1:3C:254:GLU:CG   | 2.15                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:177:VAL:CG2  | 1:3F:332:ILE:CG2  | 2.62                     | 0.76              |
| 1:1I:260:VAL:HG11 | 2:4U:407:TRP:HZ2  | 1.51                     | 0.76              |
| 1:1L:280:LYS:NZ   | 1:1M:90:GLU:OE2   | 2.14                     | 0.76              |
| 2:1S:181:VAL:H    | 1:2F:258:ASN:HD22 | 0.82                     | 0.76              |
| 2:2S:394:GLN:CB   | 1:3F:348:PRO:CG   | 2.63                     | 0.76              |
| 1:4D:280:LYS:NZ   | 1:4E:90:GLU:OE2   | 2.14                     | 0.76              |
| 1:1F:2:ARG:NH2    | 2:4S:73:GLY:HA3   | 1.99                     | 0.76              |
| 1:1G:324:VAL:HG13 | 2:4T:222:PRO:O    | 1.85                     | 0.76              |
| 1:1I:348:PRO:CG   | 2:4U:394:GLN:CB   | 2.60                     | 0.76              |
| 1:1J:351:PHE:O    | 2:4V:180:THR:C    | 2.28                     | 0.76              |
| 2:1Q:100:GLY:HA3  | 1:2D:253:THR:HG22 | 1.67                     | 0.76              |
| 2:1Q:222:PRO:HG2  | 1:2D:326:LYS:HB2  | 1.66                     | 0.76              |
| 2:1X:181:VAL:CB   | 1:2L:258:ASN:CA   | 2.63                     | 0.76              |
| 2:2O:404:PHE:CD1  | 1:3B:260:VAL:O    | 2.38                     | 0.76              |
| 2:2Q:394:GLN:CA   | 1:3D:348:PRO:HG3  | 2.14                     | 0.76              |
| 2:2R:176:LYS:HE2  | 1:3E:333:ALA:CB   | 2.15                     | 0.76              |
| 1:1F:349:THR:CG2  | 2:4S:184:PRO:HG3  | 2.14                     | 0.76              |
| 1:1F:349:THR:HG23 | 2:4S:184:PRO:HG3  | 1.67                     | 0.76              |
| 2:1H:221:THR:HA   | 1:2A:324:VAL:HG11 | 1.67                     | 0.76              |
| 2:1T:101:ASN:HB2  | 1:2G:254:GLU:HG2  | 1.68                     | 0.76              |
| 2:1T:221:THR:CB   | 1:2G:324:VAL:HG21 | 2.15                     | 0.76              |
| 2:1U:178:SER:CB   | 1:2I:349:THR:HB   | 2.14                     | 0.76              |
| 2:1X:224:TYR:CE2  | 1:2L:248:LEU:HB2  | 2.21                     | 0.76              |
| 1:2D:280:LYS:NZ   | 1:2E:90:GLU:OE2   | 2.14                     | 0.76              |
| 2:2P:181:VAL:HG21 | 1:3C:314:ALA:HB1  | 1.67                     | 0.76              |
| 1:1C:326:LYS:CB   | 2:4P:222:PRO:HG2  | 2.15                     | 0.76              |
| 1:1D:326:LYS:HG2  | 2:4Q:210:TYR:CB   | 2.16                     | 0.76              |
| 1:1F:314:ALA:HB2  | 2:4S:181:VAL:HG11 | 1.67                     | 0.76              |
| 1:1I:260:VAL:HG11 | 2:4U:407:TRP:CZ2  | 2.20                     | 0.76              |
| 1:1K:329:ASN:HB2  | 2:4W:210:TYR:HE2  | 1.51                     | 0.76              |
| 1:1M:257:THR:HG21 | 2:4Y:102:ASN:HB2  | 1.67                     | 0.76              |
| 2:1V:401:ARG:CB   | 1:2J:262:TYR:OH   | 2.33                     | 0.76              |
| 2:1W:182:VAL:CG2  | 1:2K:257:THR:CG2  | 2.60                     | 0.76              |
| 2:1X:404:PHE:CE2  | 1:2L:261:PRO:HA   | 2.21                     | 0.76              |
| 2:2Y:224:TYR:HD2  | 1:3M:247:ALA:O    | 1.67                     | 0.76              |
| 1:3D:280:LYS:NZ   | 1:3E:90:GLU:OE2   | 2.14                     | 0.76              |
| 1:1E:346:TRP:O    | 2:4R:398:MET:CB   | 2.33                     | 0.76              |
| 1:1F:263:PRO:N    | 2:4S:406:HIS:CE1  | 2.54                     | 0.76              |
| 2:1O:207:GLU:CD   | 1:2B:329:ASN:HD21 | 1.94                     | 0.76              |
| 2:1U:214:PHE:CD1  | 1:2I:326:LYS:CE   | 2.68                     | 0.76              |
| 2:2W:406:HIS:NE2  | 1:3K:263:PRO:CD   | 2.49                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:100:GLY:HA2  | 1:3N:253:THR:CB   | 2.14                     | 0.76              |
| 1:1C:262:TYR:C    | 2:4P:406:HIS:CE1  | 2.62                     | 0.76              |
| 1:1D:280:LYS:NZ   | 1:1E:90:GLU:OE2   | 2.14                     | 0.76              |
| 1:1K:329:ASN:ND2  | 2:4W:207:GLU:OE1  | 2.18                     | 0.76              |
| 1:1M:248:LEU:HD13 | 5:4Y:501:GDP:C8   | 2.21                     | 0.76              |
| 1:1M:260:VAL:HB   | 2:4Y:407:TRP:NE1  | 1.99                     | 0.76              |
| 1:1M:346:TRP:CZ3  | 2:4Y:403:ALA:HB1  | 2.20                     | 0.76              |
| 2:1P:311:ARG:NH1  | 2:1P:341:SER:O    | 2.19                     | 0.76              |
| 2:1Z:404:PHE:CD1  | 1:2N:260:VAL:O    | 2.39                     | 0.76              |
| 2:2P:311:ARG:NH1  | 2:2P:341:SER:O    | 2.19                     | 0.76              |
| 2:2Z:176:LYS:HE2  | 1:3N:333:ALA:CB   | 2.14                     | 0.76              |
| 2:3P:311:ARG:NH1  | 2:3P:341:SER:O    | 2.19                     | 0.76              |
| 2:3X:311:ARG:NH1  | 2:3X:341:SER:O    | 2.19                     | 0.76              |
| 2:4P:311:ARG:NH1  | 2:4P:341:SER:O    | 2.19                     | 0.76              |
| 1:1C:346:TRP:HA   | 2:4P:397:ALA:C    | 2.11                     | 0.76              |
| 1:1C:349:THR:OG1  | 2:4P:184:PRO:HD3  | 1.85                     | 0.76              |
| 1:1D:352:LYS:CE   | 2:4Q:101:ASN:ND2  | 2.49                     | 0.76              |
| 1:1G:325:PRO:HB2  | 2:4T:224:TYR:CE1  | 2.21                     | 0.76              |
| 1:1N:348:PRO:CG   | 2:4Z:394:GLN:CB   | 2.64                     | 0.76              |
| 2:1R:11:GLN:HE22  | 1:2E:249:ASN:H    | 1.32                     | 0.76              |
| 2:1X:311:ARG:NH1  | 2:1X:341:SER:O    | 2.19                     | 0.76              |
| 2:1Z:182:VAL:HG21 | 1:2N:257:THR:HG22 | 1.65                     | 0.76              |
| 2:1Z:311:ARG:NH1  | 2:1Z:341:SER:O    | 2.19                     | 0.76              |
| 2:2O:179:ASP:OD2  | 1:3B:248:LEU:CD2  | 2.34                     | 0.76              |
| 2:2X:311:ARG:NH1  | 2:2X:341:SER:O    | 2.19                     | 0.76              |
| 2:2Y:311:ARG:NH1  | 2:2Y:341:SER:O    | 2.19                     | 0.76              |
| 2:3Y:311:ARG:NH1  | 2:3Y:341:SER:O    | 2.19                     | 0.76              |
| 2:4X:311:ARG:NH1  | 2:4X:341:SER:O    | 2.19                     | 0.76              |
| 2:4Y:311:ARG:NH1  | 2:4Y:341:SER:O    | 2.19                     | 0.76              |
| 1:1A:263:PRO:CD   | 2:4H:406:HIS:CG   | 2.63                     | 0.76              |
| 1:1D:262:TYR:CE2  | 2:4Q:403:ALA:HA   | 2.20                     | 0.76              |
| 1:1F:325:PRO:HG2  | 2:4S:224:TYR:CD1  | 2.21                     | 0.76              |
| 1:1K:348:PRO:HG3  | 2:4W:394:GLN:HB3  | 1.68                     | 0.76              |
| 2:1V:404:PHE:CZ   | 1:2J:261:PRO:HA   | 2.21                     | 0.76              |
| 2:1Y:311:ARG:NH1  | 2:1Y:341:SER:O    | 2.19                     | 0.76              |
| 2:2H:101:ASN:O    | 1:3A:257:THR:HG21 | 1.85                     | 0.76              |
| 2:2U:179:ASP:OD1  | 1:3I:353:VAL:HB   | 1.86                     | 0.76              |
| 2:2V:180:THR:CG2  | 1:3J:258:ASN:ND2  | 2.37                     | 0.76              |
| 5:2W:501:GDP:H8   | 1:3K:248:LEU:CD1  | 1.99                     | 0.76              |
| 2:2Z:311:ARG:NH1  | 2:2Z:341:SER:O    | 2.19                     | 0.76              |
| 2:3Z:311:ARG:NH1  | 2:3Z:341:SER:O    | 2.19                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:329:ASN:HD22 | 2:4P:210:TYR:HD2  | 1.34                     | 0.76              |
| 1:1E:260:VAL:CA   | 2:4R:407:TRP:HE1  | 1.98                     | 0.76              |
| 1:1F:257:THR:HG21 | 2:4S:102:ASN:CA   | 2.14                     | 0.76              |
| 1:1F:260:VAL:HG11 | 2:4S:407:TRP:CZ2  | 2.20                     | 0.76              |
| 1:1G:261:PRO:C    | 2:4T:406:HIS:CD2  | 2.64                     | 0.76              |
| 1:1K:353:VAL:CB   | 2:4W:179:ASP:OD1  | 2.31                     | 0.76              |
| 2:1Q:311:ARG:NH1  | 2:1Q:341:SER:O    | 2.19                     | 0.76              |
| 2:2Q:311:ARG:NH1  | 2:2Q:341:SER:O    | 2.19                     | 0.76              |
| 2:2T:404:PHE:CE1  | 1:3G:261:PRO:N    | 2.54                     | 0.76              |
| 2:2V:221:THR:CA   | 1:3J:324:VAL:HG11 | 2.16                     | 0.76              |
| 2:4H:311:ARG:NH1  | 2:4H:341:SER:O    | 2.19                     | 0.76              |
| 2:4Q:311:ARG:NH1  | 2:4Q:341:SER:O    | 2.19                     | 0.76              |
| 2:4Z:311:ARG:NH1  | 2:4Z:341:SER:O    | 2.19                     | 0.76              |
| 1:1A:2:ARG:CD     | 2:4H:72:PRO:HD2   | 2.16                     | 0.75              |
| 1:1C:332:ILE:HB   | 2:4P:177:VAL:HG21 | 1.68                     | 0.75              |
| 1:1F:352:LYS:HA   | 2:4S:179:ASP:O    | 1.85                     | 0.75              |
| 1:1G:325:PRO:HB3  | 2:4T:224:TYR:CZ   | 2.21                     | 0.75              |
| 1:1I:346:TRP:CD2  | 2:4U:403:ALA:HB2  | 2.20                     | 0.75              |
| 1:1J:260:VAL:HG11 | 2:4V:407:TRP:HZ2  | 1.51                     | 0.75              |
| 1:1L:329:ASN:ND2  | 2:4X:207:GLU:OE1  | 2.18                     | 0.75              |
| 2:1O:311:ARG:NH1  | 2:1O:341:SER:O    | 2.19                     | 0.75              |
| 2:1V:181:VAL:CG2  | 1:2J:258:ASN:HB3  | 2.12                     | 0.75              |
| 2:1V:221:THR:CA   | 1:2J:324:VAL:CG1  | 2.54                     | 0.75              |
| 2:1Z:11:GLN:HE22  | 1:2N:249:ASN:H    | 1.35                     | 0.75              |
| 1:2B:280:LYS:NZ   | 1:2C:90:GLU:OE2   | 2.14                     | 0.75              |
| 2:2H:311:ARG:NH1  | 2:2H:341:SER:O    | 2.19                     | 0.75              |
| 2:2S:177:VAL:HG23 | 1:3F:332:ILE:HG21 | 1.63                     | 0.75              |
| 2:2V:406:HIS:NE2  | 1:3J:263:PRO:CD   | 2.48                     | 0.75              |
| 2:2X:71:GLU:HB2   | 1:3L:2:ARG:HD3    | 1.67                     | 0.75              |
| 2:2X:406:HIS:NE2  | 1:3L:262:TYR:C    | 2.45                     | 0.75              |
| 5:2X:501:GDP:H8   | 1:3L:248:LEU:CD1  | 2.00                     | 0.75              |
| 2:3H:311:ARG:NH1  | 2:3H:341:SER:O    | 2.19                     | 0.75              |
| 2:3Q:311:ARG:NH1  | 2:3Q:341:SER:O    | 2.19                     | 0.75              |
| 1:4B:280:LYS:NZ   | 1:4C:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:1D:325:PRO:CB   | 2:4Q:224:TYR:CE1  | 2.68                     | 0.75              |
| 1:1G:253:THR:C    | 2:4T:100:GLY:HA2  | 2.10                     | 0.75              |
| 1:1G:254:GLU:CA   | 2:4T:100:GLY:C    | 2.56                     | 0.75              |
| 1:1G:325:PRO:O    | 2:4T:210:TYR:OH   | 2.05                     | 0.75              |
| 1:1L:260:VAL:HB   | 2:4X:407:TRP:NE1  | 2.02                     | 0.75              |
| 2:2P:404:PHE:CE2  | 1:3C:261:PRO:HB3  | 2.21                     | 0.75              |
| 2:2S:394:GLN:CA   | 1:3F:348:PRO:HG3  | 2.16                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2X:401:ARG:O    | 1:3L:262:TYR:OH   | 2.01                     | 0.75              |
| 1:3B:280:LYS:NZ   | 1:3C:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:4J:280:LYS:NZ   | 1:4K:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:1B:280:LYS:NZ   | 1:1C:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:1D:2:ARG:HG3    | 2:4Q:72:PRO:CG    | 2.15                     | 0.75              |
| 1:1F:333:ALA:HB1  | 2:4S:176:LYS:HE2  | 1.68                     | 0.75              |
| 2:1H:311:ARG:NH1  | 2:1H:341:SER:O    | 2.19                     | 0.75              |
| 2:1P:100:GLY:HA3  | 1:2C:253:THR:HG22 | 1.67                     | 0.75              |
| 2:1X:100:GLY:CA   | 1:2L:253:THR:HG22 | 2.12                     | 0.75              |
| 2:1Z:100:GLY:HA3  | 1:2N:253:THR:HG21 | 1.64                     | 0.75              |
| 1:2J:280:LYS:NZ   | 1:2K:90:GLU:OE2   | 2.14                     | 0.75              |
| 2:2H:394:GLN:HA   | 1:3A:348:PRO:HG3  | 1.68                     | 0.75              |
| 2:2O:311:ARG:NH1  | 2:2O:341:SER:O    | 2.19                     | 0.75              |
| 2:2P:406:HIS:NE2  | 1:3C:263:PRO:N    | 2.35                     | 0.75              |
| 2:2S:407:TRP:HE1  | 1:3F:260:VAL:HB   | 1.51                     | 0.75              |
| 2:2T:177:VAL:CG2  | 1:3G:332:ILE:CG2  | 2.64                     | 0.75              |
| 2:2U:180:THR:HG23 | 1:3I:258:ASN:HD21 | 0.73                     | 0.75              |
| 2:2X:394:GLN:HG2  | 1:3L:348:PRO:CB   | 2.15                     | 0.75              |
| 2:2Y:406:HIS:CG   | 1:3M:263:PRO:HD3  | 2.19                     | 0.75              |
| 2:3O:311:ARG:NH1  | 2:3O:341:SER:O    | 2.19                     | 0.75              |
| 1:1C:254:GLU:HB3  | 2:4P:101:ASN:HB2  | 1.67                     | 0.75              |
| 1:1C:326:LYS:CE   | 2:4P:214:PHE:HB2  | 2.16                     | 0.75              |
| 1:1D:325:PRO:O    | 2:4Q:210:TYR:OH   | 2.03                     | 0.75              |
| 1:1E:257:THR:CG2  | 2:4R:102:ASN:HB2  | 2.16                     | 0.75              |
| 1:1F:260:VAL:CG1  | 2:4S:407:TRP:NE1  | 2.46                     | 0.75              |
| 1:1J:348:PRO:HG3  | 2:4V:394:GLN:CA   | 2.16                     | 0.75              |
| 1:1L:261:PRO:HA   | 2:4X:404:PHE:CD1  | 2.21                     | 0.75              |
| 1:1N:262:TYR:CZ   | 2:4Z:403:ALA:HA   | 2.22                     | 0.75              |
| 1:3J:280:LYS:NZ   | 1:3K:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:1C:346:TRP:HA   | 2:4P:397:ALA:HB1  | 1.69                     | 0.75              |
| 1:1E:254:GLU:HG2  | 2:4R:100:GLY:C    | 2.11                     | 0.75              |
| 1:1F:260:VAL:CB   | 2:4S:407:TRP:CZ2  | 2.69                     | 0.75              |
| 1:1F:349:THR:HG23 | 2:4S:184:PRO:CG   | 2.15                     | 0.75              |
| 1:1I:261:PRO:HA   | 2:4U:404:PHE:CA   | 2.17                     | 0.75              |
| 1:1I:346:TRP:CA   | 2:4U:397:ALA:O    | 2.34                     | 0.75              |
| 1:1J:346:TRP:HA   | 2:4V:397:ALA:O    | 1.86                     | 0.75              |
| 2:1Z:100:GLY:HA3  | 1:2N:253:THR:CB   | 2.17                     | 0.75              |
| 2:2H:404:PHE:CD1  | 1:3A:261:PRO:HA   | 2.20                     | 0.75              |
| 2:2H:406:HIS:NE2  | 1:3A:263:PRO:N    | 2.35                     | 0.75              |
| 2:2P:177:VAL:CG2  | 1:3C:332:ILE:HG21 | 2.16                     | 0.75              |
| 2:2V:394:GLN:CB   | 1:3J:348:PRO:HG3  | 2.15                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4O:311:ARG:NH1  | 2:4O:341:SER:O    | 2.19                     | 0.75              |
| 1:1A:253:THR:CG2  | 2:4H:100:GLY:HA3  | 2.14                     | 0.75              |
| 1:1B:325:PRO:O    | 2:4O:210:TYR:CZ   | 2.40                     | 0.75              |
| 1:1C:254:GLU:CA   | 2:4P:100:GLY:C    | 2.59                     | 0.75              |
| 1:1E:2:ARG:CG     | 2:4R:72:PRO:CD    | 2.64                     | 0.75              |
| 1:1G:260:VAL:CG1  | 2:4T:407:TRP:CZ2  | 2.70                     | 0.75              |
| 1:1I:348:PRO:HD2  | 2:4U:398:MET:HG3  | 1.68                     | 0.75              |
| 1:1J:254:GLU:N    | 2:4V:100:GLY:HA2  | 2.02                     | 0.75              |
| 1:1J:326:LYS:CB   | 2:4V:222:PRO:HG2  | 2.17                     | 0.75              |
| 1:1K:260:VAL:CB   | 2:4W:407:TRP:CZ2  | 2.68                     | 0.75              |
| 2:1P:401:ARG:HH22 | 1:2C:435:VAL:HA   | 1.50                     | 0.75              |
| 2:2H:404:PHE:HE1  | 1:3A:260:VAL:N    | 1.84                     | 0.75              |
| 2:2P:100:GLY:CA   | 1:3C:253:THR:CB   | 2.65                     | 0.75              |
| 2:2U:100:GLY:HA2  | 1:3I:253:THR:HB   | 1.69                     | 0.75              |
| 2:2Y:394:GLN:HG2  | 1:3M:348:PRO:CB   | 2.15                     | 0.75              |
| 1:1A:346:TRP:HB2  | 2:4H:397:ALA:O    | 1.85                     | 0.75              |
| 1:1C:346:TRP:CH2  | 2:4P:403:ALA:HB1  | 2.22                     | 0.75              |
| 1:1D:347:CYS:HA   | 2:4Q:398:MET:HG2  | 1.68                     | 0.75              |
| 1:1D:435:VAL:O    | 2:4Q:401:ARG:NH2  | 2.13                     | 0.75              |
| 1:1E:262:TYR:CE2  | 2:4R:403:ALA:HA   | 2.22                     | 0.75              |
| 1:1F:347:CYS:HA   | 2:4S:398:MET:CG   | 2.17                     | 0.75              |
| 1:1I:329:ASN:HD22 | 2:4U:210:TYR:HD2  | 1.30                     | 0.75              |
| 1:1J:280:LYS:NZ   | 1:1K:90:GLU:OE2   | 2.14                     | 0.75              |
| 1:1J:332:ILE:CG2  | 2:4V:177:VAL:CG2  | 2.64                     | 0.75              |
| 2:1P:180:THR:HG23 | 1:2C:258:ASN:HD21 | 1.50                     | 0.75              |
| 2:2H:100:GLY:HA2  | 1:3A:253:THR:CB   | 2.17                     | 0.75              |
| 2:2R:214:PHE:CB   | 1:3E:326:LYS:HE2  | 2.15                     | 0.75              |
| 2:2X:177:VAL:HG23 | 1:3L:332:ILE:HG21 | 1.69                     | 0.75              |
| 2:3W:311:ARG:NH1  | 2:3W:341:SER:O    | 2.19                     | 0.75              |
| 1:1G:349:THR:HG23 | 2:4T:184:PRO:CG   | 2.17                     | 0.75              |
| 1:1K:348:PRO:HG3  | 2:4W:394:GLN:CB   | 2.16                     | 0.75              |
| 2:1W:311:ARG:NH1  | 2:1W:341:SER:O    | 2.19                     | 0.75              |
| 2:1X:404:PHE:CD2  | 1:2L:261:PRO:HA   | 2.20                     | 0.75              |
| 2:2H:224:TYR:HE2  | 1:3A:248:LEU:HB2  | 1.51                     | 0.75              |
| 2:2O:404:PHE:HE1  | 1:3B:260:VAL:N    | 1.84                     | 0.75              |
| 2:2W:311:ARG:NH1  | 2:2W:341:SER:O    | 2.19                     | 0.75              |
| 1:1E:261:PRO:C    | 2:4R:404:PHE:H    | 1.94                     | 0.75              |
| 1:1F:2:ARG:HG3    | 2:4S:72:PRO:CG    | 2.17                     | 0.75              |
| 1:1I:261:PRO:C    | 2:4U:406:HIS:CD2  | 2.63                     | 0.75              |
| 1:1J:346:TRP:HZ3  | 2:4V:404:PHE:CE2  | 2.05                     | 0.75              |
| 2:1R:311:ARG:NH1  | 2:1R:341:SER:O    | 2.19                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1S:100:GLY:HA2  | 1:2F:253:THR:HB   | 1.69                     | 0.75              |
| 2:1S:221:THR:OG1  | 1:2F:324:VAL:HG22 | 1.86                     | 0.75              |
| 2:1U:224:TYR:CE2  | 1:2I:248:LEU:HB2  | 2.22                     | 0.75              |
| 2:1V:214:PHE:CD1  | 1:2J:326:LYS:CE   | 2.68                     | 0.75              |
| 2:2R:311:ARG:NH1  | 2:2R:341:SER:O    | 2.19                     | 0.75              |
| 2:3R:311:ARG:NH1  | 2:3R:341:SER:O    | 2.19                     | 0.75              |
| 2:4R:311:ARG:NH1  | 2:4R:341:SER:O    | 2.19                     | 0.75              |
| 2:4W:311:ARG:NH1  | 2:4W:341:SER:O    | 2.19                     | 0.75              |
| 1:1C:349:THR:HG21 | 2:4P:184:PRO:HD3  | 1.69                     | 0.74              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:N    | 2.02                     | 0.74              |
| 1:1K:245:ASP:OD2  | 2:4W:77:SER:CB    | 2.34                     | 0.74              |
| 1:1L:329:ASN:ND2  | 2:4X:210:TYR:HD2  | 1.83                     | 0.74              |
| 2:1T:311:ARG:NH1  | 2:1T:341:SER:O    | 2.19                     | 0.74              |
| 1:4A:90:GLU:OE2   | 1:4N:280:LYS:NZ   | 2.14                     | 0.74              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:HA   | 2.17                     | 0.74              |
| 1:1E:333:ALA:CB   | 2:4R:176:LYS:HE2  | 2.17                     | 0.74              |
| 1:1F:332:ILE:HG22 | 2:4S:177:VAL:CG2  | 1.99                     | 0.74              |
| 1:1J:326:LYS:HA   | 2:4V:210:TYR:CE1  | 2.22                     | 0.74              |
| 1:1J:346:TRP:CZ3  | 2:4V:404:PHE:CE2  | 2.76                     | 0.74              |
| 1:1L:332:ILE:CG2  | 2:4X:177:VAL:HG23 | 2.16                     | 0.74              |
| 2:1U:11:GLN:HE22  | 1:2I:249:ASN:HB2  | 1.51                     | 0.74              |
| 2:2H:179:ASP:OD2  | 1:3A:248:LEU:CD2  | 2.36                     | 0.74              |
| 2:2W:401:ARG:O    | 1:3K:262:TYR:OH   | 2.03                     | 0.74              |
| 2:3S:311:ARG:NH1  | 2:3S:341:SER:O    | 2.19                     | 0.74              |
| 2:3T:311:ARG:NH1  | 2:3T:341:SER:O    | 2.19                     | 0.74              |
| 2:4S:311:ARG:NH1  | 2:4S:341:SER:O    | 2.19                     | 0.74              |
| 2:4T:311:ARG:NH1  | 2:4T:341:SER:O    | 2.19                     | 0.74              |
| 1:1B:351:PHE:O    | 2:4O:180:THR:C    | 2.30                     | 0.74              |
| 1:1I:245:ASP:OD2  | 2:4U:77:SER:HB2   | 1.86                     | 0.74              |
| 1:1K:254:GLU:HA   | 2:4W:100:GLY:C    | 2.12                     | 0.74              |
| 2:1W:178:SER:HB3  | 1:2K:349:THR:HB   | 1.69                     | 0.74              |
| 2:1X:181:VAL:CG2  | 1:2L:258:ASN:C    | 2.50                     | 0.74              |
| 2:2O:407:TRP:HE1  | 1:3B:260:VAL:HB   | 1.52                     | 0.74              |
| 2:2Q:394:GLN:CB   | 1:3D:348:PRO:HG3  | 2.18                     | 0.74              |
| 2:2S:311:ARG:NH1  | 2:2S:341:SER:O    | 2.19                     | 0.74              |
| 2:2T:311:ARG:NH1  | 2:2T:341:SER:O    | 2.19                     | 0.74              |
| 2:2U:100:GLY:CA   | 1:3I:253:THR:CG2  | 2.64                     | 0.74              |
| 2:2U:311:ARG:NH1  | 2:2U:341:SER:O    | 2.19                     | 0.74              |
| 2:2U:406:HIS:CE1  | 1:3I:263:PRO:N    | 2.56                     | 0.74              |
| 2:2V:311:ARG:NH1  | 2:2V:341:SER:O    | 2.19                     | 0.74              |
| 2:2Z:210:TYR:HD2  | 1:3N:329:ASN:HD22 | 1.35                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3U:311:ARG:NH1  | 2:3U:341:SER:O    | 2.19                     | 0.74              |
| 2:3V:311:ARG:NH1  | 2:3V:341:SER:O    | 2.19                     | 0.74              |
| 2:4U:311:ARG:NH1  | 2:4U:341:SER:O    | 2.19                     | 0.74              |
| 2:4V:311:ARG:NH1  | 2:4V:341:SER:O    | 2.19                     | 0.74              |
| 1:1A:257:THR:CB   | 2:4H:100:GLY:O    | 2.35                     | 0.74              |
| 1:1G:435:VAL:C    | 2:4T:401:ARG:NH2  | 2.44                     | 0.74              |
| 1:1K:257:THR:CG2  | 2:4W:102:ASN:HB2  | 2.17                     | 0.74              |
| 2:1S:311:ARG:NH1  | 2:1S:341:SER:O    | 2.19                     | 0.74              |
| 2:1U:311:ARG:NH1  | 2:1U:341:SER:O    | 2.19                     | 0.74              |
| 2:1V:311:ARG:NH1  | 2:1V:341:SER:O    | 2.19                     | 0.74              |
| 2:1V:404:PHE:CZ   | 1:2J:261:PRO:CA   | 2.70                     | 0.74              |
| 1:2A:90:GLU:OE2   | 1:2N:280:LYS:NZ   | 2.14                     | 0.74              |
| 2:2T:397:ALA:O    | 1:3G:346:TRP:HB2  | 1.87                     | 0.74              |
| 2:2X:100:GLY:CA   | 1:3L:253:THR:CB   | 2.65                     | 0.74              |
| 1:1A:348:PRO:CB   | 2:4H:394:GLN:CG   | 2.63                     | 0.74              |
| 1:1C:263:PRO:HA   | 2:4P:406:HIS:CE1  | 2.22                     | 0.74              |
| 1:1D:257:THR:HG21 | 2:4Q:102:ASN:CA   | 2.18                     | 0.74              |
| 1:1D:349:THR:CG2  | 2:4Q:184:PRO:CG   | 2.66                     | 0.74              |
| 1:1J:325:PRO:HD2  | 2:4V:223:THR:HA   | 1.70                     | 0.74              |
| 2:1U:401:ARG:HH22 | 1:2I:435:VAL:HA   | 1.50                     | 0.74              |
| 2:1X:181:VAL:CG2  | 1:2L:258:ASN:CB   | 2.60                     | 0.74              |
| 2:2P:210:TYR:HD2  | 1:3C:329:ASN:HD22 | 1.36                     | 0.74              |
| 2:2P:404:PHE:H    | 1:3C:261:PRO:C    | 1.95                     | 0.74              |
| 2:2X:100:GLY:O    | 1:3L:257:THR:OG1  | 2.02                     | 0.74              |
| 2:2Y:176:LYS:HE2  | 1:3M:333:ALA:CB   | 2.17                     | 0.74              |
| 1:1D:2:ARG:HD3    | 2:4Q:72:PRO:CD    | 2.13                     | 0.74              |
| 1:1J:258:ASN:HD21 | 2:4V:180:THR:HG23 | 1.52                     | 0.74              |
| 2:2P:404:PHE:CE1  | 1:3C:260:VAL:C    | 2.65                     | 0.74              |
| 2:2T:394:GLN:CB   | 1:3G:348:PRO:CG   | 2.65                     | 0.74              |
| 2:2Z:224:TYR:HD2  | 1:3N:247:ALA:O    | 1.69                     | 0.74              |
| 1:3A:90:GLU:OE2   | 1:3N:280:LYS:NZ   | 2.14                     | 0.74              |
| 1:1E:261:PRO:O    | 2:4R:404:PHE:N    | 2.20                     | 0.74              |
| 1:1E:262:TYR:CE1  | 2:4R:402:LYS:O    | 2.40                     | 0.74              |
| 1:1K:349:THR:CG2  | 2:4W:184:PRO:CD   | 2.65                     | 0.74              |
| 1:1L:353:VAL:CB   | 2:4X:179:ASP:OD1  | 2.35                     | 0.74              |
| 1:1M:260:VAL:HB   | 2:4Y:407:TRP:CZ2  | 2.22                     | 0.74              |
| 2:1W:207:GLU:OE1  | 1:2K:329:ASN:ND2  | 2.21                     | 0.74              |
| 2:2R:77:SER:CB    | 1:3E:245:ASP:CG   | 2.60                     | 0.74              |
| 2:2R:177:VAL:CG2  | 1:3E:332:ILE:CG2  | 2.63                     | 0.74              |
| 2:2V:222:PRO:CG   | 1:3J:326:LYS:HB2  | 2.13                     | 0.74              |
| 2:2Y:181:VAL:HG21 | 1:3M:258:ASN:O    | 1.86                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Y:181:VAL:HG21 | 1:3M:314:ALA:HB1  | 1.70                     | 0.74              |
| 2:2Z:207:GLU:CD   | 1:3N:329:ASN:ND2  | 2.31                     | 0.74              |
| 1:1A:2:ARG:NH2    | 2:4H:73:GLY:HA3   | 2.03                     | 0.74              |
| 1:1A:90:GLU:OE2   | 1:1N:280:LYS:NZ   | 2.14                     | 0.74              |
| 1:1D:248:LEU:C    | 2:4Q:11:GLN:NE2   | 2.44                     | 0.74              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:HA   | 2.09                     | 0.74              |
| 1:1L:349:THR:HG21 | 2:4X:184:PRO:CD   | 2.11                     | 0.74              |
| 1:1M:262:TYR:CA   | 2:4Y:406:HIS:CD2  | 2.40                     | 0.74              |
| 2:2R:394:GLN:HB3  | 1:3E:348:PRO:HG2  | 1.70                     | 0.74              |
| 1:1A:258:ASN:OD1  | 2:4H:101:ASN:ND2  | 2.20                     | 0.74              |
| 1:1B:261:PRO:O    | 2:4O:404:PHE:CA   | 2.36                     | 0.74              |
| 1:1C:2:ARG:CD     | 2:4P:71:GLU:HB2   | 2.17                     | 0.74              |
| 1:1C:253:THR:HB   | 2:4P:100:GLY:CA   | 2.18                     | 0.74              |
| 1:1C:261:PRO:O    | 2:4P:404:PHE:CA   | 2.35                     | 0.74              |
| 1:1C:262:TYR:N    | 2:4P:406:HIS:NE2  | 2.35                     | 0.74              |
| 1:1C:329:ASN:HB2  | 2:4P:210:TYR:HE2  | 1.52                     | 0.74              |
| 1:1F:346:TRP:CA   | 2:4S:397:ALA:C    | 2.55                     | 0.74              |
| 1:1K:260:VAL:HG11 | 2:4W:407:TRP:HZ2  | 1.53                     | 0.74              |
| 1:1K:261:PRO:HA   | 2:4W:404:PHE:HA   | 1.70                     | 0.74              |
| 1:1K:351:PHE:O    | 2:4W:180:THR:CA   | 2.35                     | 0.74              |
| 1:1M:348:PRO:CB   | 2:4Y:394:GLN:HG2  | 2.18                     | 0.74              |
| 2:1U:181:VAL:CB   | 1:2I:258:ASN:O    | 2.35                     | 0.74              |
| 2:2H:222:PRO:O    | 1:3A:325:PRO:HD2  | 1.88                     | 0.74              |
| 2:2O:406:HIS:NE2  | 1:3B:263:PRO:N    | 2.36                     | 0.74              |
| 2:2S:72:PRO:HD2   | 1:3F:2:ARG:CG     | 2.18                     | 0.74              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:N    | 2.51                     | 0.74              |
| 1:1D:349:THR:HG21 | 2:4Q:184:PRO:CD   | 2.18                     | 0.74              |
| 1:1G:263:PRO:N    | 2:4T:406:HIS:CE1  | 2.56                     | 0.74              |
| 1:1J:260:VAL:CB   | 2:4V:407:TRP:NE1  | 2.51                     | 0.74              |
| 2:1W:11:GLN:NE2   | 1:2K:249:ASN:HB2  | 2.02                     | 0.74              |
| 2:2X:224:TYR:HD2  | 1:3L:247:ALA:O    | 1.70                     | 0.74              |
| 1:1E:257:THR:HG21 | 2:4R:102:ASN:CB   | 2.18                     | 0.73              |
| 1:1E:347:CYS:HA   | 2:4R:398:MET:CG   | 2.18                     | 0.73              |
| 1:1M:248:LEU:CA   | 2:4Y:11:GLN:HE22  | 2.01                     | 0.73              |
| 1:1M:346:TRP:CE3  | 2:4Y:403:ALA:CB   | 2.70                     | 0.73              |
| 2:1S:394:GLN:HG2  | 1:2F:348:PRO:HG3  | 1.69                     | 0.73              |
| 2:2O:401:ARG:NH2  | 1:3B:435:VAL:CA   | 2.33                     | 0.73              |
| 2:2P:177:VAL:HG23 | 1:3C:332:ILE:HG22 | 1.70                     | 0.73              |
| 2:2T:177:VAL:HG23 | 1:3G:332:ILE:HG21 | 1.67                     | 0.73              |
| 1:1A:437:VAL:O    | 2:4H:401:ARG:NH1  | 2.20                     | 0.73              |
| 1:1C:260:VAL:CG1  | 2:4P:407:TRP:NE1  | 2.49                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:2:ARG:CG     | 2:4Q:72:PRO:CD    | 2.64                     | 0.73              |
| 1:1E:435:VAL:CA   | 2:4R:401:ARG:HH21 | 1.86                     | 0.73              |
| 1:1F:348:PRO:HB2  | 2:4S:394:GLN:CD   | 2.12                     | 0.73              |
| 1:1F:434:GLU:O    | 2:4S:401:ARG:NH2  | 2.21                     | 0.73              |
| 1:1J:260:VAL:CG1  | 2:4V:407:TRP:CZ2  | 2.70                     | 0.73              |
| 2:2R:407:TRP:NE1  | 1:3E:260:VAL:HB   | 2.02                     | 0.73              |
| 1:1A:262:TYR:CZ   | 2:4H:403:ALA:HA   | 2.24                     | 0.73              |
| 1:1F:261:PRO:C    | 2:4S:406:HIS:NE2  | 2.46                     | 0.73              |
| 1:1I:349:THR:CB   | 2:4U:184:PRO:HD3  | 2.17                     | 0.73              |
| 2:1O:179:ASP:O    | 1:2B:352:LYS:HD2  | 1.86                     | 0.73              |
| 2:1P:207:GLU:OE1  | 1:2C:329:ASN:ND2  | 2.18                     | 0.73              |
| 2:1T:406:HIS:NE2  | 1:2G:263:PRO:HD3  | 2.03                     | 0.73              |
| 2:2Y:394:GLN:CG   | 1:3M:348:PRO:HG3  | 2.15                     | 0.73              |
| 1:4C:280:LYS:NZ   | 1:4D:90:GLU:OE2   | 2.14                     | 0.73              |
| 1:1A:332:ILE:HG21 | 2:4H:177:VAL:HG23 | 1.65                     | 0.73              |
| 1:1F:326:LYS:CA   | 2:4S:210:TYR:CE1  | 2.71                     | 0.73              |
| 1:1G:254:GLU:CA   | 2:4T:100:GLY:HA2  | 2.17                     | 0.73              |
| 1:1I:346:TRP:HB2  | 2:4U:398:MET:CA   | 2.16                     | 0.73              |
| 1:1M:314:ALA:HB1  | 2:4Y:181:VAL:HG21 | 1.68                     | 0.73              |
| 2:1S:181:VAL:N    | 1:2F:258:ASN:ND2  | 2.31                     | 0.73              |
| 2:1T:404:PHE:CZ   | 1:2G:261:PRO:CA   | 2.71                     | 0.73              |
| 2:2S:221:THR:OG1  | 1:3F:324:VAL:CG2  | 2.36                     | 0.73              |
| 2:2T:223:THR:HA   | 1:3G:325:PRO:CD   | 2.17                     | 0.73              |
| 2:2U:77:SER:CB    | 1:3I:245:ASP:CG   | 2.61                     | 0.73              |
| 1:1J:248:LEU:HD13 | 5:4V:501:GDP:C8   | 2.24                     | 0.73              |
| 1:1M:434:GLU:O    | 2:4Y:401:ARG:NH2  | 2.22                     | 0.73              |
| 2:1Z:224:TYR:HD2  | 1:2N:247:ALA:O    | 1.69                     | 0.73              |
| 2:2P:404:PHE:HE1  | 1:3C:260:VAL:N    | 1.86                     | 0.73              |
| 2:2S:100:GLY:HA2  | 1:3F:253:THR:HB   | 1.70                     | 0.73              |
| 2:2T:398:MET:HG2  | 1:3G:346:TRP:O    | 1.88                     | 0.73              |
| 2:2U:404:PHE:CD1  | 1:3I:260:VAL:O    | 2.41                     | 0.73              |
| 2:2X:179:ASP:OD2  | 1:3L:248:LEU:HD21 | 1.89                     | 0.73              |
| 2:2X:181:VAL:HG21 | 1:3L:258:ASN:O    | 1.87                     | 0.73              |
| 1:1A:346:TRP:HB3  | 2:4H:397:ALA:O    | 1.87                     | 0.73              |
| 1:1C:326:LYS:HA   | 2:4P:210:TYR:CE1  | 2.24                     | 0.73              |
| 1:1D:259:LEU:C    | 2:4Q:404:PHE:HE1  | 1.97                     | 0.73              |
| 1:1D:439:SER:CB   | 2:4Q:400:ARG:HD2  | 2.19                     | 0.73              |
| 1:1E:346:TRP:CE3  | 2:4R:403:ALA:CB   | 2.70                     | 0.73              |
| 1:1F:258:ASN:ND2  | 2:4S:180:THR:CG2  | 2.50                     | 0.73              |
| 1:1F:325:PRO:HG2  | 2:4S:224:TYR:CG   | 2.24                     | 0.73              |
| 1:1I:260:VAL:CB   | 2:4U:407:TRP:HZ2  | 2.01                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:332:ILE:CG2  | 2:4W:177:VAL:HG23 | 2.17                     | 0.73              |
| 1:1L:249:ASN:H    | 2:4X:11:GLN:HE22  | 0.77                     | 0.73              |
| 1:1L:263:PRO:HD3  | 2:4X:406:HIS:CD2  | 2.22                     | 0.73              |
| 1:1N:262:TYR:C    | 2:4Z:406:HIS:CE1  | 2.66                     | 0.73              |
| 2:1W:100:GLY:CA   | 1:2K:253:THR:HB   | 1.98                     | 0.73              |
| 2:2R:72:PRO:HD2   | 1:3E:2:ARG:CG     | 2.19                     | 0.73              |
| 2:2V:222:PRO:O    | 1:3J:325:PRO:HD2  | 1.88                     | 0.73              |
| 1:4A:280:LYS:NZ   | 1:4B:90:GLU:OE2   | 2.14                     | 0.73              |
| 1:1D:329:ASN:CB   | 2:4Q:210:TYR:CD2  | 2.72                     | 0.73              |
| 1:1E:329:ASN:CB   | 2:4R:210:TYR:CE2  | 2.70                     | 0.73              |
| 1:1G:329:ASN:HD22 | 2:4T:210:TYR:HD2  | 1.36                     | 0.73              |
| 1:1K:346:TRP:CE3  | 2:4W:403:ALA:HB3  | 2.22                     | 0.73              |
| 1:1L:258:ASN:ND2  | 2:4X:180:THR:HG23 | 2.03                     | 0.73              |
| 2:2X:101:ASN:HB2  | 1:3L:254:GLU:HG2  | 1.71                     | 0.73              |
| 1:1D:245:ASP:OD2  | 2:4Q:77:SER:CB    | 2.37                     | 0.73              |
| 1:1D:254:GLU:HG2  | 2:4Q:101:ASN:H    | 1.52                     | 0.73              |
| 1:1E:326:LYS:CA   | 2:4R:210:TYR:CE1  | 2.71                     | 0.73              |
| 1:1G:263:PRO:HD3  | 2:4T:406:HIS:CD2  | 2.22                     | 0.73              |
| 1:1J:254:GLU:HA   | 2:4V:100:GLY:O    | 1.89                     | 0.73              |
| 1:1J:329:ASN:CB   | 2:4V:210:TYR:CE2  | 2.71                     | 0.73              |
| 2:1R:178:SER:CB   | 1:2E:349:THR:HB   | 2.18                     | 0.73              |
| 2:1T:100:GLY:HA2  | 1:2G:253:THR:CB   | 2.17                     | 0.73              |
| 2:1X:181:VAL:CB   | 1:2L:258:ASN:HA   | 2.07                     | 0.73              |
| 2:2R:101:ASN:O    | 1:3E:257:THR:HG21 | 1.88                     | 0.73              |
| 2:2S:404:PHE:CD1  | 1:3F:261:PRO:CA   | 2.71                     | 0.73              |
| 2:2U:73:GLY:HA3   | 1:3I:2:ARG:NH2    | 2.04                     | 0.73              |
| 2:2W:100:GLY:HA2  | 1:3K:253:THR:CB   | 2.19                     | 0.73              |
| 1:1C:263:PRO:CA   | 2:4P:406:HIS:CE1  | 2.71                     | 0.73              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:CA   | 2.37                     | 0.73              |
| 1:1E:348:PRO:HD2  | 2:4R:398:MET:HG3  | 1.70                     | 0.73              |
| 1:1M:260:VAL:HG11 | 2:4Y:407:TRP:HZ2  | 1.53                     | 0.73              |
| 2:1X:221:THR:CB   | 1:2L:324:VAL:HG21 | 2.19                     | 0.73              |
| 2:2P:404:PHE:CD1  | 1:3C:261:PRO:HA   | 2.23                     | 0.73              |
| 2:2Q:401:ARG:HH21 | 1:3D:435:VAL:HA   | 1.51                     | 0.73              |
| 2:2S:404:PHE:CE1  | 1:3F:260:VAL:C    | 2.66                     | 0.73              |
| 2:2T:100:GLY:HA2  | 1:3G:253:THR:HB   | 1.71                     | 0.73              |
| 2:2T:210:TYR:HD2  | 1:3G:329:ASN:ND2  | 1.81                     | 0.73              |
| 2:2V:177:VAL:CG2  | 1:3J:332:ILE:HG21 | 2.19                     | 0.73              |
| 2:2W:179:ASP:O    | 1:3K:352:LYS:CD   | 2.36                     | 0.73              |
| 1:1G:349:THR:OG1  | 2:4T:184:PRO:HD2  | 1.88                     | 0.73              |
| 1:1I:346:TRP:CD2  | 2:4U:403:ALA:CB   | 2.72                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:260:VAL:CG1  | 2:4V:407:TRP:HZ2  | 2.01                     | 0.73              |
| 1:1K:258:ASN:HD21 | 2:4W:180:THR:HG23 | 1.53                     | 0.73              |
| 1:1L:248:LEU:HD12 | 2:4X:11:GLN:CD    | 2.13                     | 0.73              |
| 2:1Y:224:TYR:HE2  | 1:2M:248:LEU:HB2  | 1.54                     | 0.73              |
| 2:1Z:180:THR:HA   | 1:2N:352:LYS:HD3  | 1.71                     | 0.73              |
| 2:2O:406:HIS:CG   | 1:3B:263:PRO:HD3  | 2.23                     | 0.73              |
| 2:2R:406:HIS:NE2  | 1:3E:262:TYR:CA   | 2.52                     | 0.73              |
| 2:2V:177:VAL:HG23 | 1:3J:332:ILE:HG22 | 1.70                     | 0.73              |
| 2:2W:223:THR:HA   | 1:3K:325:PRO:CD   | 2.19                     | 0.73              |
| 2:2Y:404:PHE:CE1  | 1:3M:261:PRO:N    | 2.56                     | 0.73              |
| 1:1G:346:TRP:CD2  | 2:4T:403:ALA:HB2  | 2.24                     | 0.72              |
| 1:1G:346:TRP:HD1  | 2:4T:401:ARG:HG3  | 1.54                     | 0.72              |
| 1:1I:254:GLU:HG2  | 2:4U:101:ASN:N    | 2.04                     | 0.72              |
| 2:1W:221:THR:CA   | 1:2K:324:VAL:CG1  | 2.64                     | 0.72              |
| 2:2O:181:VAL:HG21 | 1:3B:314:ALA:HB1  | 1.71                     | 0.72              |
| 2:2T:73:GLY:HA3   | 1:3G:2:ARG:NH2    | 2.03                     | 0.72              |
| 2:2Z:101:ASN:HB2  | 1:3N:254:GLU:CG   | 2.19                     | 0.72              |
| 1:1E:249:ASN:N    | 2:4R:11:GLN:OE1   | 2.22                     | 0.72              |
| 1:1F:345:ASP:O    | 2:4S:397:ALA:HB1  | 1.89                     | 0.72              |
| 1:1G:263:PRO:HD3  | 2:4T:406:HIS:CB   | 2.19                     | 0.72              |
| 1:1J:258:ASN:ND2  | 2:4V:180:THR:HG23 | 2.04                     | 0.72              |
| 1:1J:260:VAL:CB   | 2:4V:407:TRP:HZ2  | 2.01                     | 0.72              |
| 1:1M:329:ASN:HB2  | 2:4Y:210:TYR:HE2  | 1.50                     | 0.72              |
| 2:2O:177:VAL:CG2  | 1:3B:332:ILE:HG21 | 2.19                     | 0.72              |
| 2:2Q:394:GLN:CB   | 1:3D:348:PRO:CG   | 2.67                     | 0.72              |
| 2:2S:73:GLY:HA3   | 1:3F:2:ARG:NH2    | 2.03                     | 0.72              |
| 2:2Y:214:PHE:CB   | 1:3M:326:LYS:CE   | 2.60                     | 0.72              |
| 2:2Y:397:ALA:O    | 1:3M:346:TRP:HB2  | 1.89                     | 0.72              |
| 1:4G:280:LYS:NZ   | 1:4I:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:4L:280:LYS:NZ   | 1:4M:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:1C:2:ARG:HG3    | 2:4P:72:PRO:CG    | 2.18                     | 0.72              |
| 1:1J:346:TRP:CD2  | 2:4V:403:ALA:HB2  | 2.24                     | 0.72              |
| 2:1R:181:VAL:CG2  | 1:2E:258:ASN:O    | 2.36                     | 0.72              |
| 2:1W:404:PHE:CZ   | 1:2K:260:VAL:C    | 2.68                     | 0.72              |
| 2:2Q:404:PHE:H    | 1:3D:261:PRO:C    | 1.95                     | 0.72              |
| 2:2Y:181:VAL:H    | 1:3M:258:ASN:HD22 | 1.37                     | 0.72              |
| 1:1B:348:PRO:HB2  | 2:4O:394:GLN:CD   | 2.14                     | 0.72              |
| 1:1D:260:VAL:O    | 2:4Q:407:TRP:NE1  | 2.21                     | 0.72              |
| 1:1F:352:LYS:CD   | 2:4S:101:ASN:ND2  | 2.51                     | 0.72              |
| 2:1V:182:VAL:HG22 | 1:2J:257:THR:HG22 | 1.71                     | 0.72              |
| 2:1Y:178:SER:OG   | 1:2M:351:PHE:O    | 2.06                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2L:280:LYS:NZ   | 1:2M:90:GLU:OE2   | 2.14                     | 0.72              |
| 2:2Q:179:ASP:OD2  | 1:3D:248:LEU:HD21 | 1.89                     | 0.72              |
| 1:1E:326:LYS:HG2  | 2:4R:210:TYR:HB3  | 1.71                     | 0.72              |
| 1:1F:248:LEU:CA   | 2:4S:11:GLN:HE22  | 2.00                     | 0.72              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:HB3  | 1.68                     | 0.72              |
| 2:1R:221:THR:OG1  | 1:2E:324:VAL:CG2  | 2.37                     | 0.72              |
| 2:1W:181:VAL:CG1  | 1:2K:258:ASN:O    | 2.37                     | 0.72              |
| 2:1X:179:ASP:O    | 1:2L:352:LYS:HD3  | 1.88                     | 0.72              |
| 2:2O:406:HIS:NE2  | 1:3B:262:TYR:C    | 2.47                     | 0.72              |
| 2:2S:176:LYS:HE2  | 1:3F:333:ALA:CB   | 2.18                     | 0.72              |
| 2:2T:221:THR:HA   | 1:3G:324:VAL:HG11 | 1.71                     | 0.72              |
| 2:2U:224:TYR:HE2  | 1:3I:248:LEU:HB2  | 1.54                     | 0.72              |
| 1:1J:262:TYR:OH   | 2:4V:401:ARG:O    | 2.06                     | 0.72              |
| 1:1L:260:VAL:HG11 | 2:4X:407:TRP:HZ2  | 1.54                     | 0.72              |
| 2:1T:181:VAL:HG23 | 1:2G:258:ASN:HB3  | 1.69                     | 0.72              |
| 1:2G:280:LYS:NZ   | 1:2I:90:GLU:OE2   | 2.14                     | 0.72              |
| 2:2H:221:THR:OG1  | 1:3A:324:VAL:CG2  | 2.38                     | 0.72              |
| 2:2V:406:HIS:NE2  | 1:3J:262:TYR:CA   | 2.53                     | 0.72              |
| 2:2Z:401:ARG:NH2  | 1:3N:434:GLU:O    | 2.22                     | 0.72              |
| 2:2Z:404:PHE:HE1  | 1:3N:260:VAL:N    | 1.87                     | 0.72              |
| 1:3L:280:LYS:NZ   | 1:3M:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:1A:435:VAL:HA   | 2:4H:401:ARG:HH21 | 1.54                     | 0.72              |
| 1:1L:2:ARG:HD3    | 2:4X:72:PRO:CD    | 2.12                     | 0.72              |
| 1:1M:261:PRO:O    | 2:4Y:406:HIS:CD2  | 2.43                     | 0.72              |
| 2:1O:181:VAL:N    | 1:2B:258:ASN:HD22 | 1.87                     | 0.72              |
| 2:1T:221:THR:HB   | 1:2G:324:VAL:HG21 | 1.71                     | 0.72              |
| 2:2Q:407:TRP:NE1  | 1:3D:260:VAL:HB   | 2.04                     | 0.72              |
| 2:2W:100:GLY:CA   | 1:3K:253:THR:HB   | 2.20                     | 0.72              |
| 1:3G:280:LYS:NZ   | 1:3I:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:1B:348:PRO:HB3  | 2:4O:394:GLN:HG2  | 1.70                     | 0.72              |
| 1:1E:2:ARG:NH2    | 2:4R:73:GLY:CA    | 2.53                     | 0.72              |
| 1:1E:280:LYS:NZ   | 1:1F:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:1G:257:THR:CB   | 2:4T:100:GLY:O    | 2.37                     | 0.72              |
| 1:1I:248:LEU:HD12 | 2:4U:11:GLN:CD    | 2.14                     | 0.72              |
| 2:1Q:214:PHE:CB   | 1:2D:326:LYS:HE2  | 2.17                     | 0.72              |
| 2:1V:224:TYR:CE2  | 1:2J:247:ALA:O    | 2.41                     | 0.72              |
| 1:2E:280:LYS:NZ   | 1:2F:90:GLU:OE2   | 2.14                     | 0.72              |
| 2:2O:101:ASN:O    | 1:3B:257:THR:HG21 | 1.90                     | 0.72              |
| 2:2U:71:GLU:HB2   | 1:3I:2:ARG:HD3    | 1.72                     | 0.72              |
| 2:2U:406:HIS:NE2  | 1:3I:263:PRO:CD   | 2.53                     | 0.72              |
| 1:1C:262:TYR:CE2  | 2:4P:403:ALA:HA   | 2.24                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:261:PRO:O    | 2:4Q:404:PHE:CA   | 2.38                     | 0.72              |
| 1:1I:326:LYS:CB   | 2:4U:222:PRO:HG2  | 2.19                     | 0.72              |
| 1:1N:437:VAL:O    | 2:4Z:401:ARG:NH1  | 2.23                     | 0.72              |
| 2:1S:100:GLY:HA3  | 1:2F:253:THR:HG21 | 1.70                     | 0.72              |
| 2:1W:404:PHE:N    | 1:2K:261:PRO:O    | 2.20                     | 0.72              |
| 2:1Z:404:PHE:CE1  | 1:2N:260:VAL:C    | 2.66                     | 0.72              |
| 2:2P:179:ASP:OD2  | 1:3C:248:LEU:CD2  | 2.37                     | 0.72              |
| 2:2R:404:PHE:H    | 1:3E:261:PRO:C    | 1.97                     | 0.72              |
| 2:2V:177:VAL:HG23 | 1:3J:332:ILE:HG21 | 1.71                     | 0.72              |
| 2:2W:214:PHE:CB   | 1:3K:326:LYS:CE   | 2.57                     | 0.72              |
| 2:2Z:181:VAL:HG21 | 1:3N:314:ALA:HB1  | 1.72                     | 0.72              |
| 1:1A:260:VAL:O    | 2:4H:407:TRP:NE1  | 2.23                     | 0.72              |
| 1:1C:326:LYS:HG2  | 2:4P:210:TYR:HB3  | 1.72                     | 0.72              |
| 1:1D:263:PRO:HA   | 2:4Q:406:HIS:CE1  | 2.24                     | 0.72              |
| 1:1E:439:SER:CB   | 2:4R:400:ARG:HD2  | 2.19                     | 0.72              |
| 1:1G:280:LYS:NZ   | 1:1I:90:GLU:OE2   | 2.14                     | 0.72              |
| 1:1K:348:PRO:HD2  | 2:4W:398:MET:CG   | 2.20                     | 0.72              |
| 1:1M:254:GLU:HA   | 2:4Y:100:GLY:C    | 2.15                     | 0.72              |
| 2:1W:178:SER:OG   | 1:2K:351:PHE:O    | 2.07                     | 0.72              |
| 2:2O:100:GLY:HA3  | 1:3B:253:THR:CB   | 2.20                     | 0.72              |
| 2:2P:394:GLN:CA   | 1:3C:348:PRO:HG3  | 2.19                     | 0.72              |
| 2:2P:401:ARG:NH2  | 1:3C:434:GLU:O    | 2.23                     | 0.72              |
| 2:2T:72:PRO:HD2   | 1:3G:2:ARG:CG     | 2.20                     | 0.72              |
| 1:1B:260:VAL:C    | 2:4O:404:PHE:CD1  | 2.67                     | 0.71              |
| 1:1B:262:TYR:C    | 2:4O:406:HIS:CE1  | 2.67                     | 0.71              |
| 1:1C:262:TYR:CE1  | 2:4P:402:LYS:O    | 2.43                     | 0.71              |
| 1:1C:346:TRP:HD1  | 2:4P:401:ARG:HG3  | 1.51                     | 0.71              |
| 1:1C:346:TRP:CZ3  | 2:4P:403:ALA:CB   | 2.72                     | 0.71              |
| 1:1D:345:ASP:O    | 2:4Q:397:ALA:HB1  | 1.90                     | 0.71              |
| 1:1I:352:LYS:HD3  | 2:4U:101:ASN:HD22 | 1.55                     | 0.71              |
| 1:1M:329:ASN:CB   | 2:4Y:210:TYR:CE2  | 2.72                     | 0.71              |
| 1:1N:346:TRP:O    | 2:4Z:398:MET:HG3  | 1.89                     | 0.71              |
| 2:2T:406:HIS:CE1  | 1:3G:263:PRO:N    | 2.58                     | 0.71              |
| 2:2W:71:GLU:HB2   | 1:3K:2:ARG:HD3    | 1.72                     | 0.71              |
| 2:2X:404:PHE:CD1  | 1:3L:261:PRO:CA   | 2.73                     | 0.71              |
| 1:1E:325:PRO:HB3  | 2:4R:224:TYR:CZ   | 2.25                     | 0.71              |
| 1:1G:332:ILE:HB   | 2:4T:177:VAL:CG2  | 2.20                     | 0.71              |
| 1:1N:261:PRO:HB3  | 2:4Z:404:PHE:CZ   | 2.25                     | 0.71              |
| 2:2O:100:GLY:CA   | 1:3B:253:THR:CG2  | 2.65                     | 0.71              |
| 2:2S:394:GLN:HB3  | 1:3F:348:PRO:HG2  | 1.71                     | 0.71              |
| 2:2V:404:PHE:CZ   | 1:3J:261:PRO:HB3  | 2.25                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2W:210:TYR:HD2  | 1:3K:329:ASN:ND2  | 1.88                     | 0.71              |
| 1:4E:280:LYS:NZ   | 1:4F:90:GLU:OE2   | 2.14                     | 0.71              |
| 1:1A:325:PRO:CD   | 2:4H:223:THR:HA   | 2.19                     | 0.71              |
| 1:1B:263:PRO:CA   | 2:4O:406:HIS:CE1  | 2.73                     | 0.71              |
| 1:1D:324:VAL:HG21 | 2:4Q:221:THR:OG1  | 1.91                     | 0.71              |
| 1:1F:258:ASN:OD1  | 2:4S:101:ASN:ND2  | 2.23                     | 0.71              |
| 1:1I:346:TRP:HA   | 2:4U:397:ALA:C    | 2.14                     | 0.71              |
| 2:1S:404:PHE:CE1  | 1:2F:261:PRO:HA   | 2.24                     | 0.71              |
| 2:1V:180:THR:CG2  | 1:2J:258:ASN:HD21 | 2.03                     | 0.71              |
| 2:1Y:404:PHE:HE1  | 1:2M:260:VAL:H    | 1.38                     | 0.71              |
| 2:2P:404:PHE:CD1  | 1:3C:260:VAL:O    | 2.43                     | 0.71              |
| 2:2Q:404:PHE:CE1  | 1:3D:260:VAL:C    | 2.68                     | 0.71              |
| 1:1D:2:ARG:NH2    | 2:4Q:73:GLY:CA    | 2.52                     | 0.71              |
| 1:1D:326:LYS:CB   | 2:4Q:222:PRO:HG2  | 2.20                     | 0.71              |
| 1:1D:352:LYS:HD3  | 2:4Q:101:ASN:ND2  | 2.06                     | 0.71              |
| 1:1F:348:PRO:HD2  | 2:4S:398:MET:CG   | 2.21                     | 0.71              |
| 1:1G:348:PRO:HD2  | 2:4T:398:MET:SD   | 2.29                     | 0.71              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:HG3  | 1.86                     | 0.71              |
| 1:1L:326:LYS:HB2  | 2:4X:222:PRO:HG2  | 1.70                     | 0.71              |
| 1:1M:346:TRP:CZ3  | 2:4Y:404:PHE:CE2  | 2.78                     | 0.71              |
| 1:1N:257:THR:HB   | 2:4Z:100:GLY:O    | 1.90                     | 0.71              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:CA   | 2.20                     | 0.71              |
| 2:1H:214:PHE:CB   | 1:2A:326:LYS:HE2  | 2.19                     | 0.71              |
| 2:1T:181:VAL:HB   | 1:2G:258:ASN:HA   | 1.72                     | 0.71              |
| 2:1T:404:PHE:CE1  | 1:2G:261:PRO:HA   | 2.25                     | 0.71              |
| 2:1W:181:VAL:CB   | 1:2K:258:ASN:CA   | 2.67                     | 0.71              |
| 2:1Y:11:GLN:HE22  | 1:2M:249:ASN:HB2  | 1.54                     | 0.71              |
| 2:1Y:180:THR:HA   | 1:2M:352:LYS:HD3  | 1.71                     | 0.71              |
| 2:2Q:394:GLN:HG2  | 1:3D:348:PRO:HB2  | 1.71                     | 0.71              |
| 2:2T:398:MET:CG   | 1:3G:346:TRP:O    | 2.38                     | 0.71              |
| 2:2V:214:PHE:CB   | 1:3J:326:LYS:CE   | 2.59                     | 0.71              |
| 1:1B:314:ALA:HB2  | 2:4O:181:VAL:HG11 | 1.70                     | 0.71              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:CD1  | 2.73                     | 0.71              |
| 1:1F:254:GLU:HG2  | 2:4S:101:ASN:H    | 1.54                     | 0.71              |
| 2:1T:221:THR:OG1  | 1:2G:324:VAL:HG21 | 1.90                     | 0.71              |
| 2:1T:224:TYR:HE2  | 1:2G:248:LEU:HB2  | 1.55                     | 0.71              |
| 2:1W:181:VAL:HG11 | 1:2K:258:ASN:O    | 1.89                     | 0.71              |
| 2:2V:406:HIS:CE1  | 1:3J:263:PRO:N    | 2.58                     | 0.71              |
| 1:3E:280:LYS:NZ   | 1:3F:90:GLU:OE2   | 2.14                     | 0.71              |
| 1:1A:257:THR:HG21 | 2:4H:101:ASN:O    | 1.90                     | 0.71              |
| 1:1A:262:TYR:C    | 2:4H:406:HIS:CE1  | 2.69                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:435:VAL:C    | 2:4H:401:ARG:HH22 | 1.98                     | 0.71              |
| 1:1B:257:THR:HG21 | 2:4O:101:ASN:O    | 1.90                     | 0.71              |
| 1:1C:346:TRP:CA   | 2:4P:397:ALA:C    | 2.63                     | 0.71              |
| 2:1U:221:THR:CA   | 1:2I:324:VAL:CG1  | 2.53                     | 0.71              |
| 2:2Q:394:GLN:HB3  | 1:3D:348:PRO:HG2  | 1.73                     | 0.71              |
| 2:2S:100:GLY:CA   | 1:3F:253:THR:HB   | 2.20                     | 0.71              |
| 2:2S:407:TRP:NE1  | 1:3F:260:VAL:HB   | 2.06                     | 0.71              |
| 2:2U:397:ALA:O    | 1:3I:346:TRP:CB   | 2.39                     | 0.71              |
| 1:1A:348:PRO:HG3  | 2:4H:394:GLN:CG   | 2.18                     | 0.71              |
| 1:1A:352:LYS:HA   | 2:4H:179:ASP:O    | 1.90                     | 0.71              |
| 1:1F:2:ARG:NH1    | 2:4S:71:GLU:HG3   | 2.05                     | 0.71              |
| 1:1G:254:GLU:N    | 2:4T:100:GLY:CA   | 2.53                     | 0.71              |
| 1:1G:254:GLU:HG2  | 2:4T:100:GLY:C    | 2.14                     | 0.71              |
| 1:1G:435:VAL:CA   | 2:4T:401:ARG:NH2  | 2.53                     | 0.71              |
| 1:1I:260:VAL:CG1  | 2:4U:407:TRP:HZ2  | 2.03                     | 0.71              |
| 1:1I:348:PRO:HG3  | 2:4U:394:GLN:HA   | 1.71                     | 0.71              |
| 1:1M:348:PRO:HG3  | 2:4Y:394:GLN:CA   | 2.19                     | 0.71              |
| 2:1H:180:THR:CG2  | 1:2A:258:ASN:HD21 | 2.02                     | 0.71              |
| 2:1V:404:PHE:CE2  | 1:2J:261:PRO:CA   | 2.74                     | 0.71              |
| 2:2O:404:PHE:H    | 1:3B:261:PRO:C    | 1.96                     | 0.71              |
| 2:2W:177:VAL:HG23 | 1:3K:332:ILE:HG21 | 1.71                     | 0.71              |
| 1:1C:329:ASN:CB   | 2:4P:210:TYR:CD2  | 2.74                     | 0.71              |
| 1:1E:329:ASN:CB   | 2:4R:210:TYR:CD2  | 2.73                     | 0.71              |
| 1:1K:260:VAL:CG1  | 2:4W:407:TRP:HZ2  | 2.03                     | 0.71              |
| 2:1W:11:GLN:HE22  | 1:2K:249:ASN:CB   | 2.04                     | 0.71              |
| 2:1X:221:THR:OG1  | 1:2L:324:VAL:CG2  | 2.38                     | 0.71              |
| 2:2R:73:GLY:HA3   | 1:3E:2:ARG:NH2    | 2.06                     | 0.71              |
| 1:1A:333:ALA:CB   | 2:4H:176:LYS:HE2  | 2.19                     | 0.71              |
| 1:1I:254:GLU:CA   | 2:4U:100:GLY:HA2  | 2.21                     | 0.71              |
| 2:2T:210:TYR:CE2  | 1:3G:329:ASN:HB2  | 2.26                     | 0.71              |
| 2:2W:222:PRO:CG   | 1:3K:326:LYS:HB2  | 2.14                     | 0.71              |
| 2:2X:180:THR:CG2  | 1:3L:258:ASN:ND2  | 2.38                     | 0.71              |
| 1:1A:2:ARG:CG     | 2:4H:72:PRO:HD2   | 2.20                     | 0.71              |
| 1:1A:261:PRO:HB3  | 2:4H:404:PHE:CD2  | 2.26                     | 0.71              |
| 1:1C:253:THR:C    | 2:4P:100:GLY:HA3  | 2.16                     | 0.71              |
| 1:1C:332:ILE:CB   | 2:4P:177:VAL:CG2  | 2.69                     | 0.71              |
| 1:1G:2:ARG:CD     | 2:4T:72:PRO:CD    | 2.61                     | 0.71              |
| 1:1G:260:VAL:HG11 | 2:4T:407:TRP:HZ2  | 1.54                     | 0.71              |
| 1:1M:346:TRP:HZ3  | 2:4Y:404:PHE:CE2  | 2.09                     | 0.71              |
| 2:1S:406:HIS:NE2  | 1:2F:263:PRO:HD3  | 2.04                     | 0.71              |
| 2:1Y:181:VAL:CB   | 1:2M:258:ASN:CA   | 2.69                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2H:181:VAL:HG21 | 1:3A:314:ALA:HB1  | 1.73                     | 0.71              |
| 2:2O:404:PHE:CD1  | 1:3B:261:PRO:HA   | 2.24                     | 0.71              |
| 2:2Q:72:PRO:HD2   | 1:3D:2:ARG:CG     | 2.21                     | 0.71              |
| 2:2R:404:PHE:CE1  | 1:3E:260:VAL:C    | 2.68                     | 0.71              |
| 2:2T:72:PRO:HD2   | 1:3G:2:ARG:HD3    | 1.73                     | 0.71              |
| 2:2T:394:GLN:HA   | 1:3G:348:PRO:HG3  | 1.72                     | 0.71              |
| 2:2X:214:PHE:CB   | 1:3L:326:LYS:CE   | 2.57                     | 0.71              |
| 1:1C:260:VAL:HG12 | 2:4P:406:HIS:CE1  | 2.26                     | 0.70              |
| 1:1F:263:PRO:N    | 2:4S:406:HIS:CD2  | 2.59                     | 0.70              |
| 1:1G:326:LYS:HA   | 2:4T:210:TYR:CD1  | 2.26                     | 0.70              |
| 1:1I:332:ILE:HB   | 2:4U:177:VAL:HG21 | 1.71                     | 0.70              |
| 1:1L:346:TRP:HZ3  | 2:4X:404:PHE:HE2  | 1.38                     | 0.70              |
| 2:1S:214:PHE:CG   | 1:2F:326:LYS:HE2  | 2.26                     | 0.70              |
| 2:1T:222:PRO:CG   | 1:2G:326:LYS:HB2  | 2.21                     | 0.70              |
| 2:2X:406:HIS:NE2  | 1:3L:263:PRO:CD   | 2.54                     | 0.70              |
| 2:2Y:181:VAL:CB   | 1:3M:258:ASN:O    | 2.39                     | 0.70              |
| 2:2Y:221:THR:CA   | 1:3M:324:VAL:HG11 | 2.20                     | 0.70              |
| 2:2Z:100:GLY:CA   | 1:3N:253:THR:HG22 | 2.07                     | 0.70              |
| 1:1C:314:ALA:CB   | 2:4P:181:VAL:HG11 | 2.21                     | 0.70              |
| 1:1E:257:THR:HB   | 2:4R:100:GLY:O    | 1.90                     | 0.70              |
| 1:1G:326:LYS:CB   | 2:4T:222:PRO:HG2  | 2.21                     | 0.70              |
| 2:1H:101:ASN:CB   | 1:2A:254:GLU:HG2  | 2.20                     | 0.70              |
| 2:1S:100:GLY:CA   | 1:2F:253:THR:HG22 | 2.19                     | 0.70              |
| 2:1V:11:GLN:NE2   | 1:2J:249:ASN:HB2  | 2.07                     | 0.70              |
| 2:2Q:100:GLY:CA   | 1:3D:253:THR:CB   | 2.69                     | 0.70              |
| 2:2Q:101:ASN:O    | 1:3D:257:THR:HG21 | 1.91                     | 0.70              |
| 2:2U:398:MET:HG2  | 1:3I:346:TRP:O    | 1.91                     | 0.70              |
| 2:2X:77:SER:CB    | 1:3L:245:ASP:OD1  | 2.38                     | 0.70              |
| 1:1F:2:ARG:HH11   | 2:4S:71:GLU:HB2   | 1.55                     | 0.70              |
| 1:1F:353:VAL:CG2  | 2:4S:179:ASP:OD1  | 2.39                     | 0.70              |
| 1:1G:325:PRO:HG2  | 2:4T:224:TYR:CG   | 2.26                     | 0.70              |
| 1:1J:249:ASN:H    | 2:4V:11:GLN:CD    | 1.97                     | 0.70              |
| 2:1R:181:VAL:N    | 1:2E:258:ASN:HD22 | 1.83                     | 0.70              |
| 2:2H:397:ALA:O    | 1:3A:346:TRP:CB   | 2.38                     | 0.70              |
| 2:2R:394:GLN:CG   | 1:3E:348:PRO:HG3  | 2.20                     | 0.70              |
| 1:1L:263:PRO:N    | 2:4X:406:HIS:CE1  | 2.59                     | 0.70              |
| 1:1L:348:PRO:HD2  | 2:4X:398:MET:SD   | 2.31                     | 0.70              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:HG3  | 1.89                     | 0.70              |
| 1:1N:324:VAL:CG2  | 2:4Z:221:THR:OG1  | 2.39                     | 0.70              |
| 2:1T:394:GLN:HG2  | 1:2G:348:PRO:CG   | 2.21                     | 0.70              |
| 2:2O:210:TYR:HD2  | 1:3B:329:ASN:HD22 | 1.40                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2O:221:THR:HA   | 1:3B:324:VAL:HG11 | 1.71                     | 0.70              |
| 2:2U:177:VAL:HG23 | 1:3I:332:ILE:HG21 | 1.69                     | 0.70              |
| 1:1B:326:LYS:HA   | 2:4O:210:TYR:CD1  | 2.25                     | 0.70              |
| 1:1B:346:TRP:CD1  | 2:4O:401:ARG:HG3  | 2.27                     | 0.70              |
| 1:1D:332:ILE:HG21 | 2:4Q:177:VAL:HG22 | 1.72                     | 0.70              |
| 1:1G:254:GLU:HA   | 2:4T:100:GLY:CA   | 2.21                     | 0.70              |
| 1:1J:260:VAL:HG11 | 2:4V:407:TRP:CZ2  | 2.26                     | 0.70              |
| 1:1L:329:ASN:HB2  | 2:4X:210:TYR:HE2  | 1.53                     | 0.70              |
| 1:1L:332:ILE:CG2  | 2:4X:177:VAL:CG2  | 2.69                     | 0.70              |
| 2:1S:224:TYR:HD2  | 1:2F:247:ALA:O    | 1.74                     | 0.70              |
| 2:1X:221:THR:HB   | 1:2L:324:VAL:HG21 | 1.72                     | 0.70              |
| 2:2H:210:TYR:HD2  | 1:3A:329:ASN:HD22 | 1.39                     | 0.70              |
| 2:2S:72:PRO:HD2   | 1:3F:2:ARG:HD3    | 1.72                     | 0.70              |
| 2:2X:176:LYS:HE2  | 1:3L:333:ALA:CB   | 2.21                     | 0.70              |
| 2:2Z:181:VAL:HG21 | 1:3N:258:ASN:O    | 1.91                     | 0.70              |
| 2:2Z:181:VAL:CB   | 1:3N:258:ASN:O    | 2.40                     | 0.70              |
| 1:1D:346:TRP:CB   | 2:4Q:398:MET:HA   | 2.17                     | 0.70              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:N    | 2.07                     | 0.70              |
| 1:1F:261:PRO:HB3  | 2:4S:404:PHE:CD2  | 2.27                     | 0.70              |
| 1:1F:326:LYS:CB   | 2:4S:222:PRO:HG2  | 2.22                     | 0.70              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:CA   | 2.40                     | 0.70              |
| 2:1H:401:ARG:HB3  | 1:2A:262:TYR:OH   | 1.91                     | 0.70              |
| 2:1X:11:GLN:HE22  | 1:2L:249:ASN:CB   | 2.05                     | 0.70              |
| 2:1Z:181:VAL:CG2  | 1:2N:258:ASN:O    | 2.40                     | 0.70              |
| 2:1Z:182:VAL:HG21 | 1:2N:257:THR:CG2  | 2.22                     | 0.70              |
| 2:2Q:77:SER:CB    | 1:3D:245:ASP:OD1  | 2.39                     | 0.70              |
| 2:2W:77:SER:HB3   | 1:3K:245:ASP:CG   | 2.16                     | 0.70              |
| 1:1B:351:PHE:HB2  | 2:4O:178:SER:OG   | 1.91                     | 0.70              |
| 1:1D:260:VAL:C    | 2:4Q:404:PHE:CD1  | 2.69                     | 0.70              |
| 1:1D:326:LYS:CE   | 2:4Q:210:TYR:O    | 2.39                     | 0.70              |
| 1:1D:332:ILE:CB   | 2:4Q:177:VAL:HG21 | 2.20                     | 0.70              |
| 1:1E:2:ARG:CD     | 2:4R:71:GLU:HB2   | 2.22                     | 0.70              |
| 1:1E:260:VAL:CG1  | 2:4R:406:HIS:HE1  | 2.03                     | 0.70              |
| 1:1F:329:ASN:CG   | 2:4S:207:GLU:OE1  | 2.35                     | 0.70              |
| 1:1G:346:TRP:HB3  | 2:4T:397:ALA:O    | 1.90                     | 0.70              |
| 2:2Q:401:ARG:C    | 1:3D:262:TYR:HH   | 1.92                     | 0.70              |
| 2:2Q:404:PHE:HE1  | 1:3D:260:VAL:N    | 1.90                     | 0.70              |
| 2:2T:180:THR:CG2  | 1:3G:258:ASN:ND2  | 2.36                     | 0.70              |
| 2:2Z:406:HIS:CG   | 1:3N:263:PRO:HD3  | 2.23                     | 0.70              |
| 1:1C:326:LYS:HE2  | 2:4P:214:PHE:HB2  | 1.72                     | 0.70              |
| 1:1E:260:VAL:HG11 | 2:4R:407:TRP:CZ2  | 2.27                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:254:GLU:CA   | 2:4S:100:GLY:HA2  | 2.21                     | 0.70              |
| 2:1U:179:ASP:O    | 1:2I:352:LYS:HD3  | 1.91                     | 0.70              |
| 2:1Z:100:GLY:CA   | 1:2N:253:THR:CG2  | 2.65                     | 0.70              |
| 2:2S:398:MET:HG2  | 1:3F:346:TRP:O    | 1.91                     | 0.70              |
| 2:2T:214:PHE:CB   | 1:3G:326:LYS:CE   | 2.69                     | 0.70              |
| 2:2U:404:PHE:CZ   | 1:3I:261:PRO:HB3  | 2.27                     | 0.70              |
| 2:2V:71:GLU:HB2   | 1:3J:2:ARG:HD3    | 1.74                     | 0.70              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:N    | 2.25                     | 0.70              |
| 1:1D:346:TRP:CZ3  | 2:4Q:403:ALA:HB1  | 2.25                     | 0.70              |
| 1:1D:353:VAL:CA   | 2:4Q:179:ASP:OD1  | 2.39                     | 0.70              |
| 1:1F:326:LYS:HG2  | 2:4S:210:TYR:CG   | 2.27                     | 0.70              |
| 1:1F:332:ILE:CB   | 2:4S:177:VAL:HG23 | 2.22                     | 0.70              |
| 1:1G:348:PRO:CD   | 2:4T:398:MET:HG3  | 2.22                     | 0.70              |
| 1:1K:329:ASN:CB   | 2:4W:210:TYR:CE2  | 2.74                     | 0.70              |
| 1:1L:346:TRP:CZ3  | 2:4X:403:ALA:CB   | 2.75                     | 0.70              |
| 2:1V:221:THR:CB   | 1:2J:324:VAL:CG2  | 2.70                     | 0.70              |
| 2:1Y:180:THR:HG23 | 1:2M:258:ASN:HD21 | 1.57                     | 0.70              |
| 2:2H:224:TYR:HD2  | 1:3A:247:ALA:O    | 1.74                     | 0.70              |
| 2:2H:406:HIS:CG   | 1:3A:263:PRO:HD3  | 2.25                     | 0.70              |
| 2:2R:407:TRP:HE1  | 1:3E:260:VAL:CB   | 2.05                     | 0.70              |
| 2:2S:404:PHE:H    | 1:3F:261:PRO:C    | 2.00                     | 0.70              |
| 2:2U:222:PRO:CG   | 1:3I:326:LYS:CB   | 2.70                     | 0.70              |
| 2:2Y:406:HIS:NE2  | 1:3M:262:TYR:C    | 2.50                     | 0.70              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:CG   | 2.74                     | 0.70              |
| 1:1C:352:LYS:HA   | 2:4P:179:ASP:C    | 2.16                     | 0.70              |
| 1:1E:256:GLN:HB2  | 2:4R:407:TRP:CH2  | 2.27                     | 0.70              |
| 1:1G:260:VAL:CG1  | 2:4T:407:TRP:HE1  | 2.04                     | 0.70              |
| 1:1G:332:ILE:HG21 | 2:4T:177:VAL:CG2  | 2.21                     | 0.70              |
| 1:1L:254:GLU:HA   | 2:4X:100:GLY:C    | 2.17                     | 0.70              |
| 1:1N:346:TRP:CB   | 2:4Z:397:ALA:O    | 2.40                     | 0.70              |
| 2:1S:221:THR:OG1  | 1:2F:324:VAL:HG21 | 1.91                     | 0.70              |
| 2:1V:214:PHE:CB   | 1:2J:326:LYS:CE   | 2.48                     | 0.70              |
| 1:1G:349:THR:O    | 2:4T:181:VAL:CA   | 2.39                     | 0.69              |
| 1:1I:263:PRO:N    | 2:4U:406:HIS:CE1  | 2.59                     | 0.69              |
| 2:1X:404:PHE:N    | 1:2L:261:PRO:O    | 2.20                     | 0.69              |
| 2:2H:179:ASP:OD1  | 1:3A:353:VAL:HB   | 1.91                     | 0.69              |
| 2:2S:210:TYR:CE2  | 1:3F:329:ASN:HB2  | 2.27                     | 0.69              |
| 2:2S:398:MET:CG   | 1:3F:346:TRP:O    | 2.39                     | 0.69              |
| 2:2W:100:GLY:CA   | 1:3K:253:THR:CB   | 2.70                     | 0.69              |
| 2:2Y:222:PRO:HG2  | 1:3M:326:LYS:CB   | 2.22                     | 0.69              |
| 1:1A:351:PHE:O    | 2:4H:180:THR:N    | 2.25                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:263:PRO:CA   | 2:4Q:406:HIS:CE1  | 2.75                     | 0.69              |
| 1:1G:352:LYS:HD3  | 2:4T:101:ASN:HD22 | 1.54                     | 0.69              |
| 1:1G:353:VAL:CG2  | 2:4T:179:ASP:OD1  | 2.40                     | 0.69              |
| 1:1J:346:TRP:CB   | 2:4V:398:MET:HA   | 2.20                     | 0.69              |
| 2:1T:179:ASP:OD2  | 1:2G:248:LEU:HD21 | 1.92                     | 0.69              |
| 2:1T:404:PHE:CE2  | 1:2G:261:PRO:HA   | 2.27                     | 0.69              |
| 2:1X:11:GLN:NE2   | 1:2L:249:ASN:HB2  | 2.06                     | 0.69              |
| 2:2T:394:GLN:CA   | 1:3G:348:PRO:HG3  | 2.22                     | 0.69              |
| 2:2Z:181:VAL:H    | 1:3N:258:ASN:HD22 | 1.40                     | 0.69              |
| 1:1B:262:TYR:OH   | 2:4O:401:ARG:C    | 2.35                     | 0.69              |
| 1:1D:346:TRP:CB   | 2:4Q:397:ALA:C    | 2.62                     | 0.69              |
| 1:1I:314:ALA:HB1  | 2:4U:181:VAL:HG21 | 1.74                     | 0.69              |
| 1:1N:348:PRO:CG   | 2:4Z:394:GLN:HG2  | 2.22                     | 0.69              |
| 2:1U:222:PRO:HG2  | 1:2I:326:LYS:HB2  | 1.72                     | 0.69              |
| 2:1U:404:PHE:CD2  | 1:2I:261:PRO:HA   | 2.27                     | 0.69              |
| 2:2Q:222:PRO:HG2  | 1:3D:326:LYS:CB   | 2.22                     | 0.69              |
| 2:2W:404:PHE:CD1  | 1:3K:260:VAL:C    | 2.70                     | 0.69              |
| 2:2X:181:VAL:CG2  | 1:3L:258:ASN:O    | 2.40                     | 0.69              |
| 2:2Y:181:VAL:CG2  | 1:3M:258:ASN:O    | 2.40                     | 0.69              |
| 1:1A:254:GLU:HA   | 2:4H:100:GLY:C    | 2.16                     | 0.69              |
| 1:1B:325:PRO:HD2  | 2:4O:223:THR:HA   | 1.72                     | 0.69              |
| 1:1B:346:TRP:HA   | 2:4O:397:ALA:HB1  | 1.72                     | 0.69              |
| 1:1C:2:ARG:NH2    | 2:4P:73:GLY:CA    | 2.55                     | 0.69              |
| 1:1D:254:GLU:HG2  | 2:4Q:100:GLY:C    | 2.17                     | 0.69              |
| 1:1F:248:LEU:C    | 2:4S:11:GLN:NE2   | 2.31                     | 0.69              |
| 1:1L:346:TRP:CZ3  | 2:4X:404:PHE:HE2  | 2.09                     | 0.69              |
| 1:1M:351:PHE:O    | 2:4Y:180:THR:CA   | 2.39                     | 0.69              |
| 2:2H:401:ARG:NH2  | 1:3A:434:GLU:O    | 2.26                     | 0.69              |
| 2:2T:100:GLY:HA2  | 1:3G:253:THR:C    | 2.18                     | 0.69              |
| 2:2T:176:LYS:HE2  | 1:3G:333:ALA:CB   | 2.22                     | 0.69              |
| 1:1E:349:THR:HG21 | 2:4R:184:PRO:CG   | 2.22                     | 0.69              |
| 1:1F:256:GLN:HB2  | 2:4S:407:TRP:CH2  | 2.27                     | 0.69              |
| 1:1K:332:ILE:CG2  | 2:4W:177:VAL:CG2  | 2.70                     | 0.69              |
| 1:1L:351:PHE:O    | 2:4X:180:THR:CA   | 2.40                     | 0.69              |
| 2:1X:179:ASP:O    | 1:2L:352:LYS:CE   | 2.40                     | 0.69              |
| 2:2O:77:SER:HB3   | 1:3B:245:ASP:CG   | 2.18                     | 0.69              |
| 2:2P:101:ASN:O    | 1:3C:257:THR:HG21 | 1.92                     | 0.69              |
| 2:2Q:101:ASN:HB2  | 1:3D:254:GLU:CG   | 2.22                     | 0.69              |
| 1:1A:261:PRO:O    | 2:4H:404:PHE:CA   | 2.41                     | 0.69              |
| 1:1E:325:PRO:HB2  | 2:4R:224:TYR:CE1  | 2.26                     | 0.69              |
| 1:1E:326:LYS:CE   | 2:4R:210:TYR:O    | 2.38                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:261:PRO:HA   | 2:4Y:404:PHE:HA   | 1.75                     | 0.69              |
| 1:1N:332:ILE:HG21 | 2:4Z:177:VAL:CG2  | 2.21                     | 0.69              |
| 2:2U:177:VAL:CG2  | 1:3I:332:ILE:CG2  | 2.69                     | 0.69              |
| 2:2W:177:VAL:CG2  | 1:3K:332:ILE:HG21 | 2.22                     | 0.69              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:CG   | 2.76                     | 0.69              |
| 1:1D:2:ARG:HG3    | 2:4Q:72:PRO:CD    | 2.22                     | 0.69              |
| 1:1F:2:ARG:CG     | 2:4S:72:PRO:CD    | 2.71                     | 0.69              |
| 1:1L:329:ASN:CB   | 2:4X:210:TYR:CE2  | 2.75                     | 0.69              |
| 2:1Q:180:THR:HG23 | 1:2D:258:ASN:HD21 | 1.57                     | 0.69              |
| 2:2V:73:GLY:HA3   | 1:3J:2:ARG:NH2    | 2.07                     | 0.69              |
| 1:1B:260:VAL:O    | 2:4O:407:TRP:HD1  | 1.76                     | 0.69              |
| 1:1C:2:ARG:CG     | 2:4P:72:PRO:CD    | 2.71                     | 0.69              |
| 1:1C:258:ASN:O    | 2:4P:181:VAL:HB   | 1.93                     | 0.69              |
| 1:1D:245:ASP:OD2  | 2:4Q:77:SER:HB2   | 1.91                     | 0.69              |
| 1:1D:352:LYS:HA   | 2:4Q:179:ASP:C    | 2.17                     | 0.69              |
| 1:1E:253:THR:HG22 | 2:4R:100:GLY:HA3  | 1.73                     | 0.69              |
| 1:1G:346:TRP:CD1  | 2:4T:401:ARG:HG3  | 2.27                     | 0.69              |
| 1:1I:325:PRO:HB2  | 2:4U:224:TYR:CE1  | 2.28                     | 0.69              |
| 1:1I:435:VAL:C    | 2:4U:401:ARG:HH22 | 1.99                     | 0.69              |
| 1:1K:260:VAL:CB   | 2:4W:407:TRP:HZ2  | 2.06                     | 0.69              |
| 1:1K:260:VAL:CG1  | 2:4W:407:TRP:CZ2  | 2.75                     | 0.69              |
| 2:1O:181:VAL:N    | 1:2B:258:ASN:ND2  | 2.39                     | 0.69              |
| 2:1P:222:PRO:HG2  | 1:2C:326:LYS:HB2  | 1.75                     | 0.69              |
| 2:1Y:404:PHE:HE1  | 1:2M:260:VAL:N    | 1.91                     | 0.69              |
| 2:1Z:404:PHE:HE1  | 1:2N:260:VAL:N    | 1.90                     | 0.69              |
| 2:2T:101:ASN:ND2  | 1:3G:258:ASN:OD1  | 2.25                     | 0.69              |
| 2:2U:72:PRO:HD2   | 1:3I:2:ARG:CG     | 2.23                     | 0.69              |
| 2:2U:394:GLN:CB   | 1:3I:348:PRO:CG   | 2.70                     | 0.69              |
| 2:2U:404:PHE:CD1  | 1:3I:260:VAL:C    | 2.71                     | 0.69              |
| 2:2V:404:PHE:CD1  | 1:3J:260:VAL:C    | 2.70                     | 0.69              |
| 2:2Y:207:GLU:CD   | 1:3M:329:ASN:ND2  | 2.36                     | 0.69              |
| 1:1A:260:VAL:CG1  | 2:4H:407:TRP:HE1  | 2.05                     | 0.69              |
| 1:1B:262:TYR:CZ   | 2:4O:403:ALA:HA   | 2.28                     | 0.69              |
| 1:1D:254:GLU:CB   | 2:4Q:101:ASN:HB2  | 2.23                     | 0.69              |
| 1:1F:249:ASN:N    | 2:4S:11:GLN:OE1   | 2.26                     | 0.69              |
| 1:1F:254:GLU:CA   | 2:4S:100:GLY:CA   | 2.71                     | 0.69              |
| 1:1F:352:LYS:CE   | 2:4S:101:ASN:HD22 | 2.06                     | 0.69              |
| 1:1K:258:ASN:ND2  | 2:4W:180:THR:HG23 | 2.07                     | 0.69              |
| 2:1O:401:ARG:NH2  | 1:2B:435:VAL:HA   | 2.05                     | 0.69              |
| 2:1T:100:GLY:HA2  | 1:2G:253:THR:CG2  | 2.23                     | 0.69              |
| 2:1T:214:PHE:CD1  | 1:2G:326:LYS:CE   | 2.76                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:1Z:224:TYR:CE2  | 1:2N:247:ALA:O   | 2.46                     | 0.69              |
| 2:2H:406:HIS:NE2  | 1:3A:262:TYR:C   | 2.50                     | 0.69              |
| 2:2S:180:THR:CG2  | 1:3F:258:ASN:ND2 | 2.36                     | 0.69              |
| 2:2S:404:PHE:CE1  | 1:3F:261:PRO:N   | 2.61                     | 0.69              |
| 2:2T:398:MET:HA   | 1:3G:346:TRP:HB2 | 1.75                     | 0.69              |
| 2:2U:397:ALA:O    | 1:3I:346:TRP:HB2 | 1.93                     | 0.69              |
| 1:1B:262:TYR:C    | 2:4O:406:HIS:CD2 | 2.68                     | 0.69              |
| 1:1C:326:LYS:HB2  | 2:4P:222:PRO:HG2 | 1.75                     | 0.69              |
| 1:1D:346:TRP:CZ3  | 2:4Q:403:ALA:HB3 | 2.27                     | 0.69              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:CA  | 2.62                     | 0.69              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:H   | 2.06                     | 0.69              |
| 1:1G:346:TRP:CH2  | 2:4T:403:ALA:CB  | 2.66                     | 0.69              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:CB  | 2.41                     | 0.69              |
| 1:1K:349:THR:HB   | 2:4W:180:THR:O   | 1.93                     | 0.69              |
| 1:1N:348:PRO:HG2  | 2:4Z:394:GLN:HB3 | 1.73                     | 0.69              |
| 1:1N:349:THR:HG21 | 2:4Z:184:PRO:HD3 | 1.73                     | 0.69              |
| 2:1S:222:PRO:CG   | 1:2F:326:LYS:HB2 | 2.23                     | 0.69              |
| 2:2S:398:MET:HA   | 1:3F:346:TRP:HB2 | 1.75                     | 0.69              |
| 1:1E:261:PRO:CB   | 2:4R:404:PHE:H   | 2.05                     | 0.68              |
| 1:1E:326:LYS:CB   | 2:4R:222:PRO:HG2 | 2.22                     | 0.68              |
| 1:1F:262:TYR:N    | 2:4S:406:HIS:CD2 | 2.50                     | 0.68              |
| 1:1G:346:TRP:CD2  | 2:4T:403:ALA:CB  | 2.76                     | 0.68              |
| 1:1J:260:VAL:HG12 | 2:4V:406:HIS:HE1 | 1.59                     | 0.68              |
| 2:1U:181:VAL:CG2  | 1:2I:258:ASN:C   | 2.62                     | 0.68              |
| 2:2Q:101:ASN:HB2  | 1:3D:254:GLU:HG2 | 1.73                     | 0.68              |
| 2:2V:404:PHE:CE1  | 1:3J:261:PRO:CA  | 2.75                     | 0.68              |
| 1:1C:439:SER:CB   | 2:4P:400:ARG:HD2 | 2.22                     | 0.68              |
| 1:1E:352:LYS:CD   | 2:4R:101:ASN:ND2 | 2.55                     | 0.68              |
| 1:1I:260:VAL:HG12 | 2:4U:406:HIS:CE1 | 2.28                     | 0.68              |
| 1:1J:346:TRP:CD2  | 2:4V:403:ALA:CB  | 2.75                     | 0.68              |
| 2:2H:100:GLY:HA3  | 1:3A:253:THR:CB  | 2.22                     | 0.68              |
| 2:2O:401:ARG:NH2  | 1:3B:434:GLU:O   | 2.26                     | 0.68              |
| 2:2Z:394:GLN:CG   | 1:3N:348:PRO:HG3 | 2.20                     | 0.68              |
| 2:2Z:406:HIS:NE2  | 1:3N:262:TYR:C   | 2.51                     | 0.68              |
| 1:1C:261:PRO:CA   | 2:4P:404:PHE:CA  | 2.68                     | 0.68              |
| 2:1V:404:PHE:CZ   | 1:2J:260:VAL:C   | 2.72                     | 0.68              |
| 2:2Q:406:HIS:CD2  | 1:3D:262:TYR:HA  | 2.28                     | 0.68              |
| 2:2W:404:PHE:CE1  | 1:3K:261:PRO:CA  | 2.76                     | 0.68              |
| 2:2Y:404:PHE:HE1  | 1:3M:260:VAL:N   | 1.91                     | 0.68              |
| 2:2Z:179:ASP:OD2  | 1:3N:248:LEU:CD2 | 2.42                     | 0.68              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:CB  | 2.23                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:260:VAL:CB   | 2:4R:407:TRP:CE2  | 2.64                     | 0.68              |
| 1:1F:262:TYR:CE2  | 2:4S:403:ALA:HA   | 2.28                     | 0.68              |
| 1:1F:326:LYS:HA   | 2:4S:210:TYR:CZ   | 2.28                     | 0.68              |
| 1:1I:325:PRO:HD2  | 2:4U:223:THR:HA   | 1.75                     | 0.68              |
| 1:1L:245:ASP:OD2  | 2:4X:77:SER:CB    | 2.40                     | 0.68              |
| 1:1N:261:PRO:O    | 2:4Z:404:PHE:HA   | 1.93                     | 0.68              |
| 2:2O:180:THR:CG2  | 1:3B:258:ASN:ND2  | 2.38                     | 0.68              |
| 2:2Q:73:GLY:HA3   | 1:3D:2:ARG:NH2    | 2.09                     | 0.68              |
| 2:2U:214:PHE:CB   | 1:3I:326:LYS:CE   | 2.64                     | 0.68              |
| 2:2W:224:TYR:HD2  | 1:3K:247:ALA:O    | 1.76                     | 0.68              |
| 2:2Z:180:THR:CG2  | 1:3N:258:ASN:ND2  | 2.39                     | 0.68              |
| 1:1B:257:THR:OG1  | 2:4O:100:GLY:O    | 2.11                     | 0.68              |
| 1:1I:325:PRO:HB3  | 2:4U:224:TYR:CZ   | 2.28                     | 0.68              |
| 1:1L:349:THR:HB   | 2:4X:180:THR:O    | 1.94                     | 0.68              |
| 1:1M:262:TYR:OH   | 2:4Y:401:ARG:O    | 2.09                     | 0.68              |
| 1:1M:346:TRP:CZ3  | 2:4Y:404:PHE:HE2  | 2.11                     | 0.68              |
| 1:1N:348:PRO:CG   | 2:4Z:394:GLN:CG   | 2.71                     | 0.68              |
| 2:2H:181:VAL:CB   | 1:3A:258:ASN:O    | 2.41                     | 0.68              |
| 2:2P:100:GLY:HA3  | 1:3C:253:THR:CB   | 2.22                     | 0.68              |
| 2:2P:394:GLN:HG2  | 1:3C:348:PRO:HB2  | 1.74                     | 0.68              |
| 2:2R:401:ARG:HH21 | 1:3E:435:VAL:HA   | 1.54                     | 0.68              |
| 2:2T:404:PHE:CD1  | 1:3G:260:VAL:O    | 2.46                     | 0.68              |
| 2:2U:101:ASN:ND2  | 1:3I:258:ASN:OD1  | 2.26                     | 0.68              |
| 1:1B:249:ASN:N    | 2:4O:11:GLN:NE2   | 1.78                     | 0.68              |
| 1:1D:2:ARG:HG3    | 2:4Q:72:PRO:HD2   | 1.74                     | 0.68              |
| 1:1E:2:ARG:CD     | 2:4R:72:PRO:CD    | 2.61                     | 0.68              |
| 1:1E:325:PRO:HG2  | 2:4R:224:TYR:CG   | 2.28                     | 0.68              |
| 1:1E:332:ILE:CB   | 2:4R:177:VAL:HG21 | 2.17                     | 0.68              |
| 1:1G:325:PRO:O    | 2:4T:210:TYR:CZ   | 2.47                     | 0.68              |
| 1:1I:283:HIS:HA   | 1:1J:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1L:257:THR:CG2  | 2:4X:102:ASN:HB2  | 2.24                     | 0.68              |
| 2:1T:207:GLU:CD   | 1:2G:329:ASN:HD21 | 2.01                     | 0.68              |
| 2:1T:401:ARG:HH22 | 1:2G:435:VAL:HA   | 1.59                     | 0.68              |
| 2:1X:182:VAL:CG2  | 1:2L:257:THR:CG2  | 2.58                     | 0.68              |
| 2:2R:72:PRO:HD2   | 1:3E:2:ARG:HD3    | 1.76                     | 0.68              |
| 2:2T:100:GLY:CA   | 1:3G:253:THR:CG2  | 2.70                     | 0.68              |
| 2:2U:398:MET:CG   | 1:3I:346:TRP:O    | 2.42                     | 0.68              |
| 2:2U:403:ALA:HA   | 1:3I:262:TYR:CZ   | 2.29                     | 0.68              |
| 2:2V:406:HIS:CD2  | 1:3J:262:TYR:HA   | 2.29                     | 0.68              |
| 2:2X:181:VAL:HB   | 1:3L:258:ASN:O    | 1.94                     | 0.68              |
| 1:3I:283:HIS:HA   | 1:3J:62:VAL:HG11  | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:248:LEU:HD13 | 5:4Q:501:GDP:H8   | 0.92                     | 0.68              |
| 1:1D:253:THR:HB   | 2:4Q:100:GLY:CA   | 2.23                     | 0.68              |
| 1:1E:348:PRO:HG3  | 2:4R:394:GLN:C    | 2.19                     | 0.68              |
| 1:1F:351:PHE:O    | 2:4S:181:VAL:N    | 2.26                     | 0.68              |
| 1:2I:283:HIS:HA   | 1:2J:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:2J:283:HIS:HA   | 1:2K:62:VAL:HG11  | 1.76                     | 0.68              |
| 2:2O:181:VAL:HB   | 1:3B:258:ASN:O    | 1.94                     | 0.68              |
| 2:2O:224:TYR:HE2  | 1:3B:248:LEU:HB2  | 1.57                     | 0.68              |
| 1:3J:283:HIS:HA   | 1:3K:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:4I:283:HIS:HA   | 1:4J:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1D:349:THR:OG1  | 2:4Q:184:PRO:HD2  | 1.94                     | 0.68              |
| 1:1E:332:ILE:HG21 | 2:4R:177:VAL:HG22 | 1.73                     | 0.68              |
| 1:1I:263:PRO:HD3  | 2:4U:406:HIS:CD2  | 2.29                     | 0.68              |
| 1:1J:245:ASP:OD2  | 2:4V:77:SER:HB2   | 1.93                     | 0.68              |
| 1:1J:283:HIS:HA   | 1:1K:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1K:346:TRP:CH2  | 2:4W:403:ALA:HB1  | 2.29                     | 0.68              |
| 2:1S:11:GLN:HE22  | 1:2F:249:ASN:H    | 1.41                     | 0.68              |
| 2:1S:404:PHE:CZ   | 1:2F:261:PRO:HA   | 2.29                     | 0.68              |
| 2:1Z:401:ARG:O    | 1:2N:262:TYR:OH   | 2.11                     | 0.68              |
| 2:2Q:101:ASN:N    | 1:3D:254:GLU:HG2  | 2.08                     | 0.68              |
| 2:2V:100:GLY:CA   | 1:3J:253:THR:HB   | 2.24                     | 0.68              |
| 2:2X:181:VAL:H    | 1:3L:258:ASN:HD22 | 1.41                     | 0.68              |
| 2:2Y:181:VAL:HB   | 1:3M:258:ASN:O    | 1.93                     | 0.68              |
| 1:1B:346:TRP:CA   | 2:4O:397:ALA:O    | 2.42                     | 0.68              |
| 1:1C:346:TRP:CB   | 2:4P:397:ALA:C    | 2.66                     | 0.68              |
| 1:1D:261:PRO:HB3  | 2:4Q:404:PHE:CE2  | 2.29                     | 0.68              |
| 1:1D:329:ASN:CB   | 2:4Q:210:TYR:CE2  | 2.77                     | 0.68              |
| 1:1F:329:ASN:HD22 | 2:4S:210:TYR:HD2  | 1.42                     | 0.68              |
| 1:1G:257:THR:HG21 | 2:4T:102:ASN:CA   | 2.23                     | 0.68              |
| 1:1J:352:LYS:HD3  | 2:4V:101:ASN:ND2  | 2.09                     | 0.68              |
| 2:1U:404:PHE:HE1  | 1:2I:260:VAL:C    | 1.99                     | 0.68              |
| 1:2G:283:HIS:HA   | 1:2I:62:VAL:HG11  | 1.76                     | 0.68              |
| 2:2U:221:THR:CA   | 1:3I:324:VAL:HG11 | 2.24                     | 0.68              |
| 2:2W:221:THR:CB   | 1:3K:324:VAL:HG21 | 2.24                     | 0.68              |
| 2:2W:394:GLN:CB   | 1:3K:348:PRO:HG3  | 2.23                     | 0.68              |
| 2:2X:404:PHE:CD1  | 1:3L:260:VAL:C    | 2.70                     | 0.68              |
| 2:2Y:224:TYR:CD2  | 1:3M:247:ALA:O    | 2.47                     | 0.68              |
| 1:3A:62:VAL:HG11  | 1:3N:283:HIS:HA   | 1.76                     | 0.68              |
| 1:3A:283:HIS:HA   | 1:3B:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:3G:283:HIS:HA   | 1:3I:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:4G:283:HIS:HA   | 1:4I:62:VAL:HG11  | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4J:283:HIS:HA   | 1:4K:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1A:283:HIS:HA   | 1:1B:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1D:329:ASN:HD22 | 2:4Q:210:TYR:HD2  | 1.42                     | 0.68              |
| 1:1E:2:ARG:HH11   | 2:4R:71:GLU:HB2   | 1.59                     | 0.68              |
| 1:1E:326:LYS:HG2  | 2:4R:210:TYR:CG   | 2.29                     | 0.68              |
| 1:1G:263:PRO:CD   | 2:4T:406:HIS:CD2  | 2.77                     | 0.68              |
| 1:1G:352:LYS:CD   | 2:4T:101:ASN:ND2  | 2.57                     | 0.68              |
| 1:1J:257:THR:HG21 | 2:4V:102:ASN:CB   | 2.22                     | 0.68              |
| 1:1K:261:PRO:HA   | 2:4W:404:PHE:CD1  | 2.28                     | 0.68              |
| 2:1V:207:GLU:OE2  | 1:2J:329:ASN:ND2  | 2.25                     | 0.68              |
| 1:2A:62:VAL:HG11  | 1:2N:283:HIS:HA   | 1.76                     | 0.68              |
| 2:2Q:407:TRP:HE1  | 1:3D:260:VAL:CB   | 2.07                     | 0.68              |
| 2:2R:394:GLN:HG2  | 1:3E:348:PRO:HB2  | 1.72                     | 0.68              |
| 2:2X:221:THR:CB   | 1:3L:324:VAL:HG21 | 2.23                     | 0.68              |
| 2:2Z:404:PHE:CE1  | 1:3N:261:PRO:N    | 2.62                     | 0.68              |
| 1:4A:62:VAL:HG11  | 1:4N:283:HIS:HA   | 1.76                     | 0.68              |
| 1:4A:283:HIS:HA   | 1:4B:62:VAL:HG11  | 1.76                     | 0.68              |
| 1:1A:62:VAL:HG11  | 1:1N:283:HIS:HA   | 1.76                     | 0.67              |
| 1:1B:283:HIS:HA   | 1:1C:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1B:349:THR:OG1  | 2:4O:184:PRO:CD   | 2.42                     | 0.67              |
| 1:1B:349:THR:HG21 | 2:4O:184:PRO:HD3  | 1.75                     | 0.67              |
| 1:1C:259:LEU:C    | 2:4P:404:PHE:HE1  | 2.02                     | 0.67              |
| 1:1D:346:TRP:HB2  | 2:4Q:397:ALA:C    | 2.19                     | 0.67              |
| 1:1E:348:PRO:CG   | 2:4R:394:GLN:HG2  | 2.23                     | 0.67              |
| 1:1G:283:HIS:HA   | 1:1I:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1I:263:PRO:CD   | 2:4U:406:HIS:CG   | 2.74                     | 0.67              |
| 1:1I:351:PHE:O    | 2:4U:180:THR:N    | 2.27                     | 0.67              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:HA   | 1.94                     | 0.67              |
| 2:1W:181:VAL:CG2  | 1:2K:258:ASN:CA   | 2.72                     | 0.67              |
| 1:2B:283:HIS:HA   | 1:2C:62:VAL:HG11  | 1.76                     | 0.67              |
| 2:2T:100:GLY:CA   | 1:3G:253:THR:HB   | 2.24                     | 0.67              |
| 2:2T:404:PHE:CD1  | 1:3G:260:VAL:C    | 2.72                     | 0.67              |
| 2:2W:404:PHE:CZ   | 1:3K:261:PRO:HB3  | 2.28                     | 0.67              |
| 2:2Y:100:GLY:O    | 1:3M:257:THR:OG1  | 2.12                     | 0.67              |
| 1:1A:249:ASN:H    | 2:4H:11:GLN:CD    | 1.97                     | 0.67              |
| 1:1D:261:PRO:C    | 2:4Q:404:PHE:HA   | 2.19                     | 0.67              |
| 1:1D:346:TRP:HA   | 2:4Q:397:ALA:HB1  | 1.76                     | 0.67              |
| 1:1F:261:PRO:C    | 2:4S:406:HIS:CD2  | 2.72                     | 0.67              |
| 1:1G:351:PHE:O    | 2:4T:181:VAL:N    | 2.27                     | 0.67              |
| 1:1J:263:PRO:N    | 2:4V:406:HIS:CE1  | 2.62                     | 0.67              |
| 1:1K:283:HIS:HA   | 1:1L:62:VAL:HG11  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1L:248:LEU:HD13 | 5:4X:501:GDP:C8   | 2.29                     | 0.67              |
| 1:1N:248:LEU:CD1  | 5:4Z:501:GDP:H8   | 2.07                     | 0.67              |
| 2:1Y:394:GLN:HG2  | 1:2M:348:PRO:HG3  | 1.76                     | 0.67              |
| 2:1Z:181:VAL:HB   | 1:2N:258:ASN:CA   | 2.23                     | 0.67              |
| 1:2A:283:HIS:HA   | 1:2B:62:VAL:HG11  | 1.76                     | 0.67              |
| 2:2H:177:VAL:CG2  | 1:3A:332:ILE:HG21 | 2.23                     | 0.67              |
| 2:2U:100:GLY:HA2  | 1:3I:253:THR:C    | 2.19                     | 0.67              |
| 2:2X:177:VAL:CG2  | 1:3L:332:ILE:HG21 | 2.25                     | 0.67              |
| 2:2Z:181:VAL:HB   | 1:3N:258:ASN:O    | 1.93                     | 0.67              |
| 2:2Z:224:TYR:CD2  | 1:3N:247:ALA:O    | 2.47                     | 0.67              |
| 1:3B:283:HIS:HA   | 1:3C:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:4B:283:HIS:HA   | 1:4C:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1B:326:LYS:HE2  | 2:4O:210:TYR:O    | 1.93                     | 0.67              |
| 1:1C:283:HIS:HA   | 1:1D:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1C:346:TRP:HB2  | 2:4P:397:ALA:C    | 2.19                     | 0.67              |
| 1:1G:324:VAL:HG13 | 2:4T:222:PRO:C    | 2.19                     | 0.67              |
| 1:1I:349:THR:OG1  | 2:4U:184:PRO:CD   | 2.43                     | 0.67              |
| 1:1K:260:VAL:CB   | 2:4W:407:TRP:HE1  | 2.06                     | 0.67              |
| 1:1M:260:VAL:CB   | 2:4Y:407:TRP:HE1  | 2.07                     | 0.67              |
| 2:2H:180:THR:CG2  | 1:3A:258:ASN:ND2  | 2.38                     | 0.67              |
| 2:2H:401:ARG:NH2  | 1:3A:435:VAL:CA   | 2.38                     | 0.67              |
| 2:2H:404:PHE:CD1  | 1:3A:260:VAL:C    | 2.73                     | 0.67              |
| 2:2T:180:THR:HG23 | 1:3G:258:ASN:HD21 | 0.72                     | 0.67              |
| 2:2Z:404:PHE:CD1  | 1:3N:260:VAL:C    | 2.72                     | 0.67              |
| 1:3C:283:HIS:HA   | 1:3D:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:3K:283:HIS:HA   | 1:3L:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1C:346:TRP:HA   | 2:4P:397:ALA:O    | 1.93                     | 0.67              |
| 1:1C:349:THR:CB   | 2:4P:184:PRO:HD3  | 2.25                     | 0.67              |
| 1:1D:261:PRO:HA   | 2:4Q:404:PHE:CD1  | 2.29                     | 0.67              |
| 1:1E:2:ARG:HG3    | 2:4R:72:PRO:CD    | 2.25                     | 0.67              |
| 1:1E:329:ASN:ND2  | 2:4R:207:GLU:CD   | 2.51                     | 0.67              |
| 1:1F:348:PRO:HG3  | 2:4S:394:GLN:C    | 2.18                     | 0.67              |
| 1:2C:283:HIS:HA   | 1:2D:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:2K:283:HIS:HA   | 1:2L:62:VAL:HG11  | 1.76                     | 0.67              |
| 2:2H:404:PHE:H    | 1:3A:261:PRO:C    | 1.99                     | 0.67              |
| 2:2Q:404:PHE:CD1  | 1:3D:260:VAL:O    | 2.47                     | 0.67              |
| 2:2U:210:TYR:CE2  | 1:3I:329:ASN:HB2  | 2.30                     | 0.67              |
| 2:2U:222:PRO:O    | 1:3I:325:PRO:HD2  | 1.95                     | 0.67              |
| 2:2X:181:VAL:CB   | 1:3L:258:ASN:O    | 2.42                     | 0.67              |
| 2:2Y:404:PHE:CD1  | 1:3M:260:VAL:C    | 2.71                     | 0.67              |
| 1:4C:283:HIS:HA   | 1:4D:62:VAL:HG11  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:4K:283:HIS:HA   | 1:4L:62:VAL:HG11 | 1.76                     | 0.67              |
| 1:1D:283:HIS:HA   | 1:1E:62:VAL:HG11 | 1.76                     | 0.67              |
| 1:1F:261:PRO:CB   | 2:4S:404:PHE:H   | 2.08                     | 0.67              |
| 1:1F:346:TRP:CE2  | 2:4S:403:ALA:HB2 | 2.30                     | 0.67              |
| 1:1I:346:TRP:C    | 2:4U:398:MET:HG2 | 2.17                     | 0.67              |
| 1:1I:348:PRO:CD   | 2:4U:398:MET:HG3 | 2.23                     | 0.67              |
| 1:1K:263:PRO:N    | 2:4W:406:HIS:CE1 | 2.63                     | 0.67              |
| 2:1W:404:PHE:CE2  | 1:2K:261:PRO:CA  | 2.76                     | 0.67              |
| 1:2F:283:HIS:HA   | 1:2G:62:VAL:HG11 | 1.76                     | 0.67              |
| 2:2Q:77:SER:CB    | 1:3D:245:ASP:CG  | 2.67                     | 0.67              |
| 2:2S:100:GLY:HA2  | 1:3F:253:THR:C   | 2.19                     | 0.67              |
| 2:2S:101:ASN:ND2  | 1:3F:258:ASN:OD1 | 2.28                     | 0.67              |
| 2:2Y:180:THR:CG2  | 1:3M:258:ASN:ND2 | 2.38                     | 0.67              |
| 1:1A:261:PRO:O    | 2:4H:404:PHE:HA  | 1.94                     | 0.67              |
| 1:1B:253:THR:HB   | 2:4O:100:GLY:CA  | 2.24                     | 0.67              |
| 1:1F:260:VAL:CG1  | 2:4S:407:TRP:CZ2 | 2.78                     | 0.67              |
| 1:1M:348:PRO:HG2  | 2:4Y:394:GLN:HB3 | 1.77                     | 0.67              |
| 2:1U:406:HIS:NE2  | 1:2I:263:PRO:HD3 | 2.09                     | 0.67              |
| 1:2D:283:HIS:HA   | 1:2E:62:VAL:HG11 | 1.76                     | 0.67              |
| 2:2O:179:ASP:O    | 1:3B:352:LYS:CD  | 2.34                     | 0.67              |
| 2:2P:72:PRO:HD2   | 1:3C:2:ARG:CG    | 2.25                     | 0.67              |
| 2:2P:401:ARG:C    | 1:3C:262:TYR:HH  | 1.92                     | 0.67              |
| 2:2R:223:THR:HA   | 1:3E:325:PRO:HD2 | 1.77                     | 0.67              |
| 2:2S:100:GLY:O    | 1:3F:257:THR:OG1 | 2.09                     | 0.67              |
| 2:2U:406:HIS:CE1  | 1:3I:263:PRO:CA  | 2.78                     | 0.67              |
| 2:2W:181:VAL:HG21 | 1:3K:258:ASN:O   | 1.93                     | 0.67              |
| 2:2Z:214:PHE:CB   | 1:3N:326:LYS:CE  | 2.65                     | 0.67              |
| 2:2Z:394:GLN:HA   | 1:3N:348:PRO:HG3 | 1.77                     | 0.67              |
| 1:3D:283:HIS:HA   | 1:3E:62:VAL:HG11 | 1.76                     | 0.67              |
| 1:4F:283:HIS:HA   | 1:4G:62:VAL:HG11 | 1.76                     | 0.67              |
| 1:1B:258:ASN:O    | 2:4O:181:VAL:HB  | 1.95                     | 0.67              |
| 1:1D:349:THR:HG23 | 2:4Q:184:PRO:HG3 | 1.75                     | 0.67              |
| 1:1F:2:ARG:CD     | 2:4S:72:PRO:CD   | 2.57                     | 0.67              |
| 1:1F:326:LYS:HG2  | 2:4S:210:TYR:CB  | 2.24                     | 0.67              |
| 1:1G:2:ARG:HG3    | 2:4T:72:PRO:CG   | 2.24                     | 0.67              |
| 1:1L:261:PRO:HA   | 2:4X:404:PHE:HA  | 1.76                     | 0.67              |
| 1:1M:2:ARG:HD3    | 2:4Y:72:PRO:CD   | 2.13                     | 0.67              |
| 2:1S:214:PHE:CG   | 1:2F:326:LYS:CE  | 2.77                     | 0.67              |
| 2:2H:181:VAL:HB   | 1:3A:258:ASN:O   | 1.93                     | 0.67              |
| 2:2P:394:GLN:CB   | 1:3C:348:PRO:HG3 | 2.25                     | 0.67              |
| 2:2P:407:TRP:NE1  | 1:3C:260:VAL:HB  | 2.09                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:221:THR:OG1  | 1:3E:324:VAL:CG2  | 2.43                     | 0.67              |
| 2:2U:176:LYS:HE2  | 1:3I:333:ALA:CB   | 2.24                     | 0.67              |
| 2:2W:176:LYS:HE2  | 1:3K:333:ALA:CB   | 2.23                     | 0.67              |
| 2:2X:223:THR:HA   | 1:3L:325:PRO:HD2  | 1.77                     | 0.67              |
| 1:3F:283:HIS:HA   | 1:3G:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:4D:283:HIS:HA   | 1:4E:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1C:349:THR:CG2  | 2:4P:184:PRO:HD3  | 2.25                     | 0.67              |
| 1:1E:262:TYR:N    | 2:4R:406:HIS:CD2  | 2.58                     | 0.67              |
| 1:1F:283:HIS:HA   | 1:1G:62:VAL:HG11  | 1.76                     | 0.67              |
| 1:1I:348:PRO:HB2  | 2:4U:394:GLN:HG2  | 1.75                     | 0.67              |
| 2:1X:404:PHE:HE1  | 1:2L:260:VAL:H    | 1.41                     | 0.67              |
| 2:1Z:181:VAL:CB   | 1:2N:258:ASN:O    | 2.43                     | 0.67              |
| 2:2P:394:GLN:CB   | 1:3C:348:PRO:CG   | 2.73                     | 0.67              |
| 1:1A:324:VAL:CG2  | 2:4H:221:THR:OG1  | 2.40                     | 0.67              |
| 1:1B:248:LEU:HD11 | 5:4O:501:GDP:H8   | 1.57                     | 0.67              |
| 1:1B:329:ASN:CB   | 2:4O:210:TYR:CD2  | 2.78                     | 0.67              |
| 1:1C:254:GLU:CB   | 2:4P:101:ASN:HB2  | 2.24                     | 0.67              |
| 1:1C:332:ILE:CB   | 2:4P:177:VAL:HG23 | 2.24                     | 0.67              |
| 1:1E:329:ASN:HB3  | 2:4R:210:TYR:CD2  | 2.29                     | 0.67              |
| 1:1F:254:GLU:HA   | 2:4S:100:GLY:CA   | 2.25                     | 0.67              |
| 1:1F:329:ASN:CB   | 2:4S:210:TYR:CD2  | 2.77                     | 0.67              |
| 1:1G:254:GLU:CA   | 2:4T:100:GLY:CA   | 2.73                     | 0.67              |
| 1:1G:326:LYS:HA   | 2:4T:210:TYR:CZ   | 2.30                     | 0.67              |
| 1:1I:349:THR:CG2  | 2:4U:184:PRO:CG   | 2.73                     | 0.67              |
| 1:1J:248:LEU:HD13 | 5:4V:501:GDP:H8   | 1.58                     | 0.67              |
| 1:1K:263:PRO:HD3  | 2:4W:406:HIS:CD2  | 2.29                     | 0.67              |
| 1:1M:261:PRO:CA   | 2:4Y:404:PHE:CD1  | 2.77                     | 0.67              |
| 1:1M:263:PRO:CD   | 2:4Y:406:HIS:CD2  | 2.78                     | 0.67              |
| 1:1N:263:PRO:CD   | 2:4Z:406:HIS:CG   | 2.69                     | 0.67              |
| 2:2S:223:THR:HA   | 1:3F:325:PRO:CD   | 2.25                     | 0.67              |
| 2:2T:224:TYR:HE2  | 1:3G:248:LEU:HB2  | 1.60                     | 0.67              |
| 1:1A:349:THR:HG21 | 2:4H:184:PRO:HD3  | 1.77                     | 0.67              |
| 1:1B:346:TRP:HB2  | 2:4O:398:MET:CA   | 2.20                     | 0.67              |
| 1:1D:249:ASN:N    | 2:4Q:11:GLN:OE1   | 2.27                     | 0.67              |
| 1:1F:439:SER:CB   | 2:4S:400:ARG:HD2  | 2.24                     | 0.67              |
| 1:1G:249:ASN:N    | 2:4T:11:GLN:CD    | 2.36                     | 0.67              |
| 1:1G:253:THR:C    | 2:4T:100:GLY:HA3  | 2.19                     | 0.67              |
| 1:1G:346:TRP:CE2  | 2:4T:403:ALA:HB2  | 2.29                     | 0.67              |
| 1:1J:261:PRO:C    | 2:4V:406:HIS:CD2  | 2.69                     | 0.67              |
| 1:1K:329:ASN:ND2  | 2:4W:210:TYR:HD2  | 1.90                     | 0.67              |
| 1:1L:260:VAL:CG1  | 2:4X:407:TRP:HZ2  | 2.07                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:245:ASP:OD2  | 2:4Y:77:SER:CB    | 2.43                     | 0.67              |
| 1:1M:349:THR:HG21 | 2:4Y:184:PRO:CD   | 2.18                     | 0.67              |
| 2:1X:71:GLU:HB2   | 1:2L:2:ARG:HD3    | 1.76                     | 0.67              |
| 2:2Q:177:VAL:CG2  | 1:3D:332:ILE:CG2  | 2.68                     | 0.67              |
| 1:1D:253:THR:CG2  | 2:4Q:100:GLY:HA3  | 2.24                     | 0.66              |
| 1:1E:332:ILE:HG22 | 2:4R:177:VAL:CG2  | 1.98                     | 0.66              |
| 1:1G:247:ALA:O    | 2:4T:15:GLN:NE2   | 2.28                     | 0.66              |
| 1:1L:260:VAL:CB   | 2:4X:407:TRP:CZ2  | 2.77                     | 0.66              |
| 1:1M:346:TRP:HZ3  | 2:4Y:404:PHE:HE2  | 1.42                     | 0.66              |
| 2:2R:100:GLY:CA   | 1:3E:253:THR:CB   | 2.73                     | 0.66              |
| 2:2R:101:ASN:N    | 1:3E:254:GLU:HG2  | 2.10                     | 0.66              |
| 2:2V:222:PRO:CG   | 1:3J:326:LYS:CB   | 2.69                     | 0.66              |
| 1:1B:263:PRO:HA   | 2:4O:406:HIS:CE1  | 2.30                     | 0.66              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:N    | 2.09                     | 0.66              |
| 1:1E:349:THR:O    | 2:4R:181:VAL:HA   | 1.95                     | 0.66              |
| 1:1F:261:PRO:O    | 2:4S:406:HIS:CD2  | 2.48                     | 0.66              |
| 1:1F:349:THR:HG21 | 2:4S:184:PRO:CG   | 2.23                     | 0.66              |
| 1:1I:435:VAL:HA   | 2:4U:401:ARG:NH2  | 2.10                     | 0.66              |
| 1:1K:346:TRP:HZ3  | 2:4W:404:PHE:HE2  | 1.40                     | 0.66              |
| 1:1L:283:HIS:HA   | 1:1M:62:VAL:HG11  | 1.76                     | 0.66              |
| 2:1H:394:GLN:HG2  | 1:2A:348:PRO:CG   | 2.25                     | 0.66              |
| 2:1T:100:GLY:CA   | 1:2G:253:THR:HG21 | 2.19                     | 0.66              |
| 2:1U:221:THR:OG1  | 1:2I:324:VAL:HG21 | 1.94                     | 0.66              |
| 2:2R:100:GLY:O    | 1:3E:254:GLU:HA   | 1.95                     | 0.66              |
| 1:3L:283:HIS:HA   | 1:3M:62:VAL:HG11  | 1.76                     | 0.66              |
| 1:1B:348:PRO:HG3  | 2:4O:394:GLN:CG   | 2.16                     | 0.66              |
| 1:1E:283:HIS:HA   | 1:1F:62:VAL:HG11  | 1.76                     | 0.66              |
| 1:1F:260:VAL:CG1  | 2:4S:406:HIS:HE1  | 2.05                     | 0.66              |
| 1:1I:247:ALA:O    | 2:4U:15:GLN:NE2   | 2.28                     | 0.66              |
| 1:1J:348:PRO:CB   | 2:4V:394:GLN:HG2  | 2.25                     | 0.66              |
| 2:1O:214:PHE:CB   | 1:2B:326:LYS:HE2  | 2.25                     | 0.66              |
| 2:2S:406:HIS:CE1  | 1:3F:263:PRO:N    | 2.63                     | 0.66              |
| 2:2Z:100:GLY:HA3  | 1:3N:253:THR:CB   | 2.26                     | 0.66              |
| 1:1D:326:LYS:CA   | 2:4Q:210:TYR:CD1  | 2.77                     | 0.66              |
| 1:1F:2:ARG:NH2    | 2:4S:73:GLY:CA    | 2.59                     | 0.66              |
| 1:1F:332:ILE:CB   | 2:4S:177:VAL:HG21 | 2.22                     | 0.66              |
| 1:1G:347:CYS:HA   | 2:4T:398:MET:CG   | 2.25                     | 0.66              |
| 1:1I:260:VAL:CB   | 2:4U:407:TRP:CE2  | 2.67                     | 0.66              |
| 1:1I:325:PRO:CB   | 2:4U:224:TYR:CE1  | 2.78                     | 0.66              |
| 1:1N:253:THR:C    | 2:4Z:100:GLY:HA2  | 2.20                     | 0.66              |
| 1:1N:262:TYR:N    | 2:4Z:406:HIS:NE2  | 2.43                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1P:101:ASN:HB2  | 1:2C:254:GLU:HG2  | 1.77                     | 0.66              |
| 2:1S:222:PRO:O    | 1:2F:325:PRO:HD2  | 1.94                     | 0.66              |
| 2:1X:404:PHE:HE1  | 1:2L:260:VAL:N    | 1.92                     | 0.66              |
| 1:2L:283:HIS:HA   | 1:2M:62:VAL:HG11  | 1.76                     | 0.66              |
| 2:2O:222:PRO:O    | 1:3B:325:PRO:HD2  | 1.94                     | 0.66              |
| 2:2R:180:THR:CG2  | 1:3E:258:ASN:ND2  | 2.36                     | 0.66              |
| 2:2S:407:TRP:HE1  | 1:3F:260:VAL:CB   | 2.09                     | 0.66              |
| 2:2V:100:GLY:CA   | 1:3J:253:THR:CB   | 2.74                     | 0.66              |
| 1:1C:254:GLU:N    | 2:4P:100:GLY:CA   | 2.57                     | 0.66              |
| 1:1E:326:LYS:CA   | 2:4R:210:TYR:CD1  | 2.77                     | 0.66              |
| 1:1E:349:THR:HG21 | 2:4R:184:PRO:HG3  | 1.77                     | 0.66              |
| 1:1F:257:THR:CB   | 2:4S:100:GLY:O    | 2.44                     | 0.66              |
| 1:1G:434:GLU:O    | 2:4T:401:ARG:NH2  | 2.29                     | 0.66              |
| 1:1K:248:LEU:HD13 | 5:4W:501:GDP:C8   | 2.30                     | 0.66              |
| 1:1K:348:PRO:HG3  | 2:4W:394:GLN:CA   | 2.25                     | 0.66              |
| 2:1V:394:GLN:HG2  | 1:2J:348:PRO:HG2  | 1.76                     | 0.66              |
| 2:1X:180:THR:HG23 | 1:2L:258:ASN:HD21 | 1.59                     | 0.66              |
| 1:2E:283:HIS:HA   | 1:2F:62:VAL:HG11  | 1.76                     | 0.66              |
| 2:2T:394:GLN:HB3  | 1:3G:348:PRO:HG2  | 1.76                     | 0.66              |
| 1:3E:283:HIS:HA   | 1:3F:62:VAL:HG11  | 1.76                     | 0.66              |
| 1:4E:283:HIS:HA   | 1:4F:62:VAL:HG11  | 1.76                     | 0.66              |
| 1:4L:283:HIS:HA   | 1:4M:62:VAL:HG11  | 1.76                     | 0.66              |
| 1:1B:2:ARG:HG3    | 2:4O:72:PRO:CG    | 2.25                     | 0.66              |
| 1:1B:348:PRO:HG2  | 2:4O:394:GLN:CB   | 2.06                     | 0.66              |
| 1:1G:260:VAL:CG1  | 2:4T:407:TRP:NE1  | 2.59                     | 0.66              |
| 1:1N:248:LEU:CD1  | 5:4Z:501:GDP:C8   | 2.79                     | 0.66              |
| 2:1S:214:PHE:CD1  | 1:2F:326:LYS:HE3  | 2.30                     | 0.66              |
| 2:1U:180:THR:C    | 1:2I:258:ASN:ND2  | 2.54                     | 0.66              |
| 2:1U:222:PRO:CG   | 1:2I:326:LYS:HB2  | 2.25                     | 0.66              |
| 2:1V:404:PHE:CZ   | 1:2J:261:PRO:N    | 2.63                     | 0.66              |
| 2:1Y:404:PHE:N    | 1:2M:261:PRO:O    | 2.26                     | 0.66              |
| 2:2S:404:PHE:CD1  | 1:3F:260:VAL:C    | 2.73                     | 0.66              |
| 2:2W:181:VAL:HB   | 1:3K:258:ASN:O    | 1.95                     | 0.66              |
| 1:1B:324:VAL:CG1  | 2:4O:222:PRO:O    | 2.44                     | 0.66              |
| 1:1C:326:LYS:HG2  | 2:4P:210:TYR:CB   | 2.26                     | 0.66              |
| 1:1E:352:LYS:CE   | 2:4R:101:ASN:HD22 | 2.06                     | 0.66              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:CG   | 2.31                     | 0.66              |
| 1:1I:254:GLU:HA   | 2:4U:100:GLY:CA   | 2.24                     | 0.66              |
| 1:1J:260:VAL:CB   | 2:4V:407:TRP:HE1  | 1.94                     | 0.66              |
| 1:1K:326:LYS:HA   | 2:4W:210:TYR:CE1  | 2.31                     | 0.66              |
| 2:2O:221:THR:OG1  | 1:3B:324:VAL:CG2  | 2.44                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:101:ASN:N    | 1:3C:254:GLU:HG2  | 2.10                     | 0.66              |
| 2:2V:176:LYS:HE2  | 1:3J:333:ALA:CB   | 2.24                     | 0.66              |
| 2:2V:179:ASP:OD1  | 1:3J:353:VAL:HB   | 1.96                     | 0.66              |
| 2:2V:403:ALA:HA   | 1:3J:262:TYR:CZ   | 2.31                     | 0.66              |
| 2:2V:406:HIS:CE1  | 1:3J:263:PRO:CA   | 2.78                     | 0.66              |
| 1:1E:261:PRO:C    | 2:4R:404:PHE:HA   | 2.19                     | 0.66              |
| 2:2O:177:VAL:HG23 | 1:3B:332:ILE:HG22 | 1.78                     | 0.66              |
| 2:2P:397:ALA:HB1  | 1:3C:346:TRP:HA   | 1.78                     | 0.66              |
| 2:2V:100:GLY:HA2  | 1:3J:253:THR:CB   | 2.25                     | 0.66              |
| 2:2X:397:ALA:O    | 1:3L:346:TRP:HB2  | 1.95                     | 0.66              |
| 2:2Y:181:VAL:N    | 1:3M:258:ASN:HD22 | 1.93                     | 0.66              |
| 1:1A:253:THR:C    | 2:4H:100:GLY:CA   | 2.69                     | 0.66              |
| 1:1C:260:VAL:HG12 | 2:4P:407:TRP:HE1  | 1.61                     | 0.66              |
| 1:1E:353:VAL:CA   | 2:4R:179:ASP:OD1  | 2.44                     | 0.66              |
| 1:1F:329:ASN:HB3  | 2:4S:210:TYR:CD2  | 2.31                     | 0.66              |
| 1:1N:329:ASN:ND2  | 2:4Z:210:TYR:CD2  | 2.54                     | 0.66              |
| 2:1P:214:PHE:CB   | 1:2C:326:LYS:HE2  | 2.24                     | 0.66              |
| 2:2R:404:PHE:CD1  | 1:3E:260:VAL:O    | 2.49                     | 0.66              |
| 2:2U:100:GLY:CA   | 1:3I:253:THR:HB   | 2.26                     | 0.66              |
| 2:2Y:177:VAL:CG2  | 1:3M:332:ILE:HG21 | 2.26                     | 0.66              |
| 1:1C:332:ILE:HB   | 2:4P:177:VAL:CG2  | 2.25                     | 0.66              |
| 1:1G:326:LYS:CA   | 2:4T:210:TYR:CE1  | 2.78                     | 0.66              |
| 1:1I:253:THR:C    | 2:4U:100:GLY:HA2  | 2.22                     | 0.66              |
| 1:1L:324:VAL:HG21 | 2:4X:221:THR:OG1  | 1.95                     | 0.66              |
| 2:1R:221:THR:OG1  | 1:2E:324:VAL:HG21 | 1.95                     | 0.66              |
| 2:1V:404:PHE:N    | 1:2J:261:PRO:O    | 2.24                     | 0.66              |
| 2:2Q:100:GLY:O    | 1:3D:254:GLU:HA   | 1.94                     | 0.66              |
| 2:2U:404:PHE:CA   | 1:3I:261:PRO:O    | 2.44                     | 0.66              |
| 2:2V:73:GLY:HA3   | 1:3J:2:ARG:CZ     | 2.26                     | 0.66              |
| 2:2Z:181:VAL:N    | 1:3N:258:ASN:HD22 | 1.94                     | 0.66              |
| 1:1A:2:ARG:HG3    | 2:4H:72:PRO:HG2   | 1.79                     | 0.65              |
| 1:1A:261:PRO:N    | 2:4H:404:PHE:CE1  | 2.64                     | 0.65              |
| 1:1F:254:GLU:HB3  | 2:4S:101:ASN:HB2  | 1.77                     | 0.65              |
| 1:1G:352:LYS:CE   | 2:4T:101:ASN:ND2  | 2.59                     | 0.65              |
| 1:1I:349:THR:HG23 | 2:4U:184:PRO:CG   | 2.25                     | 0.65              |
| 2:2R:11:GLN:CD    | 1:3E:249:ASN:H    | 2.00                     | 0.65              |
| 2:2S:404:PHE:CD1  | 1:3F:260:VAL:O    | 2.49                     | 0.65              |
| 2:2Y:101:ASN:HB2  | 1:3M:254:GLU:CG   | 2.25                     | 0.65              |
| 2:2Z:177:VAL:CG2  | 1:3N:332:ILE:HG21 | 2.25                     | 0.65              |
| 1:1C:325:PRO:HG2  | 2:4P:224:TYR:CD1  | 2.32                     | 0.65              |
| 1:1D:261:PRO:CA   | 2:4Q:404:PHE:CD1  | 2.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:2:ARG:HH11   | 2:4T:71:GLU:HB2   | 1.60                     | 0.65              |
| 1:1I:261:PRO:CA   | 2:4U:404:PHE:HA   | 2.22                     | 0.65              |
| 2:1V:182:VAL:CG2  | 1:2J:257:THR:CG2  | 2.72                     | 0.65              |
| 2:2P:404:PHE:CD1  | 1:3C:260:VAL:C    | 2.74                     | 0.65              |
| 2:2T:406:HIS:CE1  | 1:3G:263:PRO:CA   | 2.80                     | 0.65              |
| 1:1C:353:VAL:CA   | 2:4P:179:ASP:OD1  | 2.43                     | 0.65              |
| 1:1C:435:VAL:CA   | 2:4P:401:ARG:HH21 | 1.91                     | 0.65              |
| 1:1D:248:LEU:HA   | 2:4Q:11:GLN:NE2   | 2.12                     | 0.65              |
| 1:1G:326:LYS:HG2  | 2:4T:210:TYR:CG   | 2.31                     | 0.65              |
| 2:2R:404:PHE:CD1  | 1:3E:260:VAL:C    | 2.74                     | 0.65              |
| 2:2W:73:GLY:HA3   | 1:3K:2:ARG:NH2    | 2.10                     | 0.65              |
| 2:2Z:181:VAL:CG2  | 1:3N:258:ASN:O    | 2.45                     | 0.65              |
| 1:1D:257:THR:HG21 | 2:4Q:102:ASN:HA   | 1.79                     | 0.65              |
| 1:1E:352:LYS:HD3  | 2:4R:101:ASN:HD21 | 1.61                     | 0.65              |
| 1:1F:2:ARG:HD3    | 2:4S:71:GLU:HB2   | 1.77                     | 0.65              |
| 1:1F:349:THR:OG1  | 2:4S:181:VAL:O    | 2.11                     | 0.65              |
| 1:1L:348:PRO:HG3  | 2:4X:394:GLN:CA   | 2.26                     | 0.65              |
| 1:1M:248:LEU:HD12 | 2:4Y:11:GLN:CD    | 2.21                     | 0.65              |
| 2:1S:179:ASP:O    | 1:2F:352:LYS:HD2  | 1.97                     | 0.65              |
| 2:1X:181:VAL:CG2  | 1:2L:258:ASN:CA   | 2.75                     | 0.65              |
| 2:1Y:401:ARG:NH2  | 1:2M:435:VAL:HA   | 1.96                     | 0.65              |
| 2:2P:180:THR:CG2  | 1:3C:258:ASN:ND2  | 2.37                     | 0.65              |
| 2:2T:403:ALA:HA   | 1:3G:262:TYR:CZ   | 2.32                     | 0.65              |
| 1:1F:262:TYR:OH   | 2:4S:402:LYS:C    | 2.40                     | 0.65              |
| 1:1F:262:TYR:CE1  | 2:4S:402:LYS:O    | 2.49                     | 0.65              |
| 1:1K:346:TRP:CD2  | 2:4W:403:ALA:HB2  | 2.31                     | 0.65              |
| 2:1P:100:GLY:HA2  | 1:2C:253:THR:HB   | 1.77                     | 0.65              |
| 2:1U:181:VAL:HG23 | 1:2I:258:ASN:CB   | 2.24                     | 0.65              |
| 2:1V:404:PHE:HE1  | 1:2J:260:VAL:C    | 1.98                     | 0.65              |
| 2:1W:221:THR:CB   | 1:2K:324:VAL:CG2  | 2.75                     | 0.65              |
| 2:2O:404:PHE:CD1  | 1:3B:260:VAL:C    | 2.73                     | 0.65              |
| 2:2Q:404:PHE:CD1  | 1:3D:260:VAL:C    | 2.74                     | 0.65              |
| 1:1B:262:TYR:N    | 2:4O:406:HIS:NE2  | 2.44                     | 0.65              |
| 1:1G:349:THR:HG23 | 2:4T:184:PRO:HG3  | 1.77                     | 0.65              |
| 1:1J:263:PRO:HD3  | 2:4V:406:HIS:CD2  | 2.31                     | 0.65              |
| 2:1W:214:PHE:CD1  | 1:2K:326:LYS:CE   | 2.77                     | 0.65              |
| 2:1W:404:PHE:CZ   | 1:2K:261:PRO:N    | 2.65                     | 0.65              |
| 2:2H:407:TRP:HE1  | 1:3A:260:VAL:HB   | 1.62                     | 0.65              |
| 2:2P:394:GLN:HB3  | 1:3C:348:PRO:HG2  | 1.79                     | 0.65              |
| 2:2V:101:ASN:ND2  | 1:3J:258:ASN:OD1  | 2.29                     | 0.65              |
| 1:1D:261:PRO:CA   | 2:4Q:404:PHE:CG   | 2.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:435:VAL:O    | 2:4U:401:ARG:NH2  | 2.30                     | 0.65              |
| 1:1K:260:VAL:HG11 | 2:4W:407:TRP:CZ2  | 2.31                     | 0.65              |
| 1:1M:348:PRO:CG   | 2:4Y:394:GLN:CB   | 2.70                     | 0.65              |
| 1:1N:261:PRO:O    | 2:4Z:404:PHE:N    | 2.29                     | 0.65              |
| 2:1W:179:ASP:O    | 1:2K:352:LYS:CE   | 2.44                     | 0.65              |
| 2:1X:180:THR:HA   | 1:2L:352:LYS:HD3  | 1.79                     | 0.65              |
| 2:2O:181:VAL:CB   | 1:3B:258:ASN:O    | 2.45                     | 0.65              |
| 1:1C:329:ASN:HB2  | 2:4P:210:TYR:CD2  | 2.32                     | 0.65              |
| 1:1C:332:ILE:HG21 | 2:4P:177:VAL:HG23 | 1.43                     | 0.65              |
| 1:1E:349:THR:HG23 | 2:4R:184:PRO:CG   | 2.21                     | 0.65              |
| 2:1T:180:THR:CA   | 1:2G:258:ASN:HD21 | 2.10                     | 0.65              |
| 2:1U:180:THR:HG23 | 1:2I:258:ASN:HD21 | 1.62                     | 0.65              |
| 2:2R:51:VAL:O     | 2:2R:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:2V:77:SER:CB    | 1:3J:245:ASP:CG   | 2.69                     | 0.65              |
| 2:3O:51:VAL:O     | 2:3O:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:4R:51:VAL:O     | 2:4R:64:ARG:NH1   | 2.30                     | 0.65              |
| 1:1A:326:LYS:HE2  | 2:4H:214:PHE:CB   | 2.25                     | 0.65              |
| 1:1B:349:THR:OG1  | 2:4O:184:PRO:HD3  | 1.96                     | 0.65              |
| 1:1E:262:TYR:OH   | 2:4R:402:LYS:C    | 2.39                     | 0.65              |
| 1:1G:353:VAL:HG23 | 2:4T:179:ASP:HA   | 1.79                     | 0.65              |
| 1:1I:348:PRO:HB2  | 2:4U:394:GLN:CG   | 2.27                     | 0.65              |
| 2:1O:51:VAL:O     | 2:1O:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:1R:51:VAL:O     | 2:1R:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:1R:404:PHE:CE1  | 1:2E:261:PRO:HA   | 2.31                     | 0.65              |
| 2:1V:101:ASN:O    | 1:2J:257:THR:HG21 | 1.97                     | 0.65              |
| 2:2O:51:VAL:O     | 2:2O:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:2Q:179:ASP:OD2  | 1:3D:248:LEU:CD2  | 2.44                     | 0.65              |
| 2:3R:51:VAL:O     | 2:3R:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:4P:51:VAL:O     | 2:4P:64:ARG:NH1   | 2.30                     | 0.65              |
| 1:1B:351:PHE:O    | 2:4O:180:THR:CA   | 2.45                     | 0.65              |
| 1:1C:422:ARG:HH12 | 1:1C:426:ALA:HB2  | 1.62                     | 0.65              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:HA   | 1.96                     | 0.65              |
| 1:1E:261:PRO:O    | 2:4R:404:PHE:CA   | 2.44                     | 0.65              |
| 1:1G:332:ILE:CB   | 2:4T:177:VAL:CG2  | 2.74                     | 0.65              |
| 1:1K:245:ASP:OD2  | 2:4W:77:SER:HB3   | 1.87                     | 0.65              |
| 1:1L:314:ALA:HB1  | 2:4X:181:VAL:HG21 | 1.78                     | 0.65              |
| 1:1L:329:ASN:ND2  | 2:4X:210:TYR:CD2  | 2.57                     | 0.65              |
| 2:1T:214:PHE:CG   | 1:2G:326:LYS:HE3  | 2.29                     | 0.65              |
| 2:1X:179:ASP:C    | 1:2L:352:LYS:HD2  | 2.20                     | 0.65              |
| 1:2N:422:ARG:HH12 | 1:2N:426:ALA:HB2  | 1.62                     | 0.65              |
| 2:2P:51:VAL:O     | 2:2P:64:ARG:NH1   | 2.30                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:73:GLY:HA3   | 1:3C:2:ARG:NH2    | 2.12                     | 0.65              |
| 2:2U:222:PRO:CG   | 1:3I:326:LYS:HB2  | 2.17                     | 0.65              |
| 2:2V:397:ALA:O    | 1:3J:346:TRP:CB   | 2.45                     | 0.65              |
| 2:2X:222:PRO:CG   | 1:3L:326:LYS:HB2  | 2.20                     | 0.65              |
| 1:3N:422:ARG:HH12 | 1:3N:426:ALA:HB2  | 1.62                     | 0.65              |
| 2:3P:51:VAL:O     | 2:3P:64:ARG:NH1   | 2.30                     | 0.65              |
| 2:4O:51:VAL:O     | 2:4O:64:ARG:NH1   | 2.30                     | 0.65              |
| 1:1D:435:VAL:CA   | 2:4Q:401:ARG:HH21 | 1.82                     | 0.64              |
| 1:1E:259:LEU:C    | 2:4R:404:PHE:HE1  | 2.04                     | 0.64              |
| 1:1E:353:VAL:CG2  | 2:4R:179:ASP:OD1  | 2.44                     | 0.64              |
| 1:1F:314:ALA:CB   | 2:4S:181:VAL:HG11 | 2.27                     | 0.64              |
| 1:1K:351:PHE:O    | 2:4W:180:THR:C    | 2.39                     | 0.64              |
| 1:1N:422:ARG:HH12 | 1:1N:426:ALA:HB2  | 1.63                     | 0.64              |
| 2:1H:422:GLU:OE2  | 2:1H:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:1Q:401:ARG:HH22 | 1:2D:435:VAL:HA   | 1.63                     | 0.64              |
| 2:2H:422:GLU:OE2  | 2:2H:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:2Q:397:ALA:HB1  | 1:3D:346:TRP:HA   | 1.78                     | 0.64              |
| 2:2V:72:PRO:HD2   | 1:3J:2:ARG:CG     | 2.27                     | 0.64              |
| 2:2W:73:GLY:HA3   | 1:3K:2:ARG:CZ     | 2.27                     | 0.64              |
| 2:2W:181:VAL:CG2  | 1:3K:258:ASN:O    | 2.45                     | 0.64              |
| 1:3C:422:ARG:HH12 | 1:3C:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:3H:422:GLU:OE2  | 2:3H:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:3O:422:GLU:OE2  | 2:3O:426:ASN:ND2  | 2.30                     | 0.64              |
| 1:4B:422:ARG:HH12 | 1:4B:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:4N:422:ARG:HH12 | 1:4N:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:4H:422:GLU:OE2  | 2:4H:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:4O:422:GLU:OE2  | 2:4O:426:ASN:ND2  | 2.30                     | 0.64              |
| 1:1A:349:THR:O    | 2:4H:181:VAL:HA   | 1.97                     | 0.64              |
| 1:1B:260:VAL:HG12 | 2:4O:407:TRP:HE1  | 1.62                     | 0.64              |
| 1:1C:261:PRO:HA   | 2:4P:404:PHE:CB   | 2.27                     | 0.64              |
| 1:1D:326:LYS:CA   | 2:4Q:210:TYR:CE1  | 2.80                     | 0.64              |
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:CG   | 2.75                     | 0.64              |
| 1:1G:349:THR:CG2  | 2:4T:184:PRO:HG3  | 2.27                     | 0.64              |
| 1:1I:324:VAL:CG1  | 2:4U:222:PRO:O    | 2.44                     | 0.64              |
| 2:1O:422:GLU:OE2  | 2:1O:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:1P:51:VAL:O     | 2:1P:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1S:404:PHE:CD1  | 1:2F:260:VAL:O    | 2.50                     | 0.64              |
| 2:1S:422:GLU:OE2  | 2:1S:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:1U:404:PHE:CE2  | 1:2I:261:PRO:CA   | 2.80                     | 0.64              |
| 2:1W:180:THR:HG23 | 1:2K:258:ASN:HD21 | 1.60                     | 0.64              |
| 1:2B:422:ARG:HH12 | 1:2B:426:ALA:HB2  | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2C:422:ARG:HH12 | 1:2C:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:2J:422:ARG:HH12 | 1:2J:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:2O:422:GLU:OE2  | 2:2O:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:2P:181:VAL:HB   | 1:3C:258:ASN:O    | 1.95                     | 0.64              |
| 2:2R:398:MET:CG   | 1:3E:346:TRP:O    | 2.46                     | 0.64              |
| 2:2S:422:GLU:OE2  | 2:2S:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:2V:397:ALA:O    | 1:3J:346:TRP:HB2  | 1.97                     | 0.64              |
| 2:2W:397:ALA:O    | 1:3K:346:TRP:HB2  | 1.97                     | 0.64              |
| 2:2Z:181:VAL:H    | 1:3N:258:ASN:ND2  | 1.95                     | 0.64              |
| 1:3B:422:ARG:HH12 | 1:3B:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:3S:422:GLU:OE2  | 2:3S:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:4C:422:ARG:HH12 | 1:4C:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:4S:422:GLU:OE2  | 2:4S:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:1B:257:THR:CB   | 2:4O:100:GLY:O    | 2.46                     | 0.64              |
| 1:1B:262:TYR:CE2  | 2:4O:403:ALA:HA   | 2.32                     | 0.64              |
| 1:1B:325:PRO:CD   | 2:4O:223:THR:HA   | 2.27                     | 0.64              |
| 1:1C:2:ARG:HG3    | 2:4P:72:PRO:HD2   | 1.78                     | 0.64              |
| 1:1C:260:VAL:O    | 2:4P:407:TRP:NE1  | 2.29                     | 0.64              |
| 1:1C:260:VAL:N    | 2:4P:404:PHE:HE1  | 1.94                     | 0.64              |
| 1:1J:422:ARG:HH12 | 1:1J:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:CG   | 2.27                     | 0.64              |
| 2:1Q:51:VAL:O     | 2:1Q:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1T:51:VAL:O     | 2:1T:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1V:178:SER:CB   | 1:2J:349:THR:HB   | 2.28                     | 0.64              |
| 2:2H:181:VAL:H    | 1:3A:258:ASN:HD22 | 1.46                     | 0.64              |
| 2:2T:407:TRP:HE1  | 1:3G:260:VAL:HB   | 1.60                     | 0.64              |
| 2:2U:181:VAL:HB   | 1:3I:258:ASN:O    | 1.98                     | 0.64              |
| 2:2X:223:THR:HA   | 1:3L:325:PRO:CD   | 2.27                     | 0.64              |
| 2:2Z:397:ALA:O    | 1:3N:346:TRP:CB   | 2.44                     | 0.64              |
| 2:3Z:422:GLU:OE2  | 2:3Z:426:ASN:ND2  | 2.30                     | 0.64              |
| 1:4J:422:ARG:HH12 | 1:4J:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:4Z:51:VAL:O     | 2:4Z:64:ARG:NH1   | 2.30                     | 0.64              |
| 1:1A:2:ARG:HD3    | 2:4H:71:GLU:HB2   | 1.80                     | 0.64              |
| 1:1A:254:GLU:HA   | 2:4H:100:GLY:O    | 1.96                     | 0.64              |
| 1:1A:324:VAL:HG13 | 2:4H:222:PRO:C    | 2.21                     | 0.64              |
| 1:1A:348:PRO:HB2  | 2:4H:394:GLN:CD   | 2.23                     | 0.64              |
| 1:1B:422:ARG:HH12 | 1:1B:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1D:248:LEU:CA   | 2:4Q:11:GLN:NE2   | 2.60                     | 0.64              |
| 1:1E:329:ASN:HD22 | 2:4R:210:TYR:HD2  | 1.44                     | 0.64              |
| 1:1G:352:LYS:HA   | 2:4T:179:ASP:O    | 1.96                     | 0.64              |
| 1:1I:346:TRP:CZ3  | 2:4U:404:PHE:CE2  | 2.85                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:261:PRO:O    | 2:4W:406:HIS:NE2  | 2.29                     | 0.64              |
| 1:1M:257:THR:CG2  | 2:4Y:102:ASN:HB2  | 2.27                     | 0.64              |
| 1:1N:258:ASN:OD1  | 2:4Z:101:ASN:ND2  | 2.31                     | 0.64              |
| 2:1T:422:GLU:OE2  | 2:1T:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:1Y:401:ARG:CB   | 1:2M:262:TYR:HH   | 2.03                     | 0.64              |
| 2:1Z:422:GLU:OE2  | 2:1Z:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:2Q:51:VAL:O     | 2:2Q:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:2R:422:GLU:OE2  | 2:2R:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:2T:51:VAL:O     | 2:2T:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:2T:422:GLU:OE2  | 2:2T:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:2Y:181:VAL:H    | 1:3M:258:ASN:ND2  | 1.96                     | 0.64              |
| 2:2Z:51:VAL:O     | 2:2Z:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:2Z:422:GLU:OE2  | 2:2Z:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:3F:422:ARG:HH12 | 1:3F:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:3J:422:ARG:HH12 | 1:3J:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:3Q:51:VAL:O     | 2:3Q:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:3T:51:VAL:O     | 2:3T:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:3T:422:GLU:OE2  | 2:3T:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:3Z:51:VAL:O     | 2:3Z:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:4T:51:VAL:O     | 2:4T:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:4Z:422:GLU:OE2  | 2:4Z:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:1C:253:THR:CB   | 2:4P:100:GLY:CA   | 2.75                     | 0.64              |
| 1:1F:422:ARG:HH12 | 1:1F:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1I:254:GLU:HG2  | 2:4U:100:GLY:C    | 2.23                     | 0.64              |
| 1:1I:329:ASN:OD1  | 2:4U:177:VAL:CG1  | 2.45                     | 0.64              |
| 1:1L:260:VAL:CG1  | 2:4X:407:TRP:CZ2  | 2.80                     | 0.64              |
| 1:1M:329:ASN:ND2  | 2:4Y:210:TYR:CD2  | 2.54                     | 0.64              |
| 1:1N:260:VAL:HB   | 2:4Z:407:TRP:NE1  | 2.13                     | 0.64              |
| 2:1R:100:GLY:HA2  | 1:2E:253:THR:HB   | 1.79                     | 0.64              |
| 2:1R:180:THR:HG23 | 1:2E:258:ASN:HD21 | 1.61                     | 0.64              |
| 2:1R:422:GLU:OE2  | 2:1R:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:1Z:51:VAL:O     | 2:1Z:64:ARG:NH1   | 2.30                     | 0.64              |
| 1:2E:422:ARG:HH12 | 1:2E:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:2H:51:VAL:O     | 2:2H:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:2Q:100:GLY:HA3  | 1:3D:253:THR:CB   | 2.26                     | 0.64              |
| 2:2R:181:VAL:HB   | 1:3E:258:ASN:O    | 1.98                     | 0.64              |
| 2:2R:210:TYR:CE2  | 1:3E:329:ASN:HB2  | 2.33                     | 0.64              |
| 2:3H:51:VAL:O     | 2:3H:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:3R:422:GLU:OE2  | 2:3R:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:4Q:51:VAL:O     | 2:4Q:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:4R:422:GLU:OE2  | 2:4R:426:ASN:ND2  | 2.30                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4T:422:GLU:OE2  | 2:4T:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:1B:260:VAL:O    | 2:4O:407:TRP:NE1  | 2.30                     | 0.64              |
| 1:1C:2:ARG:HH11   | 2:4P:71:GLU:HG3   | 1.62                     | 0.64              |
| 1:1E:257:THR:HG21 | 2:4R:102:ASN:HA   | 1.78                     | 0.64              |
| 1:1E:422:ARG:HH12 | 1:1E:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1G:329:ASN:OD1  | 2:4T:177:VAL:CG1  | 2.46                     | 0.64              |
| 1:1G:351:PHE:HB2  | 2:4T:178:SER:OG   | 1.97                     | 0.64              |
| 1:1K:346:TRP:CZ3  | 2:4W:404:PHE:HE2  | 2.11                     | 0.64              |
| 2:1H:51:VAL:O     | 2:1H:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1H:179:ASP:O    | 1:2A:352:LYS:CD   | 2.44                     | 0.64              |
| 2:1S:224:TYR:CD2  | 1:2F:247:ALA:O    | 2.51                     | 0.64              |
| 2:1W:404:PHE:CZ   | 1:2K:261:PRO:CA   | 2.80                     | 0.64              |
| 2:1X:181:VAL:CB   | 1:2L:258:ASN:C    | 2.71                     | 0.64              |
| 2:1X:404:PHE:CZ   | 1:2L:260:VAL:C    | 2.74                     | 0.64              |
| 1:2F:422:ARG:HH12 | 1:2F:426:ALA:HB2  | 1.63                     | 0.64              |
| 1:2K:422:ARG:HH12 | 1:2K:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:2T:222:PRO:CG   | 1:3G:326:LYS:CB   | 2.75                     | 0.64              |
| 2:2W:181:VAL:CB   | 1:3K:258:ASN:O    | 2.46                     | 0.64              |
| 1:3E:422:ARG:HH12 | 1:3E:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:4E:422:ARG:HH12 | 1:4E:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:4F:422:ARG:HH12 | 1:4F:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:4H:51:VAL:O     | 2:4H:64:ARG:NH1   | 2.30                     | 0.64              |
| 1:1D:326:LYS:CE   | 2:4Q:214:PHE:HB2  | 2.27                     | 0.64              |
| 1:1K:346:TRP:HA   | 2:4W:397:ALA:O    | 1.98                     | 0.64              |
| 1:1K:422:ARG:HH12 | 1:1K:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1L:260:VAL:CB   | 2:4X:407:TRP:HE1  | 2.11                     | 0.64              |
| 1:1N:2:ARG:CD     | 2:4Z:72:PRO:HD2   | 2.24                     | 0.64              |
| 2:1S:51:VAL:O     | 2:1S:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1U:101:ASN:O    | 1:2I:257:THR:HG21 | 1.97                     | 0.64              |
| 2:1V:224:TYR:OH   | 1:2J:248:LEU:HD22 | 1.96                     | 0.64              |
| 2:2H:394:GLN:CG   | 1:3A:348:PRO:HG3  | 2.25                     | 0.64              |
| 2:2Q:394:GLN:CG   | 1:3D:348:PRO:HG3  | 2.24                     | 0.64              |
| 2:2S:221:THR:HA   | 1:3F:324:VAL:HG11 | 1.79                     | 0.64              |
| 2:2S:394:GLN:HB3  | 1:3F:348:PRO:CG   | 2.25                     | 0.64              |
| 2:2V:181:VAL:HB   | 1:3J:258:ASN:O    | 1.96                     | 0.64              |
| 2:2Z:404:PHE:H    | 1:3N:261:PRO:C    | 2.02                     | 0.64              |
| 1:3K:422:ARG:HH12 | 1:3K:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:4K:422:ARG:HH12 | 1:4K:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1C:349:THR:CG2  | 2:4P:184:PRO:HG3  | 2.27                     | 0.64              |
| 1:1G:349:THR:OG1  | 2:4T:184:PRO:HD3  | 1.95                     | 0.64              |
| 1:1J:349:THR:HB   | 2:4V:180:THR:O    | 1.98                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:262:TYR:OH   | 2:4W:401:ARG:O    | 2.15                     | 0.64              |
| 2:1P:422:GLU:OE2  | 2:1P:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:1U:422:GLU:OE2  | 2:1U:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:1V:180:THR:HG23 | 1:2J:258:ASN:HD21 | 1.61                     | 0.64              |
| 2:2H:224:TYR:CD2  | 1:3A:247:ALA:O    | 2.50                     | 0.64              |
| 2:2O:397:ALA:HB1  | 1:3B:346:TRP:HA   | 1.78                     | 0.64              |
| 2:2P:179:ASP:O    | 1:3C:352:LYS:CD   | 2.40                     | 0.64              |
| 2:2S:51:VAL:O     | 2:2S:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:2S:181:VAL:HB   | 1:3F:258:ASN:O    | 1.98                     | 0.64              |
| 2:2T:100:GLY:CA   | 1:3G:253:THR:HG22 | 2.12                     | 0.64              |
| 2:2U:72:PRO:HG2   | 1:3I:2:ARG:HG3    | 1.80                     | 0.64              |
| 2:2W:222:PRO:CG   | 1:3K:326:LYS:CB   | 2.74                     | 0.64              |
| 2:2Y:422:GLU:OE2  | 2:2Y:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:3P:422:GLU:OE2  | 2:3P:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:3S:51:VAL:O     | 2:3S:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:4Y:422:GLU:OE2  | 2:4Y:426:ASN:ND2  | 2.30                     | 0.64              |
| 1:1D:326:LYS:HB3  | 2:4Q:222:PRO:HG2  | 1.80                     | 0.64              |
| 1:1D:349:THR:HG21 | 2:4Q:184:PRO:HG3  | 1.78                     | 0.64              |
| 1:1E:324:VAL:HG21 | 2:4R:221:THR:OG1  | 1.98                     | 0.64              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:N    | 2.60                     | 0.64              |
| 1:1F:348:PRO:CD   | 2:4S:398:MET:HG3  | 2.28                     | 0.64              |
| 1:1G:2:ARG:NH2    | 2:4T:73:GLY:HA3   | 2.12                     | 0.64              |
| 1:1G:325:PRO:HD2  | 2:4T:223:THR:HA   | 1.80                     | 0.64              |
| 1:1I:422:ARG:HH12 | 1:1I:426:ALA:HB2  | 1.62                     | 0.64              |
| 1:1J:348:PRO:HG2  | 2:4V:394:GLN:HB3  | 1.77                     | 0.64              |
| 1:1K:254:GLU:N    | 2:4W:100:GLY:HA2  | 2.12                     | 0.64              |
| 1:1K:326:LYS:HB2  | 2:4W:222:PRO:HG2  | 1.79                     | 0.64              |
| 1:1L:332:ILE:HG22 | 2:4X:177:VAL:CG2  | 2.25                     | 0.64              |
| 2:1S:180:THR:HG23 | 1:2F:258:ASN:HD21 | 1.63                     | 0.64              |
| 2:1V:422:GLU:OE2  | 2:1V:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:1Y:51:VAL:O     | 2:1Y:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1Y:404:PHE:CD2  | 1:2M:261:PRO:HA   | 2.33                     | 0.64              |
| 2:1Y:422:GLU:OE2  | 2:1Y:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:2H:397:ALA:HB1  | 1:3A:346:TRP:HA   | 1.79                     | 0.64              |
| 2:2O:224:TYR:HD2  | 1:3B:247:ALA:O    | 1.81                     | 0.64              |
| 2:2P:422:GLU:OE2  | 2:2P:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:2Q:181:VAL:HB   | 1:3D:258:ASN:O    | 1.97                     | 0.64              |
| 2:2R:397:ALA:HB1  | 1:3E:346:TRP:HA   | 1.79                     | 0.64              |
| 2:2U:422:GLU:OE2  | 2:2U:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:2V:177:VAL:CG2  | 1:3J:332:ILE:CG2  | 2.76                     | 0.64              |
| 2:2V:422:GLU:OE2  | 2:2V:426:ASN:ND2  | 2.31                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:222:PRO:HG2  | 1:3N:326:LYS:CB   | 2.28                     | 0.64              |
| 1:3M:422:ARG:HH12 | 1:3M:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:3U:422:GLU:OE2  | 2:3U:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:3V:422:GLU:OE2  | 2:3V:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:3Y:422:GLU:OE2  | 2:3Y:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:4M:422:ARG:HH12 | 1:4M:426:ALA:HB2  | 1.62                     | 0.64              |
| 2:4P:422:GLU:OE2  | 2:4P:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:4S:51:VAL:O     | 2:4S:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:4V:422:GLU:OE2  | 2:4V:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:1A:263:PRO:CA   | 2:4H:406:HIS:CE1  | 2.80                     | 0.64              |
| 1:1E:346:TRP:CD1  | 2:4R:401:ARG:CG   | 2.79                     | 0.64              |
| 1:1F:260:VAL:HG11 | 2:4S:407:TRP:HZ2  | 1.62                     | 0.64              |
| 1:1G:346:TRP:C    | 2:4T:398:MET:HG2  | 2.20                     | 0.64              |
| 1:1L:346:TRP:CE3  | 2:4X:403:ALA:HB3  | 2.31                     | 0.64              |
| 1:1M:346:TRP:CZ3  | 2:4Y:403:ALA:CB   | 2.80                     | 0.64              |
| 2:1O:71:GLU:HB2   | 1:2B:2:ARG:HD3    | 1.80                     | 0.64              |
| 2:1X:51:VAL:O     | 2:1X:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:1X:422:GLU:OE2  | 2:1X:426:ASN:ND2  | 2.31                     | 0.64              |
| 1:2M:422:ARG:HH12 | 1:2M:426:ALA:HB2  | 1.63                     | 0.64              |
| 2:2R:394:GLN:HB3  | 1:3E:348:PRO:CG   | 2.28                     | 0.64              |
| 2:2S:100:GLY:CA   | 1:3F:253:THR:CG2  | 2.74                     | 0.64              |
| 2:2T:404:PHE:CA   | 1:3G:261:PRO:O    | 2.45                     | 0.64              |
| 2:2V:221:THR:CB   | 1:3J:324:VAL:HG21 | 2.27                     | 0.64              |
| 2:2W:101:ASN:HB2  | 1:3K:254:GLU:HG2  | 1.80                     | 0.64              |
| 2:2Y:51:VAL:O     | 2:2Y:64:ARG:NH1   | 2.30                     | 0.64              |
| 2:3X:422:GLU:OE2  | 2:3X:426:ASN:ND2  | 2.30                     | 0.64              |
| 2:4U:422:GLU:OE2  | 2:4U:426:ASN:ND2  | 2.31                     | 0.64              |
| 2:4Y:51:VAL:O     | 2:4Y:64:ARG:NH1   | 2.30                     | 0.64              |
| 1:1C:263:PRO:HD3  | 2:4P:406:HIS:CB   | 2.25                     | 0.63              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:CB   | 2.28                     | 0.63              |
| 1:1I:326:LYS:HE2  | 2:4U:210:TYR:O    | 1.98                     | 0.63              |
| 1:1L:348:PRO:CB   | 2:4X:394:GLN:HG2  | 2.28                     | 0.63              |
| 1:1M:422:ARG:HH12 | 1:1M:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:1H:224:TYR:CD2  | 1:2A:247:ALA:O    | 2.51                     | 0.63              |
| 2:1Y:221:THR:OG1  | 1:2M:324:VAL:HG22 | 1.98                     | 0.63              |
| 1:2I:422:ARG:HH12 | 1:2I:426:ALA:HB2  | 1.62                     | 0.63              |
| 2:2Q:11:GLN:CD    | 1:3D:249:ASN:H    | 2.02                     | 0.63              |
| 2:2U:51:VAL:O     | 2:2U:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:2U:404:PHE:CE1  | 1:3I:261:PRO:CA   | 2.80                     | 0.63              |
| 5:2U:501:GDP:H8   | 1:3I:248:LEU:HD11 | 1.63                     | 0.63              |
| 2:2X:51:VAL:O     | 2:2X:64:ARG:NH1   | 2.30                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2X:422:GLU:OE2  | 2:2X:426:ASN:ND2  | 2.31                     | 0.63              |
| 2:2Y:221:THR:CB   | 1:3M:324:VAL:HG21 | 2.27                     | 0.63              |
| 1:3I:422:ARG:HH12 | 1:3I:426:ALA:HB2  | 1.62                     | 0.63              |
| 2:3X:51:VAL:O     | 2:3X:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:3Y:51:VAL:O     | 2:3Y:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:4U:51:VAL:O     | 2:4U:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:4X:51:VAL:O     | 2:4X:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:4X:422:GLU:OE2  | 2:4X:426:ASN:ND2  | 2.31                     | 0.63              |
| 1:1A:348:PRO:HB2  | 2:4H:394:GLN:CG   | 2.25                     | 0.63              |
| 1:1B:348:PRO:HG3  | 2:4O:394:GLN:HG2  | 1.80                     | 0.63              |
| 1:1B:352:LYS:HA   | 2:4O:179:ASP:C    | 2.23                     | 0.63              |
| 1:1C:261:PRO:N    | 2:4P:404:PHE:CD1  | 2.65                     | 0.63              |
| 1:1D:349:THR:CG2  | 2:4Q:184:PRO:CD   | 2.74                     | 0.63              |
| 1:1F:352:LYS:HD3  | 2:4S:101:ASN:HD22 | 1.62                     | 0.63              |
| 1:1J:348:PRO:HD2  | 2:4V:398:MET:HG3  | 1.78                     | 0.63              |
| 2:1R:394:GLN:HG2  | 1:2E:348:PRO:HG3  | 1.80                     | 0.63              |
| 2:1U:51:VAL:O     | 2:1U:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:2R:404:PHE:HE1  | 1:3E:260:VAL:N    | 1.95                     | 0.63              |
| 2:2T:401:ARG:NH2  | 1:3G:435:VAL:CA   | 2.45                     | 0.63              |
| 2:2V:51:VAL:O     | 2:2V:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:2V:404:PHE:CA   | 1:3J:261:PRO:O    | 2.45                     | 0.63              |
| 2:2W:406:HIS:CE1  | 1:3K:263:PRO:N    | 2.65                     | 0.63              |
| 2:3U:51:VAL:O     | 2:3U:64:ARG:NH1   | 2.30                     | 0.63              |
| 1:4G:422:ARG:HH12 | 1:4G:426:ALA:HB2  | 1.63                     | 0.63              |
| 1:4I:422:ARG:HH12 | 1:4I:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:4V:51:VAL:O     | 2:4V:64:ARG:NH1   | 2.30                     | 0.63              |
| 1:1C:257:THR:HG21 | 2:4P:101:ASN:O    | 1.98                     | 0.63              |
| 1:1E:353:VAL:CG2  | 2:4R:179:ASP:HA   | 2.28                     | 0.63              |
| 1:1G:256:GLN:HB2  | 2:4T:407:TRP:CH2  | 2.33                     | 0.63              |
| 1:1L:422:ARG:HH12 | 1:1L:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:1R:178:SER:HB3  | 1:2E:349:THR:HB   | 1.79                     | 0.63              |
| 2:1S:101:ASN:HB2  | 1:2F:254:GLU:HG2  | 1.81                     | 0.63              |
| 2:1Y:182:VAL:HG22 | 1:2M:257:THR:HG22 | 1.79                     | 0.63              |
| 2:1Z:404:PHE:HE1  | 1:2N:260:VAL:H    | 1.45                     | 0.63              |
| 1:2G:422:ARG:HH12 | 1:2G:426:ALA:HB2  | 1.62                     | 0.63              |
| 2:2O:72:PRO:HD2   | 1:3B:2:ARG:CG     | 2.29                     | 0.63              |
| 2:2P:221:THR:HA   | 1:3C:324:VAL:HG11 | 1.79                     | 0.63              |
| 2:2P:401:ARG:HH21 | 1:3C:435:VAL:HA   | 1.53                     | 0.63              |
| 2:2S:100:GLY:CA   | 1:3F:253:THR:CB   | 2.76                     | 0.63              |
| 2:2S:394:GLN:HG2  | 1:3F:348:PRO:HB2  | 1.78                     | 0.63              |
| 2:2T:407:TRP:NE1  | 1:3G:260:VAL:HB   | 2.13                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2U:72:PRO:HD2   | 1:3I:2:ARG:HD3    | 1.79                     | 0.63              |
| 2:2U:398:MET:HA   | 1:3I:346:TRP:HB2  | 1.79                     | 0.63              |
| 2:2W:179:ASP:OD2  | 1:3K:248:LEU:HD21 | 1.99                     | 0.63              |
| 1:3L:422:ARG:HH12 | 1:3L:426:ALA:HB2  | 1.62                     | 0.63              |
| 2:3V:51:VAL:O     | 2:3V:64:ARG:NH1   | 2.30                     | 0.63              |
| 1:1B:261:PRO:O    | 2:4O:404:PHE:HA   | 1.97                     | 0.63              |
| 1:1B:261:PRO:N    | 2:4O:404:PHE:CE1  | 2.66                     | 0.63              |
| 1:1N:257:THR:HG21 | 2:4Z:101:ASN:O    | 1.98                     | 0.63              |
| 2:1Q:422:GLU:OE2  | 2:1Q:426:ASN:ND2  | 2.30                     | 0.63              |
| 2:1T:221:THR:CA   | 1:2G:324:VAL:CG1  | 2.60                     | 0.63              |
| 2:1V:406:HIS:CE1  | 1:2J:263:PRO:HB3  | 2.32                     | 0.63              |
| 2:1W:51:VAL:O     | 2:1W:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:1Y:224:TYR:CE2  | 1:2M:248:LEU:HB2  | 2.34                     | 0.63              |
| 2:2P:224:TYR:HE2  | 1:3C:248:LEU:HB2  | 1.62                     | 0.63              |
| 2:2Q:422:GLU:OE2  | 2:2Q:426:ASN:ND2  | 2.30                     | 0.63              |
| 2:2T:394:GLN:HB3  | 1:3G:348:PRO:CG   | 2.27                     | 0.63              |
| 2:2U:100:GLY:CA   | 1:3I:253:THR:CB   | 2.76                     | 0.63              |
| 2:2W:51:VAL:O     | 2:2W:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:2X:73:GLY:HA3   | 1:3L:2:ARG:NH2    | 2.14                     | 0.63              |
| 1:3G:422:ARG:HH12 | 1:3G:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:3Q:422:GLU:OE2  | 2:3Q:426:ASN:ND2  | 2.31                     | 0.63              |
| 2:3W:51:VAL:O     | 2:3W:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:3W:422:GLU:OE2  | 2:3W:426:ASN:ND2  | 2.30                     | 0.63              |
| 2:4W:51:VAL:O     | 2:4W:64:ARG:NH1   | 2.30                     | 0.63              |
| 1:1A:422:ARG:HH12 | 1:1A:426:ALA:HB2  | 1.62                     | 0.63              |
| 1:1C:346:TRP:CH2  | 2:4P:403:ALA:CB   | 2.81                     | 0.63              |
| 1:1D:346:TRP:CE3  | 2:4Q:403:ALA:HB3  | 2.34                     | 0.63              |
| 1:1G:348:PRO:HB2  | 2:4T:394:GLN:CD   | 2.22                     | 0.63              |
| 1:1G:422:ARG:HH12 | 1:1G:426:ALA:HB2  | 1.62                     | 0.63              |
| 1:1I:253:THR:C    | 2:4U:100:GLY:CA   | 2.72                     | 0.63              |
| 1:1M:260:VAL:HG11 | 2:4Y:407:TRP:CZ2  | 2.33                     | 0.63              |
| 2:1H:179:ASP:CG   | 1:2A:248:LEU:HD21 | 2.22                     | 0.63              |
| 2:1P:179:ASP:OD2  | 1:2C:248:LEU:HD21 | 1.97                     | 0.63              |
| 2:1V:51:VAL:O     | 2:1V:64:ARG:NH1   | 2.30                     | 0.63              |
| 2:1W:422:GLU:OE2  | 2:1W:426:ASN:ND2  | 2.31                     | 0.63              |
| 1:2L:422:ARG:HH12 | 1:2L:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:2W:422:GLU:OE2  | 2:2W:426:ASN:ND2  | 2.31                     | 0.63              |
| 2:2X:404:PHE:HE1  | 1:3L:260:VAL:N    | 1.96                     | 0.63              |
| 1:4L:422:ARG:HH12 | 1:4L:426:ALA:HB2  | 1.62                     | 0.63              |
| 2:4Q:422:GLU:OE2  | 2:4Q:426:ASN:ND2  | 2.31                     | 0.63              |
| 2:4W:422:GLU:OE2  | 2:4W:426:ASN:ND2  | 2.31                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:248:LEU:C    | 2:4O:11:GLN:HE22  | 1.96                     | 0.63              |
| 1:1C:261:PRO:C    | 2:4P:404:PHE:HA   | 2.23                     | 0.63              |
| 1:1E:248:LEU:CD1  | 5:4R:501:GDP:C8   | 2.50                     | 0.63              |
| 1:1I:248:LEU:CD1  | 5:4U:501:GDP:H8   | 2.12                     | 0.63              |
| 1:1J:254:GLU:CA   | 2:4V:100:GLY:HA2  | 2.29                     | 0.63              |
| 1:1J:329:ASN:ND2  | 2:4V:210:TYR:HD2  | 1.95                     | 0.63              |
| 1:1J:347:CYS:HA   | 2:4V:398:MET:HG2  | 1.79                     | 0.63              |
| 2:1Y:179:ASP:O    | 1:2M:352:LYS:CE   | 2.45                     | 0.63              |
| 2:2Q:401:ARG:HH22 | 1:3D:435:VAL:C    | 2.06                     | 0.63              |
| 2:2U:73:GLY:HA3   | 1:3I:2:ARG:CZ     | 2.29                     | 0.63              |
| 1:3A:422:ARG:HH12 | 1:3A:426:ALA:HB2  | 1.62                     | 0.63              |
| 1:1B:2:ARG:HG3    | 2:4O:72:PRO:HG2   | 1.79                     | 0.63              |
| 1:1D:256:GLN:HB2  | 2:4Q:407:TRP:CH2  | 2.34                     | 0.63              |
| 1:1D:329:ASN:HB3  | 2:4Q:210:TYR:CD2  | 2.33                     | 0.63              |
| 1:1D:347:CYS:HA   | 2:4Q:398:MET:CG   | 2.28                     | 0.63              |
| 1:1I:346:TRP:HZ3  | 2:4U:404:PHE:CE2  | 2.17                     | 0.63              |
| 1:1K:439:SER:OG   | 2:4W:401:ARG:HD3  | 1.97                     | 0.63              |
| 2:1W:224:TYR:OH   | 1:2K:248:LEU:HD22 | 1.98                     | 0.63              |
| 1:2A:422:ARG:HH12 | 1:2A:426:ALA:HB2  | 1.63                     | 0.63              |
| 2:2Q:406:HIS:NE2  | 1:3D:262:TYR:CA   | 2.62                     | 0.63              |
| 2:2X:404:PHE:HD1  | 1:3L:260:VAL:O    | 1.82                     | 0.63              |
| 1:1A:257:THR:HB   | 2:4H:100:GLY:O    | 1.99                     | 0.63              |
| 1:1A:262:TYR:N    | 2:4H:406:HIS:NE2  | 2.47                     | 0.63              |
| 1:1C:262:TYR:CZ   | 2:4P:403:ALA:HA   | 2.33                     | 0.63              |
| 1:1G:325:PRO:HG2  | 2:4T:224:TYR:CD1  | 2.34                     | 0.63              |
| 1:1J:261:PRO:HA   | 2:4V:404:PHE:CD1  | 2.33                     | 0.63              |
| 1:1K:346:TRP:CD2  | 2:4W:403:ALA:CB   | 2.82                     | 0.63              |
| 2:1P:179:ASP:O    | 1:2C:352:LYS:HD2  | 1.99                     | 0.63              |
| 2:1R:404:PHE:CE1  | 1:2E:260:VAL:C    | 2.76                     | 0.63              |
| 2:1R:406:HIS:NE2  | 1:2E:263:PRO:HD3  | 2.12                     | 0.63              |
| 2:2P:77:SER:CB    | 1:3C:245:ASP:OD1  | 2.47                     | 0.63              |
| 2:2V:72:PRO:HG2   | 1:3J:2:ARG:HG3    | 1.81                     | 0.63              |
| 2:2V:398:MET:HG2  | 1:3J:346:TRP:O    | 1.99                     | 0.63              |
| 2:2W:404:PHE:HD1  | 1:3K:260:VAL:O    | 1.81                     | 0.63              |
| 2:2X:404:PHE:CE1  | 1:3L:261:PRO:CA   | 2.82                     | 0.63              |
| 1:4A:422:ARG:HH12 | 1:4A:426:ALA:HB2  | 1.62                     | 0.63              |
| 1:1D:422:ARG:HH12 | 1:1D:426:ALA:HB2  | 1.62                     | 0.63              |
| 1:1E:352:LYS:HD2  | 2:4R:179:ASP:O    | 1.99                     | 0.63              |
| 1:1F:352:LYS:HD3  | 2:4S:101:ASN:HD21 | 1.62                     | 0.63              |
| 2:1R:100:GLY:CA   | 1:2E:253:THR:CG2  | 2.76                     | 0.63              |
| 2:1T:180:THR:HG23 | 1:2G:258:ASN:HD21 | 1.63                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2O:394:GLN:CA   | 1:3B:348:PRO:HG3  | 2.26                     | 0.63              |
| 2:2P:222:PRO:HG2  | 1:3C:326:LYS:CB   | 2.29                     | 0.63              |
| 2:2Q:221:THR:OG1  | 1:3D:324:VAL:CG2  | 2.47                     | 0.63              |
| 2:2R:101:ASN:ND2  | 1:3E:258:ASN:OD1  | 2.32                     | 0.63              |
| 2:2R:404:PHE:CD1  | 1:3E:261:PRO:CA   | 2.80                     | 0.63              |
| 2:2R:404:PHE:CE1  | 1:3E:261:PRO:N    | 2.67                     | 0.63              |
| 2:2S:397:ALA:HB1  | 1:3F:346:TRP:HA   | 1.80                     | 0.63              |
| 2:2Y:397:ALA:HB1  | 1:3M:346:TRP:HA   | 1.81                     | 0.63              |
| 1:1F:326:LYS:CE   | 2:4S:210:TYR:O    | 2.46                     | 0.62              |
| 1:1G:258:ASN:OD1  | 2:4T:101:ASN:HB3  | 1.99                     | 0.62              |
| 1:1L:262:TYR:OH   | 2:4X:401:ARG:O    | 2.15                     | 0.62              |
| 2:1V:181:VAL:CG2  | 1:2J:258:ASN:CA   | 2.77                     | 0.62              |
| 2:1V:207:GLU:OE1  | 1:2J:329:ASN:ND2  | 2.32                     | 0.62              |
| 2:2H:182:VAL:HG21 | 1:3A:257:THR:HG22 | 1.79                     | 0.62              |
| 1:1C:253:THR:CB   | 2:4P:100:GLY:HA3  | 2.29                     | 0.62              |
| 1:1C:326:LYS:HB3  | 2:4P:222:PRO:HG2  | 1.81                     | 0.62              |
| 1:1J:314:ALA:HB1  | 2:4V:181:VAL:HG21 | 1.81                     | 0.62              |
| 1:1L:260:VAL:HG11 | 2:4X:407:TRP:CZ2  | 2.34                     | 0.62              |
| 2:1T:401:ARG:HB3  | 1:2G:262:TYR:OH   | 1.99                     | 0.62              |
| 2:2V:100:GLY:HA2  | 1:3J:253:THR:C    | 2.24                     | 0.62              |
| 2:2V:394:GLN:CB   | 1:3J:348:PRO:CG   | 2.76                     | 0.62              |
| 1:3D:422:ARG:HH12 | 1:3D:426:ALA:HB2  | 1.62                     | 0.62              |
| 1:1B:260:VAL:CG1  | 2:4O:407:TRP:NE1  | 2.62                     | 0.62              |
| 1:1B:326:LYS:HE3  | 2:4O:214:PHE:HB2  | 1.81                     | 0.62              |
| 1:1C:248:LEU:HD13 | 5:4P:501:GDP:N7   | 2.11                     | 0.62              |
| 1:1C:326:LYS:CE   | 2:4P:210:TYR:O    | 2.48                     | 0.62              |
| 1:1E:263:PRO:HA   | 2:4R:406:HIS:CE1  | 2.34                     | 0.62              |
| 2:1U:180:THR:CG2  | 1:2I:258:ASN:HD21 | 2.12                     | 0.62              |
| 2:1V:181:VAL:CB   | 1:2J:258:ASN:HA   | 2.18                     | 0.62              |
| 1:2D:422:ARG:HH12 | 1:2D:426:ALA:HB2  | 1.62                     | 0.62              |
| 2:2R:179:ASP:OD2  | 1:3E:248:LEU:HD21 | 1.98                     | 0.62              |
| 2:2R:401:ARG:HH22 | 1:3E:435:VAL:C    | 2.07                     | 0.62              |
| 2:2T:181:VAL:HB   | 1:3G:258:ASN:O    | 1.98                     | 0.62              |
| 2:2U:406:HIS:NE2  | 1:3I:262:TYR:HA   | 2.13                     | 0.62              |
| 2:2V:179:ASP:O    | 1:3J:352:LYS:CD   | 2.42                     | 0.62              |
| 1:4D:422:ARG:HH12 | 1:4D:426:ALA:HB2  | 1.62                     | 0.62              |
| 1:1A:261:PRO:HA   | 2:4H:404:PHE:CA   | 2.30                     | 0.62              |
| 1:1B:2:ARG:NH1    | 2:4O:71:GLU:HG3   | 2.13                     | 0.62              |
| 1:1C:257:THR:HG21 | 2:4P:102:ASN:CA   | 2.29                     | 0.62              |
| 1:1E:2:ARG:NH1    | 2:4R:71:GLU:CG    | 2.63                     | 0.62              |
| 2:1H:181:VAL:HG23 | 1:2A:258:ASN:HB3  | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:404:PHE:CE1  | 1:2I:261:PRO:HA   | 2.34                     | 0.62              |
| 2:1X:214:PHE:CD1  | 1:2L:326:LYS:HE3  | 2.35                     | 0.62              |
| 2:2P:100:GLY:O    | 1:3C:254:GLU:HA   | 1.99                     | 0.62              |
| 2:2R:398:MET:HA   | 1:3E:346:TRP:HB2  | 1.81                     | 0.62              |
| 2:2W:177:VAL:HG23 | 1:3K:332:ILE:HG22 | 1.78                     | 0.62              |
| 2:2W:406:HIS:CE1  | 1:3K:263:PRO:CA   | 2.81                     | 0.62              |
| 1:1G:352:LYS:CD   | 2:4T:101:ASN:HD22 | 2.12                     | 0.62              |
| 1:1L:180:ALA:HB3  | 1:1L:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1L:348:PRO:HD2  | 2:4X:398:MET:CG   | 2.29                     | 0.62              |
| 1:1M:180:ALA:HB3  | 1:1M:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1M:348:PRO:HD2  | 2:4Y:398:MET:SD   | 2.40                     | 0.62              |
| 1:1M:435:VAL:HA   | 2:4Y:401:ARG:NH2  | 2.13                     | 0.62              |
| 1:2L:180:ALA:HB3  | 1:2L:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:2M:180:ALA:HB3  | 1:2M:183:GLU:HG3  | 1.82                     | 0.62              |
| 2:2H:181:VAL:HG21 | 1:3A:258:ASN:O    | 1.99                     | 0.62              |
| 2:2Q:180:THR:CG2  | 1:3D:258:ASN:ND2  | 2.36                     | 0.62              |
| 2:2T:100:GLY:CA   | 1:3G:253:THR:CB   | 2.77                     | 0.62              |
| 2:2V:221:THR:C    | 1:3J:324:VAL:HG11 | 2.25                     | 0.62              |
| 2:2X:77:SER:HB3   | 1:3L:245:ASP:CG   | 2.24                     | 0.62              |
| 2:2X:224:TYR:CD2  | 1:3L:247:ALA:O    | 2.52                     | 0.62              |
| 1:3L:180:ALA:HB3  | 1:3L:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4M:180:ALA:HB3  | 1:4M:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1B:260:VAL:HB   | 2:4O:407:TRP:CE2  | 2.33                     | 0.62              |
| 1:1B:262:TYR:CE1  | 2:4O:402:LYS:O    | 2.53                     | 0.62              |
| 1:1D:346:TRP:O    | 2:4Q:398:MET:CB   | 2.47                     | 0.62              |
| 1:1E:254:GLU:CA   | 2:4R:100:GLY:CA   | 2.77                     | 0.62              |
| 1:1E:346:TRP:CB   | 2:4R:397:ALA:C    | 2.68                     | 0.62              |
| 1:1E:352:LYS:HE2  | 2:4R:101:ASN:ND2  | 2.13                     | 0.62              |
| 1:1F:258:ASN:OD1  | 2:4S:101:ASN:HB3  | 1.99                     | 0.62              |
| 1:1F:352:LYS:CD   | 2:4S:101:ASN:HD22 | 2.12                     | 0.62              |
| 1:1J:348:PRO:CD   | 2:4V:398:MET:HG3  | 2.30                     | 0.62              |
| 1:1M:254:GLU:N    | 2:4Y:100:GLY:HA2  | 2.14                     | 0.62              |
| 5:1Z:501:GDP:C8   | 1:2N:248:LEU:HD13 | 2.34                     | 0.62              |
| 1:2N:180:ALA:HB3  | 1:2N:183:GLU:HG3  | 1.82                     | 0.62              |
| 2:2H:77:SER:HB3   | 1:3A:245:ASP:CG   | 2.25                     | 0.62              |
| 2:2H:181:VAL:N    | 1:3A:258:ASN:HD22 | 1.97                     | 0.62              |
| 2:2R:100:GLY:HA2  | 1:3E:253:THR:C    | 2.24                     | 0.62              |
| 2:2T:404:PHE:CZ   | 1:3G:261:PRO:HB3  | 2.34                     | 0.62              |
| 2:2U:394:GLN:HA   | 1:3I:348:PRO:HG3  | 1.80                     | 0.62              |
| 1:3M:180:ALA:HB3  | 1:3M:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4L:180:ALA:HB3  | 1:4L:183:GLU:HG3  | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4N:180:ALA:HB3  | 1:4N:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1C:248:LEU:HD11 | 5:4P:501:GDP:H8   | 1.56                     | 0.62              |
| 1:1F:407:TRP:CE3  | 2:1S:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1I:332:ILE:HG22 | 2:4U:177:VAL:CG2  | 2.13                     | 0.62              |
| 1:1I:407:TRP:CE3  | 2:1U:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1J:407:TRP:CE3  | 2:1V:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1K:407:TRP:CE3  | 2:1W:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:CA   | 2.47                     | 0.62              |
| 1:1M:351:PHE:O    | 2:4Y:180:THR:N    | 2.33                     | 0.62              |
| 2:1W:404:PHE:CZ   | 1:2K:261:PRO:HA   | 2.34                     | 0.62              |
| 2:1X:214:PHE:CB   | 1:2L:326:LYS:CE   | 2.60                     | 0.62              |
| 2:1Y:214:PHE:CG   | 1:2M:326:LYS:HE3  | 2.33                     | 0.62              |
| 1:2F:407:TRP:CE3  | 2:2S:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:2I:407:TRP:CE3  | 2:2U:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:2K:407:TRP:CE3  | 2:2W:257:VAL:HG22 | 2.35                     | 0.62              |
| 2:2V:101:ASN:C    | 1:3J:257:THR:HG21 | 2.24                     | 0.62              |
| 2:2Z:179:ASP:OD1  | 1:3N:353:VAL:HB   | 1.99                     | 0.62              |
| 1:3B:180:ALA:HB3  | 1:3B:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:3F:407:TRP:CE3  | 2:3S:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3J:180:ALA:HB3  | 1:3J:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:3J:407:TRP:CE3  | 2:3V:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3K:407:TRP:CE3  | 2:3W:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3N:180:ALA:HB3  | 1:3N:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4F:407:TRP:CE3  | 2:4S:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:4J:407:TRP:CE3  | 2:4V:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1A:180:ALA:HB3  | 1:1A:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1B:180:ALA:HB3  | 1:1B:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1C:352:LYS:CE   | 2:4P:101:ASN:ND2  | 2.63                     | 0.62              |
| 1:1E:325:PRO:HB3  | 2:4R:224:TYR:CE1  | 2.35                     | 0.62              |
| 1:1F:439:SER:HB2  | 2:4S:400:ARG:HD2  | 1.81                     | 0.62              |
| 1:1G:407:TRP:CE3  | 2:1T:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1I:353:VAL:CG2  | 2:4U:179:ASP:OD1  | 2.47                     | 0.62              |
| 1:1J:348:PRO:CG   | 2:4V:394:GLN:CB   | 2.73                     | 0.62              |
| 2:1S:404:PHE:CZ   | 1:2F:261:PRO:CA   | 2.82                     | 0.62              |
| 2:1T:178:SER:HB3  | 1:2G:349:THR:CB   | 2.27                     | 0.62              |
| 2:1Y:181:VAL:CG2  | 1:2M:258:ASN:C    | 2.66                     | 0.62              |
| 1:2B:180:ALA:HB3  | 1:2B:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:2J:180:ALA:HB3  | 1:2J:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:2J:407:TRP:CE3  | 2:2V:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:2K:180:ALA:HB3  | 1:2K:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:2L:407:TRP:CE3  | 2:2X:257:VAL:HG22 | 2.35                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:398:MET:HG2  | 1:3E:346:TRP:O    | 1.98                     | 0.62              |
| 1:3A:180:ALA:HB3  | 1:3A:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:3G:407:TRP:CE3  | 2:3T:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3I:407:TRP:CE3  | 2:3U:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3K:180:ALA:HB3  | 1:3K:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4B:180:ALA:HB3  | 1:4B:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4J:180:ALA:HB3  | 1:4J:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4K:407:TRP:CE3  | 2:4W:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1D:257:THR:HG21 | 2:4Q:102:ASN:HB2  | 1.82                     | 0.62              |
| 1:1D:260:VAL:CG1  | 2:4Q:406:HIS:HE1  | 2.12                     | 0.62              |
| 1:1D:326:LYS:HA   | 2:4Q:210:TYR:CG   | 2.35                     | 0.62              |
| 1:1I:180:ALA:HB3  | 1:1I:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1J:180:ALA:HB3  | 1:1J:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1K:180:ALA:HB3  | 1:1K:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:1L:407:TRP:CE3  | 2:1X:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1N:180:ALA:HB3  | 1:1N:183:GLU:HG3  | 1.82                     | 0.62              |
| 2:1U:182:VAL:CG2  | 1:2I:257:THR:HG22 | 2.30                     | 0.62              |
| 2:1Z:181:VAL:CG1  | 1:2N:258:ASN:O    | 2.47                     | 0.62              |
| 2:1Z:222:PRO:O    | 1:2N:325:PRO:HD2  | 2.00                     | 0.62              |
| 1:2A:180:ALA:HB3  | 1:2A:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:2G:407:TRP:CE3  | 2:2T:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:2I:180:ALA:HB3  | 1:2I:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:3L:407:TRP:CE3  | 2:3X:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:4G:407:TRP:CE3  | 2:4T:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:4I:180:ALA:HB3  | 1:4I:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4I:407:TRP:CE3  | 2:4U:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:4K:180:ALA:HB3  | 1:4K:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4L:407:TRP:CE3  | 2:4X:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1A:254:GLU:N    | 2:4H:100:GLY:HA2  | 2.14                     | 0.62              |
| 1:1B:329:ASN:HB2  | 2:4O:210:TYR:CD2  | 2.35                     | 0.62              |
| 1:1B:439:SER:CB   | 2:4O:400:ARG:HD2  | 2.29                     | 0.62              |
| 1:1C:2:ARG:HG3    | 2:4P:72:PRO:CD    | 2.29                     | 0.62              |
| 1:1E:407:TRP:CE3  | 2:1R:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1G:262:TYR:C    | 2:4T:406:HIS:CD2  | 2.60                     | 0.62              |
| 1:1G:348:PRO:HB3  | 2:4T:394:GLN:HG2  | 1.76                     | 0.62              |
| 1:1N:2:ARG:HG3    | 2:4Z:72:PRO:HG2   | 1.81                     | 0.62              |
| 2:1S:221:THR:CB   | 1:2F:324:VAL:HG21 | 2.30                     | 0.62              |
| 2:2H:181:VAL:H    | 1:3A:258:ASN:ND2  | 1.98                     | 0.62              |
| 2:2S:72:PRO:HD2   | 1:3F:2:ARG:CD     | 2.28                     | 0.62              |
| 2:2S:224:TYR:HE2  | 1:3F:248:LEU:HB2  | 1.65                     | 0.62              |
| 2:2W:404:PHE:CE2  | 1:3K:261:PRO:CB   | 2.79                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2W:406:HIS:NE2  | 1:3K:262:TYR:CA   | 2.63                     | 0.62              |
| 1:3E:407:TRP:CE3  | 2:3R:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:3I:180:ALA:HB3  | 1:3I:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4A:180:ALA:HB3  | 1:4A:183:GLU:HG3  | 1.82                     | 0.62              |
| 1:4E:407:TRP:CE3  | 2:4R:257:VAL:HG22 | 2.35                     | 0.62              |
| 1:1D:2:ARG:HH11   | 2:4Q:71:GLU:HG3   | 1.61                     | 0.61              |
| 1:1I:2:ARG:CG     | 2:4U:72:PRO:HD2   | 2.30                     | 0.61              |
| 1:1I:325:PRO:HG2  | 2:4U:224:TYR:CG   | 2.34                     | 0.61              |
| 1:1J:352:LYS:HD3  | 2:4V:101:ASN:HD22 | 1.62                     | 0.61              |
| 1:2E:407:TRP:CE3  | 2:2R:257:VAL:HG22 | 2.35                     | 0.61              |
| 2:2O:394:GLN:HG2  | 1:3B:348:PRO:HB2  | 1.81                     | 0.61              |
| 1:1D:257:THR:CG2  | 2:4Q:102:ASN:HB2  | 2.30                     | 0.61              |
| 1:1D:261:PRO:N    | 2:4Q:404:PHE:CD1  | 2.67                     | 0.61              |
| 1:1F:346:TRP:CD2  | 2:4S:403:ALA:HB2  | 2.35                     | 0.61              |
| 1:1F:352:LYS:HE2  | 2:4S:101:ASN:ND2  | 2.15                     | 0.61              |
| 1:1G:260:VAL:CB   | 2:4T:407:TRP:HZ2  | 2.10                     | 0.61              |
| 1:1M:349:THR:O    | 2:4Y:181:VAL:CA   | 2.35                     | 0.61              |
| 1:1N:351:PHE:O    | 2:4Z:180:THR:N    | 2.33                     | 0.61              |
| 2:1U:182:VAL:HG21 | 1:2I:257:THR:CG2  | 2.30                     | 0.61              |
| 2:1W:181:VAL:CG2  | 1:2K:258:ASN:CB   | 2.67                     | 0.61              |
| 2:1W:406:HIS:CE1  | 1:2K:263:PRO:HB3  | 2.35                     | 0.61              |
| 2:2H:404:PHE:CE1  | 1:3A:261:PRO:N    | 2.68                     | 0.61              |
| 2:2P:222:PRO:O    | 1:3C:325:PRO:HD2  | 2.00                     | 0.61              |
| 2:2S:406:HIS:CE1  | 1:3F:263:PRO:CA   | 2.83                     | 0.61              |
| 1:3M:407:TRP:CE3  | 2:3Y:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:4M:407:TRP:CE3  | 2:4Y:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:1C:325:PRO:O    | 2:4P:210:TYR:OH   | 2.18                     | 0.61              |
| 1:1D:257:THR:HB   | 2:4Q:100:GLY:O    | 1.99                     | 0.61              |
| 1:1D:329:ASN:HB2  | 2:4Q:210:TYR:CD2  | 2.35                     | 0.61              |
| 1:1E:326:LYS:HB3  | 2:4R:222:PRO:HG2  | 1.81                     | 0.61              |
| 1:1E:439:SER:HB2  | 2:4R:400:ARG:HD2  | 1.82                     | 0.61              |
| 1:1J:346:TRP:CB   | 2:4V:397:ALA:O    | 2.48                     | 0.61              |
| 1:1M:407:TRP:CE3  | 2:1Y:257:VAL:HG22 | 2.35                     | 0.61              |
| 2:1O:179:ASP:OD2  | 1:2B:248:LEU:CD2  | 2.48                     | 0.61              |
| 2:1T:180:THR:CA   | 1:2G:258:ASN:ND2  | 2.63                     | 0.61              |
| 2:1Y:404:PHE:CE1  | 1:2M:260:VAL:N    | 2.68                     | 0.61              |
| 1:2M:407:TRP:CE3  | 2:2Y:257:VAL:HG22 | 2.35                     | 0.61              |
| 2:2P:221:THR:OG1  | 1:3C:324:VAL:CG2  | 2.47                     | 0.61              |
| 2:2U:101:ASN:C    | 1:3I:257:THR:HG21 | 2.24                     | 0.61              |
| 2:2Y:77:SER:CB    | 1:3M:245:ASP:OD1  | 2.45                     | 0.61              |
| 2:2Z:397:ALA:HB1  | 1:3N:346:TRP:HA   | 1.80                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:351:PHE:O    | 2:4R:181:VAL:N    | 2.32                     | 0.61              |
| 1:1F:325:PRO:CB   | 2:4S:224:TYR:CZ   | 2.83                     | 0.61              |
| 1:1G:346:TRP:O    | 2:4T:398:MET:N    | 2.33                     | 0.61              |
| 1:1L:434:GLU:O    | 2:4X:401:ARG:NH2  | 2.33                     | 0.61              |
| 2:1T:224:TYR:CE2  | 1:2G:248:LEU:HB2  | 2.35                     | 0.61              |
| 2:1V:11:GLN:HE22  | 1:2J:249:ASN:CB   | 2.11                     | 0.61              |
| 2:2H:401:ARG:C    | 1:3A:262:TYR:HH   | 1.96                     | 0.61              |
| 2:2T:397:ALA:HB1  | 1:3G:346:TRP:HA   | 1.81                     | 0.61              |
| 2:2T:404:PHE:H    | 1:3G:261:PRO:C    | 2.03                     | 0.61              |
| 2:2Y:397:ALA:O    | 1:3M:346:TRP:CB   | 2.48                     | 0.61              |
| 1:1B:329:ASN:HB2  | 2:4O:210:TYR:HE2  | 1.61                     | 0.61              |
| 1:1C:180:ALA:HB3  | 1:1C:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:1C:325:PRO:CB   | 2:4P:224:TYR:CE1  | 2.83                     | 0.61              |
| 1:1D:180:ALA:HB3  | 1:1D:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:1D:258:ASN:O    | 2:4Q:181:VAL:HB   | 2.00                     | 0.61              |
| 1:1E:2:ARG:HH22   | 2:4R:73:GLY:HA3   | 1.63                     | 0.61              |
| 1:1E:263:PRO:CA   | 2:4R:406:HIS:CE1  | 2.83                     | 0.61              |
| 1:1E:333:ALA:HB1  | 2:4R:176:LYS:HB3  | 1.80                     | 0.61              |
| 1:1F:64:ARG:NH2   | 1:1F:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1G:352:LYS:CE   | 2:4T:101:ASN:HD22 | 2.12                     | 0.61              |
| 1:1K:254:GLU:HA   | 2:4W:100:GLY:O    | 2.00                     | 0.61              |
| 1:1M:326:LYS:HA   | 2:4Y:210:TYR:CE1  | 2.35                     | 0.61              |
| 2:1P:181:VAL:N    | 1:2C:258:ASN:HD22 | 1.94                     | 0.61              |
| 1:2C:64:ARG:NH2   | 1:2C:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2C:180:ALA:HB3  | 1:2C:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:2D:180:ALA:HB3  | 1:2D:183:GLU:HG3  | 1.82                     | 0.61              |
| 2:2O:182:VAL:HG21 | 1:3B:257:THR:HG22 | 1.81                     | 0.61              |
| 2:2S:210:TYR:HD2  | 1:3F:329:ASN:ND2  | 1.89                     | 0.61              |
| 2:2U:394:GLN:CA   | 1:3I:348:PRO:HG3  | 2.30                     | 0.61              |
| 1:3C:64:ARG:NH2   | 1:3C:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3F:64:ARG:NH2   | 1:3F:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4C:64:ARG:NH2   | 1:4C:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4C:180:ALA:HB3  | 1:4C:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:4G:64:ARG:NH2   | 1:4G:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1A:261:PRO:C    | 2:4H:404:PHE:H    | 2.08                     | 0.61              |
| 1:1B:329:ASN:ND2  | 2:4O:210:TYR:HD2  | 1.95                     | 0.61              |
| 1:1B:353:VAL:HG23 | 2:4O:179:ASP:HA   | 1.81                     | 0.61              |
| 1:1C:64:ARG:NH2   | 1:1C:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1C:326:LYS:HE3  | 2:4P:214:PHE:HB2  | 1.83                     | 0.61              |
| 1:1C:349:THR:HG23 | 2:4P:394:GLN:OE1  | 2.00                     | 0.61              |
| 1:1D:64:ARG:NH2   | 1:1D:129:CYS:SG   | 2.74                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:260:VAL:HG11 | 2:4Q:407:TRP:CZ2  | 2.36                     | 0.61              |
| 1:1D:407:TRP:CE3  | 2:1Q:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:1F:180:ALA:HB3  | 1:1F:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:1G:64:ARG:NH2   | 1:1G:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1J:346:TRP:CZ3  | 2:4V:404:PHE:HE2  | 2.17                     | 0.61              |
| 1:1L:64:ARG:NH2   | 1:1L:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1N:257:THR:HG21 | 2:4Z:101:ASN:C    | 2.25                     | 0.61              |
| 1:1N:407:TRP:CE3  | 2:1Z:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:2F:64:ARG:NH2   | 1:2F:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2G:64:ARG:NH2   | 1:2G:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2L:64:ARG:NH2   | 1:2L:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2N:407:TRP:CE3  | 2:2Z:257:VAL:HG22 | 2.35                     | 0.61              |
| 2:2O:394:GLN:CG   | 1:3B:348:PRO:HG3  | 2.27                     | 0.61              |
| 2:2R:101:ASN:HB2  | 1:3E:254:GLU:CG   | 2.30                     | 0.61              |
| 5:2V:501:GDP:H8   | 1:3J:248:LEU:HD11 | 1.64                     | 0.61              |
| 1:3C:180:ALA:HB3  | 1:3C:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:3D:180:ALA:HB3  | 1:3D:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:3D:407:TRP:CE3  | 2:3Q:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:3G:64:ARG:NH2   | 1:3G:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3L:64:ARG:NH2   | 1:3L:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3N:407:TRP:CE3  | 2:3Z:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:4D:180:ALA:HB3  | 1:4D:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:4F:64:ARG:NH2   | 1:4F:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4N:407:TRP:CE3  | 2:4Z:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:1C:2:ARG:HG3    | 2:4P:72:PRO:HG2   | 1.82                     | 0.61              |
| 1:1C:325:PRO:HD2  | 2:4P:223:THR:HA   | 1.82                     | 0.61              |
| 1:1D:2:ARG:HH22   | 2:4Q:73:GLY:HA3   | 1.65                     | 0.61              |
| 1:1L:326:LYS:HA   | 2:4X:210:TYR:CE1  | 2.35                     | 0.61              |
| 1:2D:64:ARG:NH2   | 1:2D:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2D:407:TRP:CE3  | 2:2Q:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:2F:180:ALA:HB3  | 1:2F:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:2K:64:ARG:NH2   | 1:2K:129:CYS:SG   | 2.74                     | 0.61              |
| 2:2P:407:TRP:HE1  | 1:3C:260:VAL:CB   | 2.13                     | 0.61              |
| 2:2T:72:PRO:HG2   | 1:3G:2:ARG:HG3    | 1.83                     | 0.61              |
| 2:2U:397:ALA:HB1  | 1:3I:346:TRP:HA   | 1.82                     | 0.61              |
| 2:2Y:406:HIS:NE2  | 1:3M:263:PRO:CD   | 2.62                     | 0.61              |
| 1:3D:64:ARG:NH2   | 1:3D:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4D:64:ARG:NH2   | 1:4D:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4F:180:ALA:HB3  | 1:4F:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:4G:180:ALA:HB3  | 1:4G:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:4K:64:ARG:NH2   | 1:4K:129:CYS:SG   | 2.74                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4L:64:ARG:NH2   | 1:4L:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1A:64:ARG:NH2   | 1:1A:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1A:261:PRO:HA   | 2:4H:404:PHE:HA   | 1.83                     | 0.61              |
| 1:1A:263:PRO:N    | 2:4H:406:HIS:CD2  | 2.68                     | 0.61              |
| 1:1B:253:THR:CB   | 2:4O:100:GLY:CA   | 2.79                     | 0.61              |
| 1:1F:261:PRO:C    | 2:4S:404:PHE:HA   | 2.26                     | 0.61              |
| 1:1G:180:ALA:HB3  | 1:1G:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:C    | 2.25                     | 0.61              |
| 1:1I:64:ARG:NH2   | 1:1I:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1I:346:TRP:CE2  | 2:4U:403:ALA:HB2  | 2.36                     | 0.61              |
| 1:1K:64:ARG:NH2   | 1:1K:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1M:248:LEU:HD13 | 5:4Y:501:GDP:H8   | 1.64                     | 0.61              |
| 2:1H:404:PHE:CE1  | 1:2A:260:VAL:C    | 2.79                     | 0.61              |
| 2:1S:180:THR:HA   | 1:2F:258:ASN:ND2  | 2.15                     | 0.61              |
| 2:1Z:181:VAL:CA   | 1:2N:258:ASN:HD22 | 2.12                     | 0.61              |
| 2:2O:73:GLY:HA3   | 1:3B:2:ARG:NH2    | 2.15                     | 0.61              |
| 2:2O:214:PHE:CB   | 1:3B:326:LYS:CE   | 2.75                     | 0.61              |
| 2:2O:394:GLN:CB   | 1:3B:348:PRO:CG   | 2.79                     | 0.61              |
| 2:2S:100:GLY:O    | 1:3F:254:GLU:HA   | 2.00                     | 0.61              |
| 2:2U:394:GLN:HB3  | 1:3I:348:PRO:HG2  | 1.83                     | 0.61              |
| 2:2V:224:TYR:HD2  | 1:3J:247:ALA:O    | 1.84                     | 0.61              |
| 1:3F:180:ALA:HB3  | 1:3F:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:3G:180:ALA:HB3  | 1:3G:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:3I:64:ARG:NH2   | 1:3I:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3K:64:ARG:NH2   | 1:3K:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1B:261:PRO:N    | 2:4O:404:PHE:CD1  | 2.69                     | 0.61              |
| 1:1F:260:VAL:CG1  | 2:4S:407:TRP:CE2  | 2.84                     | 0.61              |
| 1:1J:332:ILE:HG22 | 2:4V:177:VAL:CG2  | 2.21                     | 0.61              |
| 1:1K:245:ASP:OD2  | 2:4W:77:SER:HB2   | 2.00                     | 0.61              |
| 1:1M:260:VAL:CG1  | 2:4Y:407:TRP:HZ2  | 2.12                     | 0.61              |
| 1:1N:261:PRO:N    | 2:4Z:404:PHE:CE1  | 2.69                     | 0.61              |
| 2:1Y:182:VAL:CG2  | 1:2M:257:THR:CG2  | 2.67                     | 0.61              |
| 1:2G:180:ALA:HB3  | 1:2G:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:2I:64:ARG:NH2   | 1:2I:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3N:64:ARG:NH2   | 1:3N:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4D:407:TRP:CE3  | 2:4Q:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:4E:180:ALA:HB3  | 1:4E:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:4N:64:ARG:NH2   | 1:4N:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1A:260:VAL:HG12 | 2:4H:407:TRP:HE1  | 1.66                     | 0.61              |
| 1:1C:435:VAL:O    | 2:4P:401:ARG:NH2  | 2.29                     | 0.61              |
| 1:1E:180:ALA:HB3  | 1:1E:183:GLU:HG3  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:211:ASP:OD1  | 1:1E:215:ARG:NH1  | 2.34                     | 0.61              |
| 1:1E:261:PRO:HA   | 2:4R:404:PHE:CD1  | 2.35                     | 0.61              |
| 1:1F:326:LYS:HB3  | 2:4S:222:PRO:HG2  | 1.83                     | 0.61              |
| 1:1J:64:ARG:NH2   | 1:1J:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1M:260:VAL:CG1  | 2:4Y:407:TRP:CZ2  | 2.83                     | 0.61              |
| 1:1M:346:TRP:CB   | 2:4Y:397:ALA:O    | 2.48                     | 0.61              |
| 1:1M:349:THR:HB   | 2:4Y:180:THR:O    | 2.00                     | 0.61              |
| 1:1N:64:ARG:NH2   | 1:1N:129:CYS:SG   | 2.74                     | 0.61              |
| 2:1Q:100:GLY:HA2  | 1:2D:253:THR:HB   | 1.82                     | 0.61              |
| 2:1Y:179:ASP:C    | 1:2M:352:LYS:HD2  | 2.23                     | 0.61              |
| 1:2A:64:ARG:NH2   | 1:2A:129:CYS:SG   | 2.74                     | 0.61              |
| 1:2A:407:TRP:CE3  | 2:2H:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:2E:180:ALA:HB3  | 1:2E:183:GLU:HG3  | 1.82                     | 0.61              |
| 1:2N:64:ARG:NH2   | 1:2N:129:CYS:SG   | 2.74                     | 0.61              |
| 2:2P:394:GLN:CG   | 1:3C:348:PRO:HG3  | 2.27                     | 0.61              |
| 2:2W:72:PRO:HD2   | 1:3K:2:ARG:CG     | 2.31                     | 0.61              |
| 1:3A:64:ARG:NH2   | 1:3A:129:CYS:SG   | 2.74                     | 0.61              |
| 1:3M:211:ASP:OD1  | 1:3M:215:ARG:NH1  | 2.34                     | 0.61              |
| 1:4A:64:ARG:NH2   | 1:4A:129:CYS:SG   | 2.74                     | 0.61              |
| 1:4A:407:TRP:CE3  | 2:4H:257:VAL:HG22 | 2.35                     | 0.61              |
| 1:4I:64:ARG:NH2   | 1:4I:129:CYS:SG   | 2.74                     | 0.61              |
| 1:1A:211:ASP:OD1  | 1:1A:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1A:326:LYS:HE3  | 2:4H:214:PHE:HB2  | 1.83                     | 0.60              |
| 1:1A:407:TRP:CE3  | 2:1H:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:1B:64:ARG:NH2   | 1:1B:129:CYS:SG   | 2.74                     | 0.60              |
| 1:1C:245:ASP:OD2  | 2:4P:77:SER:HB2   | 2.01                     | 0.60              |
| 1:1D:349:THR:HG21 | 2:4Q:184:PRO:CG   | 2.29                     | 0.60              |
| 1:1E:64:ARG:NH2   | 1:1E:129:CYS:SG   | 2.74                     | 0.60              |
| 1:1G:248:LEU:HD12 | 2:4T:11:GLN:CD    | 2.26                     | 0.60              |
| 1:1K:332:ILE:HG22 | 2:4W:177:VAL:CG2  | 2.25                     | 0.60              |
| 1:1K:348:PRO:CB   | 2:4W:394:GLN:HG2  | 2.31                     | 0.60              |
| 1:1L:262:TYR:CA   | 2:4X:406:HIS:CD2  | 2.40                     | 0.60              |
| 1:1M:211:ASP:OD1  | 1:1M:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1N:353:VAL:CB   | 2:4Z:179:ASP:OD1  | 2.47                     | 0.60              |
| 2:1Q:181:VAL:N    | 1:2D:258:ASN:HD22 | 1.93                     | 0.60              |
| 2:1R:404:PHE:CE1  | 1:2E:260:VAL:O    | 2.54                     | 0.60              |
| 2:1S:179:ASP:O    | 1:2F:352:LYS:CD   | 2.50                     | 0.60              |
| 1:2B:64:ARG:NH2   | 1:2B:129:CYS:SG   | 2.74                     | 0.60              |
| 1:2E:211:ASP:OD1  | 1:2E:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2G:211:ASP:OD1  | 1:2G:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2J:64:ARG:NH2   | 1:2J:129:CYS:SG   | 2.74                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2M:211:ASP:OD1  | 1:2M:215:ARG:NH1  | 2.34                     | 0.60              |
| 2:2X:394:GLN:CB   | 1:3L:348:PRO:HG3  | 2.30                     | 0.60              |
| 2:2Y:73:GLY:HA3   | 1:3M:2:ARG:NH2    | 2.16                     | 0.60              |
| 1:3A:211:ASP:OD1  | 1:3A:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:3A:407:TRP:CE3  | 2:3H:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:3B:64:ARG:NH2   | 1:3B:129:CYS:SG   | 2.74                     | 0.60              |
| 1:3E:180:ALA:HB3  | 1:3E:183:GLU:HG3  | 1.82                     | 0.60              |
| 1:3G:211:ASP:OD1  | 1:3G:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:3J:64:ARG:NH2   | 1:3J:129:CYS:SG   | 2.74                     | 0.60              |
| 1:4A:211:ASP:OD1  | 1:4A:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4B:64:ARG:NH2   | 1:4B:129:CYS:SG   | 2.74                     | 0.60              |
| 1:4E:211:ASP:OD1  | 1:4E:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4G:211:ASP:OD1  | 1:4G:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4M:211:ASP:OD1  | 1:4M:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1B:326:LYS:HE2  | 2:4O:214:PHE:CB   | 2.28                     | 0.60              |
| 1:1C:249:ASN:N    | 2:4P:11:GLN:CD    | 2.35                     | 0.60              |
| 1:1G:211:ASP:OD1  | 1:1G:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1G:325:PRO:CB   | 2:4T:224:TYR:CZ   | 2.83                     | 0.60              |
| 1:1G:346:TRP:CZ3  | 2:4T:403:ALA:HB3  | 2.25                     | 0.60              |
| 1:1J:439:SER:OG   | 2:4V:401:ARG:HD3  | 2.01                     | 0.60              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:HA   | 1.81                     | 0.60              |
| 2:1X:404:PHE:CE1  | 1:2L:260:VAL:N    | 2.69                     | 0.60              |
| 1:2A:211:ASP:OD1  | 1:2A:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2E:64:ARG:NH2   | 1:2E:129:CYS:SG   | 2.74                     | 0.60              |
| 1:2J:211:ASP:OD1  | 1:2J:215:ARG:NH1  | 2.34                     | 0.60              |
| 2:2S:401:ARG:HH21 | 1:3F:435:VAL:HA   | 1.62                     | 0.60              |
| 2:2U:221:THR:C    | 1:3I:324:VAL:HG11 | 2.26                     | 0.60              |
| 2:2Y:179:ASP:OD2  | 1:3M:248:LEU:CD2  | 2.49                     | 0.60              |
| 2:2Z:182:VAL:HG21 | 1:3N:257:THR:HG22 | 1.81                     | 0.60              |
| 1:3E:64:ARG:NH2   | 1:3E:129:CYS:SG   | 2.74                     | 0.60              |
| 1:3E:211:ASP:OD1  | 1:3E:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4J:64:ARG:NH2   | 1:4J:129:CYS:SG   | 2.74                     | 0.60              |
| 1:1A:257:THR:HG21 | 2:4H:101:ASN:C    | 2.26                     | 0.60              |
| 1:1C:2:ARG:HD3    | 2:4P:72:PRO:CD    | 2.23                     | 0.60              |
| 1:1E:439:SER:CB   | 2:4R:400:ARG:CD   | 2.79                     | 0.60              |
| 1:1F:260:VAL:C    | 2:4S:407:TRP:NE1  | 2.53                     | 0.60              |
| 1:1G:332:ILE:HG22 | 2:4T:177:VAL:CG2  | 2.04                     | 0.60              |
| 1:1I:348:PRO:CB   | 2:4U:394:GLN:CG   | 2.79                     | 0.60              |
| 1:1J:349:THR:CB   | 2:4V:184:PRO:HD3  | 2.31                     | 0.60              |
| 2:1U:406:HIS:CE1  | 1:2I:263:PRO:HB3  | 2.36                     | 0.60              |
| 2:1W:404:PHE:HE1  | 1:2K:260:VAL:N    | 1.99                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2T:222:PRO:O    | 1:3G:325:PRO:HD2  | 2.01                     | 0.60              |
| 2:2T:404:PHE:CD2  | 1:3G:261:PRO:HB3  | 2.36                     | 0.60              |
| 1:3J:211:ASP:OD1  | 1:3J:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4D:211:ASP:OD1  | 1:4D:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4E:64:ARG:NH2   | 1:4E:129:CYS:SG   | 2.74                     | 0.60              |
| 1:4J:211:ASP:OD1  | 1:4J:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1B:211:ASP:OD1  | 1:1B:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1C:407:TRP:CE3  | 2:1P:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:1D:211:ASP:OD1  | 1:1D:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1D:325:PRO:HB3  | 2:4Q:224:TYR:CZ   | 2.37                     | 0.60              |
| 1:1E:260:VAL:CB   | 2:4R:407:TRP:CZ2  | 2.84                     | 0.60              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:CD1  | 2.84                     | 0.60              |
| 1:1J:211:ASP:OD1  | 1:1J:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1J:247:ALA:O    | 2:4V:15:GLN:NE2   | 2.32                     | 0.60              |
| 1:1L:254:GLU:N    | 2:4X:100:GLY:HA2  | 2.16                     | 0.60              |
| 1:1M:64:ARG:NH2   | 1:1M:129:CYS:SG   | 2.74                     | 0.60              |
| 1:1M:245:ASP:OD2  | 2:4Y:77:SER:HB2   | 2.01                     | 0.60              |
| 1:1M:257:THR:OG1  | 2:4Y:100:GLY:O    | 2.20                     | 0.60              |
| 2:1U:404:PHE:CZ   | 1:2I:261:PRO:N    | 2.70                     | 0.60              |
| 1:2D:211:ASP:OD1  | 1:2D:215:ARG:NH1  | 2.34                     | 0.60              |
| 2:2H:73:GLY:HA3   | 1:3A:2:ARG:NH2    | 2.17                     | 0.60              |
| 2:2W:397:ALA:O    | 1:3K:346:TRP:CB   | 2.49                     | 0.60              |
| 2:2X:207:GLU:CD   | 1:3L:329:ASN:ND2  | 2.44                     | 0.60              |
| 1:3C:407:TRP:CE3  | 2:3P:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:3D:211:ASP:OD1  | 1:3D:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4B:211:ASP:OD1  | 1:4B:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:4B:407:TRP:CE3  | 2:4O:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:4L:211:ASP:OD1  | 1:4L:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1D:248:LEU:HD11 | 5:4Q:501:GDP:H8   | 1.61                     | 0.60              |
| 1:1D:352:LYS:CE   | 2:4Q:101:ASN:HD22 | 2.14                     | 0.60              |
| 1:1E:261:PRO:CB   | 2:4R:404:PHE:N    | 2.65                     | 0.60              |
| 1:1G:329:ASN:CB   | 2:4T:210:TYR:CD2  | 2.85                     | 0.60              |
| 1:1I:211:ASP:OD1  | 1:1I:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1K:211:ASP:OD1  | 1:1K:215:ARG:NH1  | 2.34                     | 0.60              |
| 2:1S:401:ARG:HH22 | 1:2F:435:VAL:HA   | 1.65                     | 0.60              |
| 2:1Y:11:GLN:HE22  | 1:2M:249:ASN:CB   | 2.13                     | 0.60              |
| 1:2B:211:ASP:OD1  | 1:2B:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2K:211:ASP:OD1  | 1:2K:215:ARG:NH1  | 2.34                     | 0.60              |
| 2:2S:179:ASP:OD1  | 1:3F:353:VAL:CB   | 2.46                     | 0.60              |
| 1:3B:211:ASP:OD1  | 1:3B:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:3K:211:ASP:OD1  | 1:3K:215:ARG:NH1  | 2.34                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3L:211:ASP:OD1  | 1:3L:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1A:262:TYR:HA   | 2:4H:406:HIS:HD2  | 1.53                     | 0.60              |
| 1:1A:326:LYS:HB3  | 2:4H:222:PRO:HG2  | 1.82                     | 0.60              |
| 1:1A:329:ASN:CB   | 2:4H:210:TYR:CD2  | 2.84                     | 0.60              |
| 1:1B:407:TRP:CE3  | 2:1O:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:1L:211:ASP:OD1  | 1:1L:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2B:407:TRP:CE3  | 2:2O:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:2C:407:TRP:CE3  | 2:2P:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:2I:211:ASP:OD1  | 1:2I:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2L:211:ASP:OD1  | 1:2L:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:2M:64:ARG:NH2   | 1:2M:129:CYS:SG   | 2.74                     | 0.60              |
| 2:2Q:224:TYR:HE2  | 1:3D:248:LEU:HB2  | 1.66                     | 0.60              |
| 2:2R:179:ASP:OD1  | 1:3E:353:VAL:CB   | 2.44                     | 0.60              |
| 2:2U:100:GLY:HA2  | 1:3I:253:THR:CB   | 2.31                     | 0.60              |
| 2:2W:397:ALA:HB1  | 1:3K:346:TRP:HA   | 1.82                     | 0.60              |
| 1:3B:407:TRP:CE3  | 2:3O:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:3I:211:ASP:OD1  | 1:3I:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:3M:64:ARG:NH2   | 1:3M:129:CYS:SG   | 2.74                     | 0.60              |
| 1:4C:407:TRP:CE3  | 2:4P:257:VAL:HG22 | 2.35                     | 0.60              |
| 1:4K:211:ASP:OD1  | 1:4K:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1G:248:LEU:HD11 | 5:4T:501:GDP:O1A  | 2.02                     | 0.60              |
| 1:1L:346:TRP:CH2  | 2:4X:403:ALA:HB1  | 2.36                     | 0.60              |
| 1:1N:261:PRO:HB3  | 2:4Z:404:PHE:CD2  | 2.37                     | 0.60              |
| 1:1N:261:PRO:O    | 2:4Z:404:PHE:CA   | 2.50                     | 0.60              |
| 1:1N:352:LYS:HA   | 2:4Z:179:ASP:O    | 2.01                     | 0.60              |
| 2:1U:181:VAL:HB   | 1:2I:258:ASN:CA   | 2.29                     | 0.60              |
| 2:2O:101:ASN:N    | 1:3B:254:GLU:HG2  | 2.17                     | 0.60              |
| 2:2P:100:GLY:CA   | 1:3C:253:THR:CG2  | 2.70                     | 0.60              |
| 2:2R:100:GLY:CA   | 1:3E:253:THR:CG2  | 2.76                     | 0.60              |
| 2:2R:224:TYR:HE2  | 1:3E:248:LEU:HB2  | 1.67                     | 0.60              |
| 2:2U:394:GLN:HB3  | 1:3I:348:PRO:CG   | 2.32                     | 0.60              |
| 2:2X:181:VAL:N    | 1:3L:258:ASN:HD22 | 1.99                     | 0.60              |
| 2:2Y:394:GLN:HA   | 1:3M:348:PRO:HG3  | 1.84                     | 0.60              |
| 1:4I:211:ASP:OD1  | 1:4I:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1B:2:ARG:NH2    | 2:4O:73:GLY:CA    | 2.62                     | 0.60              |
| 1:1D:262:TYR:OH   | 2:4Q:402:LYS:C    | 2.45                     | 0.60              |
| 1:1E:263:PRO:HD3  | 2:4R:406:HIS:HB3  | 1.83                     | 0.60              |
| 2:2R:72:PRO:HD2   | 1:3E:2:ARG:CD     | 2.31                     | 0.60              |
| 2:2U:404:PHE:CD2  | 1:3I:261:PRO:HB3  | 2.37                     | 0.60              |
| 2:2X:73:GLY:HA3   | 1:3L:2:ARG:CZ     | 2.30                     | 0.60              |
| 2:2X:397:ALA:HB1  | 1:3L:346:TRP:HA   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4M:64:ARG:NH2   | 1:4M:129:CYS:SG   | 2.74                     | 0.60              |
| 1:1C:349:THR:HG21 | 2:4P:184:PRO:CD   | 2.32                     | 0.60              |
| 1:1E:254:GLU:CA   | 2:4R:100:GLY:HA2  | 2.32                     | 0.60              |
| 1:1G:349:THR:HG21 | 2:4T:184:PRO:CG   | 2.29                     | 0.60              |
| 1:1I:261:PRO:HA   | 2:4U:404:PHE:CD1  | 2.36                     | 0.60              |
| 1:1I:349:THR:OG1  | 2:4U:184:PRO:HD2  | 2.01                     | 0.60              |
| 1:1K:249:ASN:H    | 2:4W:11:GLN:CD    | 2.07                     | 0.60              |
| 2:1H:404:PHE:CD1  | 1:2A:260:VAL:O    | 2.55                     | 0.60              |
| 2:1Q:221:THR:OG1  | 1:2D:324:VAL:HG21 | 2.01                     | 0.60              |
| 2:1V:222:PRO:HG2  | 1:2J:326:LYS:HB2  | 1.84                     | 0.60              |
| 2:1X:401:ARG:O    | 1:2L:262:TYR:HE1  | 1.85                     | 0.60              |
| 2:1Z:182:VAL:CG2  | 1:2N:257:THR:HG22 | 2.31                     | 0.60              |
| 1:2N:211:ASP:OD1  | 1:2N:215:ARG:NH1  | 2.34                     | 0.60              |
| 5:2S:501:GDP:H8   | 1:3F:248:LEU:HD11 | 1.66                     | 0.60              |
| 2:2T:179:ASP:O    | 1:3G:352:LYS:HA   | 2.02                     | 0.60              |
| 2:2T:406:HIS:NE2  | 1:3G:262:TYR:HA   | 2.13                     | 0.60              |
| 1:1A:260:VAL:C    | 2:4H:404:PHE:CD1  | 2.80                     | 0.60              |
| 1:1D:348:PRO:HD2  | 2:4Q:398:MET:HG3  | 1.82                     | 0.60              |
| 1:1E:258:ASN:ND2  | 2:4R:182:VAL:HG22 | 2.17                     | 0.60              |
| 1:1G:258:ASN:OD1  | 2:4T:101:ASN:ND2  | 2.35                     | 0.60              |
| 1:1J:329:ASN:OD1  | 2:4V:177:VAL:CG1  | 2.50                     | 0.60              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:CA   | 2.50                     | 0.60              |
| 2:1S:178:SER:HB3  | 1:2F:349:THR:CB   | 2.31                     | 0.60              |
| 2:2V:397:ALA:HB1  | 1:3J:346:TRP:HA   | 1.83                     | 0.60              |
| 1:4N:211:ASP:OD1  | 1:4N:215:ARG:NH1  | 2.34                     | 0.60              |
| 1:1B:326:LYS:HB3  | 2:4O:222:PRO:HG2  | 1.81                     | 0.59              |
| 1:1E:257:THR:CB   | 2:4R:100:GLY:O    | 2.50                     | 0.59              |
| 1:1E:326:LYS:HA   | 2:4R:210:TYR:CZ   | 2.34                     | 0.59              |
| 1:1N:211:ASP:OD1  | 1:1N:215:ARG:NH1  | 2.34                     | 0.59              |
| 2:1W:101:ASN:O    | 1:2K:257:THR:HG21 | 2.01                     | 0.59              |
| 2:1W:179:ASP:OD2  | 1:2K:248:LEU:CD2  | 2.36                     | 0.59              |
| 2:2P:181:VAL:CB   | 1:3C:258:ASN:O    | 2.49                     | 0.59              |
| 2:2T:72:PRO:HD2   | 1:3G:2:ARG:CD     | 2.30                     | 0.59              |
| 2:2V:210:TYR:CE2  | 1:3J:329:ASN:HB2  | 2.37                     | 0.59              |
| 2:2Z:221:THR:CA   | 1:3N:324:VAL:HG11 | 2.28                     | 0.59              |
| 1:3N:211:ASP:OD1  | 1:3N:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:1F:211:ASP:OD1  | 1:1F:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:1N:348:PRO:HG3  | 2:4Z:394:GLN:HG2  | 1.84                     | 0.59              |
| 2:1P:207:GLU:CD   | 1:2C:329:ASN:HD21 | 2.09                     | 0.59              |
| 2:1R:100:GLY:CA   | 1:2E:253:THR:HG22 | 2.32                     | 0.59              |
| 1:2F:211:ASP:OD1  | 1:2F:215:ARG:NH1  | 2.34                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2T:406:HIS:NE2  | 1:3G:263:PRO:CD   | 2.60                     | 0.59              |
| 2:2X:397:ALA:O    | 1:3L:346:TRP:CB   | 2.50                     | 0.59              |
| 2:2Y:404:PHE:CD1  | 1:3M:261:PRO:CA   | 2.82                     | 0.59              |
| 1:4C:211:ASP:OD1  | 1:4C:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:1A:2:ARG:HG3    | 2:4H:72:PRO:CG    | 2.32                     | 0.59              |
| 1:1B:254:GLU:HB3  | 2:4O:101:ASN:HB2  | 1.84                     | 0.59              |
| 1:1C:211:ASP:OD1  | 1:1C:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:1D:257:THR:HG21 | 2:4Q:102:ASN:CB   | 2.32                     | 0.59              |
| 1:1E:247:ALA:O    | 2:4R:15:GLN:OE1   | 2.19                     | 0.59              |
| 1:1J:260:VAL:CB   | 2:4V:407:TRP:CE2  | 2.79                     | 0.59              |
| 1:1K:314:ALA:HB1  | 2:4W:181:VAL:HG21 | 1.83                     | 0.59              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:CB   | 2.48                     | 0.59              |
| 1:1L:351:PHE:O    | 2:4X:180:THR:C    | 2.45                     | 0.59              |
| 1:1M:260:VAL:CB   | 2:4Y:407:TRP:CZ2  | 2.84                     | 0.59              |
| 2:1Q:221:THR:OG1  | 1:2D:324:VAL:CG2  | 2.49                     | 0.59              |
| 1:2C:211:ASP:OD1  | 1:2C:215:ARG:NH1  | 2.34                     | 0.59              |
| 2:2S:101:ASN:N    | 1:3F:254:GLU:HG2  | 2.17                     | 0.59              |
| 2:2W:101:ASN:ND2  | 1:3K:258:ASN:OD1  | 2.33                     | 0.59              |
| 2:2W:403:ALA:HA   | 1:3K:262:TYR:CZ   | 2.37                     | 0.59              |
| 5:2W:501:GDP:H8   | 1:3K:248:LEU:HD11 | 1.66                     | 0.59              |
| 1:3C:211:ASP:OD1  | 1:3C:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:3F:211:ASP:OD1  | 1:3F:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:4F:211:ASP:OD1  | 1:4F:215:ARG:NH1  | 2.34                     | 0.59              |
| 1:1B:260:VAL:C    | 2:4O:404:PHE:CE1  | 2.80                     | 0.59              |
| 1:1F:247:ALA:O    | 2:4S:15:GLN:NE2   | 2.35                     | 0.59              |
| 2:1H:11:GLN:NE2   | 1:2A:249:ASN:H    | 1.97                     | 0.59              |
| 2:1Y:11:GLN:NE2   | 1:2M:249:ASN:HB2  | 2.17                     | 0.59              |
| 2:1Z:394:GLN:HG2  | 1:2N:348:PRO:HG2  | 1.84                     | 0.59              |
| 2:2H:72:PRO:HD2   | 1:3A:2:ARG:CG     | 2.32                     | 0.59              |
| 2:2O:11:GLN:HE22  | 1:3B:249:ASN:H    | 0.65                     | 0.59              |
| 2:2O:100:GLY:HA2  | 1:3B:253:THR:CB   | 2.22                     | 0.59              |
| 2:2O:394:GLN:CB   | 1:3B:348:PRO:HG3  | 2.31                     | 0.59              |
| 2:2R:221:THR:HA   | 1:3E:324:VAL:HG11 | 1.83                     | 0.59              |
| 1:1C:260:VAL:HG12 | 2:4P:406:HIS:HE1  | 1.65                     | 0.59              |
| 1:1D:262:TYR:CZ   | 2:4Q:403:ALA:HA   | 2.37                     | 0.59              |
| 1:1F:2:ARG:HH22   | 2:4S:73:GLY:HA3   | 1.67                     | 0.59              |
| 1:1I:326:LYS:HA   | 2:4U:210:TYR:CZ   | 2.37                     | 0.59              |
| 1:1I:329:ASN:ND2  | 2:4U:210:TYR:HD2  | 2.00                     | 0.59              |
| 1:1J:254:GLU:HA   | 2:4V:100:GLY:CA   | 2.32                     | 0.59              |
| 1:1J:346:TRP:CA   | 2:4V:397:ALA:O    | 2.50                     | 0.59              |
| 1:1K:260:VAL:CB   | 2:4W:407:TRP:NE1  | 2.63                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:329:ASN:ND2  | 2:4W:210:TYR:CD2  | 2.62                     | 0.59              |
| 2:1Q:275:LEU:H    | 2:1Q:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1Y:100:GLY:CA   | 1:2M:253:THR:HG22 | 2.24                     | 0.59              |
| 2:1Z:207:GLU:OE2  | 1:2N:329:ASN:ND2  | 2.35                     | 0.59              |
| 2:2R:275:LEU:H    | 2:2R:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2S:404:PHE:CA   | 1:3F:261:PRO:O    | 2.49                     | 0.59              |
| 2:2U:406:HIS:CG   | 1:3I:263:PRO:CD   | 2.77                     | 0.59              |
| 2:2Y:176:LYS:CE   | 1:3M:333:ALA:HB1  | 2.32                     | 0.59              |
| 1:1B:260:VAL:N    | 2:4O:404:PHE:HE1  | 1.99                     | 0.59              |
| 1:1C:261:PRO:O    | 2:4P:404:PHE:HA   | 2.02                     | 0.59              |
| 1:1E:254:GLU:CA   | 2:4R:100:GLY:O    | 2.29                     | 0.59              |
| 1:1E:260:VAL:C    | 2:4R:407:TRP:HE1  | 2.10                     | 0.59              |
| 1:1E:324:VAL:CG1  | 2:4R:222:PRO:C    | 2.71                     | 0.59              |
| 1:1E:352:LYS:HA   | 2:4R:179:ASP:C    | 2.27                     | 0.59              |
| 1:1F:325:PRO:HD2  | 2:4S:223:THR:HA   | 1.85                     | 0.59              |
| 1:1I:263:PRO:HD3  | 2:4U:406:HIS:CB   | 2.33                     | 0.59              |
| 1:1I:351:PHE:O    | 2:4U:181:VAL:N    | 2.35                     | 0.59              |
| 1:1K:248:LEU:HD13 | 5:4W:501:GDP:H8   | 1.67                     | 0.59              |
| 2:1R:275:LEU:H    | 2:1R:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2Q:275:LEU:H    | 2:2Q:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2S:404:PHE:HE1  | 1:3F:260:VAL:N    | 2.00                     | 0.59              |
| 2:3P:275:LEU:H    | 2:3P:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3R:275:LEU:H    | 2:3R:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3S:275:LEU:H    | 2:3S:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4R:275:LEU:H    | 2:4R:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4S:275:LEU:H    | 2:4S:294:GLN:HE22 | 1.51                     | 0.59              |
| 1:1I:351:PHE:O    | 2:4U:180:THR:HA   | 2.01                     | 0.59              |
| 1:1L:261:PRO:CA   | 2:4X:404:PHE:CD1  | 2.86                     | 0.59              |
| 1:1M:262:TYR:CZ   | 2:4Y:403:ALA:HA   | 2.37                     | 0.59              |
| 2:1P:275:LEU:H    | 2:1P:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1S:275:LEU:H    | 2:1S:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2H:11:GLN:HE22  | 1:3A:249:ASN:H    | 0.68                     | 0.59              |
| 2:2P:77:SER:CB    | 1:3C:245:ASP:CG   | 2.75                     | 0.59              |
| 2:2P:275:LEU:H    | 2:2P:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2P:401:ARG:HH22 | 1:3C:435:VAL:C    | 2.10                     | 0.59              |
| 2:2Q:72:PRO:HD2   | 1:3D:2:ARG:HD3    | 1.85                     | 0.59              |
| 2:2Q:221:THR:HA   | 1:3D:324:VAL:HG11 | 1.83                     | 0.59              |
| 2:2S:275:LEU:H    | 2:2S:294:GLN:HE22 | 1.51                     | 0.59              |
| 5:2T:501:GDP:H8   | 1:3G:248:LEU:HD11 | 1.64                     | 0.59              |
| 2:2V:398:MET:CG   | 1:3J:346:TRP:O    | 2.50                     | 0.59              |
| 2:2V:404:PHE:HD1  | 1:3J:260:VAL:O    | 1.82                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2W:404:PHE:CA  | 1:3K:261:PRO:O    | 2.50                     | 0.59              |
| 2:2Z:275:LEU:H   | 2:2Z:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3Q:275:LEU:H   | 2:3Q:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3Z:275:LEU:H   | 2:3Z:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4P:275:LEU:H   | 2:4P:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4Q:275:LEU:H   | 2:4Q:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4T:275:LEU:H   | 2:4T:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4Z:275:LEU:H   | 2:4Z:294:GLN:HE22 | 1.51                     | 0.59              |
| 1:1C:349:THR:CG2 | 2:4P:184:PRO:CG   | 2.81                     | 0.59              |
| 1:1D:261:PRO:CB  | 2:4Q:404:PHE:H    | 2.14                     | 0.59              |
| 2:1O:275:LEU:H   | 2:1O:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1U:11:GLN:NE2  | 1:2I:249:ASN:HB2  | 2.17                     | 0.59              |
| 2:1U:224:TYR:OH  | 1:2I:248:LEU:HD22 | 2.03                     | 0.59              |
| 2:1W:181:VAL:CB  | 1:2K:258:ASN:C    | 2.72                     | 0.59              |
| 2:2Q:179:ASP:OD1 | 1:3D:353:VAL:CB   | 2.46                     | 0.59              |
| 2:2S:179:ASP:O   | 1:3F:352:LYS:HA   | 2.03                     | 0.59              |
| 2:2W:404:PHE:HE1 | 1:3K:260:VAL:N    | 2.01                     | 0.59              |
| 2:2Y:275:LEU:H   | 2:2Y:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4H:275:LEU:H   | 2:4H:294:GLN:HE22 | 1.51                     | 0.59              |
| 1:1F:325:PRO:HB3 | 2:4S:224:TYR:CE1  | 2.38                     | 0.59              |
| 1:1L:348:PRO:HG2 | 2:4X:394:GLN:HB3  | 1.85                     | 0.59              |
| 1:1L:439:SER:OG  | 2:4X:401:ARG:HD3  | 2.02                     | 0.59              |
| 2:1T:11:GLN:HE22 | 1:2G:249:ASN:H    | 1.50                     | 0.59              |
| 2:1T:101:ASN:O   | 1:2G:257:THR:HG21 | 2.02                     | 0.59              |
| 2:1T:275:LEU:H   | 2:1T:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1V:275:LEU:H   | 2:1V:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1W:100:GLY:O   | 1:2K:253:THR:HG22 | 2.03                     | 0.59              |
| 2:1X:275:LEU:H   | 2:1X:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1Z:275:LEU:H   | 2:1Z:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2H:275:LEU:H   | 2:2H:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2O:275:LEU:H   | 2:2O:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2P:214:PHE:CB  | 1:3C:326:LYS:CE   | 2.78                     | 0.59              |
| 2:2S:406:HIS:CD2 | 1:3F:262:TYR:CA   | 2.86                     | 0.59              |
| 2:2T:275:LEU:H   | 2:2T:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2W:179:ASP:OD1 | 1:3K:353:VAL:HB   | 2.03                     | 0.59              |
| 2:2W:181:VAL:H   | 1:3K:258:ASN:HD22 | 1.50                     | 0.59              |
| 2:2W:275:LEU:H   | 2:2W:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3H:275:LEU:H   | 2:3H:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3O:275:LEU:H   | 2:3O:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3T:275:LEU:H   | 2:3T:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4O:275:LEU:H   | 2:4O:294:GLN:HE22 | 1.51                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4Y:275:LEU:H    | 2:4Y:294:GLN:HE22 | 1.51                     | 0.59              |
| 1:1C:347:CYS:HA   | 2:4P:398:MET:HG2  | 1.85                     | 0.59              |
| 1:1D:260:VAL:HG12 | 2:4Q:407:TRP:HE1  | 1.63                     | 0.59              |
| 1:1G:345:ASP:O    | 2:4T:397:ALA:HB1  | 2.02                     | 0.59              |
| 1:1I:434:GLU:O    | 2:4U:401:ARG:NH2  | 2.36                     | 0.59              |
| 1:1J:351:PHE:O    | 2:4V:180:THR:N    | 2.36                     | 0.59              |
| 2:1H:275:LEU:H    | 2:1H:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1O:101:ASN:HB2  | 1:2B:254:GLU:CG   | 2.33                     | 0.59              |
| 2:1W:275:LEU:H    | 2:1W:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:1Y:275:LEU:H    | 2:1Y:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2R:214:PHE:CB   | 1:3E:326:LYS:CE   | 2.78                     | 0.59              |
| 2:2V:275:LEU:H    | 2:2V:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2X:275:LEU:H    | 2:2X:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:2Z:73:GLY:HA3   | 1:3N:2:ARG:NH2    | 2.17                     | 0.59              |
| 2:2Z:176:LYS:CE   | 1:3N:333:ALA:HB1  | 2.31                     | 0.59              |
| 2:3X:275:LEU:H    | 2:3X:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:3Y:275:LEU:H    | 2:3Y:294:GLN:HE22 | 1.51                     | 0.59              |
| 2:4X:275:LEU:H    | 2:4X:294:GLN:HE22 | 1.51                     | 0.59              |
| 1:1C:332:ILE:HG21 | 2:4P:177:VAL:HG22 | 1.80                     | 0.58              |
| 1:1D:352:LYS:HD3  | 2:4Q:101:ASN:HD21 | 1.68                     | 0.58              |
| 1:1F:247:ALA:C    | 2:4S:15:GLN:HE22  | 2.11                     | 0.58              |
| 1:1G:329:ASN:HB3  | 2:4T:210:TYR:CD2  | 2.37                     | 0.58              |
| 2:2O:222:PRO:HG2  | 1:3B:326:LYS:CB   | 2.33                     | 0.58              |
| 2:2R:406:HIS:CE1  | 1:3E:263:PRO:N    | 2.71                     | 0.58              |
| 2:2U:100:GLY:O    | 1:3I:257:THR:CB   | 2.50                     | 0.58              |
| 2:2Z:401:ARG:NH2  | 1:3N:435:VAL:CA   | 2.44                     | 0.58              |
| 2:3V:275:LEU:H    | 2:3V:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:3W:275:LEU:H    | 2:3W:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:4U:275:LEU:H    | 2:4U:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:4V:275:LEU:H    | 2:4V:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:4W:275:LEU:H    | 2:4W:294:GLN:HE22 | 1.51                     | 0.58              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:CD1  | 2.38                     | 0.58              |
| 1:1G:439:SER:CB   | 2:4T:400:ARG:HD2  | 2.33                     | 0.58              |
| 2:1Q:178:SER:CB   | 1:2D:349:THR:HB   | 2.33                     | 0.58              |
| 2:1R:401:ARG:HH22 | 1:2E:435:VAL:HA   | 1.67                     | 0.58              |
| 2:1S:224:TYR:HE2  | 1:2F:248:LEU:HB2  | 1.68                     | 0.58              |
| 2:1X:178:SER:HB3  | 1:2L:349:THR:HB   | 1.85                     | 0.58              |
| 2:1X:214:PHE:HB2  | 1:2L:326:LYS:CE   | 2.19                     | 0.58              |
| 2:1X:222:PRO:HD2  | 1:2L:324:VAL:CG1  | 2.33                     | 0.58              |
| 2:1Z:404:PHE:CE1  | 1:2N:260:VAL:N    | 2.71                     | 0.58              |
| 2:2R:101:ASN:HB2  | 1:3E:254:GLU:HG2  | 1.83                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:223:THR:HA   | 1:3E:325:PRO:CD   | 2.33                     | 0.58              |
| 2:2V:181:VAL:CB   | 1:3J:258:ASN:O    | 2.51                     | 0.58              |
| 2:3U:275:LEU:H    | 2:3U:294:GLN:HE22 | 1.51                     | 0.58              |
| 1:1B:332:ILE:HB   | 2:4O:177:VAL:HG21 | 1.85                     | 0.58              |
| 1:1C:245:ASP:OD2  | 2:4P:77:SER:CB    | 2.50                     | 0.58              |
| 1:1F:332:ILE:HG21 | 2:4S:177:VAL:HG22 | 1.82                     | 0.58              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:CB   | 2.51                     | 0.58              |
| 1:1N:2:ARG:NH2    | 2:4Z:73:GLY:HA3   | 2.18                     | 0.58              |
| 2:1H:224:TYR:HD2  | 1:2A:247:ALA:O    | 1.85                     | 0.58              |
| 2:1S:179:ASP:OD2  | 1:2F:248:LEU:HD21 | 2.04                     | 0.58              |
| 2:1U:275:LEU:H    | 2:1U:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:1V:207:GLU:CD   | 1:2J:329:ASN:ND2  | 2.54                     | 0.58              |
| 2:2O:407:TRP:NE1  | 1:3B:260:VAL:HB   | 2.18                     | 0.58              |
| 2:2S:403:ALA:HA   | 1:3F:262:TYR:CZ   | 2.38                     | 0.58              |
| 2:2T:407:TRP:HE1  | 1:3G:260:VAL:CG1  | 2.16                     | 0.58              |
| 2:2U:179:ASP:O    | 1:3I:352:LYS:CD   | 2.48                     | 0.58              |
| 2:2U:275:LEU:H    | 2:2U:294:GLN:HE22 | 1.51                     | 0.58              |
| 2:2W:394:GLN:CB   | 1:3K:348:PRO:CG   | 2.82                     | 0.58              |
| 1:1C:345:ASP:O    | 2:4P:397:ALA:HB1  | 2.03                     | 0.58              |
| 1:1D:2:ARG:HG3    | 2:4Q:72:PRO:HG2   | 1.86                     | 0.58              |
| 1:1D:260:VAL:N    | 2:4Q:404:PHE:HE1  | 2.01                     | 0.58              |
| 1:1D:346:TRP:CD1  | 2:4Q:401:ARG:CG   | 2.82                     | 0.58              |
| 1:1E:260:VAL:C    | 2:4R:404:PHE:CD1  | 2.81                     | 0.58              |
| 1:1F:326:LYS:HG2  | 2:4S:210:TYR:HB3  | 1.83                     | 0.58              |
| 1:1G:261:PRO:HB3  | 2:4T:404:PHE:CD2  | 2.38                     | 0.58              |
| 1:1G:262:TYR:OH   | 2:4T:402:LYS:C    | 2.47                     | 0.58              |
| 1:1I:2:ARG:HG3    | 2:4U:72:PRO:CG    | 2.34                     | 0.58              |
| 1:1L:260:VAL:CB   | 2:4X:407:TRP:HZ2  | 2.15                     | 0.58              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:HA   | 2.02                     | 0.58              |
| 2:1O:100:GLY:CA   | 1:2B:253:THR:HB   | 2.32                     | 0.58              |
| 2:2H:394:GLN:CA   | 1:3A:348:PRO:HG3  | 2.34                     | 0.58              |
| 2:2P:182:VAL:HG21 | 1:3C:257:THR:HG22 | 1.85                     | 0.58              |
| 2:2T:214:PHE:HB2  | 1:3G:326:LYS:HE3  | 1.84                     | 0.58              |
| 2:2W:207:GLU:CD   | 1:3K:329:ASN:ND2  | 2.51                     | 0.58              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:H    | 2.17                     | 0.58              |
| 1:1D:253:THR:CB   | 2:4Q:100:GLY:HA3  | 2.32                     | 0.58              |
| 1:1D:351:PHE:CB   | 2:4Q:178:SER:OG   | 2.46                     | 0.58              |
| 1:1E:346:TRP:CE2  | 2:4R:403:ALA:HB2  | 2.39                     | 0.58              |
| 1:1G:333:ALA:HB1  | 2:4T:176:LYS:HE2  | 1.85                     | 0.58              |
| 1:1I:249:ASN:N    | 2:4U:11:GLN:CD    | 2.52                     | 0.58              |
| 1:1I:324:VAL:HG13 | 2:4U:222:PRO:O    | 2.01                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1L:349:THR:CG2  | 2:4X:184:PRO:CD   | 2.73                     | 0.58              |
| 1:1M:326:LYS:HB3  | 2:4Y:222:PRO:HG2  | 1.84                     | 0.58              |
| 1:1M:351:PHE:O    | 2:4Y:180:THR:C    | 2.45                     | 0.58              |
| 2:2H:181:VAL:CG2  | 1:3A:258:ASN:O    | 2.51                     | 0.58              |
| 2:2S:407:TRP:HE1  | 1:3F:260:VAL:CG1  | 2.16                     | 0.58              |
| 2:2U:404:PHE:HA   | 1:3I:261:PRO:O    | 2.03                     | 0.58              |
| 2:2W:101:ASN:C    | 1:3K:257:THR:HG21 | 2.29                     | 0.58              |
| 2:2Z:221:THR:CB   | 1:3N:324:VAL:HG21 | 2.32                     | 0.58              |
| 1:1D:326:LYS:HB2  | 2:4Q:222:PRO:HG2  | 1.86                     | 0.58              |
| 1:1D:439:SER:CB   | 2:4Q:400:ARG:CD   | 2.82                     | 0.58              |
| 1:1G:314:ALA:HB2  | 2:4T:181:VAL:HG11 | 1.84                     | 0.58              |
| 2:1Y:221:THR:OG1  | 1:2M:324:VAL:CG2  | 2.52                     | 0.58              |
| 2:2H:222:PRO:HG2  | 1:3A:326:LYS:CB   | 2.32                     | 0.58              |
| 2:2O:401:ARG:C    | 1:3B:262:TYR:HH   | 1.96                     | 0.58              |
| 2:2P:406:HIS:CD2  | 1:3C:262:TYR:HA   | 2.38                     | 0.58              |
| 2:2Q:214:PHE:CB   | 1:3D:326:LYS:CE   | 2.79                     | 0.58              |
| 2:2R:207:GLU:CD   | 1:3E:329:ASN:ND2  | 2.41                     | 0.58              |
| 2:2S:100:GLY:CA   | 1:3F:253:THR:C    | 2.76                     | 0.58              |
| 1:1B:346:TRP:HA   | 2:4O:397:ALA:C    | 2.29                     | 0.58              |
| 1:1C:257:THR:CB   | 2:4P:100:GLY:O    | 2.52                     | 0.58              |
| 1:1E:326:LYS:CB   | 2:4R:210:TYR:CD1  | 2.87                     | 0.58              |
| 1:1F:248:LEU:HD11 | 5:4S:501:GDP:O1A  | 2.04                     | 0.58              |
| 1:1F:348:PRO:HD2  | 2:4S:398:MET:SD   | 2.44                     | 0.58              |
| 1:1G:260:VAL:CG1  | 2:4T:407:TRP:HZ2  | 2.12                     | 0.58              |
| 1:1G:261:PRO:HA   | 2:4T:404:PHE:CD1  | 2.38                     | 0.58              |
| 2:1Q:221:THR:CA   | 1:2D:324:VAL:HG11 | 2.26                     | 0.58              |
| 2:1S:207:GLU:CD   | 1:2F:329:ASN:HD21 | 2.12                     | 0.58              |
| 2:1Y:404:PHE:CE2  | 1:2M:261:PRO:HA   | 2.39                     | 0.58              |
| 2:2T:221:THR:CA   | 1:3G:324:VAL:HG11 | 2.33                     | 0.58              |
| 2:2V:101:ASN:O    | 1:3J:257:THR:CG2  | 2.48                     | 0.58              |
| 2:2X:72:PRO:HD2   | 1:3L:2:ARG:CG     | 2.34                     | 0.58              |
| 2:2Z:77:SER:HB3   | 1:3N:245:ASP:CG   | 2.27                     | 0.58              |
| 1:1A:254:GLU:HG2  | 2:4H:101:ASN:N    | 2.19                     | 0.58              |
| 1:1C:332:ILE:CB   | 2:4P:177:VAL:HG21 | 2.31                     | 0.58              |
| 1:1D:253:THR:CB   | 2:4Q:100:GLY:CA   | 2.81                     | 0.58              |
| 1:1D:262:TYR:CZ   | 2:4Q:402:LYS:C    | 2.82                     | 0.58              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:CD1  | 2.87                     | 0.58              |
| 1:1F:261:PRO:O    | 2:4S:404:PHE:N    | 2.37                     | 0.58              |
| 1:1J:325:PRO:HB3  | 2:4V:224:TYR:CZ   | 2.39                     | 0.58              |
| 1:1K:352:LYS:HD3  | 2:4W:101:ASN:ND2  | 2.19                     | 0.58              |
| 1:1L:245:ASP:OD2  | 2:4X:77:SER:HB2   | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:346:TRP:CE3  | 2:4Y:403:ALA:HB3  | 2.37                     | 0.58              |
| 2:1Y:221:THR:CB   | 1:2M:324:VAL:HG21 | 2.33                     | 0.58              |
| 2:2P:394:GLN:CB   | 1:3C:348:PRO:HG2  | 2.34                     | 0.58              |
| 1:1C:254:GLU:HG2  | 2:4P:100:GLY:C    | 2.29                     | 0.58              |
| 1:1J:325:PRO:HB2  | 2:4V:224:TYR:CE1  | 2.38                     | 0.58              |
| 1:1M:260:VAL:CB   | 2:4Y:407:TRP:NE1  | 2.66                     | 0.58              |
| 2:1V:181:VAL:CB   | 1:2J:258:ASN:CA   | 2.80                     | 0.58              |
| 2:2Q:404:PHE:CE1  | 1:3D:261:PRO:N    | 2.72                     | 0.58              |
| 2:2U:404:PHE:H    | 1:3I:261:PRO:C    | 2.07                     | 0.58              |
| 1:1A:348:PRO:HB3  | 2:4H:394:GLN:HG2  | 1.82                     | 0.58              |
| 1:1C:329:ASN:CB   | 2:4P:210:TYR:CE2  | 2.84                     | 0.58              |
| 1:1G:262:TYR:CE2  | 2:4T:403:ALA:HA   | 2.39                     | 0.58              |
| 1:1I:325:PRO:O    | 2:4U:210:TYR:OH   | 2.18                     | 0.58              |
| 1:1K:324:VAL:HG21 | 2:4W:221:THR:OG1  | 2.03                     | 0.58              |
| 1:1L:248:LEU:HD13 | 5:4X:501:GDP:H8   | 1.68                     | 0.58              |
| 1:1N:260:VAL:CB   | 2:4Z:407:TRP:HE1  | 2.17                     | 0.58              |
| 2:1H:100:GLY:CA   | 1:2A:253:THR:CB   | 2.79                     | 0.58              |
| 2:1S:394:GLN:HG2  | 1:2F:348:PRO:CG   | 2.33                     | 0.58              |
| 2:1T:11:GLN:HE22  | 1:2G:249:ASN:HB2  | 1.69                     | 0.58              |
| 2:1X:181:VAL:HB   | 1:2L:258:ASN:C    | 2.29                     | 0.58              |
| 2:1Y:100:GLY:CA   | 1:2M:253:THR:HG21 | 2.11                     | 0.58              |
| 2:2H:214:PHE:CB   | 1:3A:326:LYS:CE   | 2.70                     | 0.58              |
| 2:2V:181:VAL:HG21 | 1:3J:258:ASN:O    | 2.03                     | 0.58              |
| 2:2W:221:THR:C    | 1:3K:324:VAL:HG11 | 2.28                     | 0.58              |
| 2:2X:406:HIS:CE1  | 1:3L:263:PRO:CA   | 2.86                     | 0.58              |
| 2:2Y:182:VAL:HG21 | 1:3M:257:THR:HG22 | 1.84                     | 0.58              |
| 2:2Z:343:PHE:HB3  | 2:2Z:350:ASN:HD21 | 1.69                     | 0.58              |
| 1:3G:79:ARG:NH2   | 1:3G:92:LEU:O     | 2.37                     | 0.58              |
| 2:3Y:343:PHE:HB3  | 2:3Y:350:ASN:HD21 | 1.69                     | 0.58              |
| 1:4G:79:ARG:NH2   | 1:4G:92:LEU:O     | 2.37                     | 0.58              |
| 2:4Y:343:PHE:HB3  | 2:4Y:350:ASN:HD21 | 1.69                     | 0.58              |
| 2:4Z:343:PHE:HB3  | 2:4Z:350:ASN:HD21 | 1.69                     | 0.58              |
| 1:1B:2:ARG:CD     | 2:4O:71:GLU:HB2   | 2.31                     | 0.57              |
| 1:1D:352:LYS:CD   | 2:4Q:101:ASN:ND2  | 2.66                     | 0.57              |
| 1:1E:263:PRO:N    | 2:4R:406:HIS:CG   | 2.72                     | 0.57              |
| 1:1F:346:TRP:CD2  | 2:4S:403:ALA:CB   | 2.87                     | 0.57              |
| 1:1G:79:ARG:NH2   | 1:1G:92:LEU:O     | 2.37                     | 0.57              |
| 2:1S:404:PHE:CD1  | 1:2F:261:PRO:HA   | 2.38                     | 0.57              |
| 2:1X:343:PHE:HB3  | 2:1X:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:1Y:343:PHE:HB3  | 2:1Y:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:1Z:343:PHE:HB3  | 2:1Z:350:ASN:HD21 | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2D:79:ARG:NH2   | 1:2D:92:LEU:O     | 2.37                     | 0.57              |
| 1:2G:79:ARG:NH2   | 1:2G:92:LEU:O     | 2.37                     | 0.57              |
| 2:2H:343:PHE:HB3  | 2:2H:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:2O:224:TYR:CD2  | 1:3B:247:ALA:O    | 2.56                     | 0.57              |
| 2:2O:404:PHE:CE1  | 1:3B:261:PRO:N    | 2.72                     | 0.57              |
| 2:2V:207:GLU:CD   | 1:3J:329:ASN:ND2  | 2.55                     | 0.57              |
| 2:2Y:343:PHE:HB3  | 2:2Y:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:3Z:343:PHE:HB3  | 2:3Z:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:1B:326:LYS:HA   | 2:4O:210:TYR:CE1  | 2.39                     | 0.57              |
| 1:1D:79:ARG:NH2   | 1:1D:92:LEU:O     | 2.37                     | 0.57              |
| 1:1E:348:PRO:HD2  | 2:4R:398:MET:CG   | 2.34                     | 0.57              |
| 1:1G:439:SER:HB2  | 2:4T:400:ARG:HD2  | 1.86                     | 0.57              |
| 1:1I:254:GLU:CA   | 2:4U:100:GLY:CA   | 2.82                     | 0.57              |
| 1:1J:332:ILE:HB   | 2:4V:177:VAL:HG21 | 1.85                     | 0.57              |
| 2:1O:222:PRO:HG2  | 1:2B:326:LYS:HB2  | 1.85                     | 0.57              |
| 2:1X:404:PHE:CE2  | 1:2L:261:PRO:CA   | 2.87                     | 0.57              |
| 2:2W:72:PRO:HG2   | 1:3K:2:ARG:HG3    | 1.86                     | 0.57              |
| 2:2X:343:PHE:HB3  | 2:2X:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:2Z:77:SER:CB    | 1:3N:245:ASP:OD1  | 2.49                     | 0.57              |
| 1:3D:79:ARG:NH2   | 1:3D:92:LEU:O     | 2.37                     | 0.57              |
| 1:3K:79:ARG:NH2   | 1:3K:92:LEU:O     | 2.37                     | 0.57              |
| 2:4X:343:PHE:HB3  | 2:4X:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:1B:257:THR:HB   | 2:4O:100:GLY:O    | 2.04                     | 0.57              |
| 1:1E:261:PRO:HB3  | 2:4R:404:PHE:CE2  | 2.39                     | 0.57              |
| 1:1G:247:ALA:C    | 2:4T:15:GLN:HE22  | 2.12                     | 0.57              |
| 1:1G:349:THR:O    | 2:4T:181:VAL:O    | 2.23                     | 0.57              |
| 1:1I:79:ARG:NH2   | 1:1I:92:LEU:O     | 2.37                     | 0.57              |
| 1:1K:79:ARG:NH2   | 1:1K:92:LEU:O     | 2.37                     | 0.57              |
| 1:1K:348:PRO:HG2  | 2:4W:394:GLN:HB3  | 1.85                     | 0.57              |
| 1:1M:253:THR:C    | 2:4Y:100:GLY:HA2  | 2.28                     | 0.57              |
| 2:1T:181:VAL:CB   | 1:2G:258:ASN:O    | 2.52                     | 0.57              |
| 2:1T:343:PHE:HB3  | 2:1T:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:1U:181:VAL:CG2  | 1:2I:258:ASN:HB3  | 2.29                     | 0.57              |
| 1:2K:79:ARG:NH2   | 1:2K:92:LEU:O     | 2.38                     | 0.57              |
| 2:2T:73:GLY:HA3   | 1:3G:2:ARG:CZ     | 2.34                     | 0.57              |
| 2:2T:100:GLY:CA   | 1:3G:253:THR:C    | 2.78                     | 0.57              |
| 2:2T:179:ASP:OD1  | 1:3G:353:VAL:CB   | 2.52                     | 0.57              |
| 2:2T:343:PHE:HB3  | 2:2T:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:2T:407:TRP:HE1  | 1:3G:260:VAL:CB   | 2.15                     | 0.57              |
| 2:2W:406:HIS:CD2  | 1:3K:262:TYR:HA   | 2.39                     | 0.57              |
| 2:2X:177:VAL:HG23 | 1:3L:332:ILE:HG22 | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3I:79:ARG:NH2   | 1:3I:92:LEU:O     | 2.37                     | 0.57              |
| 2:3H:343:PHE:HB3  | 2:3H:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:3T:343:PHE:HB3  | 2:3T:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:3X:343:PHE:HB3  | 2:3X:350:ASN:HD21 | 1.70                     | 0.57              |
| 1:4D:79:ARG:NH2   | 1:4D:92:LEU:O     | 2.38                     | 0.57              |
| 1:4K:79:ARG:NH2   | 1:4K:92:LEU:O     | 2.37                     | 0.57              |
| 2:4H:343:PHE:HB3  | 2:4H:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:1B:248:LEU:HD13 | 5:4O:501:GDP:N7   | 2.13                     | 0.57              |
| 1:1C:254:GLU:HG2  | 2:4P:101:ASN:H    | 1.67                     | 0.57              |
| 1:1C:346:TRP:HA   | 2:4P:397:ALA:CB   | 2.34                     | 0.57              |
| 1:1D:260:VAL:HG12 | 2:4Q:407:TRP:NE1  | 2.20                     | 0.57              |
| 1:1E:245:ASP:OD1  | 2:4R:77:SER:OG    | 2.22                     | 0.57              |
| 1:1F:326:LYS:CA   | 2:4S:210:TYR:CD1  | 2.85                     | 0.57              |
| 1:1J:346:TRP:C    | 2:4V:398:MET:HG2  | 2.18                     | 0.57              |
| 1:1M:261:PRO:HB3  | 2:4Y:404:PHE:CE2  | 2.40                     | 0.57              |
| 1:1M:325:PRO:CD   | 2:4Y:223:THR:HA   | 2.30                     | 0.57              |
| 2:1H:343:PHE:HB3  | 2:1H:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:1R:179:ASP:O    | 1:2E:352:LYS:HD2  | 2.04                     | 0.57              |
| 2:1W:343:PHE:HB3  | 2:1W:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:1X:100:GLY:O    | 1:2L:253:THR:HG22 | 2.04                     | 0.57              |
| 1:2I:79:ARG:NH2   | 1:2I:92:LEU:O     | 2.37                     | 0.57              |
| 2:2S:404:PHE:CD2  | 1:3F:261:PRO:HB3  | 2.38                     | 0.57              |
| 2:2U:179:ASP:O    | 1:3I:352:LYS:HA   | 2.04                     | 0.57              |
| 2:3W:343:PHE:HB3  | 2:3W:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:4I:79:ARG:NH2   | 1:4I:92:LEU:O     | 2.37                     | 0.57              |
| 2:4W:343:PHE:HB3  | 2:4W:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:1C:325:PRO:CD   | 2:4P:223:THR:HA   | 2.35                     | 0.57              |
| 1:1D:2:ARG:NH1    | 2:4Q:71:GLU:CG    | 2.63                     | 0.57              |
| 1:1D:326:LYS:HG2  | 2:4Q:210:TYR:CG   | 2.40                     | 0.57              |
| 1:1I:435:VAL:HA   | 2:4U:401:ARG:HH21 | 1.67                     | 0.57              |
| 1:1L:79:ARG:NH2   | 1:1L:92:LEU:O     | 2.37                     | 0.57              |
| 2:1H:100:GLY:HA3  | 1:2A:253:THR:HG21 | 1.82                     | 0.57              |
| 2:1S:180:THR:HA   | 1:2F:258:ASN:HD21 | 1.69                     | 0.57              |
| 2:1W:222:PRO:HD2  | 1:2K:324:VAL:CG1  | 2.35                     | 0.57              |
| 2:2T:406:HIS:CG   | 1:3G:263:PRO:CD   | 2.77                     | 0.57              |
| 2:2W:343:PHE:HB3  | 2:2W:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:2Y:404:PHE:HD1  | 1:3M:260:VAL:O    | 1.84                     | 0.57              |
| 2:4T:343:PHE:HB3  | 2:4T:350:ASN:HD21 | 1.70                     | 0.57              |
| 1:1C:326:LYS:CA   | 2:4P:210:TYR:CD1  | 2.87                     | 0.57              |
| 1:1C:348:PRO:CG   | 2:4P:394:GLN:HA   | 2.10                     | 0.57              |
| 1:1D:349:THR:HG23 | 2:4Q:184:PRO:CG   | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:79:ARG:NH2   | 1:1E:92:LEU:O     | 2.37                     | 0.57              |
| 1:1E:261:PRO:CA   | 2:4R:404:PHE:CG   | 2.86                     | 0.57              |
| 1:1F:253:THR:HG22 | 2:4S:100:GLY:HA3  | 1.86                     | 0.57              |
| 1:1F:333:ALA:HB1  | 2:4S:176:LYS:HB3  | 1.85                     | 0.57              |
| 1:1F:349:THR:O    | 2:4S:181:VAL:O    | 2.23                     | 0.57              |
| 1:1I:2:ARG:CD     | 2:4U:72:PRO:CD    | 2.69                     | 0.57              |
| 1:1N:248:LEU:HA   | 2:4Z:11:GLN:NE2   | 2.19                     | 0.57              |
| 2:1V:222:PRO:CG   | 1:2J:326:LYS:HB2  | 2.34                     | 0.57              |
| 2:1V:343:PHE:HB3  | 2:1V:350:ASN:HD21 | 1.69                     | 0.57              |
| 1:2E:79:ARG:NH2   | 1:2E:92:LEU:O     | 2.37                     | 0.57              |
| 2:2Q:11:GLN:NE2   | 1:3D:249:ASN:N    | 2.08                     | 0.57              |
| 2:2S:407:TRP:CD1  | 1:3F:260:VAL:O    | 2.58                     | 0.57              |
| 2:2T:100:GLY:O    | 1:3G:257:THR:CB   | 2.52                     | 0.57              |
| 2:2T:101:ASN:C    | 1:3G:257:THR:HG21 | 2.29                     | 0.57              |
| 2:2V:406:HIS:NE2  | 1:3J:262:TYR:HA   | 2.19                     | 0.57              |
| 2:2W:100:GLY:HA2  | 1:3K:253:THR:C    | 2.30                     | 0.57              |
| 2:2X:404:PHE:CE2  | 1:3L:261:PRO:CB   | 2.83                     | 0.57              |
| 1:3E:79:ARG:NH2   | 1:3E:92:LEU:O     | 2.37                     | 0.57              |
| 2:3U:343:PHE:HB3  | 2:3U:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:3Y:69:ASP:OD2   | 2:3Y:74:THR:OG1   | 2.19                     | 0.57              |
| 1:1D:333:ALA:HB1  | 2:4Q:176:LYS:HB3  | 1.85                     | 0.57              |
| 1:1E:2:ARG:HH11   | 2:4R:71:GLU:HG3   | 1.70                     | 0.57              |
| 1:1E:435:VAL:CA   | 2:4R:401:ARG:HH22 | 1.90                     | 0.57              |
| 1:1G:326:LYS:HB3  | 2:4T:222:PRO:HG2  | 1.86                     | 0.57              |
| 1:1I:263:PRO:CD   | 2:4U:406:HIS:CD2  | 2.87                     | 0.57              |
| 1:1J:254:GLU:HG2  | 2:4V:101:ASN:N    | 2.20                     | 0.57              |
| 1:1N:249:ASN:N    | 2:4Z:11:GLN:NE2   | 1.97                     | 0.57              |
| 2:1O:11:GLN:NE2   | 1:2B:249:ASN:H    | 1.97                     | 0.57              |
| 2:1O:343:PHE:HB3  | 2:1O:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:1U:343:PHE:HB3  | 2:1U:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:1V:316:ALA:HB3  | 2:1V:378:ILE:HB   | 1.87                     | 0.57              |
| 1:2F:79:ARG:NH2   | 1:2F:92:LEU:O     | 2.37                     | 0.57              |
| 2:2O:343:PHE:HB3  | 2:2O:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:2Q:101:ASN:ND2  | 1:3D:258:ASN:OD1  | 2.38                     | 0.57              |
| 2:2Q:223:THR:HA   | 1:3D:325:PRO:HD2  | 1.87                     | 0.57              |
| 2:2U:343:PHE:HB3  | 2:2U:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:2Y:69:ASP:OD2   | 2:2Y:74:THR:OG1   | 2.20                     | 0.57              |
| 2:2Y:77:SER:HB3   | 1:3M:245:ASP:CG   | 2.28                     | 0.57              |
| 2:2Y:316:ALA:HB3  | 2:2Y:378:ILE:HB   | 1.87                     | 0.57              |
| 2:3V:343:PHE:HB3  | 2:3V:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:3Y:316:ALA:HB3  | 2:3Y:378:ILE:HB   | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4E:79:ARG:NH2   | 1:4E:92:LEU:O     | 2.37                     | 0.57              |
| 1:4F:79:ARG:NH2   | 1:4F:92:LEU:O     | 2.37                     | 0.57              |
| 2:4O:343:PHE:HB3  | 2:4O:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:4V:343:PHE:HB3  | 2:4V:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:4Y:316:ALA:HB3  | 2:4Y:378:ILE:HB   | 1.87                     | 0.57              |
| 1:1A:324:VAL:HG13 | 2:4H:222:PRO:O    | 2.04                     | 0.57              |
| 1:1C:314:ALA:HB1  | 2:4P:181:VAL:CG2  | 2.23                     | 0.57              |
| 1:1D:258:ASN:ND2  | 2:4Q:182:VAL:HG22 | 2.20                     | 0.57              |
| 1:1D:325:PRO:HG2  | 2:4Q:224:TYR:CG   | 2.39                     | 0.57              |
| 1:1D:346:TRP:CE3  | 2:4Q:403:ALA:CB   | 2.87                     | 0.57              |
| 1:1E:260:VAL:CG1  | 2:4R:407:TRP:CE2  | 2.87                     | 0.57              |
| 1:1F:79:ARG:NH2   | 1:1F:92:LEU:O     | 2.37                     | 0.57              |
| 1:1I:254:GLU:HG2  | 2:4U:100:GLY:CA   | 2.34                     | 0.57              |
| 1:1I:258:ASN:OD1  | 2:4U:101:ASN:HB3  | 2.05                     | 0.57              |
| 1:1L:346:TRP:HA   | 2:4X:397:ALA:O    | 2.05                     | 0.57              |
| 2:1Y:316:ALA:HB3  | 2:1Y:378:ILE:HB   | 1.87                     | 0.57              |
| 2:2Q:100:GLY:HA2  | 1:3D:253:THR:C    | 2.30                     | 0.57              |
| 2:2V:181:VAL:CG2  | 1:3J:258:ASN:O    | 2.52                     | 0.57              |
| 2:2V:316:ALA:HB3  | 2:2V:378:ILE:HB   | 1.87                     | 0.57              |
| 2:2V:343:PHE:HB3  | 2:2V:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:2X:221:THR:OG1  | 1:3L:324:VAL:HG22 | 2.03                     | 0.57              |
| 2:2Y:179:ASP:OD1  | 1:3M:353:VAL:HB   | 2.04                     | 0.57              |
| 2:2Z:72:PRO:HD2   | 1:3N:2:ARG:CG     | 2.34                     | 0.57              |
| 2:3O:343:PHE:HB3  | 2:3O:350:ASN:HD21 | 1.70                     | 0.57              |
| 2:3V:316:ALA:HB3  | 2:3V:378:ILE:HB   | 1.87                     | 0.57              |
| 2:4S:283:TYR:OH   | 2:4T:85:GLN:O     | 2.18                     | 0.57              |
| 2:4S:343:PHE:HB3  | 2:4S:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:4U:343:PHE:HB3  | 2:4U:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:4W:339:ASN:HB3  | 2:4W:342:TYR:HB2  | 1.87                     | 0.57              |
| 1:1A:260:VAL:C    | 2:4H:404:PHE:CE1  | 2.83                     | 0.57              |
| 1:1D:314:ALA:HB1  | 2:4Q:181:VAL:CG2  | 2.26                     | 0.57              |
| 1:1D:349:THR:HG23 | 2:4Q:394:GLN:OE1  | 2.05                     | 0.57              |
| 1:1E:254:GLU:CB   | 2:4R:101:ASN:HB2  | 2.33                     | 0.57              |
| 1:1F:260:VAL:HG21 | 2:4S:407:TRP:HZ2  | 1.69                     | 0.57              |
| 1:1F:261:PRO:HB2  | 2:4S:404:PHE:H    | 1.69                     | 0.57              |
| 1:1F:329:ASN:OD1  | 2:4S:177:VAL:CG1  | 2.53                     | 0.57              |
| 1:1G:2:ARG:CG     | 2:4T:72:PRO:CD    | 2.82                     | 0.57              |
| 1:1M:263:PRO:CD   | 2:4Y:406:HIS:CG   | 2.77                     | 0.57              |
| 1:1N:352:LYS:HD2  | 2:4Z:179:ASP:O    | 2.04                     | 0.57              |
| 2:1H:100:GLY:CA   | 1:2A:253:THR:CG2  | 2.78                     | 0.57              |
| 2:1H:207:GLU:CD   | 1:2A:329:ASN:ND2  | 2.46                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1H:339:ASN:HB3  | 2:1H:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:1R:339:ASN:HB3  | 2:1R:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:1V:339:ASN:HB3  | 2:1V:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:1Y:205:ASP:OD2  | 2:1Y:304:ALA:N    | 2.35                     | 0.57              |
| 2:2H:339:ASN:HB3  | 2:2H:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2O:394:GLN:HB3  | 1:3B:348:PRO:HG2  | 1.86                     | 0.57              |
| 2:2Q:404:PHE:CD1  | 1:3D:261:PRO:CA   | 2.88                     | 0.57              |
| 2:2R:339:ASN:HB3  | 2:2R:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2S:343:PHE:HB3  | 2:2S:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:2U:221:THR:CB   | 1:3I:324:VAL:HG21 | 2.34                     | 0.57              |
| 2:2W:11:GLN:HE22  | 1:3K:249:ASN:CA   | 2.15                     | 0.57              |
| 2:2W:339:ASN:HB3  | 2:2W:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2X:222:PRO:CG   | 1:3L:326:LYS:CB   | 2.81                     | 0.57              |
| 2:2X:404:PHE:CZ   | 1:3L:261:PRO:HB3  | 2.36                     | 0.57              |
| 1:3F:79:ARG:NH2   | 1:3F:92:LEU:O     | 2.38                     | 0.57              |
| 2:4H:339:ASN:HB3  | 2:4H:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:4O:339:ASN:HB3  | 2:4O:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:4V:316:ALA:HB3  | 2:4V:378:ILE:HB   | 1.87                     | 0.57              |
| 2:4V:339:ASN:HB3  | 2:4V:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:4X:339:ASN:HB3  | 2:4X:342:TYR:HB2  | 1.87                     | 0.57              |
| 1:1B:349:THR:CG2  | 2:4O:184:PRO:HD3  | 2.35                     | 0.57              |
| 1:1E:260:VAL:HG12 | 2:4R:407:TRP:NE1  | 2.18                     | 0.57              |
| 1:1F:324:VAL:HG21 | 2:4S:221:THR:OG1  | 2.04                     | 0.57              |
| 1:1G:251:ASP:OD2  | 2:4T:71:GLU:HB3   | 2.04                     | 0.57              |
| 1:1G:254:GLU:HG2  | 2:4T:100:GLY:CA   | 2.34                     | 0.57              |
| 1:1G:260:VAL:CG1  | 2:4T:407:TRP:CE2  | 2.87                     | 0.57              |
| 1:1G:262:TYR:N    | 2:4T:406:HIS:CD2  | 2.50                     | 0.57              |
| 1:1M:346:TRP:CH2  | 2:4Y:403:ALA:HB1  | 2.38                     | 0.57              |
| 1:1N:260:VAL:HG11 | 2:4Z:407:TRP:HZ2  | 1.69                     | 0.57              |
| 2:1O:339:ASN:HB3  | 2:1O:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:1P:343:PHE:HB3  | 2:1P:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:1Q:339:ASN:HB3  | 2:1Q:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:1R:221:THR:HA   | 1:2E:324:VAL:CG1  | 2.19                     | 0.57              |
| 2:1W:339:ASN:HB3  | 2:1W:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2H:177:VAL:HG23 | 1:3A:332:ILE:HG22 | 1.84                     | 0.57              |
| 2:2O:339:ASN:HB3  | 2:2O:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2P:343:PHE:HB3  | 2:2P:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:2Q:71:GLU:HG3   | 1:3D:2:ARG:NH1    | 2.20                     | 0.57              |
| 2:2S:283:TYR:OH   | 2:2T:85:GLN:O     | 2.18                     | 0.57              |
| 2:2S:406:HIS:CD2  | 1:3F:263:PRO:N    | 2.71                     | 0.57              |
| 2:2T:394:GLN:HG2  | 1:3G:348:PRO:HB2  | 1.85                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2V:339:ASN:HB3 | 2:2V:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2W:77:SER:CB   | 1:3K:245:ASP:CG   | 2.77                     | 0.57              |
| 2:2X:339:ASN:HB3 | 2:2X:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:2Y:223:THR:HA  | 1:3M:325:PRO:HD2  | 1.87                     | 0.57              |
| 2:3H:339:ASN:HB3 | 2:3H:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:3Q:339:ASN:HB3 | 2:3Q:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:3R:339:ASN:HB3 | 2:3R:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:3S:343:PHE:HB3 | 2:3S:350:ASN:HD21 | 1.69                     | 0.57              |
| 2:3V:339:ASN:HB3 | 2:3V:342:TYR:HB2  | 1.87                     | 0.57              |
| 2:3W:339:ASN:HB3 | 2:3W:342:TYR:HB2  | 1.87                     | 0.57              |
| 1:1B:346:TRP:CH2 | 2:4O:403:ALA:HB1  | 2.40                     | 0.56              |
| 1:1C:349:THR:CG2 | 2:4P:394:GLN:OE1  | 2.53                     | 0.56              |
| 1:1F:261:PRO:C   | 2:4S:404:PHE:H    | 2.13                     | 0.56              |
| 1:1G:254:GLU:HG2 | 2:4T:101:ASN:H    | 1.69                     | 0.56              |
| 1:1L:260:VAL:CB  | 2:4X:407:TRP:NE1  | 2.68                     | 0.56              |
| 2:1S:339:ASN:HB3 | 2:1S:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:1T:316:ALA:HB3 | 2:1T:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1U:339:ASN:HB3 | 2:1U:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:1V:406:HIS:NE2 | 1:2J:263:PRO:HD3  | 2.20                     | 0.56              |
| 2:1Y:339:ASN:HB3 | 2:1Y:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:1Z:339:ASN:HB3 | 2:1Z:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2H:394:GLN:CG  | 1:3A:348:PRO:HG2  | 2.34                     | 0.56              |
| 2:2P:339:ASN:HB3 | 2:2P:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2Q:339:ASN:HB3 | 2:2Q:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2S:214:PHE:CB  | 1:3F:326:LYS:CE   | 2.74                     | 0.56              |
| 2:2S:222:PRO:O   | 1:3F:325:PRO:HD2  | 2.05                     | 0.56              |
| 2:2S:339:ASN:HB3 | 2:2S:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2T:404:PHE:HA  | 1:3G:261:PRO:O    | 2.05                     | 0.56              |
| 2:2X:101:ASN:HB2 | 1:3L:254:GLU:CG   | 2.34                     | 0.56              |
| 2:2X:181:VAL:H   | 1:3L:258:ASN:ND2  | 2.03                     | 0.56              |
| 2:2Y:339:ASN:HB3 | 2:2Y:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2Z:339:ASN:HB3 | 2:2Z:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3O:339:ASN:HB3 | 2:3O:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3P:343:PHE:HB3 | 2:3P:350:ASN:HD21 | 1.70                     | 0.56              |
| 2:3S:339:ASN:HB3 | 2:3S:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3T:316:ALA:HB3 | 2:3T:378:ILE:HB   | 1.87                     | 0.56              |
| 2:3U:339:ASN:HB3 | 2:3U:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3X:339:ASN:HB3 | 2:3X:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3Y:339:ASN:HB3 | 2:3Y:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3Z:339:ASN:HB3 | 2:3Z:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4P:339:ASN:HB3 | 2:4P:342:TYR:HB2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4P:343:PHE:HB3  | 2:4P:350:ASN:HD21 | 1.70                     | 0.56              |
| 2:4Q:339:ASN:HB3  | 2:4Q:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4R:339:ASN:HB3  | 2:4R:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4T:316:ALA:HB3  | 2:4T:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4T:339:ASN:HB3  | 2:4T:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4U:339:ASN:HB3  | 2:4U:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4Y:339:ASN:HB3  | 2:4Y:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:4Z:339:ASN:HB3  | 2:4Z:342:TYR:HB2  | 1.87                     | 0.56              |
| 1:1A:261:PRO:HB3  | 2:4H:404:PHE:CZ   | 2.39                     | 0.56              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:HA   | 2.35                     | 0.56              |
| 1:1D:257:THR:CB   | 2:4Q:100:GLY:O    | 2.53                     | 0.56              |
| 1:1G:261:PRO:CA   | 2:4T:404:PHE:CA   | 2.77                     | 0.56              |
| 2:1H:181:VAL:CG2  | 1:2A:258:ASN:HB3  | 2.35                     | 0.56              |
| 2:1H:316:ALA:HB3  | 2:1H:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1P:339:ASN:HB3  | 2:1P:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:1R:221:THR:OG1  | 1:2E:324:VAL:HG22 | 2.04                     | 0.56              |
| 2:1S:343:PHE:HB3  | 2:1S:350:ASN:HD21 | 1.70                     | 0.56              |
| 2:1T:339:ASN:HB3  | 2:1T:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:1W:71:GLU:HB2   | 1:2K:2:ARG:HD3    | 1.87                     | 0.56              |
| 2:1X:339:ASN:HB3  | 2:1X:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2O:77:SER:CB    | 1:3B:245:ASP:OD1  | 2.51                     | 0.56              |
| 2:2P:401:ARG:C    | 1:3C:262:TYR:OH   | 2.45                     | 0.56              |
| 2:2S:401:ARG:HH22 | 1:3F:435:VAL:C    | 2.13                     | 0.56              |
| 2:2T:316:ALA:HB3  | 2:2T:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2T:339:ASN:HB3  | 2:2T:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2U:339:ASN:HB3  | 2:2U:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:2Y:394:GLN:CG   | 1:3M:348:PRO:HG2  | 2.34                     | 0.56              |
| 2:3P:339:ASN:HB3  | 2:3P:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3S:283:TYR:OH   | 2:3T:85:GLN:O     | 2.18                     | 0.56              |
| 2:3T:339:ASN:HB3  | 2:3T:342:TYR:HB2  | 1.87                     | 0.56              |
| 2:3Y:205:ASP:OD2  | 2:3Y:304:ALA:N    | 2.35                     | 0.56              |
| 2:4H:316:ALA:HB3  | 2:4H:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4S:339:ASN:HB3  | 2:4S:342:TYR:HB2  | 1.87                     | 0.56              |
| 1:1B:257:THR:HG21 | 2:4O:101:ASN:C    | 2.30                     | 0.56              |
| 1:1C:257:THR:HB   | 2:4P:100:GLY:O    | 2.04                     | 0.56              |
| 1:1C:326:LYS:HA   | 2:4P:210:TYR:CG   | 2.40                     | 0.56              |
| 1:1C:329:ASN:HB3  | 2:4P:210:TYR:CD2  | 2.41                     | 0.56              |
| 1:1E:326:LYS:HA   | 2:4R:210:TYR:CG   | 2.40                     | 0.56              |
| 1:1F:333:ALA:CB   | 2:4S:176:LYS:HE2  | 2.35                     | 0.56              |
| 1:1F:347:CYS:CA   | 2:4S:398:MET:HG2  | 2.30                     | 0.56              |
| 1:1J:79:ARG:NH2   | 1:1J:92:LEU:O     | 2.37                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:79:ARG:NH2   | 1:1M:92:LEU:O     | 2.37                     | 0.56              |
| 1:1M:254:GLU:HA   | 2:4Y:100:GLY:O    | 2.04                     | 0.56              |
| 1:1N:254:GLU:HA   | 2:4Z:100:GLY:C    | 2.30                     | 0.56              |
| 2:1S:283:TYR:OH   | 2:1T:85:GLN:O     | 2.18                     | 0.56              |
| 2:1W:179:ASP:CG   | 1:2K:248:LEU:HD21 | 2.24                     | 0.56              |
| 2:1W:316:ALA:HB3  | 2:1W:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1W:404:PHE:HE1  | 1:2K:260:VAL:H    | 1.53                     | 0.56              |
| 1:2C:79:ARG:NH2   | 1:2C:92:LEU:O     | 2.37                     | 0.56              |
| 1:2J:79:ARG:NH2   | 1:2J:92:LEU:O     | 2.37                     | 0.56              |
| 1:2M:79:ARG:NH2   | 1:2M:92:LEU:O     | 2.38                     | 0.56              |
| 2:2H:316:ALA:HB3  | 2:2H:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2Q:222:PRO:O    | 1:3D:325:PRO:HD2  | 2.05                     | 0.56              |
| 2:2Q:343:PHE:HB3  | 2:2Q:350:ASN:HD21 | 1.70                     | 0.56              |
| 2:2R:100:GLY:HA3  | 1:3E:253:THR:CB   | 2.32                     | 0.56              |
| 2:2R:100:GLY:CA   | 1:3E:253:THR:C    | 2.77                     | 0.56              |
| 2:2U:404:PHE:HD1  | 1:3I:260:VAL:O    | 1.85                     | 0.56              |
| 2:2W:316:ALA:HB3  | 2:2W:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2X:404:PHE:CD2  | 1:3L:261:PRO:HA   | 2.39                     | 0.56              |
| 2:2Y:205:ASP:OD2  | 2:2Y:304:ALA:N    | 2.35                     | 0.56              |
| 1:3C:79:ARG:NH2   | 1:3C:92:LEU:O     | 2.37                     | 0.56              |
| 1:3J:79:ARG:NH2   | 1:3J:92:LEU:O     | 2.37                     | 0.56              |
| 1:3M:79:ARG:NH2   | 1:3M:92:LEU:O     | 2.38                     | 0.56              |
| 2:3H:316:ALA:HB3  | 2:3H:378:ILE:HB   | 1.87                     | 0.56              |
| 2:3Q:343:PHE:HB3  | 2:3Q:350:ASN:HD21 | 1.69                     | 0.56              |
| 2:3W:316:ALA:HB3  | 2:3W:378:ILE:HB   | 1.87                     | 0.56              |
| 1:4C:79:ARG:NH2   | 1:4C:92:LEU:O     | 2.37                     | 0.56              |
| 1:4J:79:ARG:NH2   | 1:4J:92:LEU:O     | 2.37                     | 0.56              |
| 1:4M:79:ARG:NH2   | 1:4M:92:LEU:O     | 2.37                     | 0.56              |
| 2:4Q:343:PHE:HB3  | 2:4Q:350:ASN:HD21 | 1.69                     | 0.56              |
| 2:4W:316:ALA:HB3  | 2:4W:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4Y:205:ASP:OD2  | 2:4Y:304:ALA:N    | 2.35                     | 0.56              |
| 1:1A:248:LEU:HD13 | 5:4H:501:GDP:N7   | 2.19                     | 0.56              |
| 1:1B:261:PRO:C    | 2:4O:404:PHE:HA   | 2.30                     | 0.56              |
| 1:1C:261:PRO:N    | 2:4P:404:PHE:CE1  | 2.73                     | 0.56              |
| 1:1D:325:PRO:HB2  | 2:4Q:224:TYR:CE1  | 2.39                     | 0.56              |
| 1:1E:326:LYS:HG3  | 2:4R:210:TYR:HA   | 1.86                     | 0.56              |
| 1:1E:346:TRP:HB2  | 2:4R:397:ALA:C    | 2.31                     | 0.56              |
| 1:1G:2:ARG:NH2    | 2:4T:73:GLY:CA    | 2.68                     | 0.56              |
| 1:1L:346:TRP:CD2  | 2:4X:403:ALA:HB2  | 2.41                     | 0.56              |
| 1:1N:263:PRO:CD   | 2:4Z:406:HIS:NE2  | 2.68                     | 0.56              |
| 2:1Q:343:PHE:HB3  | 2:1Q:350:ASN:HD21 | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Z:401:ARG:HB3  | 1:2N:262:TYR:HH   | 1.70                     | 0.56              |
| 2:2P:404:PHE:CE1  | 1:3C:261:PRO:N    | 2.74                     | 0.56              |
| 2:2Z:394:GLN:CG   | 1:3N:348:PRO:HG2  | 2.34                     | 0.56              |
| 2:2Z:404:PHE:CD1  | 1:3N:261:PRO:CA   | 2.88                     | 0.56              |
| 1:1C:79:ARG:NH2   | 1:1C:92:LEU:O     | 2.37                     | 0.56              |
| 1:1F:261:PRO:O    | 2:4S:404:PHE:CA   | 2.54                     | 0.56              |
| 1:1G:346:TRP:CA   | 2:4T:397:ALA:C    | 2.71                     | 0.56              |
| 1:1I:350:GLY:C    | 2:4U:181:VAL:HG22 | 2.30                     | 0.56              |
| 1:1N:435:VAL:CA   | 2:4Z:401:ARG:NH2  | 2.68                     | 0.56              |
| 2:1R:404:PHE:CD1  | 1:2E:261:PRO:HA   | 2.40                     | 0.56              |
| 2:2R:343:PHE:HB3  | 2:2R:350:ASN:HD21 | 1.69                     | 0.56              |
| 2:2R:406:HIS:CE1  | 1:3E:263:PRO:CA   | 2.88                     | 0.56              |
| 2:2S:222:PRO:C    | 1:3F:324:VAL:HG13 | 2.30                     | 0.56              |
| 2:2T:221:THR:C    | 1:3G:324:VAL:HG11 | 2.31                     | 0.56              |
| 2:2T:404:PHE:HD1  | 1:3G:260:VAL:O    | 1.88                     | 0.56              |
| 2:2X:101:ASN:ND2  | 1:3L:258:ASN:OD1  | 2.39                     | 0.56              |
| 2:2X:179:ASP:OD1  | 1:3L:353:VAL:HB   | 2.06                     | 0.56              |
| 2:2Z:407:TRP:HE1  | 1:3N:260:VAL:HB   | 1.71                     | 0.56              |
| 2:3R:343:PHE:HB3  | 2:3R:350:ASN:HD21 | 1.69                     | 0.56              |
| 2:4R:343:PHE:HB3  | 2:4R:350:ASN:HD21 | 1.70                     | 0.56              |
| 1:1C:346:TRP:CZ3  | 2:4P:403:ALA:HB1  | 2.40                     | 0.56              |
| 1:1D:247:ALA:O    | 2:4Q:15:GLN:OE1   | 2.22                     | 0.56              |
| 1:1D:325:PRO:HB3  | 2:4Q:224:TYR:CE1  | 2.40                     | 0.56              |
| 1:1E:253:THR:O    | 2:4R:100:GLY:HA3  | 2.06                     | 0.56              |
| 1:1G:346:TRP:HB2  | 2:4T:397:ALA:O    | 2.03                     | 0.56              |
| 1:1M:253:THR:HG22 | 2:4Y:100:GLY:HA3  | 1.88                     | 0.56              |
| 2:1S:222:PRO:HD2  | 1:2F:326:LYS:HB3  | 1.87                     | 0.56              |
| 2:1X:316:ALA:HB3  | 2:1X:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2R:11:GLN:NE2   | 1:3E:249:ASN:N    | 2.02                     | 0.56              |
| 2:2R:406:HIS:CD2  | 1:3E:262:TYR:CA   | 2.89                     | 0.56              |
| 2:2U:101:ASN:O    | 1:3I:257:THR:CG2  | 2.50                     | 0.56              |
| 2:2V:100:GLY:O    | 1:3J:257:THR:CB   | 2.54                     | 0.56              |
| 1:1A:248:LEU:HD11 | 5:4H:501:GDP:H8   | 1.66                     | 0.56              |
| 1:1B:346:TRP:CZ3  | 2:4O:403:ALA:CB   | 2.89                     | 0.56              |
| 1:1C:254:GLU:CG   | 2:4P:101:ASN:HB2  | 2.36                     | 0.56              |
| 1:1D:324:VAL:CG1  | 2:4Q:222:PRO:C    | 2.72                     | 0.56              |
| 1:1D:325:PRO:HD2  | 2:4Q:223:THR:HA   | 1.87                     | 0.56              |
| 1:1D:326:LYS:HE2  | 2:4Q:214:PHE:HB2  | 1.87                     | 0.56              |
| 1:1E:262:TYR:CZ   | 2:4R:402:LYS:C    | 2.83                     | 0.56              |
| 1:1F:439:SER:CB   | 2:4S:400:ARG:CD   | 2.82                     | 0.56              |
| 1:1L:254:GLU:HA   | 2:4X:100:GLY:O    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1L:261:PRO:O    | 2:4X:406:HIS:NE2  | 2.34                     | 0.56              |
| 1:1M:348:PRO:HG3  | 2:4Y:394:GLN:HA   | 1.87                     | 0.56              |
| 2:1R:343:PHE:HB3  | 2:1R:350:ASN:HD21 | 1.69                     | 0.56              |
| 2:1U:404:PHE:CE2  | 1:2I:261:PRO:HB3  | 2.40                     | 0.56              |
| 2:1W:214:PHE:HB3  | 1:2K:326:LYS:HE2  | 1.78                     | 0.56              |
| 2:2H:77:SER:CB    | 1:3A:245:ASP:OD1  | 2.52                     | 0.56              |
| 2:2P:71:GLU:HG3   | 1:3C:2:ARG:NH1    | 2.21                     | 0.56              |
| 2:2T:404:PHE:HE1  | 1:3G:260:VAL:N    | 2.04                     | 0.56              |
| 2:2V:404:PHE:HA   | 1:3J:261:PRO:O    | 2.05                     | 0.56              |
| 2:2X:316:ALA:HB3  | 2:2X:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2Y:72:PRO:HD2   | 1:3M:2:ARG:CG     | 2.35                     | 0.56              |
| 2:3X:316:ALA:HB3  | 2:3X:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4X:316:ALA:HB3  | 2:4X:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4Z:316:ALA:HB3  | 2:4Z:378:ILE:HB   | 1.87                     | 0.56              |
| 1:1B:326:LYS:CE   | 2:4O:214:PHE:CB   | 2.81                     | 0.56              |
| 1:1D:2:ARG:HH11   | 2:4Q:71:GLU:HB2   | 1.71                     | 0.56              |
| 1:1D:248:LEU:HD13 | 5:4Q:501:GDP:N7   | 2.15                     | 0.56              |
| 1:1F:346:TRP:CD1  | 2:4S:401:ARG:CG   | 2.86                     | 0.56              |
| 2:1O:316:ALA:HB3  | 2:1O:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1Q:207:GLU:OE1  | 1:2D:329:ASN:ND2  | 2.33                     | 0.56              |
| 2:1R:316:ALA:HB3  | 2:1R:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1X:401:ARG:HH22 | 1:2L:435:VAL:CA   | 2.05                     | 0.56              |
| 2:1Z:316:ALA:HB3  | 2:1Z:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2O:316:ALA:HB3  | 2:2O:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2O:394:GLN:CG   | 1:3B:348:PRO:HG2  | 2.35                     | 0.56              |
| 2:2O:394:GLN:OE1  | 1:3B:349:THR:CG2  | 2.54                     | 0.56              |
| 2:2P:176:LYS:CE   | 1:3C:333:ALA:HB1  | 2.32                     | 0.56              |
| 2:2Q:401:ARG:C    | 1:3D:262:TYR:OH   | 2.46                     | 0.56              |
| 2:2R:316:ALA:HB3  | 2:2R:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2V:404:PHE:H    | 1:3J:261:PRO:C    | 2.08                     | 0.56              |
| 2:2V:404:PHE:HE1  | 1:3J:260:VAL:N    | 2.04                     | 0.56              |
| 2:2X:11:GLN:HE22  | 1:3L:249:ASN:CA   | 2.18                     | 0.56              |
| 2:2X:394:GLN:CG   | 1:3L:348:PRO:HG2  | 2.36                     | 0.56              |
| 2:2Z:316:ALA:HB3  | 2:2Z:378:ILE:HB   | 1.87                     | 0.56              |
| 2:3R:316:ALA:HB3  | 2:3R:378:ILE:HB   | 1.87                     | 0.56              |
| 2:3Z:316:ALA:HB3  | 2:3Z:378:ILE:HB   | 1.87                     | 0.56              |
| 2:4R:316:ALA:HB3  | 2:4R:378:ILE:HB   | 1.87                     | 0.56              |
| 1:1B:326:LYS:HG2  | 2:4O:210:TYR:HB3  | 1.87                     | 0.56              |
| 1:1D:245:ASP:OD1  | 2:4Q:77:SER:OG    | 2.23                     | 0.56              |
| 1:1D:352:LYS:HE2  | 2:4Q:101:ASN:ND2  | 2.19                     | 0.56              |
| 1:1I:251:ASP:OD2  | 2:4U:71:GLU:HB3   | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:346:TRP:HA   | 2:4V:397:ALA:C    | 2.29                     | 0.56              |
| 2:1P:316:ALA:HB3  | 2:1P:378:ILE:HB   | 1.87                     | 0.56              |
| 2:1T:214:PHE:CB   | 1:2G:326:LYS:CE   | 2.63                     | 0.56              |
| 2:1V:178:SER:OG   | 1:2J:351:PHE:O    | 2.21                     | 0.56              |
| 2:1V:181:VAL:CG1  | 1:2J:258:ASN:O    | 2.52                     | 0.56              |
| 2:2S:100:GLY:C    | 1:3F:254:GLU:HA   | 2.31                     | 0.56              |
| 2:4O:316:ALA:HB3  | 2:4O:378:ILE:HB   | 1.87                     | 0.56              |
| 1:1D:263:PRO:HD3  | 2:4Q:406:HIS:HB3  | 1.87                     | 0.56              |
| 5:1H:501:GDP:C8   | 1:2A:248:LEU:HD13 | 2.41                     | 0.56              |
| 2:1X:394:GLN:CD   | 1:2L:349:THR:HG23 | 2.31                     | 0.56              |
| 2:2P:316:ALA:HB3  | 2:2P:378:ILE:HB   | 1.87                     | 0.56              |
| 2:2Q:210:TYR:CE2  | 1:3D:329:ASN:HB2  | 2.41                     | 0.56              |
| 2:2V:394:GLN:HA   | 1:3J:348:PRO:HG3  | 1.87                     | 0.56              |
| 2:3O:316:ALA:HB3  | 2:3O:378:ILE:HB   | 1.87                     | 0.56              |
| 2:3P:316:ALA:HB3  | 2:3P:378:ILE:HB   | 1.87                     | 0.56              |
| 1:4A:79:ARG:NH2   | 1:4A:92:LEU:O     | 2.37                     | 0.56              |
| 2:4P:316:ALA:HB3  | 2:4P:378:ILE:HB   | 1.87                     | 0.56              |
| 1:1A:79:ARG:NH2   | 1:1A:92:LEU:O     | 2.37                     | 0.55              |
| 1:1D:260:VAL:CB   | 2:4Q:407:TRP:CE2  | 2.78                     | 0.55              |
| 1:1D:326:LYS:HE3  | 2:4Q:214:PHE:HB2  | 1.88                     | 0.55              |
| 1:1F:260:VAL:HG12 | 2:4S:407:TRP:NE1  | 2.20                     | 0.55              |
| 1:1F:326:LYS:CB   | 2:4S:210:TYR:CD1  | 2.90                     | 0.55              |
| 1:1G:260:VAL:C    | 2:4T:407:TRP:NE1  | 2.42                     | 0.55              |
| 1:1K:434:GLU:O    | 2:4W:401:ARG:NH2  | 2.39                     | 0.55              |
| 1:1M:346:TRP:CB   | 2:4Y:398:MET:HA   | 2.23                     | 0.55              |
| 2:1R:101:ASN:HB2  | 1:2E:254:GLU:HG2  | 1.87                     | 0.55              |
| 2:1R:222:PRO:CG   | 1:2E:326:LYS:HB2  | 2.31                     | 0.55              |
| 2:1S:276:THR:HG22 | 2:1S:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1V:100:GLY:CA   | 1:2J:253:THR:CB   | 2.56                     | 0.55              |
| 1:2A:79:ARG:NH2   | 1:2A:92:LEU:O     | 2.37                     | 0.55              |
| 1:2C:195:LEU:HD12 | 1:2C:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:2O:276:THR:HG22 | 2:2O:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2O:401:ARG:C    | 1:3B:262:TYR:OH   | 2.48                     | 0.55              |
| 2:2Q:100:GLY:HA2  | 1:3D:253:THR:CB   | 2.33                     | 0.55              |
| 2:2R:222:PRO:O    | 1:3E:325:PRO:HD2  | 2.06                     | 0.55              |
| 2:2T:404:PHE:CE1  | 1:3G:261:PRO:CA   | 2.88                     | 0.55              |
| 1:3A:79:ARG:NH2   | 1:3A:92:LEU:O     | 2.37                     | 0.55              |
| 2:4O:276:THR:HG22 | 2:4O:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:4T:276:THR:HG22 | 2:4T:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:1D:254:GLU:CA   | 2:4Q:100:GLY:O    | 2.32                     | 0.55              |
| 1:1D:261:PRO:O    | 2:4Q:404:PHE:HA   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:346:TRP:HA   | 2:4Q:397:ALA:CB   | 2.36                     | 0.55              |
| 1:1E:262:TYR:CZ   | 2:4R:402:LYS:O    | 2.59                     | 0.55              |
| 1:1F:2:ARG:HG3    | 2:4S:72:PRO:CD    | 2.35                     | 0.55              |
| 1:1G:261:PRO:CB   | 2:4T:404:PHE:H    | 2.20                     | 0.55              |
| 1:1G:329:ASN:ND2  | 2:4T:210:TYR:HD2  | 2.05                     | 0.55              |
| 1:1I:332:ILE:HB   | 2:4U:177:VAL:CG2  | 2.36                     | 0.55              |
| 1:1K:439:SER:OG   | 2:4W:401:ARG:CD   | 2.54                     | 0.55              |
| 1:1L:195:LEU:HD12 | 1:1L:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:1H:181:VAL:CG2  | 1:2A:258:ASN:O    | 2.53                     | 0.55              |
| 2:1O:276:THR:HG22 | 2:1O:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1R:224:TYR:HD2  | 1:2E:247:ALA:O    | 1.90                     | 0.55              |
| 1:2L:195:LEU:HD12 | 1:2L:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:2M:195:LEU:HD12 | 1:2M:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:2Q:71:GLU:HB2   | 1:3D:2:ARG:CD     | 2.29                     | 0.55              |
| 2:2R:222:PRO:C    | 1:3E:324:VAL:HG13 | 2.31                     | 0.55              |
| 2:2R:407:TRP:HE1  | 1:3E:260:VAL:CG1  | 2.18                     | 0.55              |
| 2:2S:207:GLU:CD   | 1:3F:329:ASN:ND2  | 2.48                     | 0.55              |
| 2:2S:276:THR:HG22 | 2:2S:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2S:316:ALA:HB3  | 2:2S:378:ILE:HB   | 1.87                     | 0.55              |
| 2:2T:276:THR:HG22 | 2:2T:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2U:407:TRP:HE1  | 1:3I:260:VAL:CG1  | 2.20                     | 0.55              |
| 2:2V:101:ASN:HB2  | 1:3J:254:GLU:HG2  | 1.88                     | 0.55              |
| 1:3C:195:LEU:HD12 | 1:3C:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:3N:79:ARG:NH2   | 1:3N:92:LEU:O     | 2.37                     | 0.55              |
| 2:3O:276:THR:HG22 | 2:3O:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:3S:276:THR:HG22 | 2:3S:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:3S:316:ALA:HB3  | 2:3S:378:ILE:HB   | 1.87                     | 0.55              |
| 2:3T:276:THR:HG22 | 2:3T:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:4F:195:LEU:HD12 | 1:4F:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:4N:79:ARG:NH2   | 1:4N:92:LEU:O     | 2.37                     | 0.55              |
| 2:4S:276:THR:HG22 | 2:4S:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:4S:316:ALA:HB3  | 2:4S:378:ILE:HB   | 1.87                     | 0.55              |
| 1:1A:348:PRO:HG3  | 2:4H:394:GLN:HG2  | 1.77                     | 0.55              |
| 1:1B:253:THR:HB   | 2:4O:100:GLY:HA2  | 1.86                     | 0.55              |
| 1:1B:324:VAL:CG2  | 2:4O:221:THR:OG1  | 2.48                     | 0.55              |
| 1:1C:195:LEU:HD12 | 1:1C:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1C:349:THR:HG21 | 2:4P:184:PRO:HG3  | 1.88                     | 0.55              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:N    | 2.22                     | 0.55              |
| 1:1F:346:TRP:CZ2  | 2:4S:403:ALA:CB   | 2.90                     | 0.55              |
| 1:1I:195:LEU:HD12 | 1:1I:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1I:326:LYS:HG2  | 2:4U:210:TYR:CG   | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:260:VAL:HG12 | 2:4W:406:HIS:HE1  | 1.71                     | 0.55              |
| 1:1M:195:LEU:HD12 | 1:1M:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1N:79:ARG:NH2   | 1:1N:92:LEU:O     | 2.37                     | 0.55              |
| 2:1S:100:GLY:HA2  | 1:2F:253:THR:CB   | 2.35                     | 0.55              |
| 2:1T:276:THR:HG22 | 2:1T:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1U:178:SER:HB3  | 1:2I:349:THR:CB   | 2.31                     | 0.55              |
| 2:1Y:401:ARG:O    | 1:2M:262:TYR:HE1  | 1.90                     | 0.55              |
| 1:2F:195:LEU:HD12 | 1:2F:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:2I:195:LEU:HD12 | 1:2I:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:2N:79:ARG:NH2   | 1:2N:92:LEU:O     | 2.37                     | 0.55              |
| 2:2H:276:THR:HG22 | 2:2H:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2T:407:TRP:CD1  | 1:3G:260:VAL:O    | 2.60                     | 0.55              |
| 2:2U:407:TRP:HE1  | 1:3I:260:VAL:HB   | 1.70                     | 0.55              |
| 2:2V:222:PRO:HD2  | 1:3J:326:LYS:HB3  | 1.89                     | 0.55              |
| 2:2Y:73:GLY:HA3   | 1:3M:2:ARG:CZ     | 2.36                     | 0.55              |
| 2:2Z:100:GLY:O    | 1:3N:257:THR:OG1  | 2.19                     | 0.55              |
| 1:3F:195:LEU:HD12 | 1:3F:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:3L:195:LEU:HD12 | 1:3L:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:3M:195:LEU:HD12 | 1:3M:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:3H:276:THR:HG22 | 2:3H:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:4B:79:ARG:NH2   | 1:4B:92:LEU:O     | 2.37                     | 0.55              |
| 1:4C:195:LEU:HD12 | 1:4C:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:4I:195:LEU:HD12 | 1:4I:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:4L:195:LEU:HD12 | 1:4L:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:4M:195:LEU:HD12 | 1:4M:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:4H:276:THR:HG22 | 2:4H:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:1B:79:ARG:NH2   | 1:1B:92:LEU:O     | 2.38                     | 0.55              |
| 1:1B:346:TRP:HB2  | 2:4O:397:ALA:C    | 2.29                     | 0.55              |
| 1:1F:195:LEU:HD12 | 1:1F:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1F:353:VAL:CG2  | 2:4S:179:ASP:HA   | 2.35                     | 0.55              |
| 1:1G:249:ASN:N    | 2:4T:11:GLN:OE1   | 2.39                     | 0.55              |
| 1:1I:325:PRO:CB   | 2:4U:224:TYR:CZ   | 2.90                     | 0.55              |
| 1:1J:326:LYS:HB2  | 2:4V:222:PRO:HG2  | 1.85                     | 0.55              |
| 1:1J:346:TRP:O    | 2:4V:398:MET:HG3  | 1.94                     | 0.55              |
| 1:1K:247:ALA:O    | 2:4W:15:GLN:NE2   | 2.39                     | 0.55              |
| 2:1H:276:THR:HG22 | 2:1H:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1Q:101:ASN:HB2  | 1:2D:254:GLU:HG2  | 1.87                     | 0.55              |
| 2:1S:316:ALA:HB3  | 2:1S:378:ILE:HB   | 1.87                     | 0.55              |
| 2:1U:316:ALA:HB3  | 2:1U:378:ILE:HB   | 1.87                     | 0.55              |
| 2:1X:182:VAL:HG21 | 1:2L:257:THR:HG21 | 1.86                     | 0.55              |
| 1:2B:79:ARG:NH2   | 1:2B:92:LEU:O     | 2.38                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2N:195:LEU:HD12 | 1:2N:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:2O:181:VAL:H    | 1:3B:258:ASN:HD22 | 1.55                     | 0.55              |
| 2:2P:224:TYR:HD2  | 1:3C:247:ALA:O    | 1.89                     | 0.55              |
| 2:2Q:406:HIS:CD2  | 1:3D:263:PRO:N    | 2.75                     | 0.55              |
| 2:2R:100:GLY:C    | 1:3E:254:GLU:HA   | 2.31                     | 0.55              |
| 2:2T:397:ALA:O    | 1:3G:346:TRP:HB3  | 2.07                     | 0.55              |
| 1:3B:79:ARG:NH2   | 1:3B:92:LEU:O     | 2.38                     | 0.55              |
| 1:3I:195:LEU:HD12 | 1:3I:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:3U:316:ALA:HB3  | 2:3U:378:ILE:HB   | 1.87                     | 0.55              |
| 1:4N:195:LEU:HD12 | 1:4N:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:4Q:69:ASP:OD2   | 2:4Q:74:THR:OG1   | 2.19                     | 0.55              |
| 1:1A:262:TYR:CE2  | 2:4H:403:ALA:HA   | 2.42                     | 0.55              |
| 1:1B:349:THR:HG23 | 2:4O:394:GLN:OE1  | 2.06                     | 0.55              |
| 1:1E:195:LEU:HD12 | 1:1E:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1E:261:PRO:N    | 2:4R:404:PHE:CD1  | 2.74                     | 0.55              |
| 1:1E:262:TYR:CZ   | 2:4R:403:ALA:HA   | 2.41                     | 0.55              |
| 1:1G:248:LEU:C    | 2:4T:11:GLN:NE2   | 2.33                     | 0.55              |
| 1:1G:422:ARG:NH1  | 1:1G:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1I:257:THR:HG21 | 2:4U:102:ASN:CA   | 2.37                     | 0.55              |
| 1:1J:346:TRP:HZ3  | 2:4V:404:PHE:HE2  | 1.48                     | 0.55              |
| 1:1J:349:THR:HG23 | 2:4V:184:PRO:CG   | 2.37                     | 0.55              |
| 1:1K:195:LEU:HD12 | 1:1K:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1L:351:PHE:O    | 2:4X:180:THR:N    | 2.40                     | 0.55              |
| 2:1H:182:VAL:HG21 | 1:2A:257:THR:HG22 | 1.88                     | 0.55              |
| 2:1R:276:THR:HG22 | 2:1R:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1T:404:PHE:CD1  | 1:2G:261:PRO:HA   | 2.41                     | 0.55              |
| 2:1X:276:THR:HG22 | 2:1X:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1X:404:PHE:CZ   | 1:2L:261:PRO:N    | 2.75                     | 0.55              |
| 2:1Z:205:ASP:OD2  | 2:1Z:304:ALA:N    | 2.35                     | 0.55              |
| 1:2G:422:ARG:NH1  | 1:2G:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:2K:195:LEU:HD12 | 1:2K:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:2H:394:GLN:CB   | 1:3A:348:PRO:CG   | 2.84                     | 0.55              |
| 2:2R:397:ALA:O    | 1:3E:346:TRP:HB3  | 2.06                     | 0.55              |
| 2:2S:72:PRO:HG2   | 1:3F:2:ARG:HG3    | 1.89                     | 0.55              |
| 2:2T:100:GLY:HA2  | 1:3G:253:THR:CB   | 2.35                     | 0.55              |
| 2:2U:11:GLN:HE22  | 1:3I:249:ASN:CA   | 2.13                     | 0.55              |
| 2:2U:316:ALA:HB3  | 2:2U:378:ILE:HB   | 1.87                     | 0.55              |
| 2:2X:210:TYR:HD2  | 1:3L:329:ASN:ND2  | 1.98                     | 0.55              |
| 2:2X:276:THR:HG22 | 2:2X:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2X:394:GLN:HA   | 1:3L:348:PRO:HG3  | 1.88                     | 0.55              |
| 2:2Y:404:PHE:CD2  | 1:3M:261:PRO:HA   | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3E:195:LEU:HD12 | 1:3E:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:3N:195:LEU:HD12 | 1:3N:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:3X:276:THR:HG22 | 2:3X:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:4K:195:LEU:HD12 | 1:4K:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:4U:316:ALA:HB3  | 2:4U:378:ILE:HB   | 1.87                     | 0.55              |
| 2:4W:276:THR:HG22 | 2:4W:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:4X:276:THR:HG22 | 2:4X:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:1B:212:ILE:HG23 | 1:1B:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:1B:346:TRP:O    | 2:4O:398:MET:CA   | 2.55                     | 0.55              |
| 1:1C:257:THR:OG1  | 2:4P:100:GLY:O    | 2.23                     | 0.55              |
| 1:1F:257:THR:HG21 | 2:4S:102:ASN:HA   | 1.88                     | 0.55              |
| 1:1I:326:LYS:HA   | 2:4U:210:TYR:CD1  | 2.41                     | 0.55              |
| 1:1I:352:LYS:HA   | 2:4U:179:ASP:O    | 2.07                     | 0.55              |
| 1:1L:348:PRO:CG   | 2:4X:394:GLN:CB   | 2.79                     | 0.55              |
| 1:1N:195:LEU:HD12 | 1:1N:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1N:348:PRO:HB2  | 2:4Z:394:GLN:CD   | 2.32                     | 0.55              |
| 2:1P:276:THR:HG22 | 2:1P:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1V:181:VAL:HG11 | 1:2J:258:ASN:O    | 2.07                     | 0.55              |
| 2:1W:276:THR:HG22 | 2:1W:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1Z:394:GLN:HG2  | 1:2N:348:PRO:HG3  | 1.86                     | 0.55              |
| 2:1Z:404:PHE:N    | 1:2N:261:PRO:O    | 2.29                     | 0.55              |
| 1:2E:195:LEU:HD12 | 1:2E:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:2K:422:ARG:NH1  | 1:2K:426:ALA:HB2  | 2.22                     | 0.55              |
| 2:2H:394:GLN:CB   | 1:3A:348:PRO:HG3  | 2.35                     | 0.55              |
| 2:2Q:398:MET:CG   | 1:3D:346:TRP:O    | 2.55                     | 0.55              |
| 2:2S:179:ASP:OD2  | 1:3F:248:LEU:HD21 | 2.06                     | 0.55              |
| 2:2U:401:ARG:NH2  | 1:3I:435:VAL:CA   | 2.51                     | 0.55              |
| 2:2W:276:THR:HG22 | 2:2W:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2Y:223:THR:HA   | 1:3M:325:PRO:CD   | 2.36                     | 0.55              |
| 2:2Y:394:GLN:CB   | 1:3M:348:PRO:HG3  | 2.35                     | 0.55              |
| 1:3F:422:ARG:NH1  | 1:3F:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:3G:422:ARG:NH1  | 1:3G:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:3J:195:LEU:HD12 | 1:3J:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:3K:195:LEU:HD12 | 1:3K:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:3P:276:THR:HG22 | 2:3P:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:3R:276:THR:HG22 | 2:3R:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:3W:276:THR:HG22 | 2:3W:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:4B:212:ILE:HG23 | 1:4B:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:4E:195:LEU:HD12 | 1:4E:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:4F:422:ARG:NH1  | 1:4F:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:4G:422:ARG:NH1  | 1:4G:426:ALA:HB2  | 2.22                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4J:195:LEU:HD12 | 1:4J:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1A:346:TRP:HA   | 2:4H:397:ALA:HB1  | 1.87                     | 0.55              |
| 1:1C:212:ILE:HG23 | 1:1C:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:1C:422:ARG:NH1  | 1:1C:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1F:261:PRO:CB   | 2:4S:404:PHE:N    | 2.70                     | 0.55              |
| 1:1F:262:TYR:CZ   | 2:4S:402:LYS:O    | 2.60                     | 0.55              |
| 1:1F:422:ARG:NH1  | 1:1F:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1I:352:LYS:CD   | 2:4U:101:ASN:HD22 | 2.19                     | 0.55              |
| 1:1J:195:LEU:HD12 | 1:1J:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:1L:212:ILE:HG23 | 1:1L:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:1L:422:ARG:NH1  | 1:1L:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1M:212:ILE:HG23 | 1:1M:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:1Q:316:ALA:HB3  | 2:1Q:378:ILE:HB   | 1.87                     | 0.55              |
| 2:1W:179:ASP:C    | 1:2K:352:LYS:HD2  | 2.26                     | 0.55              |
| 1:2B:212:ILE:HG23 | 1:2B:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:2C:422:ARG:NH1  | 1:2C:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:2F:422:ARG:NH1  | 1:2F:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:2J:195:LEU:HD12 | 1:2J:266:HIS:HE1  | 1.72                     | 0.55              |
| 1:2L:212:ILE:HG23 | 1:2L:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:2L:422:ARG:NH1  | 1:2L:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:2M:212:ILE:HG23 | 1:2M:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:2P:276:THR:HG22 | 2:2P:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2R:276:THR:HG22 | 2:2R:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:3B:212:ILE:HG23 | 1:3B:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:3C:422:ARG:NH1  | 1:3C:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:3L:422:ARG:NH1  | 1:3L:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:3M:212:ILE:HG23 | 1:3M:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:3Z:205:ASP:OD2  | 2:3Z:304:ALA:N    | 2.35                     | 0.55              |
| 1:4A:212:ILE:HG23 | 1:4A:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:4C:422:ARG:NH1  | 1:4C:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:4M:212:ILE:HG23 | 1:4M:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:4R:276:THR:HG22 | 2:4R:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:4U:276:THR:HG22 | 2:4U:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:1A:351:PHE:O    | 2:4H:180:THR:C    | 2.49                     | 0.55              |
| 1:1G:346:TRP:C    | 2:4T:398:MET:HA   | 2.32                     | 0.55              |
| 1:1G:347:CYS:CA   | 2:4T:398:MET:HG2  | 2.34                     | 0.55              |
| 1:1K:422:ARG:NH1  | 1:1K:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1L:263:PRO:CD   | 2:4X:406:HIS:CD2  | 2.89                     | 0.55              |
| 1:1M:261:PRO:O    | 2:4Y:404:PHE:HA   | 2.07                     | 0.55              |
| 1:1N:329:ASN:CB   | 2:4Z:210:TYR:CD2  | 2.89                     | 0.55              |
| 2:1Q:179:ASP:O    | 1:2D:352:LYS:HD2  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1T:404:PHE:CE2  | 1:2G:261:PRO:HB3  | 2.41                     | 0.55              |
| 1:2N:212:ILE:HG23 | 1:2N:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:2Q:181:VAL:CB   | 1:3D:258:ASN:O    | 2.54                     | 0.55              |
| 2:2Q:316:ALA:HB3  | 2:2Q:378:ILE:HB   | 1.87                     | 0.55              |
| 2:2R:179:ASP:OD2  | 1:3E:248:LEU:CD2  | 2.54                     | 0.55              |
| 2:2Z:205:ASP:OD2  | 2:2Z:304:ALA:N    | 2.35                     | 0.55              |
| 1:3A:212:ILE:HG23 | 1:3A:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:3C:212:ILE:HG23 | 1:3C:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:3K:422:ARG:NH1  | 1:3K:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:3L:212:ILE:HG23 | 1:3L:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:3Q:316:ALA:HB3  | 2:3Q:378:ILE:HB   | 1.87                     | 0.55              |
| 2:3U:276:THR:HG22 | 2:3U:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:3W:284:ARG:HD3  | 2:3W:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:3Y:276:THR:HG22 | 2:3Y:284:ARG:NH1  | 2.21                     | 0.55              |
| 1:4K:422:ARG:NH1  | 1:4K:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:4L:212:ILE:HG23 | 1:4L:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:4L:422:ARG:NH1  | 1:4L:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1A:314:ALA:HB2  | 2:4H:181:VAL:HG11 | 1.88                     | 0.55              |
| 1:1B:254:GLU:CB   | 2:4O:101:ASN:HB2  | 2.37                     | 0.55              |
| 1:1C:348:PRO:HG3  | 2:4P:394:GLN:CG   | 2.21                     | 0.55              |
| 1:1C:352:LYS:HD3  | 2:4P:101:ASN:ND2  | 2.22                     | 0.55              |
| 1:1D:261:PRO:CB   | 2:4Q:404:PHE:N    | 2.70                     | 0.55              |
| 1:1D:262:TYR:O    | 2:4Q:406:HIS:NE2  | 2.37                     | 0.55              |
| 1:1I:422:ARG:NH1  | 1:1I:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1J:253:THR:C    | 2:4V:100:GLY:HA2  | 2.31                     | 0.55              |
| 1:1J:324:VAL:HG21 | 2:4V:221:THR:OG1  | 2.07                     | 0.55              |
| 1:1K:439:SER:OG   | 2:4W:401:ARG:HG2  | 2.07                     | 0.55              |
| 1:1M:346:TRP:HA   | 2:4Y:397:ALA:O    | 2.07                     | 0.55              |
| 1:1N:212:ILE:HG23 | 1:1N:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:1H:100:GLY:HA3  | 1:2A:253:THR:CB   | 2.37                     | 0.55              |
| 2:1P:221:THR:OG1  | 1:2C:324:VAL:HG21 | 2.07                     | 0.55              |
| 2:1Q:284:ARG:HD3  | 2:1Q:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:1R:181:VAL:N    | 1:2E:258:ASN:ND2  | 2.45                     | 0.55              |
| 2:1W:284:ARG:HD3  | 2:1W:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:1Y:276:THR:HG22 | 2:1Y:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1Z:404:PHE:CE1  | 1:2N:260:VAL:O    | 2.60                     | 0.55              |
| 1:2A:212:ILE:HG23 | 1:2A:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:2C:212:ILE:HG23 | 1:2C:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:2I:422:ARG:NH1  | 1:2I:426:ALA:HB2  | 2.22                     | 0.55              |
| 2:2Q:284:ARG:HD3  | 2:2Q:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:2R:406:HIS:CD2  | 1:3E:263:PRO:N    | 2.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:397:ALA:O    | 1:3F:346:TRP:HB3  | 2.04                     | 0.55              |
| 2:2T:222:PRO:C    | 1:3G:324:VAL:HG13 | 2.32                     | 0.55              |
| 2:2U:276:THR:HG22 | 2:2U:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:2V:179:ASP:OD2  | 1:3J:248:LEU:HD21 | 2.06                     | 0.55              |
| 2:2V:398:MET:HA   | 1:3J:346:TRP:HB2  | 1.87                     | 0.55              |
| 2:2W:284:ARG:HD3  | 2:2W:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:2X:214:PHE:CG   | 1:3L:326:LYS:HE3  | 2.41                     | 0.55              |
| 1:3N:212:ILE:HG23 | 1:3N:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:4N:212:ILE:HG23 | 1:4N:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:4P:276:THR:HG22 | 2:4P:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:4Q:284:ARG:HD3  | 2:4Q:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:4Q:316:ALA:HB3  | 2:4Q:378:ILE:HB   | 1.87                     | 0.55              |
| 2:4W:284:ARG:HD3  | 2:4W:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:4X:69:ASP:OD2   | 2:4X:74:THR:OG1   | 2.20                     | 0.55              |
| 2:4Z:205:ASP:OD2  | 2:4Z:304:ALA:N    | 2.35                     | 0.55              |
| 1:1A:212:ILE:HG23 | 1:1A:216:ASN:HD22 | 1.72                     | 0.55              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:N    | 2.70                     | 0.55              |
| 1:1D:325:PRO:C    | 2:4Q:210:TYR:CZ   | 2.84                     | 0.55              |
| 1:1D:422:ARG:NH1  | 1:1D:426:ALA:HB2  | 2.22                     | 0.55              |
| 1:1E:352:LYS:HA   | 2:4R:180:THR:HA   | 1.88                     | 0.55              |
| 1:1F:2:ARG:CD     | 2:4S:71:GLU:HB2   | 2.37                     | 0.55              |
| 1:1I:332:ILE:HG21 | 2:4U:177:VAL:CG2  | 2.36                     | 0.55              |
| 1:1J:329:ASN:ND2  | 2:4V:210:TYR:CD2  | 2.67                     | 0.55              |
| 1:1J:434:GLU:O    | 2:4V:401:ARG:NH2  | 2.40                     | 0.55              |
| 1:1K:346:TRP:CB   | 2:4W:398:MET:HA   | 2.25                     | 0.55              |
| 1:1L:346:TRP:CD2  | 2:4X:403:ALA:CB   | 2.90                     | 0.55              |
| 1:1N:435:VAL:HA   | 2:4Z:401:ARG:HH22 | 1.68                     | 0.55              |
| 2:1O:284:ARG:HD3  | 2:1O:290:GLU:OE2  | 2.07                     | 0.55              |
| 2:1U:276:THR:HG22 | 2:1U:284:ARG:NH1  | 2.22                     | 0.55              |
| 2:1Z:397:ALA:O    | 1:2N:346:TRP:HB2  | 2.07                     | 0.55              |
| 1:2A:195:LEU:HD12 | 1:2A:266:HIS:HE1  | 1.72                     | 0.55              |
| 2:2O:100:GLY:O    | 1:3B:254:GLU:HA   | 2.07                     | 0.55              |
| 2:2P:177:VAL:CG2  | 1:3C:332:ILE:CG2  | 2.74                     | 0.55              |
| 2:2Q:100:GLY:CA   | 1:3D:253:THR:CG2  | 2.74                     | 0.55              |
| 2:2U:404:PHE:HE1  | 1:3I:260:VAL:N    | 2.05                     | 0.55              |
| 2:2V:404:PHE:CE2  | 1:3J:261:PRO:CB   | 2.79                     | 0.55              |
| 2:2X:69:ASP:OD2   | 2:2X:74:THR:OG1   | 2.19                     | 0.55              |
| 2:2Y:276:THR:HG22 | 2:2Y:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:3D:422:ARG:NH1  | 1:3D:426:ALA:HB2  | 2.22                     | 0.55              |
| 2:3Q:284:ARG:HD3  | 2:3Q:290:GLU:OE2  | 2.07                     | 0.55              |
| 1:4A:195:LEU:HD12 | 1:4A:266:HIS:HE1  | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4C:212:ILE:HG23 | 1:4C:216:ASN:HD22 | 1.72                     | 0.55              |
| 2:4Y:276:THR:HG22 | 2:4Y:284:ARG:NH1  | 2.22                     | 0.55              |
| 1:1C:248:LEU:C    | 2:4P:11:GLN:NE2   | 2.56                     | 0.54              |
| 1:1C:253:THR:HB   | 2:4P:100:GLY:HA2  | 1.90                     | 0.54              |
| 1:1E:261:PRO:C    | 2:4R:406:HIS:NE2  | 2.65                     | 0.54              |
| 1:1E:261:PRO:HB2  | 2:4R:404:PHE:H    | 1.71                     | 0.54              |
| 1:1G:261:PRO:CA   | 2:4T:404:PHE:CD1  | 2.90                     | 0.54              |
| 1:1G:352:LYS:HE2  | 2:4T:101:ASN:ND2  | 2.22                     | 0.54              |
| 1:1J:348:PRO:HG3  | 2:4V:394:GLN:HA   | 1.85                     | 0.54              |
| 1:1M:326:LYS:HE2  | 2:4Y:214:PHE:HB2  | 1.89                     | 0.54              |
| 1:1N:260:VAL:HG12 | 2:4Z:407:TRP:HE1  | 1.72                     | 0.54              |
| 2:1H:205:ASP:OD2  | 2:1H:304:ALA:N    | 2.35                     | 0.54              |
| 2:1O:180:THR:CG2  | 1:2B:258:ASN:HD21 | 2.16                     | 0.54              |
| 2:1Q:179:ASP:OD2  | 1:2D:248:LEU:HD21 | 2.07                     | 0.54              |
| 2:1T:404:PHE:CE1  | 1:2G:261:PRO:CA   | 2.89                     | 0.54              |
| 2:1X:411:GLU:OE2  | 1:2L:163:LYS:NZ   | 2.39                     | 0.54              |
| 1:2B:195:LEU:HD12 | 1:2B:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:2D:422:ARG:NH1  | 1:2D:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:2K:212:ILE:HG23 | 1:2K:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:2V:11:GLN:HE22  | 1:3J:249:ASN:CA   | 2.14                     | 0.54              |
| 1:3B:195:LEU:HD12 | 1:3B:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:3I:422:ARG:NH1  | 1:3I:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:3O:284:ARG:HD3  | 2:3O:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3Z:276:THR:HG22 | 2:3Z:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:4D:422:ARG:NH1  | 1:4D:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:4I:422:ARG:NH1  | 1:4I:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:4O:283:TYR:OH   | 2:4P:85:GLN:O     | 2.18                     | 0.54              |
| 2:4O:284:ARG:HD3  | 2:4O:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4Z:276:THR:HG22 | 2:4Z:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:1A:195:LEU:HD12 | 1:1A:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:1C:257:THR:HG21 | 2:4P:102:ASN:HA   | 1.89                     | 0.54              |
| 1:1F:253:THR:O    | 2:4S:100:GLY:HA3  | 2.06                     | 0.54              |
| 1:1F:260:VAL:HG12 | 2:4S:407:TRP:HE1  | 1.71                     | 0.54              |
| 1:1F:326:LYS:CG   | 2:4S:210:TYR:CD1  | 2.90                     | 0.54              |
| 1:1G:248:LEU:HA   | 2:4T:11:GLN:CD    | 2.30                     | 0.54              |
| 1:1G:324:VAL:HG21 | 2:4T:221:THR:OG1  | 2.07                     | 0.54              |
| 1:1G:326:LYS:HG2  | 2:4T:210:TYR:CD1  | 2.43                     | 0.54              |
| 1:1K:212:ILE:HG23 | 1:1K:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1K:352:LYS:HD3  | 2:4W:101:ASN:HD22 | 1.71                     | 0.54              |
| 1:1N:261:PRO:CA   | 2:4Z:404:PHE:CE1  | 2.89                     | 0.54              |
| 1:1N:349:THR:OG1  | 2:4Z:181:VAL:O    | 2.25                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:182:VAL:HG22 | 1:2I:257:THR:HG22 | 1.88                     | 0.54              |
| 2:1W:205:ASP:OD2  | 2:1W:304:ALA:N    | 2.35                     | 0.54              |
| 2:1Y:181:VAL:CB   | 1:2M:258:ASN:C    | 2.80                     | 0.54              |
| 2:1Z:276:THR:HG22 | 2:1Z:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:2E:212:ILE:HG23 | 1:2E:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:2N:422:ARG:NH1  | 1:2N:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:2O:181:VAL:H    | 1:3B:258:ASN:ND2  | 2.04                     | 0.54              |
| 2:2O:284:ARG:HD3  | 2:2O:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2Q:72:PRO:HD2   | 1:3D:2:ARG:CD     | 2.37                     | 0.54              |
| 5:2V:501:GDP:N7   | 1:3J:248:LEU:HD13 | 2.20                     | 0.54              |
| 2:2X:406:HIS:CE1  | 1:3L:263:PRO:N    | 2.74                     | 0.54              |
| 2:2Z:180:THR:HB   | 2:2Z:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:2Z:276:THR:HG22 | 2:2Z:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:3A:195:LEU:HD12 | 1:3A:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:3K:212:ILE:HG23 | 1:3K:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:3N:422:ARG:NH1  | 1:3N:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:3X:69:ASP:OD2   | 2:3X:74:THR:OG1   | 2.20                     | 0.54              |
| 1:4B:195:LEU:HD12 | 1:4B:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:4E:212:ILE:HG23 | 1:4E:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:4F:212:ILE:HG23 | 1:4F:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:4K:212:ILE:HG23 | 1:4K:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:4V:276:THR:HG22 | 2:4V:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:1B:195:LEU:HD12 | 1:1B:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:1B:245:ASP:CG   | 2:4O:77:SER:HB2   | 2.32                     | 0.54              |
| 1:1B:346:TRP:HD1  | 2:4O:401:ARG:HG3  | 1.71                     | 0.54              |
| 1:1D:212:ILE:HG23 | 1:1D:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1E:212:ILE:HG23 | 1:1E:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1F:247:ALA:O    | 2:4S:15:GLN:OE1   | 2.24                     | 0.54              |
| 1:1G:351:PHE:O    | 2:4T:180:THR:HA   | 2.01                     | 0.54              |
| 1:1I:324:VAL:HG13 | 2:4U:222:PRO:C    | 2.32                     | 0.54              |
| 1:1J:212:ILE:HG23 | 1:1J:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1J:422:ARG:NH1  | 1:1J:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:1N:253:THR:CG2  | 2:4Z:100:GLY:HA3  | 2.31                     | 0.54              |
| 1:1N:326:LYS:CB   | 2:4Z:222:PRO:CG   | 2.74                     | 0.54              |
| 1:1N:422:ARG:NH1  | 1:1N:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:1H:180:THR:HB   | 2:1H:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:1Q:181:VAL:CG2  | 1:2D:258:ASN:O    | 2.51                     | 0.54              |
| 2:1Q:276:THR:HG22 | 2:1Q:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:1T:284:ARG:HD3  | 2:1T:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:1V:276:THR:HG22 | 2:1V:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:1Z:180:THR:HB   | 2:1Z:183:GLU:HB3  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Z:284:ARG:HD3  | 2:1Z:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:2F:212:ILE:HG23 | 1:2F:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:2J:212:ILE:HG23 | 1:2J:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:2H:205:ASP:OD2  | 2:2H:304:ALA:N    | 2.35                     | 0.54              |
| 2:2O:176:LYS:CE   | 1:3B:333:ALA:HB1  | 2.31                     | 0.54              |
| 2:2Q:401:ARG:HG3  | 1:3D:346:TRP:CD1  | 2.43                     | 0.54              |
| 2:2T:284:ARG:HD3  | 2:2T:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2U:72:PRO:HD2   | 1:3I:2:ARG:CD     | 2.36                     | 0.54              |
| 2:2U:181:VAL:CB   | 1:3I:258:ASN:O    | 2.55                     | 0.54              |
| 2:2V:276:THR:HG22 | 2:2V:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:2X:176:LYS:CE   | 1:3L:333:ALA:HB1  | 2.33                     | 0.54              |
| 2:2Y:180:THR:HB   | 2:2Y:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:2Y:222:PRO:CG   | 1:3M:326:LYS:HB2  | 2.29                     | 0.54              |
| 2:2Z:394:GLN:CB   | 1:3N:348:PRO:HG3  | 2.36                     | 0.54              |
| 1:3D:212:ILE:HG23 | 1:3D:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:3E:212:ILE:HG23 | 1:3E:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:3F:212:ILE:HG23 | 1:3F:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:3H:205:ASP:OD2  | 2:3H:304:ALA:N    | 2.35                     | 0.54              |
| 2:3V:276:THR:HG22 | 2:3V:284:ARG:NH1  | 2.22                     | 0.54              |
| 1:4J:212:ILE:HG23 | 1:4J:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:4N:422:ARG:NH1  | 1:4N:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:4T:284:ARG:HD3  | 2:4T:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:1A:422:ARG:NH1  | 1:1A:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:1E:258:ASN:OD1  | 2:4R:101:ASN:HB3  | 2.08                     | 0.54              |
| 1:1E:260:VAL:CG1  | 2:4R:407:TRP:CZ2  | 2.89                     | 0.54              |
| 1:1E:325:PRO:HD2  | 2:4R:223:THR:HA   | 1.88                     | 0.54              |
| 1:1E:351:PHE:CB   | 2:4R:178:SER:OG   | 2.50                     | 0.54              |
| 1:1F:212:ILE:HG23 | 1:1F:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1F:258:ASN:ND2  | 2:4S:182:VAL:HG22 | 2.23                     | 0.54              |
| 1:1F:258:ASN:OD1  | 2:4S:101:ASN:CB   | 2.56                     | 0.54              |
| 1:1J:435:VAL:HA   | 2:4V:401:ARG:NH2  | 2.22                     | 0.54              |
| 1:1K:348:PRO:CG   | 2:4W:394:GLN:CB   | 2.80                     | 0.54              |
| 2:1O:205:ASP:OD2  | 2:1O:304:ALA:N    | 2.35                     | 0.54              |
| 2:1P:205:ASP:OD2  | 2:1P:304:ALA:N    | 2.35                     | 0.54              |
| 2:1Q:205:ASP:OD2  | 2:1Q:304:ALA:N    | 2.35                     | 0.54              |
| 2:1R:284:ARG:HD3  | 2:1R:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:1V:205:ASP:OD2  | 2:1V:304:ALA:N    | 2.35                     | 0.54              |
| 2:1V:217:LEU:HD11 | 2:1V:275:LEU:HD22 | 1.90                     | 0.54              |
| 1:2D:212:ILE:HG23 | 1:2D:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:2J:422:ARG:NH1  | 1:2J:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:2H:180:THR:HB   | 2:2H:183:GLU:HB3  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2O:283:TYR:OH   | 2:2P:85:GLN:O     | 2.18                     | 0.54              |
| 2:2Q:394:GLN:CB   | 1:3D:348:PRO:HG2  | 2.31                     | 0.54              |
| 2:2R:179:ASP:O    | 1:3E:352:LYS:HA   | 2.07                     | 0.54              |
| 2:2R:284:ARG:HD3  | 2:2R:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2S:11:GLN:NE2   | 1:3F:249:ASN:N    | 1.99                     | 0.54              |
| 2:2V:404:PHE:CD2  | 1:3J:261:PRO:HB3  | 2.40                     | 0.54              |
| 2:2W:205:ASP:OD2  | 2:2W:304:ALA:N    | 2.35                     | 0.54              |
| 2:2Y:221:THR:OG1  | 1:3M:324:VAL:HG22 | 2.07                     | 0.54              |
| 1:3I:212:ILE:HG23 | 1:3I:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:3J:212:ILE:HG23 | 1:3J:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:3H:180:THR:HB   | 2:3H:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:3O:205:ASP:OD2  | 2:3O:304:ALA:N    | 2.35                     | 0.54              |
| 2:3O:283:TYR:OH   | 2:3P:85:GLN:O     | 2.18                     | 0.54              |
| 2:3Q:205:ASP:OD2  | 2:3Q:304:ALA:N    | 2.35                     | 0.54              |
| 2:3Q:276:THR:HG22 | 2:3Q:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:3R:284:ARG:HD3  | 2:3R:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3T:284:ARG:HD3  | 2:3T:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3W:205:ASP:OD2  | 2:3W:304:ALA:N    | 2.35                     | 0.54              |
| 2:3Z:180:THR:HB   | 2:3Z:183:GLU:HB3  | 1.89                     | 0.54              |
| 1:4D:212:ILE:HG23 | 1:4D:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:4E:422:ARG:NH1  | 1:4E:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:4L:79:ARG:NH2   | 1:4L:92:LEU:O     | 2.37                     | 0.54              |
| 2:4H:180:THR:HB   | 2:4H:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4W:205:ASP:OD2  | 2:4W:304:ALA:N    | 2.35                     | 0.54              |
| 2:4Z:180:THR:HB   | 2:4Z:183:GLU:HB3  | 1.89                     | 0.54              |
| 1:1A:439:SER:CB   | 2:4H:400:ARG:HD2  | 2.38                     | 0.54              |
| 1:1D:261:PRO:C    | 2:4Q:404:PHE:N    | 2.51                     | 0.54              |
| 1:1D:349:THR:O    | 2:4Q:181:VAL:HA   | 2.07                     | 0.54              |
| 1:1I:212:ILE:HG23 | 1:1I:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1I:348:PRO:HB3  | 2:4U:394:GLN:HG2  | 1.90                     | 0.54              |
| 1:1J:254:GLU:HG2  | 2:4V:100:GLY:C    | 2.33                     | 0.54              |
| 2:1R:205:ASP:OD2  | 2:1R:304:ALA:N    | 2.35                     | 0.54              |
| 2:1S:404:PHE:CE1  | 1:2F:261:PRO:CA   | 2.91                     | 0.54              |
| 2:1X:69:ASP:OD2   | 2:1X:74:THR:OG1   | 2.20                     | 0.54              |
| 2:1X:284:ARG:HD3  | 2:1X:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:2E:422:ARG:NH1  | 1:2E:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:2L:79:ARG:NH2   | 1:2L:92:LEU:O     | 2.37                     | 0.54              |
| 2:2H:394:GLN:OE1  | 1:3A:349:THR:CG2  | 2.56                     | 0.54              |
| 2:2Q:205:ASP:OD2  | 2:2Q:304:ALA:N    | 2.35                     | 0.54              |
| 2:2Q:276:THR:HG22 | 2:2Q:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:2S:214:PHE:HB2  | 1:3F:326:LYS:HE3  | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:205:ASP:OD2  | 2:2V:304:ALA:N    | 2.35                     | 0.54              |
| 2:2V:217:LEU:HD11 | 2:2V:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:2Y:214:PHE:CG   | 1:3M:326:LYS:HE3  | 2.43                     | 0.54              |
| 2:2Y:284:ARG:HD3  | 2:2Y:290:GLU:OE2  | 2.07                     | 0.54              |
| 5:2Y:501:GDP:H8   | 1:3M:248:LEU:HD11 | 1.73                     | 0.54              |
| 1:3A:422:ARG:NH1  | 1:3A:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:3J:422:ARG:NH1  | 1:3J:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:3L:79:ARG:NH2   | 1:3L:92:LEU:O     | 2.37                     | 0.54              |
| 2:3P:205:ASP:OD2  | 2:3P:304:ALA:N    | 2.35                     | 0.54              |
| 2:3V:205:ASP:OD2  | 2:3V:304:ALA:N    | 2.35                     | 0.54              |
| 2:3X:284:ARG:HD3  | 2:3X:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3Y:180:THR:HB   | 2:3Y:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:3Y:284:ARG:HD3  | 2:3Y:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3Z:284:ARG:HD3  | 2:3Z:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:4B:422:ARG:NH1  | 1:4B:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:4I:212:ILE:HG23 | 1:4I:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:4H:205:ASP:OD2  | 2:4H:304:ALA:N    | 2.35                     | 0.54              |
| 2:4Q:276:THR:HG22 | 2:4Q:284:ARG:NH1  | 2.22                     | 0.54              |
| 2:4R:284:ARG:HD3  | 2:4R:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4Y:180:THR:HB   | 2:4Y:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4Y:284:ARG:HD3  | 2:4Y:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:1E:422:ARG:NH1  | 1:1E:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:1I:260:VAL:CG1  | 2:4U:407:TRP:HE1  | 2.20                     | 0.54              |
| 1:1J:261:PRO:HA   | 2:4V:404:PHE:CA   | 2.34                     | 0.54              |
| 1:1J:349:THR:CG2  | 2:4V:184:PRO:CG   | 2.86                     | 0.54              |
| 1:1M:332:ILE:HG21 | 2:4Y:177:VAL:CG2  | 2.38                     | 0.54              |
| 1:1N:260:VAL:HB   | 2:4Z:407:TRP:HE1  | 1.71                     | 0.54              |
| 2:1H:181:VAL:HB   | 1:2A:258:ASN:HA   | 1.88                     | 0.54              |
| 2:1O:394:GLN:HG2  | 1:2B:348:PRO:CG   | 2.37                     | 0.54              |
| 2:1Q:210:TYR:HD2  | 1:2D:329:ASN:HD22 | 1.56                     | 0.54              |
| 2:1U:284:ARG:HD3  | 2:1U:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:1W:101:ASN:HB2  | 1:2K:254:GLU:CG   | 2.11                     | 0.54              |
| 2:1Y:180:THR:HB   | 2:1Y:183:GLU:HB3  | 1.90                     | 0.54              |
| 2:1Y:284:ARG:HD3  | 2:1Y:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:2A:422:ARG:NH1  | 1:2A:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:2B:422:ARG:NH1  | 1:2B:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:2G:212:ILE:HG23 | 1:2G:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:2I:212:ILE:HG23 | 1:2I:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:2O:205:ASP:OD2  | 2:2O:304:ALA:N    | 2.35                     | 0.54              |
| 2:2P:394:GLN:OE1  | 1:3C:349:THR:CG2  | 2.55                     | 0.54              |
| 2:2R:205:ASP:OD2  | 2:2R:304:ALA:N    | 2.35                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2U:284:ARG:HD3  | 2:2U:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2X:284:ARG:HD3  | 2:2X:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2Y:404:PHE:H    | 1:3M:261:PRO:C    | 2.05                     | 0.54              |
| 2:2Z:284:ARG:HD3  | 2:2Z:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:3B:422:ARG:NH1  | 1:3B:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:3E:422:ARG:NH1  | 1:3E:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:3R:205:ASP:OD2  | 2:3R:304:ALA:N    | 2.35                     | 0.54              |
| 2:3V:217:LEU:HD11 | 2:3V:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:3X:270:PRO:HG2  | 2:3X:302:MET:HB2  | 1.90                     | 0.54              |
| 1:4G:212:ILE:HG23 | 1:4G:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:4J:422:ARG:NH1  | 1:4J:426:ALA:HB2  | 2.22                     | 0.54              |
| 2:4H:284:ARG:HD3  | 2:4H:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4V:205:ASP:OD2  | 2:4V:304:ALA:N    | 2.35                     | 0.54              |
| 2:4V:217:LEU:HD11 | 2:4V:275:LEU:HD22 | 1.90                     | 0.54              |
| 1:1A:325:PRO:O    | 2:4H:210:TYR:CZ   | 2.60                     | 0.54              |
| 1:1B:422:ARG:NH1  | 1:1B:426:ALA:HB2  | 2.22                     | 0.54              |
| 1:1I:256:GLN:HB2  | 2:4U:407:TRP:CH2  | 2.43                     | 0.54              |
| 1:1K:254:GLU:CA   | 2:4W:100:GLY:HA2  | 2.38                     | 0.54              |
| 1:1K:348:PRO:HD2  | 2:4W:398:MET:HG3  | 1.88                     | 0.54              |
| 1:1K:351:PHE:O    | 2:4W:180:THR:N    | 2.41                     | 0.54              |
| 1:1M:261:PRO:HA   | 2:4Y:404:PHE:CG   | 2.42                     | 0.54              |
| 2:1Q:394:GLN:HG2  | 1:2D:348:PRO:HG3  | 1.89                     | 0.54              |
| 2:1S:180:THR:HB   | 2:1S:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:1U:214:PHE:CB   | 1:2I:326:LYS:CE   | 2.53                     | 0.54              |
| 2:1U:221:THR:CB   | 1:2I:324:VAL:CG2  | 2.74                     | 0.54              |
| 2:1U:270:PRO:HG2  | 2:1U:302:MET:HB2  | 1.90                     | 0.54              |
| 2:1X:270:PRO:HG2  | 2:1X:302:MET:HB2  | 1.90                     | 0.54              |
| 2:1Y:181:VAL:CG2  | 1:2M:258:ASN:CA   | 2.86                     | 0.54              |
| 2:1Y:401:ARG:O    | 1:2M:262:TYR:CE1  | 2.60                     | 0.54              |
| 2:2O:11:GLN:NE2   | 1:3B:249:ASN:N    | 2.22                     | 0.54              |
| 2:2P:205:ASP:OD2  | 2:2P:304:ALA:N    | 2.35                     | 0.54              |
| 2:2Q:222:PRO:O    | 1:3D:324:VAL:HG13 | 2.08                     | 0.54              |
| 2:2Q:394:GLN:HB3  | 1:3D:348:PRO:CG   | 2.34                     | 0.54              |
| 2:2T:217:LEU:HD11 | 2:2T:275:LEU:HD22 | 1.90                     | 0.54              |
| 5:2U:501:GDP:N7   | 1:3I:248:LEU:HD13 | 2.19                     | 0.54              |
| 2:2W:217:LEU:HD11 | 2:2W:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:2X:270:PRO:HG2  | 2:2X:302:MET:HB2  | 1.90                     | 0.54              |
| 2:2X:404:PHE:CA   | 1:3L:261:PRO:O    | 2.56                     | 0.54              |
| 1:3G:212:ILE:HG23 | 1:3G:216:ASN:HD22 | 1.72                     | 0.54              |
| 2:3U:284:ARG:HD3  | 2:3U:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:4A:422:ARG:NH1  | 1:4A:426:ALA:HB2  | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4D:195:LEU:HD12 | 1:4D:266:HIS:HE1  | 1.72                     | 0.54              |
| 2:4O:205:ASP:OD2  | 2:4O:304:ALA:N    | 2.35                     | 0.54              |
| 2:4Q:205:ASP:OD2  | 2:4Q:304:ALA:N    | 2.35                     | 0.54              |
| 2:4T:217:LEU:HD11 | 2:4T:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:4X:284:ARG:HD3  | 2:4X:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4Z:284:ARG:HD3  | 2:4Z:290:GLU:OE2  | 2.07                     | 0.54              |
| 1:1A:2:ARG:CZ     | 2:4H:73:GLY:HA3   | 2.38                     | 0.54              |
| 1:1D:349:THR:CG2  | 2:4Q:394:GLN:OE1  | 2.56                     | 0.54              |
| 1:1E:253:THR:HB   | 2:4R:100:GLY:CA   | 2.37                     | 0.54              |
| 1:1G:212:ILE:HG23 | 1:1G:216:ASN:HD22 | 1.72                     | 0.54              |
| 1:1I:346:TRP:HD1  | 2:4U:401:ARG:HG3  | 1.72                     | 0.54              |
| 1:1J:350:GLY:C    | 2:4V:181:VAL:HG22 | 2.32                     | 0.54              |
| 2:1T:217:LEU:HD11 | 2:1T:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:1U:404:PHE:CE1  | 1:2I:261:PRO:N    | 2.76                     | 0.54              |
| 2:1Y:403:ALA:HA   | 1:2M:261:PRO:O    | 2.08                     | 0.54              |
| 1:2D:195:LEU:HD12 | 1:2D:266:HIS:HE1  | 1.72                     | 0.54              |
| 2:2H:284:ARG:HD3  | 2:2H:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2O:181:VAL:N    | 1:3B:258:ASN:HD22 | 2.05                     | 0.54              |
| 2:2R:404:PHE:CD2  | 1:3E:261:PRO:HB3  | 2.43                     | 0.54              |
| 2:2X:180:THR:HB   | 2:2X:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:2Y:404:PHE:CE1  | 1:3M:261:PRO:CA   | 2.91                     | 0.54              |
| 1:3D:195:LEU:HD12 | 1:3D:266:HIS:HE1  | 1.72                     | 0.54              |
| 2:3H:284:ARG:HD3  | 2:3H:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:3S:180:THR:HB   | 2:3S:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:3T:217:LEU:HD11 | 2:3T:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:3U:270:PRO:HG2  | 2:3U:302:MET:HB2  | 1.90                     | 0.54              |
| 1:4G:195:LEU:HD12 | 1:4G:266:HIS:HE1  | 1.71                     | 0.54              |
| 2:4P:205:ASP:OD2  | 2:4P:304:ALA:N    | 2.35                     | 0.54              |
| 2:4S:180:THR:HB   | 2:4S:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4U:270:PRO:HG2  | 2:4U:302:MET:HB2  | 1.90                     | 0.54              |
| 2:4W:217:LEU:HD11 | 2:4W:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:4X:180:THR:HB   | 2:4X:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4X:270:PRO:HG2  | 2:4X:302:MET:HB2  | 1.90                     | 0.54              |
| 1:1A:258:ASN:O    | 2:4H:181:VAL:HB   | 2.08                     | 0.54              |
| 1:1A:326:LYS:HA   | 2:4H:210:TYR:CD1  | 2.43                     | 0.54              |
| 1:1B:2:ARG:CZ     | 2:4O:73:GLY:HA3   | 2.37                     | 0.54              |
| 1:1D:195:LEU:HD12 | 1:1D:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:1G:195:LEU:HD12 | 1:1G:266:HIS:HE1  | 1.72                     | 0.54              |
| 1:1M:349:THR:CG2  | 2:4Y:184:PRO:CD   | 2.79                     | 0.54              |
| 1:1N:2:ARG:CG     | 2:4Z:72:PRO:HD2   | 2.38                     | 0.54              |
| 2:1T:179:ASP:O    | 1:2G:352:LYS:HD3  | 2.08                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1V:320:ARG:NH1  | 2:1V:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:2S:100:GLY:HA3  | 1:3F:253:THR:CB   | 2.38                     | 0.54              |
| 2:2S:180:THR:HB   | 2:2S:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:2U:270:PRO:HG2  | 2:2U:302:MET:HB2  | 1.90                     | 0.54              |
| 2:2U:407:TRP:NE1  | 1:3I:260:VAL:HB   | 2.23                     | 0.54              |
| 2:2V:404:PHE:CZ   | 1:3J:261:PRO:CB   | 2.91                     | 0.54              |
| 2:2W:214:PHE:CG   | 1:3K:326:LYS:HE3  | 2.43                     | 0.54              |
| 2:2W:221:THR:OG1  | 1:3K:324:VAL:HG22 | 2.04                     | 0.54              |
| 2:2W:404:PHE:CD2  | 1:3K:261:PRO:HA   | 2.41                     | 0.54              |
| 2:2Y:177:VAL:HG23 | 1:3M:332:ILE:HG22 | 1.89                     | 0.54              |
| 2:2Y:217:LEU:HD11 | 2:2Y:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:2Y:406:HIS:CE1  | 1:3M:263:PRO:CA   | 2.91                     | 0.54              |
| 1:3G:195:LEU:HD12 | 1:3G:266:HIS:HE1  | 1.71                     | 0.54              |
| 2:3W:217:LEU:HD11 | 2:3W:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:3X:180:THR:HB   | 2:3X:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4R:205:ASP:OD2  | 2:4R:304:ALA:N    | 2.35                     | 0.54              |
| 2:4S:270:PRO:HG2  | 2:4S:302:MET:HB2  | 1.90                     | 0.54              |
| 2:4U:284:ARG:HD3  | 2:4U:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4V:284:ARG:HD3  | 2:4V:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:4V:320:ARG:NH1  | 2:4V:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:4W:180:THR:HB   | 2:4W:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:4Y:217:LEU:HD11 | 2:4Y:275:LEU:HD22 | 1.90                     | 0.54              |
| 1:1C:324:VAL:CG1  | 2:4P:222:PRO:C    | 2.78                     | 0.54              |
| 1:1E:2:ARG:HG3    | 2:4R:72:PRO:HG2   | 1.90                     | 0.54              |
| 1:1E:325:PRO:CB   | 2:4R:224:TYR:CZ   | 2.90                     | 0.54              |
| 1:1I:2:ARG:HH11   | 2:4U:71:GLU:HB2   | 1.72                     | 0.54              |
| 1:1I:261:PRO:O    | 2:4U:406:HIS:HD2  | 1.88                     | 0.54              |
| 1:1M:346:TRP:O    | 2:4Y:398:MET:HA   | 2.08                     | 0.54              |
| 2:1H:284:ARG:HD3  | 2:1H:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:1H:394:GLN:HG2  | 1:2A:348:PRO:HG3  | 1.90                     | 0.54              |
| 2:1R:100:GLY:HA3  | 1:2E:253:THR:HG21 | 1.88                     | 0.54              |
| 2:1U:207:GLU:OE1  | 1:2I:329:ASN:ND2  | 2.41                     | 0.54              |
| 2:1W:180:THR:HB   | 2:1W:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:1W:320:ARG:NH1  | 2:1W:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:1Y:217:LEU:HD11 | 2:1Y:275:LEU:HD22 | 1.90                     | 0.54              |
| 2:1Y:221:THR:HB   | 1:2M:324:VAL:HG21 | 1.89                     | 0.54              |
| 1:2G:195:LEU:HD12 | 1:2G:266:HIS:HE1  | 1.72                     | 0.54              |
| 2:2O:181:VAL:HG21 | 1:3B:258:ASN:O    | 2.08                     | 0.54              |
| 2:2R:100:GLY:O    | 1:3E:257:THR:OG1  | 2.18                     | 0.54              |
| 2:2S:270:PRO:HG2  | 2:2S:302:MET:HB2  | 1.90                     | 0.54              |
| 2:2U:207:GLU:CD   | 1:3I:329:ASN:ND2  | 2.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:284:ARG:HD3  | 2:2V:290:GLU:OE2  | 2.07                     | 0.54              |
| 2:2V:320:ARG:NH1  | 2:2V:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:2W:177:VAL:CG2  | 1:3K:332:ILE:CG2  | 2.82                     | 0.54              |
| 2:2W:180:THR:HB   | 2:2W:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:2W:320:ARG:NH1  | 2:2W:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:2X:320:ARG:NH1  | 2:2X:360:PRO:HG3  | 2.23                     | 0.54              |
| 5:2X:501:GDP:H8   | 1:3L:248:LEU:HD11 | 1.69                     | 0.54              |
| 2:3O:180:THR:HB   | 2:3O:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:3V:320:ARG:NH1  | 2:3V:360:PRO:HG3  | 2.23                     | 0.54              |
| 2:3W:180:THR:HB   | 2:3W:183:GLU:HB3  | 1.89                     | 0.54              |
| 2:3Y:217:LEU:HD11 | 2:3Y:275:LEU:HD22 | 1.90                     | 0.54              |
| 1:1A:2:ARG:NH2    | 2:4H:73:GLY:CA    | 2.71                     | 0.53              |
| 1:1B:261:PRO:HA   | 2:4O:404:PHE:CB   | 2.37                     | 0.53              |
| 1:1B:349:THR:O    | 2:4O:181:VAL:HA   | 2.08                     | 0.53              |
| 1:1J:325:PRO:CB   | 2:4V:224:TYR:CE1  | 2.91                     | 0.53              |
| 1:1J:439:SER:OG   | 2:4V:401:ARG:CD   | 2.56                     | 0.53              |
| 2:1O:180:THR:HB   | 2:1O:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1R:270:PRO:HG2  | 2:1R:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1S:205:ASP:OD2  | 2:1S:304:ALA:N    | 2.35                     | 0.53              |
| 2:1T:404:PHE:CD2  | 1:2G:261:PRO:HA   | 2.43                     | 0.53              |
| 2:1W:217:LEU:HD11 | 2:1W:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:1X:180:THR:HB   | 2:1X:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1X:320:ARG:NH1  | 2:1X:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1Z:224:TYR:HE2  | 1:2N:248:LEU:HB2  | 1.72                     | 0.53              |
| 2:2O:180:THR:HB   | 2:2O:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2Q:398:MET:HA   | 1:3D:346:TRP:HB2  | 1.90                     | 0.53              |
| 2:2R:270:PRO:HG2  | 2:2R:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2S:222:PRO:CG   | 1:3F:326:LYS:CB   | 2.83                     | 0.53              |
| 2:2S:284:ARG:HD3  | 2:2S:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:2W:101:ASN:O    | 1:3K:257:THR:CG2  | 2.50                     | 0.53              |
| 2:2Z:181:VAL:N    | 1:3N:258:ASN:ND2  | 2.55                     | 0.53              |
| 2:3S:205:ASP:OD2  | 2:3S:304:ALA:N    | 2.35                     | 0.53              |
| 2:3W:320:ARG:NH1  | 2:3W:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:4O:180:THR:HB   | 2:4O:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4S:284:ARG:HD3  | 2:4S:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:4V:270:PRO:HG2  | 2:4V:302:MET:HB2  | 1.90                     | 0.53              |
| 2:4W:320:ARG:NH1  | 2:4W:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:4X:320:ARG:NH1  | 2:4X:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1B:253:THR:CB   | 2:4O:100:GLY:HA3  | 2.38                     | 0.53              |
| 1:1D:261:PRO:C    | 2:4Q:404:PHE:CA   | 2.79                     | 0.53              |
| 1:1D:353:VAL:CG2  | 2:4Q:179:ASP:OD1  | 2.54                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:257:THR:OG1  | 2:4R:102:ASN:HB2  | 2.07                     | 0.53              |
| 1:1E:260:VAL:HG11 | 2:4R:407:TRP:HZ2  | 1.71                     | 0.53              |
| 1:1J:254:GLU:HG2  | 2:4V:100:GLY:CA   | 2.38                     | 0.53              |
| 1:1L:435:VAL:HA   | 2:4X:401:ARG:NH2  | 2.24                     | 0.53              |
| 1:1N:326:LYS:HB3  | 2:4Z:222:PRO:HG2  | 1.83                     | 0.53              |
| 2:1H:270:PRO:HG2  | 2:1H:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1R:222:PRO:HD2  | 1:2E:326:LYS:HB3  | 1.90                     | 0.53              |
| 2:1S:270:PRO:HG2  | 2:1S:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1V:284:ARG:HD3  | 2:1V:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:1V:404:PHE:CE2  | 1:2J:261:PRO:HB3  | 2.44                     | 0.53              |
| 2:1W:401:ARG:O    | 1:2K:262:TYR:HE1  | 1.91                     | 0.53              |
| 2:1W:404:PHE:HE1  | 1:2K:260:VAL:C    | 2.05                     | 0.53              |
| 2:1Z:11:GLN:NE2   | 1:2N:249:ASN:H    | 2.03                     | 0.53              |
| 1:2N:319:TYR:HB3  | 1:2N:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:2H:270:PRO:HG2  | 2:2H:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2S:205:ASP:OD2  | 2:2S:304:ALA:N    | 2.35                     | 0.53              |
| 2:2V:270:PRO:HG2  | 2:2V:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2X:404:PHE:H    | 1:3L:261:PRO:C    | 2.08                     | 0.53              |
| 2:2Z:404:PHE:CD2  | 1:3N:261:PRO:HA   | 2.43                     | 0.53              |
| 1:3N:319:TYR:HB3  | 1:3N:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:3H:270:PRO:HG2  | 2:3H:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3R:270:PRO:HG2  | 2:3R:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3S:270:PRO:HG2  | 2:3S:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3S:284:ARG:HD3  | 2:3S:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:3V:270:PRO:HG2  | 2:3V:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3V:284:ARG:HD3  | 2:3V:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:3X:320:ARG:NH1  | 2:3X:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:4N:319:TYR:HB3  | 1:4N:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:4R:270:PRO:HG2  | 2:4R:302:MET:HB2  | 1.90                     | 0.53              |
| 2:4S:320:ARG:NH1  | 2:4S:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1A:329:ASN:CG   | 2:4H:207:GLU:OE1  | 2.48                     | 0.53              |
| 1:1B:2:ARG:HD3    | 2:4O:72:PRO:CD    | 2.32                     | 0.53              |
| 1:1C:249:ASN:N    | 2:4P:11:GLN:OE1   | 2.42                     | 0.53              |
| 1:1F:349:THR:CB   | 2:4S:184:PRO:CD   | 2.74                     | 0.53              |
| 1:1G:326:LYS:CG   | 2:4T:210:TYR:CD1  | 2.91                     | 0.53              |
| 1:1I:319:TYR:HB3  | 1:1I:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1I:435:VAL:C    | 2:4U:401:ARG:NH2  | 2.65                     | 0.53              |
| 1:1J:439:SER:OG   | 2:4V:401:ARG:HG2  | 2.08                     | 0.53              |
| 1:1M:333:ALA:HB1  | 2:4Y:176:LYS:HE2  | 1.91                     | 0.53              |
| 1:1N:319:TYR:HB3  | 1:1N:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1N:346:TRP:CZ3  | 2:4Z:404:PHE:HE2  | 2.27                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1N:346:TRP:HB3  | 2:4Z:397:ALA:O    | 2.06                     | 0.53              |
| 2:1P:180:THR:HB   | 2:1P:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1S:217:LEU:HD11 | 2:1S:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:1S:284:ARG:HD3  | 2:1S:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:1V:270:PRO:HG2  | 2:1V:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1W:406:HIS:CD2  | 1:2K:263:PRO:CD   | 2.87                     | 0.53              |
| 2:1W:411:GLU:OE2  | 1:2K:163:LYS:NZ   | 2.41                     | 0.53              |
| 2:2P:401:ARG:HG3  | 1:3C:346:TRP:CD1  | 2.43                     | 0.53              |
| 2:2Q:100:GLY:CA   | 1:3D:253:THR:C    | 2.81                     | 0.53              |
| 2:2T:320:ARG:NH1  | 2:2T:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:2V:401:ARG:NH2  | 1:3J:435:VAL:CA   | 2.55                     | 0.53              |
| 2:3S:217:LEU:HD11 | 2:3S:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:3S:320:ARG:NH1  | 2:3S:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:3T:320:ARG:NH1  | 2:3T:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:4I:319:TYR:HB3  | 1:4I:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:4T:320:ARG:NH1  | 2:4T:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1B:319:TYR:HB3  | 1:1B:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1C:245:ASP:CG   | 2:4P:77:SER:HB2   | 2.27                     | 0.53              |
| 1:1C:248:LEU:HA   | 2:4P:11:GLN:NE2   | 2.23                     | 0.53              |
| 1:1D:257:THR:OG1  | 2:4Q:102:ASN:HB2  | 2.08                     | 0.53              |
| 1:1D:260:VAL:CA   | 2:4Q:407:TRP:HE1  | 2.14                     | 0.53              |
| 1:1F:251:ASP:OD2  | 2:4S:71:GLU:HB3   | 2.08                     | 0.53              |
| 1:1F:346:TRP:C    | 2:4S:398:MET:HG2  | 2.28                     | 0.53              |
| 1:1I:248:LEU:HD11 | 5:4U:501:GDP:O1A  | 2.07                     | 0.53              |
| 1:1I:324:VAL:HG21 | 2:4U:221:THR:OG1  | 2.08                     | 0.53              |
| 1:1I:346:TRP:CD1  | 2:4U:401:ARG:HG3  | 2.44                     | 0.53              |
| 1:1K:261:PRO:CA   | 2:4W:404:PHE:CD1  | 2.91                     | 0.53              |
| 2:1T:181:VAL:HG21 | 1:2G:258:ASN:C    | 2.16                     | 0.53              |
| 2:1X:401:ARG:O    | 1:2L:262:TYR:CE1  | 2.60                     | 0.53              |
| 1:2B:319:TYR:HB3  | 1:2B:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:2G:319:TYR:HB3  | 1:2G:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:2I:319:TYR:HB3  | 1:2I:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:2P:284:ARG:HD3  | 2:2P:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:2R:222:PRO:O    | 1:3E:324:VAL:HG13 | 2.09                     | 0.53              |
| 2:2S:217:LEU:HD11 | 2:2S:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:2S:406:HIS:CE1  | 1:3F:263:PRO:HA   | 2.44                     | 0.53              |
| 2:2T:394:GLN:CG   | 1:3G:348:PRO:CB   | 2.81                     | 0.53              |
| 2:2U:320:ARG:NH1  | 2:2U:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:2W:222:PRO:HD2  | 1:3K:326:LYS:HB3  | 1.91                     | 0.53              |
| 1:3A:319:TYR:HB3  | 1:3A:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:3I:319:TYR:HB3  | 1:3I:323:VAL:HG21 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4A:319:TYR:HB3  | 1:4A:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:4B:319:TYR:HB3  | 1:4B:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:4G:319:TYR:HB3  | 1:4G:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:4H:270:PRO:HG2  | 2:4H:302:MET:HB2  | 1.90                     | 0.53              |
| 2:4P:284:ARG:HD3  | 2:4P:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:4S:217:LEU:HD11 | 2:4S:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:4T:180:THR:HB   | 2:4T:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4U:320:ARG:NH1  | 2:4U:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1A:319:TYR:HB3  | 1:1A:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1D:326:LYS:HG3  | 2:4Q:210:TYR:HA   | 1.89                     | 0.53              |
| 1:1I:326:LYS:HB2  | 2:4U:222:PRO:HG2  | 1.89                     | 0.53              |
| 1:1J:324:VAL:CG1  | 2:4V:222:PRO:O    | 2.57                     | 0.53              |
| 1:1K:346:TRP:O    | 2:4W:398:MET:HG3  | 1.98                     | 0.53              |
| 1:1L:346:TRP:CB   | 2:4X:397:ALA:O    | 2.57                     | 0.53              |
| 2:1P:284:ARG:HD3  | 2:1P:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:1Q:100:GLY:CA   | 1:2D:253:THR:CG2  | 2.86                     | 0.53              |
| 2:1S:221:THR:HB   | 1:2F:324:VAL:HG21 | 1.90                     | 0.53              |
| 2:1S:320:ARG:NH1  | 2:1S:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1U:205:ASP:OD2  | 2:1U:304:ALA:N    | 2.35                     | 0.53              |
| 2:1X:217:LEU:HD11 | 2:1X:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:1Y:320:ARG:NH1  | 2:1Y:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1Y:394:GLN:CD   | 1:2M:349:THR:HG23 | 2.33                     | 0.53              |
| 1:2A:319:TYR:HB3  | 1:2A:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:2O:270:PRO:HG2  | 2:2O:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2P:180:THR:HB   | 2:2P:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2Q:398:MET:HG2  | 1:3D:346:TRP:O    | 2.08                     | 0.53              |
| 2:2S:320:ARG:NH1  | 2:2S:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:2T:180:THR:HB   | 2:2T:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2T:406:HIS:CE1  | 1:3G:263:PRO:HA   | 2.43                     | 0.53              |
| 2:2V:179:ASP:O    | 1:3J:352:LYS:HA   | 2.09                     | 0.53              |
| 2:2W:394:GLN:HA   | 1:3K:348:PRO:HG3  | 1.90                     | 0.53              |
| 2:2X:217:LEU:HD11 | 2:2X:275:LEU:HD22 | 1.90                     | 0.53              |
| 1:3B:319:TYR:HB3  | 1:3B:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:3G:319:TYR:HB3  | 1:3G:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:3M:319:TYR:HB3  | 1:3M:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:3O:270:PRO:HG2  | 2:3O:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3P:180:THR:HB   | 2:3P:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:3U:205:ASP:OD2  | 2:3U:304:ALA:N    | 2.35                     | 0.53              |
| 2:3U:320:ARG:NH1  | 2:3U:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:3Y:320:ARG:NH1  | 2:3Y:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:4O:270:PRO:HG2  | 2:4O:302:MET:HB2  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4P:180:THR:HB   | 2:4P:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4S:205:ASP:OD2  | 2:4S:304:ALA:N    | 2.35                     | 0.53              |
| 2:4X:217:LEU:HD11 | 2:4X:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:4Y:320:ARG:NH1  | 2:4Y:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1B:244:PHE:HB2  | 1:1B:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1G:263:PRO:N    | 2:4T:406:HIS:CD2  | 2.77                     | 0.53              |
| 1:1K:346:TRP:CB   | 2:4W:397:ALA:O    | 2.57                     | 0.53              |
| 1:1L:245:ASP:OD2  | 2:4X:77:SER:HB3   | 1.95                     | 0.53              |
| 1:1M:319:TYR:HB3  | 1:1M:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1N:329:ASN:CB   | 2:4Z:210:TYR:CE2  | 2.89                     | 0.53              |
| 1:1N:348:PRO:CB   | 2:4Z:394:GLN:CG   | 2.81                     | 0.53              |
| 2:1O:270:PRO:HG2  | 2:1O:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1S:181:VAL:HG23 | 1:2F:258:ASN:HB3  | 1.89                     | 0.53              |
| 2:1S:214:PHE:CD1  | 1:2F:326:LYS:CE   | 2.92                     | 0.53              |
| 2:1S:228:ASN:HD21 | 5:1S:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:1T:320:ARG:NH1  | 2:1T:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1U:180:THR:HB   | 2:1U:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1U:320:ARG:NH1  | 2:1U:360:PRO:HG3  | 2.23                     | 0.53              |
| 5:1X:501:GDP:C8   | 1:2L:248:LEU:CD1  | 2.92                     | 0.53              |
| 1:2M:319:TYR:HB3  | 1:2M:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:2R:71:GLU:HG3   | 1:3E:2:ARG:NH1    | 2.23                     | 0.53              |
| 2:2U:100:GLY:CA   | 1:3I:253:THR:C    | 2.82                     | 0.53              |
| 2:2U:205:ASP:OD2  | 2:2U:304:ALA:N    | 2.35                     | 0.53              |
| 2:2U:224:TYR:HD2  | 1:3I:247:ALA:O    | 1.92                     | 0.53              |
| 2:2V:72:PRO:HD2   | 1:3J:2:ARG:HD3    | 1.89                     | 0.53              |
| 2:2X:11:GLN:NE2   | 1:3L:249:ASN:HB2  | 2.24                     | 0.53              |
| 2:2Y:270:PRO:HG2  | 2:2Y:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2Y:320:ARG:NH1  | 2:2Y:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:3B:244:PHE:HB2  | 1:3B:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:3M:422:ARG:NH1  | 1:3M:426:ALA:HB2  | 2.22                     | 0.53              |
| 2:3P:284:ARG:HD3  | 2:3P:290:GLU:OE2  | 2.07                     | 0.53              |
| 2:3W:174:SER:HB2  | 2:3W:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3X:217:LEU:HD11 | 2:3X:275:LEU:HD22 | 1.90                     | 0.53              |
| 1:4M:319:TYR:HB3  | 1:4M:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:4M:422:ARG:NH1  | 1:4M:426:ALA:HB2  | 2.22                     | 0.53              |
| 2:4Q:180:THR:HB   | 2:4Q:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4U:205:ASP:OD2  | 2:4U:304:ALA:N    | 2.35                     | 0.53              |
| 2:4X:174:SER:HB2  | 2:4X:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4Y:270:PRO:HG2  | 2:4Y:302:MET:HB2  | 1.90                     | 0.53              |
| 1:1A:261:PRO:N    | 2:4H:404:PHE:CD1  | 2.77                     | 0.53              |
| 1:1C:319:TYR:HB3  | 1:1C:323:VAL:HG21 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:247:ALA:C    | 2:4R:15:GLN:HE22  | 2.17                     | 0.53              |
| 1:1E:258:ASN:HD22 | 2:4R:182:VAL:HG22 | 1.73                     | 0.53              |
| 1:1F:346:TRP:C    | 2:4S:398:MET:HA   | 2.33                     | 0.53              |
| 1:1G:319:TYR:HB3  | 1:1G:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1I:352:LYS:CD   | 2:4U:101:ASN:ND2  | 2.68                     | 0.53              |
| 1:1N:263:PRO:CA   | 2:4Z:406:HIS:CE1  | 2.91                     | 0.53              |
| 2:1O:404:PHE:CE1  | 1:2B:260:VAL:C    | 2.87                     | 0.53              |
| 2:1Q:180:THR:HB   | 2:1Q:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1Q:404:PHE:CE1  | 1:2D:260:VAL:C    | 2.87                     | 0.53              |
| 2:1S:174:SER:HB2  | 2:1S:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1T:180:THR:HB   | 2:1T:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1U:224:TYR:CE2  | 1:2I:247:ALA:O    | 2.60                     | 0.53              |
| 2:1U:404:PHE:N    | 1:2I:261:PRO:O    | 2.33                     | 0.53              |
| 2:1W:174:SER:HB2  | 2:1W:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1W:270:PRO:HG2  | 2:1W:302:MET:HB2  | 1.90                     | 0.53              |
| 2:1X:221:THR:CB   | 1:2L:324:VAL:CG2  | 2.87                     | 0.53              |
| 2:1Y:270:PRO:HG2  | 2:1Y:302:MET:HB2  | 1.90                     | 0.53              |
| 1:2A:244:PHE:HB2  | 1:2A:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:2L:319:TYR:HB3  | 1:2L:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:2M:422:ARG:NH1  | 1:2M:426:ALA:HB2  | 2.22                     | 0.53              |
| 2:2P:179:ASP:OD1  | 1:3C:353:VAL:CB   | 2.53                     | 0.53              |
| 2:2Q:180:THR:HB   | 2:2Q:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2R:228:ASN:HD21 | 5:2R:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:2U:180:THR:HB   | 2:2U:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2W:174:SER:HB2  | 2:2W:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2Z:177:VAL:HG23 | 1:3N:332:ILE:HG22 | 1.88                     | 0.53              |
| 2:2Z:217:LEU:HD11 | 2:2Z:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:3Q:180:THR:HB   | 2:3Q:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:3R:228:ASN:HD21 | 5:3R:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:3V:174:SER:HB2  | 2:3V:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3V:180:THR:HB   | 2:3V:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:3Y:270:PRO:HG2  | 2:3Y:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3Z:217:LEU:HD11 | 2:3Z:275:LEU:HD22 | 1.90                     | 0.53              |
| 1:4L:319:TYR:HB3  | 1:4L:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:4V:180:THR:HB   | 2:4V:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4W:174:SER:HB2  | 2:4W:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4W:270:PRO:HG2  | 2:4W:302:MET:HB2  | 1.90                     | 0.53              |
| 2:4Z:217:LEU:HD11 | 2:4Z:275:LEU:HD22 | 1.90                     | 0.53              |
| 1:1C:260:VAL:C    | 2:4P:404:PHE:CE1  | 2.87                     | 0.53              |
| 1:1E:326:LYS:CE   | 2:4R:214:PHE:HB2  | 2.38                     | 0.53              |
| 1:1E:346:TRP:CZ2  | 2:4R:403:ALA:CB   | 2.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:319:TYR:HB3  | 1:1J:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:1L:319:TYR:HB3  | 1:1L:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:1R:174:SER:HB2  | 2:1R:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1R:228:ASN:HD21 | 5:1R:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:1V:174:SER:HB2  | 2:1V:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1Z:270:PRO:HG2  | 2:1Z:302:MET:HB2  | 1.90                     | 0.53              |
| 1:2B:244:PHE:HB2  | 1:2B:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:2I:244:PHE:HB2  | 1:2I:356:ASN:HD21 | 1.74                     | 0.53              |
| 2:2H:221:THR:CB   | 1:3A:324:VAL:HG21 | 2.39                     | 0.53              |
| 2:2R:320:ARG:NH1  | 2:2R:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:2R:404:PHE:CA   | 1:3E:261:PRO:O    | 2.55                     | 0.53              |
| 2:2S:174:SER:HB2  | 2:2S:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2S:228:ASN:HD21 | 5:2S:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:2V:174:SER:HB2  | 2:2V:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2V:180:THR:HB   | 2:2V:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:2V:394:GLN:CA   | 1:3J:348:PRO:HG3  | 2.38                     | 0.53              |
| 2:2W:270:PRO:HG2  | 2:2W:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2X:174:SER:HB2  | 2:2X:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2X:182:VAL:HG21 | 1:3L:257:THR:HG22 | 1.90                     | 0.53              |
| 2:2X:221:THR:C    | 1:3L:324:VAL:HG11 | 2.33                     | 0.53              |
| 1:3J:319:TYR:HB3  | 1:3J:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:3L:319:TYR:HB3  | 1:3L:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:3H:320:ARG:NH1  | 2:3H:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:3P:228:ASN:HD21 | 5:3P:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:3R:320:ARG:NH1  | 2:3R:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:3S:174:SER:HB2  | 2:3S:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3S:228:ASN:HD21 | 5:3S:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:3T:180:THR:HB   | 2:3T:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:3U:180:THR:HB   | 2:3U:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:3W:270:PRO:HG2  | 2:3W:302:MET:HB2  | 1.90                     | 0.53              |
| 2:3X:174:SER:HB2  | 2:3X:207:GLU:HB2  | 1.91                     | 0.53              |
| 1:4A:244:PHE:HB2  | 1:4A:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:4B:244:PHE:HB2  | 1:4B:356:ASN:HD21 | 1.74                     | 0.53              |
| 2:4P:228:ASN:HD21 | 5:4P:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:4R:228:ASN:HD21 | 5:4R:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:4R:320:ARG:NH1  | 2:4R:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:4S:228:ASN:HD21 | 5:4S:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:4U:180:THR:HB   | 2:4U:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:4V:174:SER:HB2  | 2:4V:207:GLU:HB2  | 1.91                     | 0.53              |
| 1:1A:244:PHE:HB2  | 1:1A:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1A:329:ASN:HB2  | 2:4H:210:TYR:CD2  | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:2:ARG:HH11   | 2:4O:71:GLU:HG3   | 1.74                     | 0.53              |
| 1:1B:257:THR:CG2  | 2:4O:101:ASN:O    | 2.57                     | 0.53              |
| 1:1E:244:PHE:HB2  | 1:1E:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1F:2:ARG:NH1    | 2:4S:71:GLU:CG    | 2.72                     | 0.53              |
| 1:1F:191:THR:HA   | 1:1F:194:THR:HG22 | 1.91                     | 0.53              |
| 1:1G:244:PHE:HB2  | 1:1G:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1I:244:PHE:HB2  | 1:1I:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1J:353:VAL:CG2  | 2:4V:179:ASP:OD1  | 2.56                     | 0.53              |
| 1:1K:257:THR:HG21 | 2:4W:102:ASN:CB   | 2.32                     | 0.53              |
| 1:1M:248:LEU:CD1  | 5:4Y:501:GDP:H8   | 2.22                     | 0.53              |
| 1:1M:329:ASN:CB   | 2:4Y:210:TYR:CD2  | 2.92                     | 0.53              |
| 1:1M:348:PRO:HD2  | 2:4Y:398:MET:CG   | 2.38                     | 0.53              |
| 1:1M:422:ARG:NH1  | 1:1M:426:ALA:HB2  | 2.22                     | 0.53              |
| 2:1H:320:ARG:NH1  | 2:1H:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1O:174:SER:HB2  | 2:1O:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1O:228:ASN:HD21 | 5:1O:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:1P:174:SER:HB2  | 2:1P:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1P:228:ASN:HD21 | 5:1P:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:1Q:228:ASN:HD21 | 5:1Q:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:1R:320:ARG:NH1  | 2:1R:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:1T:174:SER:HB2  | 2:1T:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1T:404:PHE:HE1  | 1:2G:260:VAL:C    | 2.07                     | 0.53              |
| 2:1U:174:SER:HB2  | 2:1U:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1V:180:THR:HB   | 2:1V:183:GLU:HB3  | 1.89                     | 0.53              |
| 2:1X:31:ASP:OD1   | 2:1X:35:SER:N     | 2.42                     | 0.53              |
| 2:1X:174:SER:HB2  | 2:1X:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:1X:224:TYR:OH   | 1:2L:248:LEU:HD22 | 2.09                     | 0.53              |
| 2:1X:403:ALA:HA   | 1:2L:261:PRO:O    | 2.09                     | 0.53              |
| 2:1Z:217:LEU:HD11 | 2:1Z:275:LEU:HD22 | 1.90                     | 0.53              |
| 1:2A:100:ALA:N    | 3:2A:501:GTP:O2G  | 2.41                     | 0.53              |
| 1:2C:319:TYR:HB3  | 1:2C:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:2G:244:PHE:HB2  | 1:2G:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:2J:319:TYR:HB3  | 1:2J:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:2H:320:ARG:NH1  | 2:2H:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:2O:174:SER:HB2  | 2:2O:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2O:228:ASN:HD21 | 5:2O:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:2P:406:HIS:NE2  | 1:3C:262:TYR:CA   | 2.72                     | 0.53              |
| 2:2R:407:TRP:CD1  | 1:3E:260:VAL:O    | 2.61                     | 0.53              |
| 2:2T:174:SER:HB2  | 2:2T:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2T:180:THR:N    | 1:3G:351:PHE:O    | 2.42                     | 0.53              |
| 2:2U:31:ASP:OD1   | 2:2U:35:SER:N     | 2.42                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:2U:174:SER:HB2 | 2:2U:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2V:250:ALA:HA  | 2:2V:254:LYS:HD3  | 1.91                     | 0.53              |
| 5:2W:501:GDP:N7  | 1:3K:248:LEU:HD13 | 2.23                     | 0.53              |
| 2:2X:31:ASP:OD1  | 2:2X:35:SER:N     | 2.42                     | 0.53              |
| 2:2Z:270:PRO:HG2 | 2:2Z:302:MET:HB2  | 1.90                     | 0.53              |
| 2:2Z:394:GLN:CB  | 1:3N:348:PRO:CG   | 2.87                     | 0.53              |
| 1:3A:244:PHE:HB2 | 1:3A:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:3F:191:THR:HA  | 1:3F:194:THR:HG22 | 1.91                     | 0.53              |
| 2:3P:174:SER:HB2 | 2:3P:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3T:174:SER:HB2 | 2:3T:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3U:174:SER:HB2 | 2:3U:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3X:31:ASP:OD1  | 2:3X:35:SER:N     | 2.42                     | 0.53              |
| 2:3Z:270:PRO:HG2 | 2:3Z:302:MET:HB2  | 1.90                     | 0.53              |
| 1:4A:100:ALA:N   | 3:4A:501:GTP:O2G  | 2.41                     | 0.53              |
| 1:4C:319:TYR:HB3 | 1:4C:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:4F:319:TYR:HB3 | 1:4F:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:4G:244:PHE:HB2 | 1:4G:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:4J:319:TYR:HB3 | 1:4J:323:VAL:HG21 | 1.90                     | 0.53              |
| 2:4H:320:ARG:NH1 | 2:4H:360:PRO:HG3  | 2.23                     | 0.53              |
| 2:4P:174:SER:HB2 | 2:4P:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4S:174:SER:HB2 | 2:4S:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4T:174:SER:HB2 | 2:4T:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4U:174:SER:HB2 | 2:4U:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4V:250:ALA:HA  | 2:4V:254:LYS:HD3  | 1.91                     | 0.53              |
| 1:1A:100:ALA:N   | 3:1A:501:GTP:O2G  | 2.41                     | 0.53              |
| 1:1C:244:PHE:HB2 | 1:1C:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1F:244:PHE:HB2 | 1:1F:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:1F:324:VAL:CG1 | 2:4S:222:PRO:C    | 2.75                     | 0.53              |
| 1:1J:435:VAL:C   | 2:4V:401:ARG:HH22 | 2.17                     | 0.53              |
| 1:1N:2:ARG:HG3   | 2:4Z:72:PRO:CG    | 2.39                     | 0.53              |
| 2:1T:205:ASP:OD2 | 2:1T:304:ALA:N    | 2.35                     | 0.53              |
| 2:1U:31:ASP:OD1  | 2:1U:35:SER:N     | 2.42                     | 0.53              |
| 2:1W:250:ALA:HA  | 2:1W:254:LYS:HD3  | 1.91                     | 0.53              |
| 2:1X:101:ASN:O   | 1:2L:257:THR:HG21 | 2.09                     | 0.53              |
| 2:1Y:179:ASP:O   | 1:2M:352:LYS:HD3  | 2.04                     | 0.53              |
| 2:1Z:320:ARG:NH1 | 2:1Z:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:2E:414:GLU:HG2 | 1:2E:416:GLY:H    | 1.74                     | 0.53              |
| 1:2F:244:PHE:HB2 | 1:2F:356:ASN:HD21 | 1.74                     | 0.53              |
| 2:2O:177:VAL:CG2 | 1:3B:332:ILE:CG2  | 2.80                     | 0.53              |
| 2:2O:394:GLN:CB  | 1:3B:348:PRO:HG2  | 2.38                     | 0.53              |
| 2:2O:394:GLN:OE1 | 1:3B:349:THR:HG23 | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:174:SER:HB2  | 2:2P:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2P:217:LEU:HD11 | 2:2P:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:2P:228:ASN:HD21 | 5:2P:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:2P:394:GLN:CG   | 1:3C:348:PRO:HG2  | 2.37                     | 0.53              |
| 2:2R:174:SER:HB2  | 2:2R:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:2R:210:TYR:HD2  | 1:3E:329:ASN:ND2  | 1.99                     | 0.53              |
| 2:2U:214:PHE:HB2  | 1:3I:326:LYS:HE3  | 1.84                     | 0.53              |
| 2:2W:250:ALA:HA   | 2:2W:254:LYS:HD3  | 1.91                     | 0.53              |
| 2:2Z:320:ARG:NH1  | 2:2Z:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:3A:100:ALA:N    | 3:3A:501:GTP:O2G  | 2.41                     | 0.53              |
| 1:3C:244:PHE:HB2  | 1:3C:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:3C:319:TYR:HB3  | 1:3C:323:VAL:HG21 | 1.90                     | 0.53              |
| 1:3E:414:GLU:HG2  | 1:3E:416:GLY:H    | 1.74                     | 0.53              |
| 1:3F:244:PHE:HB2  | 1:3F:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:3F:414:GLU:HG2  | 1:3F:416:GLY:H    | 1.74                     | 0.53              |
| 1:3G:244:PHE:HB2  | 1:3G:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:3I:244:PHE:HB2  | 1:3I:356:ASN:HD21 | 1.74                     | 0.53              |
| 2:3O:174:SER:HB2  | 2:3O:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3O:228:ASN:HD21 | 5:3O:501:GDP:HN1  | 1.57                     | 0.53              |
| 2:3P:217:LEU:HD11 | 2:3P:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:3Q:174:SER:HB2  | 2:3Q:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3R:174:SER:HB2  | 2:3R:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:3U:31:ASP:OD1   | 2:3U:35:SER:N     | 2.42                     | 0.53              |
| 2:3W:250:ALA:HA   | 2:3W:254:LYS:HD3  | 1.91                     | 0.53              |
| 2:3Z:320:ARG:NH1  | 2:3Z:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:4E:244:PHE:HB2  | 1:4E:356:ASN:HD21 | 1.74                     | 0.53              |
| 1:4E:414:GLU:HG2  | 1:4E:416:GLY:H    | 1.74                     | 0.53              |
| 1:4F:191:THR:HA   | 1:4F:194:THR:HG22 | 1.91                     | 0.53              |
| 2:4O:174:SER:HB2  | 2:4O:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4Q:174:SER:HB2  | 2:4Q:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4Q:217:LEU:HD11 | 2:4Q:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:4R:174:SER:HB2  | 2:4R:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4U:31:ASP:OD1   | 2:4U:35:SER:N     | 2.42                     | 0.53              |
| 2:4U:217:LEU:HD11 | 2:4U:275:LEU:HD22 | 1.90                     | 0.53              |
| 2:4X:31:ASP:OD1   | 2:4X:35:SER:N     | 2.42                     | 0.53              |
| 2:4Y:174:SER:HB2  | 2:4Y:207:GLU:HB2  | 1.91                     | 0.53              |
| 2:4Z:320:ARG:NH1  | 2:4Z:360:PRO:HG3  | 2.23                     | 0.53              |
| 1:1A:351:PHE:O    | 2:4H:180:THR:CA   | 2.57                     | 0.52              |
| 1:1B:260:VAL:O    | 2:4O:404:PHE:CD1  | 2.62                     | 0.52              |
| 1:1B:332:ILE:CB   | 2:4O:177:VAL:CG2  | 2.87                     | 0.52              |
| 1:1E:414:GLU:HG2  | 1:1E:416:GLY:H    | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:263:PRO:CD   | 2:4V:406:HIS:CG   | 2.82                     | 0.52              |
| 1:1K:347:CYS:SG   | 2:4W:181:VAL:HG13 | 2.49                     | 0.52              |
| 1:1K:348:PRO:CD   | 2:4W:398:MET:HG3  | 2.39                     | 0.52              |
| 2:1H:174:SER:HB2  | 2:1H:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:1O:320:ARG:NH1  | 2:1O:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:1P:217:LEU:HD11 | 2:1P:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:1Q:174:SER:HB2  | 2:1Q:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:1Q:217:LEU:HD11 | 2:1Q:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:1Q:270:PRO:HG2  | 2:1Q:302:MET:HB2  | 1.90                     | 0.52              |
| 2:1V:221:THR:C    | 1:2J:324:VAL:HG13 | 2.34                     | 0.52              |
| 2:1V:250:ALA:HA   | 2:1V:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:1Y:222:PRO:HD2  | 1:2M:324:VAL:CG1  | 2.39                     | 0.52              |
| 1:2C:244:PHE:HB2  | 1:2C:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:2E:244:PHE:HB2  | 1:2E:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:2F:191:THR:HA   | 1:2F:194:THR:HG22 | 1.91                     | 0.52              |
| 2:2H:181:VAL:N    | 1:3A:258:ASN:ND2  | 2.57                     | 0.52              |
| 2:2O:217:LEU:HD11 | 2:2O:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:2Q:174:SER:HB2  | 2:2Q:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:2Q:217:LEU:HD11 | 2:2Q:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:2Q:320:ARG:NH1  | 2:2Q:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:2R:71:GLU:HB2   | 1:3E:2:ARG:CD     | 2.33                     | 0.52              |
| 2:2R:100:GLY:HA2  | 1:3E:253:THR:CB   | 2.36                     | 0.52              |
| 2:2R:180:THR:HB   | 2:2R:183:GLU:HB3  | 1.89                     | 0.52              |
| 2:2Y:174:SER:HB2  | 2:2Y:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:2Z:404:PHE:HD1  | 1:3N:260:VAL:O    | 1.87                     | 0.52              |
| 1:3B:191:THR:HA   | 1:3B:194:THR:HG22 | 1.91                     | 0.52              |
| 1:3E:244:PHE:HB2  | 1:3E:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:3F:319:TYR:HB3  | 1:3F:323:VAL:HG21 | 1.90                     | 0.52              |
| 2:3H:174:SER:HB2  | 2:3H:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:3O:217:LEU:HD11 | 2:3O:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:3R:180:THR:HB   | 2:3R:183:GLU:HB3  | 1.89                     | 0.52              |
| 2:3V:250:ALA:HA   | 2:3V:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:3Y:174:SER:HB2  | 2:3Y:207:GLU:HB2  | 1.91                     | 0.52              |
| 1:4F:244:PHE:HB2  | 1:4F:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:4I:244:PHE:HB2  | 1:4I:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:4H:217:LEU:HD11 | 2:4H:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:4O:228:ASN:HD21 | 5:4O:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:4P:217:LEU:HD11 | 2:4P:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:4W:250:ALA:HA   | 2:4W:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:4Z:270:PRO:HG2  | 2:4Z:302:MET:HB2  | 1.90                     | 0.52              |
| 1:1B:191:THR:HA   | 1:1B:194:THR:HG22 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:260:VAL:CB   | 2:4O:407:TRP:NE1  | 2.44                     | 0.52              |
| 1:1D:333:ALA:CB   | 2:4Q:176:LYS:HB3  | 2.39                     | 0.52              |
| 1:1E:333:ALA:CB   | 2:4R:176:LYS:HB3  | 2.39                     | 0.52              |
| 1:1F:414:GLU:HG2  | 1:1F:416:GLY:H    | 1.74                     | 0.52              |
| 1:1G:261:PRO:HA   | 2:4T:404:PHE:CG   | 2.43                     | 0.52              |
| 1:1I:261:PRO:CA   | 2:4U:404:PHE:CD1  | 2.92                     | 0.52              |
| 1:1N:324:VAL:HG13 | 2:4Z:222:PRO:C    | 2.35                     | 0.52              |
| 2:1O:217:LEU:HD11 | 2:1O:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:1Q:320:ARG:NH1  | 2:1Q:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:1T:180:THR:CG2  | 1:2G:258:ASN:HD21 | 2.22                     | 0.52              |
| 2:1T:270:PRO:HG2  | 2:1T:302:MET:HB2  | 1.90                     | 0.52              |
| 2:1U:217:LEU:HD11 | 2:1U:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:1U:250:ALA:HA   | 2:1U:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:1Z:401:ARG:CB   | 1:2N:262:TYR:OH   | 2.47                     | 0.52              |
| 1:2C:191:THR:HA   | 1:2C:194:THR:HG22 | 1.91                     | 0.52              |
| 1:2F:414:GLU:HG2  | 1:2F:416:GLY:H    | 1.74                     | 0.52              |
| 2:2H:174:SER:HB2  | 2:2H:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:2H:217:LEU:HD11 | 2:2H:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:2O:320:ARG:NH1  | 2:2O:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:2U:217:LEU:HD11 | 2:2U:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:2U:250:ALA:HA   | 2:2U:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:2Y:11:GLN:NE2   | 1:3M:249:ASN:HB2  | 2.23                     | 0.52              |
| 1:3C:191:THR:HA   | 1:3C:194:THR:HG22 | 1.91                     | 0.52              |
| 2:3O:320:ARG:NH1  | 2:3O:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:3Q:217:LEU:HD11 | 2:3Q:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:3Q:228:ASN:HD21 | 5:3Q:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:3Q:270:PRO:HG2  | 2:3Q:302:MET:HB2  | 1.90                     | 0.52              |
| 2:3T:205:ASP:OD2  | 2:3T:304:ALA:N    | 2.35                     | 0.52              |
| 2:3U:217:LEU:HD11 | 2:3U:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:3U:250:ALA:HA   | 2:3U:254:LYS:HD3  | 1.91                     | 0.52              |
| 1:4B:191:THR:HA   | 1:4B:194:THR:HG22 | 1.91                     | 0.52              |
| 1:4F:414:GLU:HG2  | 1:4F:416:GLY:H    | 1.74                     | 0.52              |
| 2:4O:217:LEU:HD11 | 2:4O:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:4Q:228:ASN:HD21 | 5:4Q:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:4Q:320:ARG:NH1  | 2:4Q:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:4U:250:ALA:HA   | 2:4U:254:LYS:HD3  | 1.92                     | 0.52              |
| 1:1B:353:VAL:CA   | 2:4O:179:ASP:OD1  | 2.57                     | 0.52              |
| 1:1C:191:THR:HA   | 1:1C:194:THR:HG22 | 1.91                     | 0.52              |
| 1:1C:326:LYS:HE2  | 2:4P:214:PHE:CB   | 2.38                     | 0.52              |
| 1:1G:258:ASN:OD1  | 2:4T:101:ASN:CB   | 2.57                     | 0.52              |
| 2:1H:217:LEU:HD11 | 2:1H:275:LEU:HD22 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1P:165:ILE:HA   | 2:1P:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1R:31:ASP:OD1   | 2:1R:35:SER:N     | 2.42                     | 0.52              |
| 2:1R:180:THR:HB   | 2:1R:183:GLU:HB3  | 1.89                     | 0.52              |
| 2:1S:100:GLY:HA2  | 1:2F:253:THR:CG2  | 2.40                     | 0.52              |
| 2:1Y:174:SER:HB2  | 2:1Y:207:GLU:HB2  | 1.91                     | 0.52              |
| 1:2B:191:THR:HA   | 1:2B:194:THR:HG22 | 1.92                     | 0.52              |
| 1:2F:319:TYR:HB3  | 1:2F:323:VAL:HG21 | 1.90                     | 0.52              |
| 2:2P:165:ILE:HA   | 2:2P:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2Q:228:ASN:HD21 | 5:2Q:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:2Q:270:PRO:HG2  | 2:2Q:302:MET:HB2  | 1.90                     | 0.52              |
| 2:2Q:394:GLN:CG   | 1:3D:348:PRO:HG2  | 2.39                     | 0.52              |
| 2:2R:31:ASP:OD1   | 2:2R:35:SER:N     | 2.43                     | 0.52              |
| 2:2S:100:GLY:HA2  | 1:3F:253:THR:CB   | 2.37                     | 0.52              |
| 5:2T:501:GDP:N7   | 1:3G:248:LEU:HD13 | 2.20                     | 0.52              |
| 2:2U:165:ILE:HA   | 2:2U:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2Z:174:SER:HB2  | 2:2Z:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:3H:217:LEU:HD11 | 2:3H:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:3Q:320:ARG:NH1  | 2:3Q:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:3R:31:ASP:OD1   | 2:3R:35:SER:N     | 2.42                     | 0.52              |
| 2:3T:270:PRO:HG2  | 2:3T:302:MET:HB2  | 1.90                     | 0.52              |
| 1:4C:191:THR:HA   | 1:4C:194:THR:HG22 | 1.91                     | 0.52              |
| 1:4C:244:PHE:HB2  | 1:4C:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:4H:174:SER:HB2  | 2:4H:207:GLU:HB2  | 1.91                     | 0.52              |
| 2:4O:320:ARG:NH1  | 2:4O:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:4P:165:ILE:HA   | 2:4P:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4R:31:ASP:OD1   | 2:4R:35:SER:N     | 2.42                     | 0.52              |
| 2:4R:180:THR:HB   | 2:4R:183:GLU:HB3  | 1.89                     | 0.52              |
| 2:4U:165:ILE:HA   | 2:4U:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4Z:174:SER:HB2  | 2:4Z:207:GLU:HB2  | 1.91                     | 0.52              |
| 1:1B:249:ASN:N    | 2:4O:11:GLN:CD    | 2.52                     | 0.52              |
| 1:1C:248:LEU:CD2  | 2:4P:179:ASP:OD2  | 2.57                     | 0.52              |
| 1:1C:346:TRP:CZ3  | 2:4P:403:ALA:HB3  | 2.44                     | 0.52              |
| 1:1D:100:ALA:N    | 3:1D:501:GTP:O2G  | 2.41                     | 0.52              |
| 1:1E:191:THR:HA   | 1:1E:194:THR:HG22 | 1.91                     | 0.52              |
| 1:1I:254:GLU:CA   | 2:4U:100:GLY:C    | 2.73                     | 0.52              |
| 1:1I:349:THR:OG1  | 2:4U:184:PRO:HD3  | 2.09                     | 0.52              |
| 2:1O:165:ILE:HA   | 2:1O:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1Q:404:PHE:CD1  | 1:2D:261:PRO:HA   | 2.44                     | 0.52              |
| 2:1Z:174:SER:HB2  | 2:1Z:207:GLU:HB2  | 1.91                     | 0.52              |
| 1:2D:100:ALA:N    | 3:2D:501:GTP:O2G  | 2.41                     | 0.52              |
| 2:2O:77:SER:CB    | 1:3B:245:ASP:CG   | 2.82                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:11:GLN:HE22  | 1:3C:249:ASN:H    | 0.59                     | 0.52              |
| 2:2P:270:PRO:HG2  | 2:2P:302:MET:HB2  | 1.90                     | 0.52              |
| 2:2R:181:VAL:CB   | 1:3E:258:ASN:O    | 2.57                     | 0.52              |
| 2:2S:101:ASN:HB2  | 1:3F:254:GLU:CG   | 2.39                     | 0.52              |
| 2:2T:205:ASP:OD2  | 2:2T:304:ALA:N    | 2.35                     | 0.52              |
| 2:2T:270:PRO:HG2  | 2:2T:302:MET:HB2  | 1.90                     | 0.52              |
| 2:2X:394:GLN:CB   | 1:3L:348:PRO:CG   | 2.86                     | 0.52              |
| 2:2Z:31:ASP:OD1   | 2:2Z:35:SER:N     | 2.42                     | 0.52              |
| 2:3O:165:ILE:HA   | 2:3O:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3T:31:ASP:OD1   | 2:3T:35:SER:N     | 2.42                     | 0.52              |
| 2:3Z:174:SER:HB2  | 2:3Z:207:GLU:HB2  | 1.91                     | 0.52              |
| 1:4D:100:ALA:N    | 3:4D:501:GTP:O2G  | 2.41                     | 0.52              |
| 1:4G:191:THR:HA   | 1:4G:194:THR:HG22 | 1.91                     | 0.52              |
| 1:4N:244:PHE:HB2  | 1:4N:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:4O:165:ILE:HA   | 2:4O:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4P:270:PRO:HG2  | 2:4P:302:MET:HB2  | 1.90                     | 0.52              |
| 2:4Q:270:PRO:HG2  | 2:4Q:302:MET:HB2  | 1.90                     | 0.52              |
| 2:4T:31:ASP:OD1   | 2:4T:35:SER:N     | 2.42                     | 0.52              |
| 2:4T:283:TYR:OH   | 2:4U:85:GLN:O     | 2.18                     | 0.52              |
| 2:4U:228:ASN:HD21 | 5:4U:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:4W:31:ASP:OD1   | 2:4W:35:SER:N     | 2.42                     | 0.52              |
| 2:4Z:31:ASP:OD1   | 2:4Z:35:SER:N     | 2.42                     | 0.52              |
| 1:1C:256:GLN:HB2  | 2:4P:407:TRP:CH2  | 2.45                     | 0.52              |
| 1:1D:244:PHE:HB2  | 1:1D:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:1D:326:LYS:CB   | 2:4Q:210:TYR:CD1  | 2.93                     | 0.52              |
| 1:1D:439:SER:HB2  | 2:4Q:400:ARG:HD2  | 1.89                     | 0.52              |
| 1:1E:261:PRO:C    | 2:4R:406:HIS:CD2  | 2.86                     | 0.52              |
| 1:1E:325:PRO:C    | 2:4R:210:TYR:CZ   | 2.86                     | 0.52              |
| 1:1F:258:ASN:HD22 | 2:4S:182:VAL:HG22 | 1.75                     | 0.52              |
| 1:1F:319:TYR:HB3  | 1:1F:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:1I:348:PRO:HB2  | 2:4U:394:GLN:CD   | 2.33                     | 0.52              |
| 1:1I:349:THR:HB   | 2:4U:180:THR:O    | 2.10                     | 0.52              |
| 1:1J:244:PHE:HB2  | 1:1J:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:1U:165:ILE:HA   | 2:1U:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1U:228:ASN:HD21 | 5:1U:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:1W:100:GLY:C    | 1:2K:253:THR:HG22 | 2.34                     | 0.52              |
| 2:1X:165:ILE:HA   | 2:1X:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1X:250:ALA:HA   | 2:1X:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:1Z:31:ASP:OD1   | 2:1Z:35:SER:N     | 2.42                     | 0.52              |
| 2:1Z:176:LYS:HE2  | 1:2N:333:ALA:CB   | 2.40                     | 0.52              |
| 1:2D:319:TYR:HB3  | 1:2D:323:VAL:HG21 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2E:191:THR:HA   | 1:2E:194:THR:HG22 | 1.91                     | 0.52              |
| 1:2J:244:PHE:HB2  | 1:2J:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:2N:244:PHE:HB2  | 1:2N:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:2O:165:ILE:HA   | 2:2O:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2Q:222:PRO:C    | 1:3D:324:VAL:HG13 | 2.35                     | 0.52              |
| 2:2R:394:GLN:CB   | 1:3E:348:PRO:HG2  | 2.32                     | 0.52              |
| 2:2T:31:ASP:OD1   | 2:2T:35:SER:N     | 2.42                     | 0.52              |
| 2:2U:228:ASN:HD21 | 5:2U:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:2W:176:LYS:CE   | 1:3K:333:ALA:HB1  | 2.34                     | 0.52              |
| 2:2X:165:ILE:HA   | 2:2X:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2X:250:ALA:HA   | 2:2X:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:2Y:11:GLN:HE22  | 1:3M:249:ASN:H    | 0.67                     | 0.52              |
| 2:2Y:181:VAL:N    | 1:3M:258:ASN:ND2  | 2.57                     | 0.52              |
| 2:2Y:394:GLN:CB   | 1:3M:348:PRO:CG   | 2.88                     | 0.52              |
| 1:3D:100:ALA:N    | 3:3D:501:GTP:O2G  | 2.41                     | 0.52              |
| 1:3D:319:TYR:HB3  | 1:3D:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:3E:191:THR:HA   | 1:3E:194:THR:HG22 | 1.91                     | 0.52              |
| 1:3J:244:PHE:HB2  | 1:3J:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:3P:165:ILE:HA   | 2:3P:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3P:270:PRO:HG2  | 2:3P:302:MET:HB2  | 1.90                     | 0.52              |
| 2:3U:165:ILE:HA   | 2:3U:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3U:228:ASN:HD21 | 5:3U:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:3X:165:ILE:HA   | 2:3X:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3Z:31:ASP:OD1   | 2:3Z:35:SER:N     | 2.42                     | 0.52              |
| 1:4D:319:TYR:HB3  | 1:4D:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:4D:414:GLU:HG2  | 1:4D:416:GLY:H    | 1.74                     | 0.52              |
| 1:4E:191:THR:HA   | 1:4E:194:THR:HG22 | 1.91                     | 0.52              |
| 2:4T:250:ALA:HA   | 2:4T:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:4T:270:PRO:HG2  | 2:4T:302:MET:HB2  | 1.90                     | 0.52              |
| 2:4X:165:ILE:HA   | 2:4X:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:1A:414:GLU:HG2  | 1:1A:416:GLY:H    | 1.74                     | 0.52              |
| 1:1B:314:ALA:CB   | 2:4O:181:VAL:HG11 | 2.39                     | 0.52              |
| 1:1B:346:TRP:CA   | 2:4O:397:ALA:C    | 2.82                     | 0.52              |
| 1:1D:319:TYR:HB3  | 1:1D:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:1D:352:LYS:HE3  | 2:4Q:101:ASN:HD22 | 1.74                     | 0.52              |
| 1:1E:260:VAL:HB   | 2:4R:407:TRP:CZ2  | 2.36                     | 0.52              |
| 1:1G:191:THR:HA   | 1:1G:194:THR:HG22 | 1.91                     | 0.52              |
| 1:1G:258:ASN:HD21 | 2:4T:180:THR:CG2  | 2.16                     | 0.52              |
| 1:1J:348:PRO:HB2  | 2:4V:394:GLN:HG2  | 1.91                     | 0.52              |
| 1:1J:349:THR:OG1  | 2:4V:184:PRO:CD   | 2.57                     | 0.52              |
| 1:1K:319:TYR:HB3  | 1:1K:323:VAL:HG21 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:347:CYS:HA   | 2:4W:398:MET:HG2  | 1.90                     | 0.52              |
| 1:1K:439:SER:OG   | 2:4W:401:ARG:CG   | 2.58                     | 0.52              |
| 2:1H:165:ILE:HA   | 2:1H:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1P:270:PRO:HG2  | 2:1P:302:MET:HB2  | 1.90                     | 0.52              |
| 2:1R:165:ILE:HA   | 2:1R:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1R:222:PRO:O    | 1:2E:325:PRO:HD2  | 2.09                     | 0.52              |
| 2:1T:31:ASP:OD1   | 2:1T:35:SER:N     | 2.42                     | 0.52              |
| 2:1T:228:ASN:HD21 | 5:1T:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:1W:31:ASP:OD1   | 2:1W:35:SER:N     | 2.42                     | 0.52              |
| 2:1W:165:ILE:HA   | 2:1W:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:2A:414:GLU:HG2  | 1:2A:416:GLY:H    | 1.74                     | 0.52              |
| 1:2D:244:PHE:HB2  | 1:2D:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:2D:414:GLU:HG2  | 1:2D:416:GLY:H    | 1.74                     | 0.52              |
| 1:2G:191:THR:HA   | 1:2G:194:THR:HG22 | 1.91                     | 0.52              |
| 2:2Q:182:VAL:HG21 | 1:3D:257:THR:HG22 | 1.92                     | 0.52              |
| 2:2T:250:ALA:HA   | 2:2T:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:2V:214:PHE:HB2  | 1:3J:326:LYS:HE3  | 1.86                     | 0.52              |
| 2:2V:394:GLN:HB3  | 1:3J:348:PRO:HG2  | 1.91                     | 0.52              |
| 2:2W:31:ASP:OD1   | 2:2W:35:SER:N     | 2.42                     | 0.52              |
| 1:3D:244:PHE:HB2  | 1:3D:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:3D:414:GLU:HG2  | 1:3D:416:GLY:H    | 1.74                     | 0.52              |
| 1:3N:244:PHE:HB2  | 1:3N:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:3R:165:ILE:HA   | 2:3R:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3T:228:ASN:HD21 | 5:3T:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:3W:31:ASP:OD1   | 2:3W:35:SER:N     | 2.42                     | 0.52              |
| 2:3W:165:ILE:HA   | 2:3W:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3X:250:ALA:HA   | 2:3X:254:LYS:HD3  | 1.92                     | 0.52              |
| 1:4A:414:GLU:HG2  | 1:4A:416:GLY:H    | 1.74                     | 0.52              |
| 1:4B:414:GLU:HG2  | 1:4B:416:GLY:H    | 1.74                     | 0.52              |
| 1:4D:244:PHE:HB2  | 1:4D:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:4H:165:ILE:HA   | 2:4H:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4T:205:ASP:OD2  | 2:4T:304:ALA:N    | 2.35                     | 0.52              |
| 2:4T:228:ASN:HD21 | 5:4T:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:4W:165:ILE:HA   | 2:4W:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4X:250:ALA:HA   | 2:4X:254:LYS:HD3  | 1.91                     | 0.52              |
| 1:1B:245:ASP:OD2  | 2:4O:77:SER:HB2   | 2.10                     | 0.52              |
| 1:1E:261:PRO:O    | 2:4R:404:PHE:HA   | 2.09                     | 0.52              |
| 1:1E:346:TRP:CZ2  | 2:4R:403:ALA:HB2  | 2.45                     | 0.52              |
| 1:1F:262:TYR:CZ   | 2:4S:403:ALA:HA   | 2.44                     | 0.52              |
| 1:1G:2:ARG:NH1    | 2:4T:71:GLU:HG3   | 2.23                     | 0.52              |
| 1:1G:260:VAL:HG21 | 2:4T:407:TRP:HZ2  | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:262:TYR:CE1  | 2:4T:402:LYS:O    | 2.63                     | 0.52              |
| 1:1L:346:TRP:O    | 2:4X:398:MET:HG3  | 1.96                     | 0.52              |
| 1:1M:352:LYS:HA   | 2:4Y:179:ASP:O    | 2.09                     | 0.52              |
| 1:1M:414:GLU:HG2  | 1:1M:416:GLY:H    | 1.74                     | 0.52              |
| 1:1N:244:PHE:HB2  | 1:1N:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:1N:329:ASN:HB2  | 2:4Z:210:TYR:HE2  | 1.72                     | 0.52              |
| 2:1H:401:ARG:O    | 1:2A:262:TYR:OH   | 2.18                     | 0.52              |
| 2:1P:250:ALA:HA   | 2:1P:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:1R:207:GLU:CD   | 1:2E:329:ASN:HD21 | 2.18                     | 0.52              |
| 2:1S:165:ILE:HA   | 2:1S:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1T:165:ILE:HA   | 2:1T:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:1T:222:PRO:HD2  | 1:2G:326:LYS:HB3  | 1.91                     | 0.52              |
| 1:2B:414:GLU:HG2  | 1:2B:416:GLY:H    | 1.74                     | 0.52              |
| 1:2G:3:GLU:HA     | 1:2G:51:THR:HA    | 1.92                     | 0.52              |
| 2:2H:165:ILE:HA   | 2:2H:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2H:176:LYS:CE   | 1:3A:333:ALA:HB1  | 2.31                     | 0.52              |
| 2:2H:228:ASN:HD21 | 5:2H:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:2P:11:GLN:CD    | 1:3C:249:ASN:H    | 2.07                     | 0.52              |
| 2:2P:250:ALA:HA   | 2:2P:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:2R:165:ILE:HA   | 2:2R:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2S:165:ILE:HA   | 2:2S:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2T:165:ILE:HA   | 2:2T:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2T:228:ASN:HD21 | 5:2T:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:2U:406:HIS:CE1  | 1:3I:263:PRO:HA   | 2.44                     | 0.52              |
| 2:2W:165:ILE:HA   | 2:2W:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:2W:224:TYR:CD2  | 1:3K:247:ALA:O    | 2.60                     | 0.52              |
| 2:2W:398:MET:HG2  | 1:3K:346:TRP:O    | 2.09                     | 0.52              |
| 2:2W:404:PHE:CZ   | 1:3K:261:PRO:CB   | 2.93                     | 0.52              |
| 2:2Z:228:ASN:HD21 | 5:2Z:501:GDP:HN1  | 1.57                     | 0.52              |
| 1:3A:414:GLU:HG2  | 1:3A:416:GLY:H    | 1.74                     | 0.52              |
| 1:3G:191:THR:HA   | 1:3G:194:THR:HG22 | 1.91                     | 0.52              |
| 2:3H:165:ILE:HA   | 2:3H:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3P:250:ALA:HA   | 2:3P:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:3S:165:ILE:HA   | 2:3S:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:3T:250:ALA:HA   | 2:3T:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:3Z:228:ASN:HD21 | 5:3Z:501:GDP:HN1  | 1.57                     | 0.52              |
| 1:4C:414:GLU:HG2  | 1:4C:416:GLY:H    | 1.74                     | 0.52              |
| 1:4J:244:PHE:HB2  | 1:4J:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:4P:320:ARG:NH1  | 2:4P:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:4R:165:ILE:HA   | 2:4R:199:ASP:OD2  | 2.10                     | 0.52              |
| 2:4S:165:ILE:HA   | 2:4S:199:ASP:OD2  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:260:VAL:HB   | 2:4H:407:TRP:CE2  | 2.45                     | 0.52              |
| 1:1C:346:TRP:CB   | 2:4P:398:MET:HA   | 2.26                     | 0.52              |
| 1:1D:414:GLU:HG2  | 1:1D:416:GLY:H    | 1.74                     | 0.52              |
| 1:1E:254:GLU:HA   | 2:4R:100:GLY:CA   | 2.35                     | 0.52              |
| 1:1G:3:GLU:HA     | 1:1G:51:THR:HA    | 1.92                     | 0.52              |
| 1:1G:414:GLU:HG2  | 1:1G:416:GLY:H    | 1.74                     | 0.52              |
| 2:1H:228:ASN:HD21 | 5:1H:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:1P:320:ARG:NH1  | 2:1P:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:1R:179:ASP:OD2  | 1:2E:248:LEU:HD21 | 2.09                     | 0.52              |
| 2:1T:250:ALA:HA   | 2:1T:254:LYS:HD3  | 1.92                     | 0.52              |
| 1:2D:138:PHE:HZ   | 1:2D:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:2M:244:PHE:HB2  | 1:2M:356:ASN:HD21 | 1.74                     | 0.52              |
| 2:2O:250:ALA:HA   | 2:2O:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:2S:101:ASN:HB2  | 1:3F:254:GLU:HG2  | 1.90                     | 0.52              |
| 2:2S:180:THR:N    | 1:3F:351:PHE:O    | 2.43                     | 0.52              |
| 2:2U:394:GLN:NE2  | 1:3I:348:PRO:HB2  | 2.25                     | 0.52              |
| 1:3B:414:GLU:HG2  | 1:3B:416:GLY:H    | 1.74                     | 0.52              |
| 1:3G:3:GLU:HA     | 1:3G:51:THR:HA    | 1.92                     | 0.52              |
| 2:3R:217:LEU:HD11 | 2:3R:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:3T:165:ILE:HA   | 2:3T:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:4D:138:PHE:HZ   | 1:4D:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:4G:3:GLU:HA     | 1:4G:51:THR:HA    | 1.92                     | 0.52              |
| 1:4K:319:TYR:HB3  | 1:4K:323:VAL:HG21 | 1.90                     | 0.52              |
| 2:4R:217:LEU:HD11 | 2:4R:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:4Z:228:ASN:HD21 | 5:4Z:501:GDP:HN1  | 1.57                     | 0.52              |
| 1:1B:414:GLU:HG2  | 1:1B:416:GLY:H    | 1.74                     | 0.52              |
| 1:1C:260:VAL:HG11 | 2:4P:407:TRP:CZ2  | 2.44                     | 0.52              |
| 1:1D:138:PHE:HZ   | 1:1D:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:1E:2:ARG:HH11   | 2:4R:71:GLU:CB    | 2.22                     | 0.52              |
| 1:1E:262:TYR:O    | 2:4R:406:HIS:NE2  | 2.34                     | 0.52              |
| 1:1E:347:CYS:CA   | 2:4R:398:MET:HG2  | 2.36                     | 0.52              |
| 1:1F:346:TRP:CD1  | 2:4S:401:ARG:CB   | 2.93                     | 0.52              |
| 1:1I:346:TRP:HB3  | 2:4U:397:ALA:O    | 2.08                     | 0.52              |
| 1:1M:244:PHE:HB2  | 1:1M:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:1N:260:VAL:CG1  | 2:4Z:407:TRP:HE1  | 2.22                     | 0.52              |
| 2:1H:181:VAL:HG11 | 1:2A:258:ASN:O    | 2.09                     | 0.52              |
| 2:1O:250:ALA:HA   | 2:1O:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:1Q:250:ALA:HA   | 2:1Q:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:1R:217:LEU:HD11 | 2:1R:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:1V:180:THR:CB   | 1:2J:258:ASN:HD21 | 2.22                     | 0.52              |
| 2:1Z:165:ILE:HA   | 2:1Z:199:ASP:OD2  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Z:228:ASN:HD21 | 5:1Z:501:GDP:HN1  | 1.57                     | 0.52              |
| 1:2A:5:ILE:HG22   | 1:2A:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:2C:414:GLU:HG2  | 1:2C:416:GLY:H    | 1.74                     | 0.52              |
| 1:2M:414:GLU:HG2  | 1:2M:416:GLY:H    | 1.74                     | 0.52              |
| 1:2N:414:GLU:HG2  | 1:2N:416:GLY:H    | 1.74                     | 0.52              |
| 2:2O:71:GLU:HG3   | 1:3B:2:ARG:NH1    | 2.25                     | 0.52              |
| 2:2O:404:PHE:CE1  | 1:3B:260:VAL:N    | 2.72                     | 0.52              |
| 2:2P:320:ARG:NH1  | 2:2P:360:PRO:HG3  | 2.23                     | 0.52              |
| 2:2R:217:LEU:HD11 | 2:2R:275:LEU:HD22 | 1.90                     | 0.52              |
| 2:2V:394:GLN:HB3  | 1:3J:348:PRO:CG   | 2.40                     | 0.52              |
| 2:2Z:11:GLN:HE22  | 1:3N:249:ASN:H    | 0.68                     | 0.52              |
| 2:2Z:165:ILE:HA   | 2:2Z:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:3C:414:GLU:HG2  | 1:3C:416:GLY:H    | 1.74                     | 0.52              |
| 1:3D:138:PHE:HZ   | 1:3D:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:3G:414:GLU:HG2  | 1:3G:416:GLY:H    | 1.74                     | 0.52              |
| 1:3I:3:GLU:HA     | 1:3I:51:THR:HA    | 1.92                     | 0.52              |
| 1:3K:319:TYR:HB3  | 1:3K:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:3N:5:ILE:HG22   | 1:3N:64:ARG:HB3   | 1.92                     | 0.52              |
| 2:3H:228:ASN:HD21 | 5:3H:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:3O:250:ALA:HA   | 2:3O:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:3Q:250:ALA:HA   | 2:3Q:254:LYS:HD3  | 1.91                     | 0.52              |
| 2:3Z:165:ILE:HA   | 2:3Z:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:4E:138:PHE:HZ   | 1:4E:235:VAL:HG11 | 1.75                     | 0.52              |
| 2:4H:228:ASN:HD21 | 5:4H:501:GDP:HN1  | 1.57                     | 0.52              |
| 2:4P:250:ALA:HA   | 2:4P:254:LYS:HD3  | 1.92                     | 0.52              |
| 2:4T:165:ILE:HA   | 2:4T:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:1A:5:ILE:HG22   | 1:1A:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:1A:263:PRO:HA   | 2:4H:406:HIS:CE1  | 2.44                     | 0.52              |
| 1:1C:248:LEU:CA   | 2:4P:11:GLN:NE2   | 2.73                     | 0.52              |
| 1:1E:138:PHE:HZ   | 1:1E:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:1E:326:LYS:HB2  | 2:4R:222:PRO:HG2  | 1.92                     | 0.52              |
| 1:1E:349:THR:CB   | 2:4R:184:PRO:CD   | 2.75                     | 0.52              |
| 1:1F:3:GLU:HA     | 1:1F:51:THR:HA    | 1.92                     | 0.52              |
| 1:1F:260:VAL:HG21 | 2:4S:407:TRP:CZ2  | 2.45                     | 0.52              |
| 1:1F:263:PRO:HD3  | 2:4S:406:HIS:HB3  | 1.89                     | 0.52              |
| 1:1I:3:GLU:HA     | 1:1I:51:THR:HA    | 1.92                     | 0.52              |
| 1:1J:191:THR:HA   | 1:1J:194:THR:HG22 | 1.91                     | 0.52              |
| 1:1K:244:PHE:HB2  | 1:1K:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:1L:257:THR:OG1  | 2:4X:100:GLY:O    | 2.28                     | 0.52              |
| 1:1L:414:GLU:HG2  | 1:1L:416:GLY:H    | 1.74                     | 0.52              |
| 1:1M:5:ILE:HG22   | 1:1M:64:ARG:HB3   | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:348:PRO:CB   | 2:4Y:394:GLN:CG   | 2.88                     | 0.52              |
| 1:1N:349:THR:CG2  | 2:4Z:184:PRO:HD3  | 2.39                     | 0.52              |
| 1:1N:414:GLU:HG2  | 1:1N:416:GLY:H    | 1.74                     | 0.52              |
| 2:1Y:165:ILE:HA   | 2:1Y:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:2E:138:PHE:HZ   | 1:2E:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:2I:3:GLU:HA     | 1:2I:51:THR:HA    | 1.92                     | 0.52              |
| 1:2K:319:TYR:HB3  | 1:2K:323:VAL:HG21 | 1.90                     | 0.52              |
| 1:2L:5:ILE:HG22   | 1:2L:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:2N:5:ILE:HG22   | 1:2N:64:ARG:HB3   | 1.92                     | 0.52              |
| 2:2H:404:PHE:CD1  | 1:3A:261:PRO:CA   | 2.93                     | 0.52              |
| 2:2O:71:GLU:HB2   | 1:3B:2:ARG:CD     | 2.29                     | 0.52              |
| 2:2X:177:VAL:CG2  | 1:3L:332:ILE:CG2  | 2.87                     | 0.52              |
| 1:3A:5:ILE:HG22   | 1:3A:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:3E:138:PHE:HZ   | 1:3E:235:VAL:HG11 | 1.75                     | 0.52              |
| 1:3K:244:PHE:HB2  | 1:3K:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:3M:5:ILE:HG22   | 1:3M:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:3M:244:PHE:HB2  | 1:3M:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:3M:414:GLU:HG2  | 1:3M:416:GLY:H    | 1.74                     | 0.52              |
| 1:3N:414:GLU:HG2  | 1:3N:416:GLY:H    | 1.74                     | 0.52              |
| 2:3P:320:ARG:NH1  | 2:3P:360:PRO:HG3  | 2.23                     | 0.52              |
| 1:4A:5:ILE:HG22   | 1:4A:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:4G:414:GLU:HG2  | 1:4G:416:GLY:H    | 1.74                     | 0.52              |
| 1:4I:3:GLU:HA     | 1:4I:51:THR:HA    | 1.92                     | 0.52              |
| 1:4L:5:ILE:HG22   | 1:4L:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:4M:5:ILE:HG22   | 1:4M:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:4M:244:PHE:HB2  | 1:4M:356:ASN:HD21 | 1.74                     | 0.52              |
| 1:4N:5:ILE:HG22   | 1:4N:64:ARG:HB3   | 1.92                     | 0.52              |
| 1:4N:414:GLU:HG2  | 1:4N:416:GLY:H    | 1.74                     | 0.52              |
| 2:4Z:165:ILE:HA   | 2:4Z:199:ASP:OD2  | 2.10                     | 0.52              |
| 1:1A:324:VAL:HG11 | 2:4H:221:THR:HA   | 1.92                     | 0.51              |
| 1:1B:5:ILE:HG22   | 1:1B:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1C:414:GLU:HG2  | 1:1C:416:GLY:H    | 1.74                     | 0.51              |
| 1:1C:434:GLU:C    | 2:4P:401:ARG:NH2  | 2.67                     | 0.51              |
| 1:1D:325:PRO:CD   | 2:4Q:223:THR:HA   | 2.41                     | 0.51              |
| 1:1E:319:TYR:HB3  | 1:1E:323:VAL:HG21 | 1.90                     | 0.51              |
| 1:1E:346:TRP:HA   | 2:4R:397:ALA:HB1  | 1.91                     | 0.51              |
| 1:1F:261:PRO:HA   | 2:4S:404:PHE:CB   | 2.39                     | 0.51              |
| 1:1F:326:LYS:HG2  | 2:4S:210:TYR:CD1  | 2.45                     | 0.51              |
| 1:1L:5:ILE:HG22   | 1:1L:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1N:5:ILE:HG22   | 1:1N:64:ARG:HB3   | 1.92                     | 0.51              |
| 2:1P:181:VAL:N    | 1:2C:258:ASN:ND2  | 2.50                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:406:HIS:NE2  | 1:2I:263:PRO:CD   | 2.73                     | 0.51              |
| 1:2G:414:GLU:HG2  | 1:2G:416:GLY:H    | 1.74                     | 0.51              |
| 1:2J:191:THR:HA   | 1:2J:194:THR:HG22 | 1.91                     | 0.51              |
| 1:2K:100:ALA:N    | 3:2K:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:2L:414:GLU:HG2  | 1:2L:416:GLY:H    | 1.74                     | 0.51              |
| 1:2M:5:ILE:HG22   | 1:2M:64:ARG:HB3   | 1.92                     | 0.51              |
| 2:2H:101:ASN:N    | 1:3A:254:GLU:HG2  | 2.26                     | 0.51              |
| 2:2O:401:ARG:HH21 | 1:3B:435:VAL:HA   | 1.60                     | 0.51              |
| 2:2Q:250:ALA:HA   | 2:2Q:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:2R:406:HIS:CE1  | 1:3E:263:PRO:HA   | 2.46                     | 0.51              |
| 2:2S:404:PHE:HD1  | 1:3F:260:VAL:O    | 1.92                     | 0.51              |
| 2:2Y:165:ILE:HA   | 2:2Y:199:ASP:OD2  | 2.10                     | 0.51              |
| 1:3B:5:ILE:HG22   | 1:3B:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3E:319:TYR:HB3  | 1:3E:323:VAL:HG21 | 1.90                     | 0.51              |
| 1:3F:3:GLU:HA     | 1:3F:51:THR:HA    | 1.92                     | 0.51              |
| 1:3J:3:GLU:HA     | 1:3J:51:THR:HA    | 1.92                     | 0.51              |
| 1:3J:191:THR:HA   | 1:3J:194:THR:HG22 | 1.91                     | 0.51              |
| 1:3K:100:ALA:N    | 3:3K:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:3L:5:ILE:HG22   | 1:3L:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3L:414:GLU:HG2  | 1:3L:416:GLY:H    | 1.74                     | 0.51              |
| 2:3Y:165:ILE:HA   | 2:3Y:199:ASP:OD2  | 2.10                     | 0.51              |
| 1:4F:3:GLU:HA     | 1:4F:51:THR:HA    | 1.92                     | 0.51              |
| 1:4M:414:GLU:HG2  | 1:4M:416:GLY:H    | 1.74                     | 0.51              |
| 2:4O:250:ALA:HA   | 2:4O:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:4Q:250:ALA:HA   | 2:4Q:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:4S:250:ALA:HA   | 2:4S:254:LYS:HD3  | 1.91                     | 0.51              |
| 1:1E:260:VAL:HG21 | 2:4R:407:TRP:HZ2  | 1.74                     | 0.51              |
| 1:1E:348:PRO:CD   | 2:4R:398:MET:HG3  | 2.40                     | 0.51              |
| 1:1G:326:LYS:HB2  | 2:4T:222:PRO:HG2  | 1.93                     | 0.51              |
| 1:1I:224:TYR:O    | 1:1I:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1J:3:GLU:HA     | 1:1J:51:THR:HA    | 1.92                     | 0.51              |
| 1:1K:3:GLU:HA     | 1:1K:51:THR:HA    | 1.92                     | 0.51              |
| 1:1M:191:THR:HA   | 1:1M:194:THR:HG22 | 1.91                     | 0.51              |
| 2:1V:228:ASN:HD21 | 5:1V:501:GDP:HN1  | 1.57                     | 0.51              |
| 5:1W:501:GDP:C8   | 1:2K:248:LEU:CD1  | 2.93                     | 0.51              |
| 2:1Y:352:LYS:NZ   | 2:1Y:353:THR:O    | 2.44                     | 0.51              |
| 1:2B:5:ILE:HG22   | 1:2B:64:ARG:HB3   | 1.93                     | 0.51              |
| 1:2E:3:GLU:HA     | 1:2E:51:THR:HA    | 1.92                     | 0.51              |
| 1:2E:319:TYR:HB3  | 1:2E:323:VAL:HG21 | 1.90                     | 0.51              |
| 1:2F:3:GLU:HA     | 1:2F:51:THR:HA    | 1.92                     | 0.51              |
| 1:2I:224:TYR:O    | 1:2I:228:ASN:ND2  | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2J:3:GLU:HA     | 1:2J:51:THR:HA    | 1.92                     | 0.51              |
| 1:2K:224:TYR:O    | 1:2K:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:2H:250:ALA:HA   | 2:2H:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:2P:100:GLY:HA2  | 1:3C:253:THR:CB   | 2.28                     | 0.51              |
| 2:2T:72:PRO:CG    | 1:3G:2:ARG:HG3    | 2.39                     | 0.51              |
| 2:2U:222:PRO:HD2  | 1:3I:326:LYS:HB3  | 1.93                     | 0.51              |
| 1:3I:224:TYR:O    | 1:3I:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3K:224:TYR:O    | 1:3K:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:3Y:352:LYS:NZ   | 2:3Y:353:THR:O    | 2.44                     | 0.51              |
| 1:4B:5:ILE:HG22   | 1:4B:64:ARG:HB3   | 1.93                     | 0.51              |
| 1:4C:5:ILE:HG22   | 1:4C:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:4D:191:THR:HA   | 1:4D:194:THR:HG22 | 1.91                     | 0.51              |
| 1:4E:3:GLU:HA     | 1:4E:51:THR:HA    | 1.92                     | 0.51              |
| 1:4I:224:TYR:O    | 1:4I:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:4J:3:GLU:HA     | 1:4J:51:THR:HA    | 1.92                     | 0.51              |
| 1:4J:191:THR:HA   | 1:4J:194:THR:HG22 | 1.91                     | 0.51              |
| 1:4K:100:ALA:N    | 3:4K:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:4K:224:TYR:O    | 1:4K:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:4Y:165:ILE:HA   | 2:4Y:199:ASP:OD2  | 2.10                     | 0.51              |
| 1:1A:257:THR:CG2  | 2:4H:101:ASN:O    | 2.58                     | 0.51              |
| 1:1A:349:THR:CG2  | 2:4H:184:PRO:HD3  | 2.40                     | 0.51              |
| 1:1B:2:ARG:CG     | 2:4O:72:PRO:CD    | 2.82                     | 0.51              |
| 1:1C:349:THR:HG23 | 2:4P:184:PRO:HG3  | 1.91                     | 0.51              |
| 1:1E:3:GLU:HA     | 1:1E:51:THR:HA    | 1.92                     | 0.51              |
| 1:1E:348:PRO:HG2  | 2:4R:394:GLN:CB   | 1.96                     | 0.51              |
| 1:1F:138:PHE:HZ   | 1:1F:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:1F:349:THR:O    | 2:4S:181:VAL:CA   | 2.56                     | 0.51              |
| 1:1G:326:LYS:HG2  | 2:4T:210:TYR:CB   | 2.39                     | 0.51              |
| 1:1J:351:PHE:O    | 2:4V:180:THR:HA   | 2.06                     | 0.51              |
| 1:1K:5:ILE:HG22   | 1:1K:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1K:100:ALA:N    | 3:1K:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:1K:224:TYR:O    | 1:1K:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1K:329:ASN:OD1  | 2:4W:177:VAL:CG1  | 2.58                     | 0.51              |
| 1:1K:414:GLU:HG2  | 1:1K:416:GLY:H    | 1.74                     | 0.51              |
| 1:1L:253:THR:C    | 2:4X:100:GLY:HA2  | 2.36                     | 0.51              |
| 1:1M:326:LYS:CE   | 2:4Y:214:PHE:HB2  | 2.40                     | 0.51              |
| 1:1N:329:ASN:HD21 | 2:4Z:207:GLU:CD   | 2.08                     | 0.51              |
| 1:1N:435:VAL:CA   | 2:4Z:401:ARG:HH22 | 2.22                     | 0.51              |
| 2:1S:250:ALA:HA   | 2:1S:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:1T:283:TYR:OH   | 2:1U:85:GLN:O     | 2.18                     | 0.51              |
| 2:1Y:228:ASN:HD21 | 5:1Y:501:GDP:HN1  | 1.57                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Y:250:ALA:HA   | 2:1Y:254:LYS:HD3  | 1.91                     | 0.51              |
| 1:2K:244:PHE:HB2  | 1:2K:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:2M:191:THR:HA   | 1:2M:194:THR:HG22 | 1.91                     | 0.51              |
| 2:2O:31:ASP:OD1   | 2:2O:35:SER:N     | 2.42                     | 0.51              |
| 2:2S:250:ALA:HA   | 2:2S:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:2V:228:ASN:HD21 | 5:2V:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:2Y:352:LYS:NZ   | 2:2Y:353:THR:O    | 2.44                     | 0.51              |
| 1:3C:5:ILE:HG22   | 1:3C:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3D:191:THR:HA   | 1:3D:194:THR:HG22 | 1.91                     | 0.51              |
| 1:3E:3:GLU:HA     | 1:3E:51:THR:HA    | 1.92                     | 0.51              |
| 1:3J:100:ALA:N    | 3:3J:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:3K:3:GLU:HA     | 1:3K:51:THR:HA    | 1.92                     | 0.51              |
| 1:3K:5:ILE:HG22   | 1:3K:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3M:191:THR:HA   | 1:3M:194:THR:HG22 | 1.91                     | 0.51              |
| 2:3H:250:ALA:HA   | 2:3H:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:3O:31:ASP:OD1   | 2:3O:35:SER:N     | 2.42                     | 0.51              |
| 2:3S:250:ALA:HA   | 2:3S:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:3V:228:ASN:HD21 | 5:3V:501:GDP:HN1  | 1.57                     | 0.51              |
| 1:4F:224:TYR:O    | 1:4F:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:4J:100:ALA:N    | 3:4J:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:4K:5:ILE:HG22   | 1:4K:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:4K:244:PHE:HB2  | 1:4K:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:4K:414:GLU:HG2  | 1:4K:416:GLY:H    | 1.74                     | 0.51              |
| 1:4L:414:GLU:HG2  | 1:4L:416:GLY:H    | 1.74                     | 0.51              |
| 1:4M:191:THR:HA   | 1:4M:194:THR:HG22 | 1.91                     | 0.51              |
| 2:4O:31:ASP:OD1   | 2:4O:35:SER:N     | 2.42                     | 0.51              |
| 2:4V:165:ILE:HA   | 2:4V:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:4V:228:ASN:HD21 | 5:4V:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:4Y:352:LYS:NZ   | 2:4Y:353:THR:O    | 2.44                     | 0.51              |
| 1:1B:248:LEU:HB2  | 2:4O:224:TYR:HE2  | 1.75                     | 0.51              |
| 1:1B:346:TRP:HA   | 2:4O:397:ALA:O    | 2.11                     | 0.51              |
| 1:1C:5:ILE:HG22   | 1:1C:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1C:138:PHE:HZ   | 1:1C:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:1E:253:THR:CG2  | 2:4R:100:GLY:HA3  | 2.40                     | 0.51              |
| 1:1F:224:TYR:O    | 1:1F:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1F:314:ALA:HB2  | 2:4S:404:PHE:HZ   | 1.76                     | 0.51              |
| 1:1J:100:ALA:N    | 3:1J:501:GTP:O2G  | 2.41                     | 0.51              |
| 2:1H:250:ALA:HA   | 2:1H:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:1H:352:LYS:NZ   | 2:1H:353:THR:O    | 2.44                     | 0.51              |
| 2:1O:31:ASP:OD1   | 2:1O:35:SER:N     | 2.42                     | 0.51              |
| 2:1P:352:LYS:NZ   | 2:1P:353:THR:O    | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1R:250:ALA:HA   | 2:1R:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:1V:179:ASP:O    | 1:2J:352:LYS:CE   | 2.57                     | 0.51              |
| 2:1X:401:ARG:NH2  | 1:2L:435:VAL:HA   | 2.03                     | 0.51              |
| 2:1Y:182:VAL:HG21 | 1:2M:257:THR:HG21 | 1.87                     | 0.51              |
| 1:2C:5:ILE:HG22   | 1:2C:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2D:191:THR:HA   | 1:2D:194:THR:HG22 | 1.91                     | 0.51              |
| 1:2F:138:PHE:HZ   | 1:2F:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:2F:224:TYR:O    | 1:2F:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:2J:100:ALA:N    | 3:2J:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:2K:3:GLU:HA     | 1:2K:51:THR:HA    | 1.92                     | 0.51              |
| 1:2K:5:ILE:HG22   | 1:2K:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2K:414:GLU:HG2  | 1:2K:416:GLY:H    | 1.74                     | 0.51              |
| 2:2H:352:LYS:NZ   | 2:2H:353:THR:O    | 2.44                     | 0.51              |
| 2:2P:101:ASN:ND2  | 1:3C:258:ASN:OD1  | 2.43                     | 0.51              |
| 2:2P:394:GLN:OE1  | 1:3C:349:THR:HG23 | 2.09                     | 0.51              |
| 2:2Q:100:GLY:C    | 1:3D:254:GLU:HA   | 2.36                     | 0.51              |
| 2:2S:73:GLY:HA3   | 1:3F:2:ARG:CZ     | 2.40                     | 0.51              |
| 2:2V:165:ILE:HA   | 2:2V:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:2Y:228:ASN:HD21 | 5:2Y:501:GDP:HN1  | 1.57                     | 0.51              |
| 1:3F:138:PHE:HZ   | 1:3F:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:3K:414:GLU:HG2  | 1:3K:416:GLY:H    | 1.74                     | 0.51              |
| 2:3H:352:LYS:NZ   | 2:3H:353:THR:O    | 2.44                     | 0.51              |
| 2:3P:352:LYS:NZ   | 2:3P:353:THR:O    | 2.44                     | 0.51              |
| 2:3Y:228:ASN:HD21 | 5:3Y:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:3Y:250:ALA:HA   | 2:3Y:254:LYS:HD3  | 1.91                     | 0.51              |
| 1:4E:319:TYR:HB3  | 1:4E:323:VAL:HG21 | 1.90                     | 0.51              |
| 1:4F:138:PHE:HZ   | 1:4F:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:4K:3:GLU:HA     | 1:4K:51:THR:HA    | 1.92                     | 0.51              |
| 1:4N:191:THR:HA   | 1:4N:194:THR:HG22 | 1.91                     | 0.51              |
| 2:4H:250:ALA:HA   | 2:4H:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:4P:352:LYS:NZ   | 2:4P:353:THR:O    | 2.44                     | 0.51              |
| 2:4Y:228:ASN:HD21 | 5:4Y:501:GDP:HN1  | 1.57                     | 0.51              |
| 1:1D:353:VAL:CG2  | 2:4Q:179:ASP:HA   | 2.30                     | 0.51              |
| 1:1F:263:PRO:N    | 2:4S:406:HIS:CG   | 2.78                     | 0.51              |
| 1:1I:349:THR:HG23 | 2:4U:184:PRO:HG3  | 1.92                     | 0.51              |
| 1:1J:325:PRO:HG2  | 2:4V:224:TYR:CG   | 2.45                     | 0.51              |
| 1:1L:244:PHE:HB2  | 1:1L:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:1M:224:TYR:O    | 1:1M:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:1Q:404:PHE:CE1  | 1:2D:261:PRO:HA   | 2.44                     | 0.51              |
| 2:1R:352:LYS:NZ   | 2:1R:353:THR:O    | 2.44                     | 0.51              |
| 2:1S:101:ASN:O    | 1:2F:257:THR:HG21 | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1S:181:VAL:HB   | 1:2F:258:ASN:HA   | 1.92                     | 0.51              |
| 1:2C:138:PHE:HZ   | 1:2C:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:2L:244:PHE:HB2  | 1:2L:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:2M:224:TYR:O    | 1:2M:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:2P:11:GLN:NE2   | 1:3C:249:ASN:N    | 2.15                     | 0.51              |
| 2:2P:352:LYS:NZ   | 2:2P:353:THR:O    | 2.44                     | 0.51              |
| 2:2Q:31:ASP:OD1   | 2:2Q:35:SER:N     | 2.42                     | 0.51              |
| 2:2Q:352:LYS:NZ   | 2:2Q:353:THR:O    | 2.44                     | 0.51              |
| 2:2R:250:ALA:HA   | 2:2R:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:2T:100:GLY:O    | 1:3G:254:GLU:HA   | 2.09                     | 0.51              |
| 2:2T:398:MET:HG3  | 1:3G:346:TRP:O    | 2.09                     | 0.51              |
| 2:2W:181:VAL:N    | 1:3K:258:ASN:HD22 | 2.08                     | 0.51              |
| 2:2Y:250:ALA:HA   | 2:2Y:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:2Z:352:LYS:NZ   | 2:2Z:353:THR:O    | 2.44                     | 0.51              |
| 2:2Z:394:GLN:CA   | 1:3N:348:PRO:HG3  | 2.40                     | 0.51              |
| 1:3A:3:GLU:HA     | 1:3A:51:THR:HA    | 1.92                     | 0.51              |
| 1:3A:191:THR:HA   | 1:3A:194:THR:HG22 | 1.91                     | 0.51              |
| 1:3C:138:PHE:HZ   | 1:3C:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:3F:224:TYR:O    | 1:3F:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3F:283:HIS:HB3  | 1:3G:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3L:100:ALA:N    | 3:3L:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:3L:244:PHE:HB2  | 1:3L:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:3M:224:TYR:O    | 1:3M:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3N:191:THR:HA   | 1:3N:194:THR:HG22 | 1.91                     | 0.51              |
| 2:3Q:352:LYS:NZ   | 2:3Q:353:THR:O    | 2.44                     | 0.51              |
| 2:3R:250:ALA:HA   | 2:3R:254:LYS:HD3  | 1.92                     | 0.51              |
| 2:3V:165:ILE:HA   | 2:3V:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:3W:228:ASN:HD21 | 5:3W:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:3Z:352:LYS:NZ   | 2:3Z:353:THR:O    | 2.44                     | 0.51              |
| 1:4C:138:PHE:HZ   | 1:4C:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:4F:283:HIS:HB3  | 1:4G:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4L:100:ALA:N    | 3:4L:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:4M:138:PHE:HZ   | 1:4M:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:4H:352:LYS:NZ   | 2:4H:353:THR:O    | 2.44                     | 0.51              |
| 2:4O:352:LYS:NZ   | 2:4O:353:THR:O    | 2.44                     | 0.51              |
| 2:4Q:31:ASP:OD1   | 2:4Q:35:SER:N     | 2.42                     | 0.51              |
| 2:4Q:352:LYS:NZ   | 2:4Q:353:THR:O    | 2.44                     | 0.51              |
| 2:4Z:352:LYS:NZ   | 2:4Z:353:THR:O    | 2.44                     | 0.51              |
| 1:1A:3:GLU:HA     | 1:1A:51:THR:HA    | 1.92                     | 0.51              |
| 1:1A:191:THR:HA   | 1:1A:194:THR:HG22 | 1.91                     | 0.51              |
| 1:1A:261:PRO:CA   | 2:4H:404:PHE:CG   | 2.82                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:349:THR:OG1  | 2:4H:184:PRO:HD3  | 2.10                     | 0.51              |
| 1:1B:259:LEU:C    | 2:4O:404:PHE:HE1  | 2.19                     | 0.51              |
| 1:1B:283:HIS:HB3  | 1:1C:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1D:191:THR:HA   | 1:1D:194:THR:HG22 | 1.91                     | 0.51              |
| 1:1F:283:HIS:HB3  | 1:1G:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1I:260:VAL:CG1  | 2:4U:407:TRP:NE1  | 2.73                     | 0.51              |
| 1:1I:329:ASN:CB   | 2:4U:210:TYR:CD2  | 2.93                     | 0.51              |
| 1:1I:352:LYS:CE   | 2:4U:101:ASN:HD22 | 2.24                     | 0.51              |
| 1:1J:261:PRO:CA   | 2:4V:404:PHE:CD1  | 2.93                     | 0.51              |
| 1:1J:283:HIS:HB3  | 1:1K:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1K:283:HIS:HB3  | 1:1L:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1N:191:THR:HA   | 1:1N:194:THR:HG22 | 1.91                     | 0.51              |
| 2:1Q:352:LYS:NZ   | 2:1Q:353:THR:O    | 2.44                     | 0.51              |
| 2:1R:404:PHE:CZ   | 1:2E:261:PRO:HA   | 2.46                     | 0.51              |
| 2:1S:404:PHE:CE2  | 1:2F:261:PRO:HB3  | 2.45                     | 0.51              |
| 2:1V:165:ILE:HA   | 2:1V:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:1W:228:ASN:HD21 | 5:1W:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:1X:214:PHE:CD1  | 1:2L:326:LYS:CE   | 2.92                     | 0.51              |
| 2:1X:228:ASN:HD21 | 5:1X:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:1Z:352:LYS:NZ   | 2:1Z:353:THR:O    | 2.44                     | 0.51              |
| 1:2A:3:GLU:HA     | 1:2A:51:THR:HA    | 1.92                     | 0.51              |
| 1:2A:191:THR:HA   | 1:2A:194:THR:HG22 | 1.91                     | 0.51              |
| 1:2B:224:TYR:O    | 1:2B:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:2B:283:HIS:HB3  | 1:2C:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2F:283:HIS:HB3  | 1:2G:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2L:100:ALA:N    | 3:2L:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:2M:138:PHE:HZ   | 1:2M:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:2N:191:THR:HA   | 1:2N:194:THR:HG22 | 1.91                     | 0.51              |
| 2:2O:352:LYS:NZ   | 2:2O:353:THR:O    | 2.44                     | 0.51              |
| 2:2O:407:TRP:HE1  | 1:3B:260:VAL:CB   | 2.21                     | 0.51              |
| 2:2Q:394:GLN:OE1  | 1:3D:349:THR:HG23 | 2.11                     | 0.51              |
| 2:2Q:407:TRP:HE1  | 1:3D:260:VAL:CG1  | 2.22                     | 0.51              |
| 2:2R:352:LYS:NZ   | 2:2R:353:THR:O    | 2.44                     | 0.51              |
| 2:2T:181:VAL:CB   | 1:3G:258:ASN:O    | 2.58                     | 0.51              |
| 2:2W:228:ASN:HD21 | 5:2W:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:2W:352:LYS:NZ   | 2:2W:353:THR:O    | 2.44                     | 0.51              |
| 2:2X:100:GLY:HA2  | 1:3L:253:THR:C    | 2.36                     | 0.51              |
| 2:2X:228:ASN:HD21 | 5:2X:501:GDP:HN1  | 1.57                     | 0.51              |
| 1:3B:283:HIS:HB3  | 1:3C:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3J:283:HIS:HB3  | 1:3K:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3N:3:GLU:HA     | 1:3N:51:THR:HA    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3Q:31:ASP:OD1   | 2:3Q:35:SER:N     | 2.42                     | 0.51              |
| 2:3R:352:LYS:NZ   | 2:3R:353:THR:O    | 2.44                     | 0.51              |
| 1:4A:3:GLU:HA     | 1:4A:51:THR:HA    | 1.92                     | 0.51              |
| 1:4A:283:HIS:HB3  | 1:4B:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4B:283:HIS:HB3  | 1:4C:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4L:244:PHE:HB2  | 1:4L:356:ASN:HD21 | 1.74                     | 0.51              |
| 1:4M:224:TYR:O    | 1:4M:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:4N:3:GLU:HA     | 1:4N:51:THR:HA    | 1.92                     | 0.51              |
| 1:4N:138:PHE:HZ   | 1:4N:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:4R:250:ALA:HA   | 2:4R:254:LYS:HD3  | 1.91                     | 0.51              |
| 2:4W:228:ASN:HD21 | 5:4W:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:4W:352:LYS:NZ   | 2:4W:353:THR:O    | 2.44                     | 0.51              |
| 2:4Y:250:ALA:HA   | 2:4Y:254:LYS:HD3  | 1.92                     | 0.51              |
| 1:1C:324:VAL:HG11 | 2:4P:222:PRO:N    | 2.26                     | 0.51              |
| 1:1C:351:PHE:CB   | 2:4P:178:SER:OG   | 2.53                     | 0.51              |
| 1:1D:5:ILE:HG22   | 1:1D:64:ARG:HB3   | 1.93                     | 0.51              |
| 1:1D:348:PRO:HG3  | 2:4Q:394:GLN:C    | 2.28                     | 0.51              |
| 1:1E:5:ILE:HG22   | 1:1E:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1G:283:HIS:HB3  | 1:1I:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1I:2:ARG:NH2    | 2:4U:73:GLY:HA3   | 2.26                     | 0.51              |
| 1:1I:191:THR:HA   | 1:1I:194:THR:HG22 | 1.91                     | 0.51              |
| 1:1I:326:LYS:HB3  | 2:4U:222:PRO:HG2  | 1.91                     | 0.51              |
| 1:1I:347:CYS:HA   | 2:4U:398:MET:CG   | 2.39                     | 0.51              |
| 1:1M:138:PHE:HZ   | 1:1M:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:1S:352:LYS:NZ   | 2:1S:353:THR:O    | 2.44                     | 0.51              |
| 2:1U:221:THR:C    | 1:2I:324:VAL:HG13 | 2.35                     | 0.51              |
| 2:1V:404:PHE:CG   | 1:2J:261:PRO:HA   | 2.45                     | 0.51              |
| 2:1W:352:LYS:NZ   | 2:1W:353:THR:O    | 2.44                     | 0.51              |
| 1:2A:283:HIS:HB3  | 1:2B:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2G:71:GLU:HB3   | 1:2G:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:2G:283:HIS:HB3  | 1:2I:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2J:5:ILE:HG22   | 1:2J:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2J:283:HIS:HB3  | 1:2K:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2N:138:PHE:HZ   | 1:2N:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:2P:101:ASN:HB2  | 1:3C:254:GLU:CB   | 2.40                     | 0.51              |
| 2:2P:406:HIS:CD2  | 1:3C:263:PRO:N    | 2.78                     | 0.51              |
| 2:2S:352:LYS:NZ   | 2:2S:353:THR:O    | 2.44                     | 0.51              |
| 2:2S:404:PHE:CZ   | 1:3F:261:PRO:HB3  | 2.44                     | 0.51              |
| 5:2S:501:GDP:N7   | 1:3F:248:LEU:HD13 | 2.23                     | 0.51              |
| 2:2X:406:HIS:NE2  | 1:3L:262:TYR:CA   | 2.74                     | 0.51              |
| 2:2Y:101:ASN:ND2  | 1:3M:258:ASN:OD1  | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:223:THR:HA   | 1:3N:325:PRO:HD2  | 1.93                     | 0.51              |
| 1:3B:224:TYR:O    | 1:3B:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3G:283:HIS:HB3  | 1:3I:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3J:5:ILE:HG22   | 1:3J:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3K:283:HIS:HB3  | 1:3L:88:HIS:CG    | 2.46                     | 0.51              |
| 2:3W:352:LYS:NZ   | 2:3W:353:THR:O    | 2.44                     | 0.51              |
| 1:4A:191:THR:HA   | 1:4A:194:THR:HG22 | 1.91                     | 0.51              |
| 1:4G:283:HIS:HB3  | 1:4I:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4J:283:HIS:HB3  | 1:4K:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4K:191:THR:HA   | 1:4K:194:THR:HG22 | 1.91                     | 0.51              |
| 2:4S:352:LYS:NZ   | 2:4S:353:THR:O    | 2.44                     | 0.51              |
| 2:4X:228:ASN:HD21 | 5:4X:501:GDP:HN1  | 1.57                     | 0.51              |
| 1:1A:283:HIS:HB3  | 1:1B:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1B:224:TYR:O    | 1:1B:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1D:71:GLU:HB3   | 1:1D:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:1F:245:ASP:OD1  | 2:4S:77:SER:OG    | 2.28                     | 0.51              |
| 1:1G:71:GLU:HB3   | 1:1G:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:1I:103:TYR:HB2  | 1:1I:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:1K:191:THR:HA   | 1:1K:194:THR:HG22 | 1.91                     | 0.51              |
| 1:1L:100:ALA:N    | 3:1L:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:1N:138:PHE:HZ   | 1:1N:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:1N:324:VAL:HG11 | 2:4Z:221:THR:HA   | 1.91                     | 0.51              |
| 2:1Q:31:ASP:OD1   | 2:1Q:35:SER:N     | 2.42                     | 0.51              |
| 2:1V:195:VAL:HG23 | 2:1V:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:1Z:250:ALA:HA   | 2:1Z:254:LYS:HD3  | 1.91                     | 0.51              |
| 1:2D:5:ILE:HG22   | 1:2D:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2D:71:GLU:HB3   | 1:2D:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:2E:5:ILE:HG22   | 1:2E:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2E:283:HIS:HB3  | 1:2F:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2F:71:GLU:HB3   | 1:2F:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:2N:3:GLU:HA     | 1:2N:51:THR:HA    | 1.92                     | 0.51              |
| 2:2Q:174:SER:OG   | 2:2Q:177:VAL:O    | 2.29                     | 0.51              |
| 2:2R:394:GLN:CG   | 1:3E:348:PRO:HG2  | 2.41                     | 0.51              |
| 2:2S:100:GLY:O    | 1:3F:257:THR:CB   | 2.58                     | 0.51              |
| 2:2T:100:GLY:C    | 1:3G:254:GLU:HA   | 2.36                     | 0.51              |
| 2:2U:195:VAL:HG23 | 2:2U:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:2Y:174:SER:OG   | 2:2Y:177:VAL:O    | 2.29                     | 0.51              |
| 2:2Z:11:GLN:NE2   | 1:3N:249:ASN:HB2  | 2.26                     | 0.51              |
| 1:3A:283:HIS:HB3  | 1:3B:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3D:5:ILE:HG22   | 1:3D:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3D:71:GLU:HB3   | 1:3D:98:ASP:HB3   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3E:5:ILE:HG22   | 1:3E:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3G:71:GLU:HB3   | 1:3G:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:3L:138:PHE:HZ   | 1:3L:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:3M:3:GLU:HA     | 1:3M:51:THR:HA    | 1.92                     | 0.51              |
| 1:3M:138:PHE:HZ   | 1:3M:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:3N:138:PHE:HZ   | 1:3N:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:3S:352:LYS:NZ   | 2:3S:353:THR:O    | 2.44                     | 0.51              |
| 1:4B:224:TYR:O    | 1:4B:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:4E:283:HIS:HB3  | 1:4F:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4J:224:TYR:O    | 1:4J:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:4K:283:HIS:HB3  | 1:4L:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4L:138:PHE:HZ   | 1:4L:235:VAL:HG11 | 1.75                     | 0.51              |
| 2:4Q:165:ILE:HA   | 2:4Q:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:4R:352:LYS:NZ   | 2:4R:353:THR:O    | 2.44                     | 0.51              |
| 1:1C:283:HIS:HB3  | 1:1D:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1C:326:LYS:CE   | 2:4P:214:PHE:CB   | 2.88                     | 0.51              |
| 1:1D:257:THR:HG21 | 2:4Q:101:ASN:O    | 2.10                     | 0.51              |
| 1:1E:283:HIS:HB3  | 1:1F:88:HIS:CG    | 2.46                     | 0.51              |
| 1:1E:352:LYS:HE3  | 2:4R:101:ASN:HD22 | 1.73                     | 0.51              |
| 1:1F:5:ILE:HG22   | 1:1F:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:1F:326:LYS:HG3  | 2:4S:210:TYR:HA   | 1.92                     | 0.51              |
| 1:1G:138:PHE:HZ   | 1:1G:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:1G:224:TYR:O    | 1:1G:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1G:350:GLY:C    | 2:4T:181:VAL:HG22 | 2.36                     | 0.51              |
| 1:1J:224:TYR:O    | 1:1J:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1L:224:TYR:O    | 1:1L:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:1L:352:LYS:HD3  | 2:4X:101:ASN:ND2  | 2.26                     | 0.51              |
| 1:1M:348:PRO:HB2  | 2:4Y:394:GLN:CD   | 2.36                     | 0.51              |
| 1:1N:3:GLU:HA     | 1:1N:51:THR:HA    | 1.92                     | 0.51              |
| 2:1Q:406:HIS:NE2  | 1:2D:263:PRO:HD3  | 2.24                     | 0.51              |
| 2:1T:406:HIS:NE2  | 1:2G:263:PRO:CD   | 2.72                     | 0.51              |
| 2:1U:195:VAL:HG23 | 2:1U:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:1W:195:VAL:HG23 | 2:1W:196:GLU:HG2  | 1.93                     | 0.51              |
| 1:2B:100:ALA:N    | 3:2B:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:2F:5:ILE:HG22   | 1:2F:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:2G:138:PHE:HZ   | 1:2G:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:2I:103:TYR:HB2  | 1:2I:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:2I:283:HIS:HB3  | 1:2J:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2J:103:TYR:HB2  | 1:2J:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:2J:224:TYR:O    | 1:2J:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:2K:191:THR:HA   | 1:2K:194:THR:HG22 | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2K:283:HIS:HB3  | 1:2L:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2L:138:PHE:HZ   | 1:2L:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:2M:3:GLU:HA     | 1:2M:51:THR:HA    | 1.92                     | 0.51              |
| 2:2P:71:GLU:HB2   | 1:3C:2:ARG:CD     | 2.27                     | 0.51              |
| 2:2S:11:GLN:CD    | 1:3F:249:ASN:H    | 2.03                     | 0.51              |
| 2:2V:394:GLN:NE2  | 1:3J:348:PRO:HB2  | 2.26                     | 0.51              |
| 2:2W:195:VAL:HG23 | 2:2W:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:2X:195:VAL:HG23 | 2:2X:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:2X:403:ALA:HA   | 1:3L:262:TYR:CZ   | 2.46                     | 0.51              |
| 2:2Z:406:HIS:CE1  | 1:3N:263:PRO:CA   | 2.94                     | 0.51              |
| 1:3E:283:HIS:HB3  | 1:3F:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3G:138:PHE:HZ   | 1:3G:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:3I:191:THR:HA   | 1:3I:194:THR:HG22 | 1.91                     | 0.51              |
| 1:3J:224:TYR:O    | 1:3J:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3K:191:THR:HA   | 1:3K:194:THR:HG22 | 1.91                     | 0.51              |
| 2:3Q:174:SER:OG   | 2:3Q:177:VAL:O    | 2.29                     | 0.51              |
| 2:3U:195:VAL:HG23 | 2:3U:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:3X:228:ASN:HD21 | 5:3X:501:GDP:HN1  | 1.57                     | 0.51              |
| 2:3Y:174:SER:OG   | 2:3Y:177:VAL:O    | 2.29                     | 0.51              |
| 2:3Z:250:ALA:HA   | 2:3Z:254:LYS:HD3  | 1.91                     | 0.51              |
| 1:4B:100:ALA:N    | 3:4B:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:4D:5:ILE:HG22   | 1:4D:64:ARG:HB3   | 1.93                     | 0.51              |
| 1:4D:71:GLU:HB3   | 1:4D:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:4E:5:ILE:HG22   | 1:4E:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:4F:71:GLU:HB3   | 1:4F:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:4G:138:PHE:HZ   | 1:4G:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:4I:103:TYR:HB2  | 1:4I:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:4J:5:ILE:HG22   | 1:4J:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:4M:3:GLU:HA     | 1:4M:51:THR:HA    | 1.92                     | 0.51              |
| 2:4U:195:VAL:HG23 | 2:4U:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:4W:195:VAL:HG23 | 2:4W:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:4X:195:VAL:HG23 | 2:4X:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:4Y:174:SER:OG   | 2:4Y:177:VAL:O    | 2.29                     | 0.51              |
| 2:4Z:250:ALA:HA   | 2:4Z:254:LYS:HD3  | 1.92                     | 0.51              |
| 1:1D:254:GLU:CG   | 2:4Q:101:ASN:HB2  | 2.40                     | 0.51              |
| 1:1E:254:GLU:CG   | 2:4R:100:GLY:C    | 2.82                     | 0.51              |
| 1:1F:71:GLU:HB3   | 1:1F:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:1G:103:TYR:HB2  | 1:1G:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:1I:414:GLU:HG2  | 1:1I:416:GLY:H    | 1.74                     | 0.51              |
| 1:1J:5:ILE:HG22   | 1:1J:64:ARG:HB3   | 1.93                     | 0.51              |
| 1:1J:103:TYR:HB2  | 1:1J:186:ASN:HD22 | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:346:TRP:CH2  | 2:4V:404:PHE:CE2  | 2.99                     | 0.51              |
| 1:1L:138:PHE:HZ   | 1:1L:235:VAL:HG11 | 1.75                     | 0.51              |
| 1:1M:3:GLU:HA     | 1:1M:51:THR:HA    | 1.92                     | 0.51              |
| 2:1P:210:TYR:HD2  | 1:2C:329:ASN:HD22 | 1.59                     | 0.51              |
| 2:1W:404:PHE:CE1  | 1:2K:260:VAL:N    | 2.78                     | 0.51              |
| 2:1X:195:VAL:HG23 | 2:1X:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:1X:221:THR:CA   | 1:2L:324:VAL:CG1  | 2.79                     | 0.51              |
| 2:1Y:174:SER:OG   | 2:1Y:177:VAL:O    | 2.29                     | 0.51              |
| 2:1Y:401:ARG:HH22 | 1:2M:435:VAL:CA   | 2.01                     | 0.51              |
| 1:2C:283:HIS:HB3  | 1:2D:88:HIS:CG    | 2.46                     | 0.51              |
| 1:2D:224:TYR:O    | 1:2D:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:2G:224:TYR:O    | 1:2G:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:2I:191:THR:HA   | 1:2I:194:THR:HG22 | 1.91                     | 0.51              |
| 1:2I:414:GLU:HG2  | 1:2I:416:GLY:H    | 1.74                     | 0.51              |
| 1:2L:191:THR:HA   | 1:2L:194:THR:HG22 | 1.91                     | 0.51              |
| 1:2L:224:TYR:O    | 1:2L:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:2O:404:PHE:HD1  | 1:3B:260:VAL:O    | 1.93                     | 0.51              |
| 2:2Q:165:ILE:HA   | 2:2Q:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:2Q:394:GLN:OE1  | 1:3D:349:THR:CG2  | 2.59                     | 0.51              |
| 2:2Q:406:HIS:CE1  | 1:3D:263:PRO:CA   | 2.93                     | 0.51              |
| 2:2U:352:LYS:NZ   | 2:2U:353:THR:O    | 2.44                     | 0.51              |
| 2:2V:195:VAL:HG23 | 2:2V:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:2V:406:HIS:CE1  | 1:3J:263:PRO:HA   | 2.46                     | 0.51              |
| 2:2Z:250:ALA:HA   | 2:2Z:254:LYS:HD3  | 1.92                     | 0.51              |
| 1:3B:100:ALA:N    | 3:3B:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:3C:283:HIS:HB3  | 1:3D:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3E:71:GLU:HB3   | 1:3E:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:3F:5:ILE:HG22   | 1:3F:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:3F:71:GLU:HB3   | 1:3F:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:3G:224:TYR:O    | 1:3G:228:ASN:ND2  | 2.44                     | 0.51              |
| 1:3I:103:TYR:HB2  | 1:3I:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:3I:283:HIS:HB3  | 1:3J:88:HIS:CG    | 2.46                     | 0.51              |
| 1:3K:103:TYR:HB2  | 1:3K:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:3L:224:TYR:O    | 1:3L:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:3Q:165:ILE:HA   | 2:3Q:199:ASP:OD2  | 2.10                     | 0.51              |
| 2:3U:352:LYS:NZ   | 2:3U:353:THR:O    | 2.44                     | 0.51              |
| 2:3V:195:VAL:HG23 | 2:3V:196:GLU:HG2  | 1.93                     | 0.51              |
| 2:3W:195:VAL:HG23 | 2:3W:196:GLU:HG2  | 1.93                     | 0.51              |
| 1:4A:88:HIS:CG    | 1:4N:283:HIS:HB3  | 2.46                     | 0.51              |
| 1:4B:3:GLU:HA     | 1:4B:51:THR:HA    | 1.92                     | 0.51              |
| 1:4D:224:TYR:O    | 1:4D:228:ASN:ND2  | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4E:100:ALA:N    | 3:4E:501:GTP:O2G  | 2.41                     | 0.51              |
| 1:4F:5:ILE:HG22   | 1:4F:64:ARG:HB3   | 1.92                     | 0.51              |
| 1:4G:71:GLU:HB3   | 1:4G:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:4I:71:GLU:HB3   | 1:4I:98:ASP:HB3   | 1.93                     | 0.51              |
| 1:4I:191:THR:HA   | 1:4I:194:THR:HG22 | 1.91                     | 0.51              |
| 1:4I:283:HIS:HB3  | 1:4J:88:HIS:CG    | 2.46                     | 0.51              |
| 1:4I:414:GLU:HG2  | 1:4I:416:GLY:H    | 1.74                     | 0.51              |
| 1:4K:103:TYR:HB2  | 1:4K:186:ASN:HD22 | 1.76                     | 0.51              |
| 1:4L:224:TYR:O    | 1:4L:228:ASN:ND2  | 2.44                     | 0.51              |
| 2:4P:31:ASP:OD1   | 2:4P:35:SER:N     | 2.42                     | 0.51              |
| 2:4U:352:LYS:NZ   | 2:4U:353:THR:O    | 2.44                     | 0.51              |
| 2:4V:195:VAL:HG23 | 2:4V:196:GLU:HG2  | 1.93                     | 0.51              |
| 1:1A:253:THR:HB   | 2:4H:100:GLY:CA   | 2.41                     | 0.50              |
| 1:1B:100:ALA:N    | 3:1B:501:GTP:O2G  | 2.41                     | 0.50              |
| 1:1B:261:PRO:CA   | 2:4O:404:PHE:CA   | 2.86                     | 0.50              |
| 1:1B:349:THR:CB   | 2:4O:184:PRO:HD3  | 2.42                     | 0.50              |
| 1:1C:3:GLU:HA     | 1:1C:51:THR:HA    | 1.92                     | 0.50              |
| 1:1C:261:PRO:C    | 2:4P:404:PHE:CA   | 2.82                     | 0.50              |
| 1:1E:71:GLU:HB3   | 1:1E:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1E:100:ALA:N    | 3:1E:501:GTP:O2G  | 2.41                     | 0.50              |
| 1:1G:5:ILE:HG22   | 1:1G:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:1J:261:PRO:CA   | 2:4V:404:PHE:HA   | 2.37                     | 0.50              |
| 1:1K:103:TYR:HB2  | 1:1K:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1K:254:GLU:HA   | 2:4W:100:GLY:CA   | 2.41                     | 0.50              |
| 1:1K:346:TRP:CH2  | 2:4W:404:PHE:CE2  | 2.99                     | 0.50              |
| 1:1L:191:THR:HA   | 1:1L:194:THR:HG22 | 1.91                     | 0.50              |
| 1:1L:283:HIS:HB3  | 1:1M:88:HIS:CG    | 2.46                     | 0.50              |
| 1:1L:439:SER:OG   | 2:4X:401:ARG:HG2  | 2.11                     | 0.50              |
| 1:1M:249:ASN:H    | 2:4Y:11:GLN:CD    | 2.07                     | 0.50              |
| 2:1P:31:ASP:OD1   | 2:1P:35:SER:N     | 2.42                     | 0.50              |
| 2:1P:306:ASP:HB3  | 2:1P:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1Q:306:ASP:HB3  | 2:1Q:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1U:352:LYS:NZ   | 2:1U:353:THR:O    | 2.44                     | 0.50              |
| 2:1W:306:ASP:HB3  | 2:1W:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:2B:3:GLU:HA     | 1:2B:51:THR:HA    | 1.92                     | 0.50              |
| 1:2C:3:GLU:HA     | 1:2C:51:THR:HA    | 1.92                     | 0.50              |
| 1:2E:71:GLU:HB3   | 1:2E:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:2E:100:ALA:N    | 3:2E:501:GTP:O2G  | 2.41                     | 0.50              |
| 1:2G:103:TYR:HB2  | 1:2G:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2K:103:TYR:HB2  | 1:2K:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:2P:31:ASP:OD1   | 2:2P:35:SER:N     | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:222:PRO:O    | 1:3C:324:VAL:HG13 | 2.12                     | 0.50              |
| 2:2P:306:ASP:HB3  | 2:2P:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2U:72:PRO:CG    | 1:3I:2:ARG:HG3    | 2.40                     | 0.50              |
| 2:2V:306:ASP:HB3  | 2:2V:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2W:210:TYR:CE2  | 1:3K:329:ASN:HB2  | 2.46                     | 0.50              |
| 2:2Y:31:ASP:OD1   | 2:2Y:35:SER:N     | 2.42                     | 0.50              |
| 1:3B:3:GLU:HA     | 1:3B:51:THR:HA    | 1.92                     | 0.50              |
| 1:3B:71:GLU:HB3   | 1:3B:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:3D:224:TYR:O    | 1:3D:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:3E:100:ALA:N    | 3:3E:501:GTP:O2G  | 2.41                     | 0.50              |
| 1:3G:5:ILE:HG22   | 1:3G:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:3G:103:TYR:HB2  | 1:3G:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3I:71:GLU:HB3   | 1:3I:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:3I:414:GLU:HG2  | 1:3I:416:GLY:H    | 1.74                     | 0.50              |
| 1:3J:103:TYR:HB2  | 1:3J:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3L:191:THR:HA   | 1:3L:194:THR:HG22 | 1.91                     | 0.50              |
| 2:3X:195:VAL:HG23 | 2:3X:196:GLU:HG2  | 1.93                     | 0.50              |
| 1:4C:283:HIS:HB3  | 1:4D:88:HIS:CG    | 2.46                     | 0.50              |
| 1:4D:3:GLU:HA     | 1:4D:51:THR:HA    | 1.92                     | 0.50              |
| 1:4G:5:ILE:HG22   | 1:4G:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:4G:224:TYR:O    | 1:4G:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:4J:103:TYR:HB2  | 1:4J:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4L:191:THR:HA   | 1:4L:194:THR:HG22 | 1.91                     | 0.50              |
| 1:4M:103:TYR:HD2  | 1:4M:413:MET:HE1  | 1.77                     | 0.50              |
| 2:4H:69:ASP:OD2   | 2:4H:74:THR:OG1   | 2.20                     | 0.50              |
| 2:4Y:31:ASP:OD1   | 2:4Y:35:SER:N     | 2.42                     | 0.50              |
| 1:1A:88:HIS:CG    | 1:1N:283:HIS:HB3  | 2.46                     | 0.50              |
| 1:1A:224:TYR:O    | 1:1A:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:1B:3:GLU:HA     | 1:1B:51:THR:HA    | 1.92                     | 0.50              |
| 1:1C:71:GLU:HB3   | 1:1C:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1D:3:GLU:HA     | 1:1D:51:THR:HA    | 1.92                     | 0.50              |
| 1:1D:224:TYR:O    | 1:1D:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:1E:224:TYR:O    | 1:1E:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:1F:263:PRO:CA   | 2:4S:406:HIS:CE1  | 2.94                     | 0.50              |
| 1:1F:346:TRP:CZ2  | 2:4S:403:ALA:HB2  | 2.47                     | 0.50              |
| 1:1I:5:ILE:HG22   | 1:1I:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:1I:71:GLU:HB3   | 1:1I:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1I:283:HIS:HB3  | 1:1J:88:HIS:CG    | 2.46                     | 0.50              |
| 1:1J:414:GLU:HG2  | 1:1J:416:GLY:H    | 1.74                     | 0.50              |
| 1:1K:348:PRO:HG3  | 2:4W:394:GLN:HA   | 1.93                     | 0.50              |
| 1:1L:3:GLU:HA     | 1:1L:51:THR:HA    | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:103:TYR:HD2  | 1:1M:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1M:261:PRO:HB3  | 2:4Y:404:PHE:CZ   | 2.46                     | 0.50              |
| 1:1N:103:TYR:HD2  | 1:1N:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1N:248:LEU:C    | 2:4Z:11:GLN:HE22  | 2.01                     | 0.50              |
| 1:1N:326:LYS:HE3  | 2:4Z:214:PHE:HB2  | 1.89                     | 0.50              |
| 2:1P:154:ILE:HG12 | 2:1P:166:MET:HE2  | 1.94                     | 0.50              |
| 2:1Q:165:ILE:HA   | 2:1Q:199:ASP:OD2  | 2.10                     | 0.50              |
| 2:1Q:283:TYR:OH   | 2:1R:85:GLN:O     | 2.18                     | 0.50              |
| 2:1R:210:TYR:HD2  | 1:2E:329:ASN:HD22 | 1.58                     | 0.50              |
| 2:1U:404:PHE:CZ   | 1:2I:260:VAL:C    | 2.86                     | 0.50              |
| 2:1Y:181:VAL:HB   | 1:2M:258:ASN:C    | 2.36                     | 0.50              |
| 5:1Z:501:GDP:C8   | 1:2N:248:LEU:CD1  | 2.93                     | 0.50              |
| 1:2A:88:HIS:CG    | 1:2N:283:HIS:HB3  | 2.46                     | 0.50              |
| 1:2A:103:TYR:HB2  | 1:2A:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2B:71:GLU:HB3   | 1:2B:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:2C:71:GLU:HB3   | 1:2C:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:2D:3:GLU:HA     | 1:2D:51:THR:HA    | 1.92                     | 0.50              |
| 1:2G:5:ILE:HG22   | 1:2G:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:2G:103:TYR:HD2  | 1:2G:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2I:71:GLU:HB3   | 1:2I:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:2J:71:GLU:HB3   | 1:2J:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:2K:138:PHE:HZ   | 1:2K:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:2M:103:TYR:HD2  | 1:2M:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2N:103:TYR:HD2  | 1:2N:413:MET:HE1  | 1.77                     | 0.50              |
| 2:2P:154:ILE:HG12 | 2:2P:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2P:404:PHE:CD1  | 1:3C:261:PRO:CA   | 2.93                     | 0.50              |
| 2:2Q:306:ASP:HB3  | 2:2Q:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2S:404:PHE:HA   | 1:3F:261:PRO:O    | 2.11                     | 0.50              |
| 2:2T:179:ASP:OD2  | 1:3G:248:LEU:HD21 | 2.10                     | 0.50              |
| 2:2W:306:ASP:HB3  | 2:2W:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:3A:88:HIS:CG    | 1:3N:283:HIS:HB3  | 2.46                     | 0.50              |
| 1:3A:103:TYR:HB2  | 1:3A:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3A:224:TYR:O    | 1:3A:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:3D:3:GLU:HA     | 1:3D:51:THR:HA    | 1.92                     | 0.50              |
| 1:3G:103:TYR:HD2  | 1:3G:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3K:138:PHE:HZ   | 1:3K:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:3L:3:GLU:HA     | 1:3L:51:THR:HA    | 1.92                     | 0.50              |
| 1:3L:283:HIS:HB3  | 1:3M:88:HIS:CG    | 2.46                     | 0.50              |
| 1:3M:103:TYR:HD2  | 1:3M:413:MET:HE1  | 1.77                     | 0.50              |
| 2:3P:31:ASP:OD1   | 2:3P:35:SER:N     | 2.43                     | 0.50              |
| 2:3P:306:ASP:HB3  | 2:3P:309:HIS:HD2  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3Q:306:ASP:HB3  | 2:3Q:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3T:195:VAL:HG23 | 2:3T:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:3V:306:ASP:HB3  | 2:3V:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3W:306:ASP:HB3  | 2:3W:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3Y:31:ASP:OD1   | 2:3Y:35:SER:N     | 2.42                     | 0.50              |
| 1:4B:71:GLU:HB3   | 1:4B:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:4C:3:GLU:HA     | 1:4C:51:THR:HA    | 1.92                     | 0.50              |
| 1:4G:103:TYR:HB2  | 1:4G:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4G:103:TYR:HD2  | 1:4G:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4I:138:PHE:HZ   | 1:4I:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:4J:71:GLU:HB3   | 1:4J:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:4K:138:PHE:HZ   | 1:4K:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:4N:103:TYR:HD2  | 1:4N:413:MET:HE1  | 1.77                     | 0.50              |
| 2:4P:306:ASP:HB3  | 2:4P:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:4Q:306:ASP:HB3  | 2:4Q:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:4R:306:ASP:HB3  | 2:4R:309:HIS:HD2  | 1.76                     | 0.50              |
| 2:4S:31:ASP:OD1   | 2:4S:35:SER:N     | 2.42                     | 0.50              |
| 2:4T:154:ILE:HG12 | 2:4T:166:MET:HE2  | 1.94                     | 0.50              |
| 2:4V:31:ASP:OD1   | 2:4V:35:SER:N     | 2.42                     | 0.50              |
| 2:4V:306:ASP:HB3  | 2:4V:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:1A:103:TYR:HB2  | 1:1A:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1B:71:GLU:HB3   | 1:1B:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1B:103:TYR:HB2  | 1:1B:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1C:326:LYS:CA   | 2:4P:210:TYR:CE1  | 2.94                     | 0.50              |
| 1:1F:254:GLU:HG2  | 2:4S:100:GLY:CA   | 2.41                     | 0.50              |
| 1:1G:103:TYR:HD2  | 1:1G:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1G:346:TRP:CZ3  | 2:4T:404:PHE:CE2  | 2.99                     | 0.50              |
| 1:1I:138:PHE:HZ   | 1:1I:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:1I:253:THR:C    | 2:4U:100:GLY:HA3  | 2.37                     | 0.50              |
| 1:1I:329:ASN:HB3  | 2:4U:210:TYR:CD2  | 2.46                     | 0.50              |
| 1:1J:71:GLU:HB3   | 1:1J:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1J:326:LYS:HE2  | 2:4V:210:TYR:O    | 2.11                     | 0.50              |
| 1:1K:138:PHE:HZ   | 1:1K:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:1L:103:TYR:HD2  | 1:1L:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1M:346:TRP:CH2  | 2:4Y:404:PHE:CE2  | 2.99                     | 0.50              |
| 1:1N:103:TYR:HB2  | 1:1N:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:1P:221:THR:OG1  | 1:2C:324:VAL:CG2  | 2.59                     | 0.50              |
| 2:1T:154:ILE:HG12 | 2:1T:166:MET:HE2  | 1.94                     | 0.50              |
| 2:1T:195:VAL:HG23 | 2:1T:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1T:352:LYS:NZ   | 2:1T:353:THR:O    | 2.44                     | 0.50              |
| 2:1U:404:PHE:HE1  | 1:2I:260:VAL:O    | 1.79                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1V:306:ASP:HB3  | 2:1V:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1Y:31:ASP:OD1   | 2:1Y:35:SER:N     | 2.42                     | 0.50              |
| 1:2B:103:TYR:HB2  | 1:2B:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2I:5:ILE:HG22   | 1:2I:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:2L:3:GLU:HA     | 1:2L:51:THR:HA    | 1.92                     | 0.50              |
| 1:2L:103:TYR:HD2  | 1:2L:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2L:283:HIS:HB3  | 1:2M:88:HIS:CG    | 2.46                     | 0.50              |
| 1:2N:103:TYR:HB2  | 1:2N:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:2H:101:ASN:CB   | 1:3A:254:GLU:HG2  | 2.35                     | 0.50              |
| 2:2H:404:PHE:CE1  | 1:3A:260:VAL:N    | 2.74                     | 0.50              |
| 2:2P:404:PHE:CE1  | 1:3C:260:VAL:N    | 2.74                     | 0.50              |
| 2:2R:207:GLU:OE1  | 1:3E:329:ASN:CG   | 2.46                     | 0.50              |
| 2:2S:31:ASP:OD1   | 2:2S:35:SER:N     | 2.42                     | 0.50              |
| 2:2S:398:MET:HG3  | 1:3F:346:TRP:O    | 2.10                     | 0.50              |
| 2:2T:154:ILE:HG12 | 2:2T:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2V:31:ASP:OD1   | 2:2V:35:SER:N     | 2.42                     | 0.50              |
| 2:2X:77:SER:CB    | 1:3L:245:ASP:CG   | 2.84                     | 0.50              |
| 2:2X:352:LYS:NZ   | 2:2X:353:THR:O    | 2.44                     | 0.50              |
| 1:3C:3:GLU:HA     | 1:3C:51:THR:HA    | 1.92                     | 0.50              |
| 1:3C:71:GLU:HB3   | 1:3C:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:3E:224:TYR:O    | 1:3E:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:3I:5:ILE:HG22   | 1:3I:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:3J:71:GLU:HB3   | 1:3J:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:3J:414:GLU:HG2  | 1:3J:416:GLY:H    | 1.74                     | 0.50              |
| 1:3N:103:TYR:HD2  | 1:3N:413:MET:HE1  | 1.77                     | 0.50              |
| 2:3P:154:ILE:HG12 | 2:3P:166:MET:HE2  | 1.94                     | 0.50              |
| 2:3T:352:LYS:NZ   | 2:3T:353:THR:O    | 2.44                     | 0.50              |
| 2:3V:31:ASP:OD1   | 2:3V:35:SER:N     | 2.42                     | 0.50              |
| 1:4A:103:TYR:HB2  | 1:4A:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4B:103:TYR:HB2  | 1:4B:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4C:71:GLU:HB3   | 1:4C:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:4E:71:GLU:HB3   | 1:4E:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:4I:5:ILE:HG22   | 1:4I:64:ARG:HB3   | 1.92                     | 0.50              |
| 1:4J:138:PHE:HZ   | 1:4J:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:4J:414:GLU:HG2  | 1:4J:416:GLY:H    | 1.74                     | 0.50              |
| 1:4L:3:GLU:HA     | 1:4L:51:THR:HA    | 1.92                     | 0.50              |
| 1:4L:103:TYR:HD2  | 1:4L:413:MET:HE1  | 1.77                     | 0.50              |
| 2:4P:154:ILE:HG12 | 2:4P:166:MET:HE2  | 1.94                     | 0.50              |
| 2:4T:195:VAL:HG23 | 2:4T:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:4W:306:ASP:HB3  | 2:4W:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:4X:352:LYS:NZ   | 2:4X:353:THR:O    | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4Z:174:SER:OG   | 2:4Z:177:VAL:O    | 2.29                     | 0.50              |
| 1:1A:248:LEU:HB2  | 2:4H:224:TYR:HE2  | 1.76                     | 0.50              |
| 1:1A:326:LYS:CB   | 2:4H:222:PRO:CG   | 2.81                     | 0.50              |
| 1:1C:245:ASP:OD1  | 2:4P:77:SER:OG    | 2.29                     | 0.50              |
| 1:1C:262:TYR:CZ   | 2:4P:402:LYS:C    | 2.90                     | 0.50              |
| 1:1E:260:VAL:HG12 | 2:4R:407:TRP:HE1  | 1.66                     | 0.50              |
| 1:1G:254:GLU:CG   | 2:4T:100:GLY:HA2  | 2.42                     | 0.50              |
| 1:1G:256:GLN:O    | 2:4T:407:TRP:CE2  | 2.65                     | 0.50              |
| 1:1I:254:GLU:CG   | 2:4U:100:GLY:HA2  | 2.41                     | 0.50              |
| 1:1J:263:PRO:CD   | 2:4V:406:HIS:CD2  | 2.94                     | 0.50              |
| 1:1K:263:PRO:CD   | 2:4W:406:HIS:CD2  | 2.95                     | 0.50              |
| 1:1M:103:TYR:HB2  | 1:1M:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1N:314:ALA:CB   | 2:4Z:181:VAL:HG21 | 2.30                     | 0.50              |
| 2:1H:404:PHE:HE1  | 1:2A:260:VAL:N    | 2.09                     | 0.50              |
| 2:1V:31:ASP:OD1   | 2:1V:35:SER:N     | 2.42                     | 0.50              |
| 2:1X:406:HIS:CE1  | 1:2L:263:PRO:HB3  | 2.46                     | 0.50              |
| 1:2A:224:TYR:O    | 1:2A:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:2B:138:PHE:HZ   | 1:2B:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:2E:224:TYR:O    | 1:2E:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:2I:138:PHE:HZ   | 1:2I:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:2J:414:GLU:HG2  | 1:2J:416:GLY:H    | 1.74                     | 0.50              |
| 1:2K:103:TYR:HD2  | 1:2K:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2M:103:TYR:HB2  | 1:2M:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:2H:69:ASP:OD2   | 2:2H:74:THR:OG1   | 2.20                     | 0.50              |
| 2:2H:100:GLY:O    | 1:3A:257:THR:OG1  | 2.27                     | 0.50              |
| 2:2H:394:GLN:OE1  | 1:3A:349:THR:HG23 | 2.10                     | 0.50              |
| 2:2O:195:VAL:HG23 | 2:2O:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2R:306:ASP:HB3  | 2:2R:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2T:101:ASN:O    | 1:3G:257:THR:CG2  | 2.54                     | 0.50              |
| 2:2T:195:VAL:HG23 | 2:2T:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2T:352:LYS:NZ   | 2:2T:353:THR:O    | 2.44                     | 0.50              |
| 1:3B:103:TYR:HB2  | 1:3B:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3C:103:TYR:HB2  | 1:3C:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3I:138:PHE:HZ   | 1:3I:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:3J:138:PHE:HZ   | 1:3J:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:3L:103:TYR:HD2  | 1:3L:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3M:103:TYR:HB2  | 1:3M:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3N:103:TYR:HB2  | 1:3N:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:3T:154:ILE:HG12 | 2:3T:166:MET:HE2  | 1.94                     | 0.50              |
| 1:4A:224:TYR:O    | 1:4A:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:4D:283:HIS:HB3  | 1:4E:88:HIS:CG    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4O:306:ASP:HB3  | 2:4O:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:1B:138:PHE:HZ   | 1:1B:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:1B:346:TRP:CB   | 2:4O:397:ALA:C    | 2.79                     | 0.50              |
| 1:1B:434:GLU:C    | 2:4O:401:ARG:NH2  | 2.69                     | 0.50              |
| 1:1C:224:TYR:O    | 1:1C:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:1D:263:PRO:N    | 2:4Q:406:HIS:CG   | 2.74                     | 0.50              |
| 1:1F:254:GLU:CG   | 2:4S:100:GLY:C    | 2.84                     | 0.50              |
| 1:1F:256:GLN:O    | 2:4S:407:TRP:CE2  | 2.64                     | 0.50              |
| 1:1F:262:TYR:OH   | 2:4S:401:ARG:C    | 2.45                     | 0.50              |
| 1:1G:262:TYR:CZ   | 2:4T:403:ALA:HA   | 2.47                     | 0.50              |
| 1:1J:138:PHE:HZ   | 1:1J:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:1K:103:TYR:HD2  | 1:1K:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1L:325:PRO:CD   | 2:4X:223:THR:HA   | 2.38                     | 0.50              |
| 2:1O:195:VAL:HG23 | 2:1O:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1O:306:ASP:HB3  | 2:1O:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1Q:207:GLU:CD   | 1:2D:329:ASN:HD21 | 2.17                     | 0.50              |
| 2:1R:306:ASP:HB3  | 2:1R:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1W:154:ILE:HG12 | 2:1W:166:MET:HE2  | 1.94                     | 0.50              |
| 2:1W:181:VAL:HB   | 1:2K:258:ASN:C    | 2.31                     | 0.50              |
| 2:1Z:174:SER:OG   | 2:1Z:177:VAL:O    | 2.29                     | 0.50              |
| 1:2A:103:TYR:HD2  | 1:2A:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2C:103:TYR:HB2  | 1:2C:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2D:283:HIS:HB3  | 1:2E:88:HIS:CG    | 2.46                     | 0.50              |
| 1:2J:138:PHE:HZ   | 1:2J:235:VAL:HG11 | 1.75                     | 0.50              |
| 2:2O:101:ASN:HB2  | 1:3B:254:GLU:CB   | 2.41                     | 0.50              |
| 2:2O:181:VAL:CG2  | 1:3B:258:ASN:O    | 2.60                     | 0.50              |
| 2:2U:179:ASP:OD2  | 1:3I:248:LEU:HD21 | 2.11                     | 0.50              |
| 2:2U:306:ASP:HB3  | 2:2U:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2W:154:ILE:HG12 | 2:2W:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2X:404:PHE:HE1  | 1:3L:260:VAL:C    | 2.15                     | 0.50              |
| 2:2Y:11:GLN:HE22  | 1:3M:249:ASN:CA   | 2.21                     | 0.50              |
| 2:2Z:174:SER:OG   | 2:2Z:177:VAL:O    | 2.29                     | 0.50              |
| 1:3B:138:PHE:HZ   | 1:3B:235:VAL:HG11 | 1.76                     | 0.50              |
| 1:3D:283:HIS:HB3  | 1:3E:88:HIS:CG    | 2.46                     | 0.50              |
| 1:3K:103:TYR:HD2  | 1:3K:413:MET:HE1  | 1.77                     | 0.50              |
| 2:3O:306:ASP:HB3  | 2:3O:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3R:306:ASP:HB3  | 2:3R:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3S:195:VAL:HG23 | 2:3S:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:3X:174:SER:OG   | 2:3X:177:VAL:O    | 2.29                     | 0.50              |
| 2:3Z:174:SER:OG   | 2:3Z:177:VAL:O    | 2.29                     | 0.50              |
| 1:4A:138:PHE:HZ   | 1:4A:235:VAL:HG11 | 1.75                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4B:138:PHE:HZ   | 1:4B:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:4C:103:TYR:HB2  | 1:4C:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4E:224:TYR:O    | 1:4E:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:4K:103:TYR:HD2  | 1:4K:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4L:283:HIS:HB3  | 1:4M:88:HIS:CG    | 2.46                     | 0.50              |
| 1:4N:103:TYR:HB2  | 1:4N:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:4O:195:VAL:HG23 | 2:4O:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:4S:195:VAL:HG23 | 2:4S:196:GLU:HG2  | 1.93                     | 0.50              |
| 1:1A:138:PHE:HZ   | 1:1A:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:1A:249:ASN:N    | 2:4H:11:GLN:NE2   | 1.88                     | 0.50              |
| 1:1C:260:VAL:N    | 2:4P:404:PHE:CE1  | 2.77                     | 0.50              |
| 1:1C:349:THR:HG21 | 2:4P:184:PRO:CG   | 2.42                     | 0.50              |
| 1:1D:103:TYR:HD2  | 1:1D:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1F:439:SER:OG   | 2:4S:400:ARG:HG3  | 2.12                     | 0.50              |
| 1:1I:326:LYS:HG2  | 2:4U:210:TYR:CD1  | 2.47                     | 0.50              |
| 1:1J:103:TYR:HD2  | 1:1J:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1K:27:GLU:OE1   | 1:1K:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:1L:103:TYR:HB2  | 1:1L:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:1R:214:PHE:CG   | 1:2E:326:LYS:HE2  | 2.46                     | 0.50              |
| 2:1S:31:ASP:OD1   | 2:1S:35:SER:N     | 2.42                     | 0.50              |
| 2:1S:69:ASP:OD2   | 2:1S:74:THR:OG1   | 2.20                     | 0.50              |
| 2:1S:154:ILE:HG12 | 2:1S:166:MET:HE2  | 1.94                     | 0.50              |
| 2:1X:174:SER:OG   | 2:1X:177:VAL:O    | 2.29                     | 0.50              |
| 2:1X:176:LYS:HE2  | 1:2L:333:ALA:HB2  | 1.93                     | 0.50              |
| 2:1X:306:ASP:HB3  | 2:1X:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1Y:195:VAL:HG23 | 2:1Y:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1Y:404:PHE:CZ   | 1:2M:260:VAL:C    | 2.89                     | 0.50              |
| 1:2A:138:PHE:HZ   | 1:2A:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:2J:103:TYR:HD2  | 1:2J:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2K:27:GLU:OE1   | 1:2K:243:ARG:NH1  | 2.44                     | 0.50              |
| 2:2H:394:GLN:HG2  | 1:3A:348:PRO:HB2  | 1.89                     | 0.50              |
| 2:2O:306:ASP:HB3  | 2:2O:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2S:69:ASP:OD2   | 2:2S:74:THR:OG1   | 2.20                     | 0.50              |
| 2:2S:394:GLN:CG   | 1:3F:348:PRO:CB   | 2.79                     | 0.50              |
| 2:2T:221:THR:CB   | 1:3G:324:VAL:HG21 | 2.41                     | 0.50              |
| 2:2U:101:ASN:HB2  | 1:3I:254:GLU:HG2  | 1.93                     | 0.50              |
| 2:2U:404:PHE:CZ   | 1:3I:261:PRO:CB   | 2.95                     | 0.50              |
| 2:2X:174:SER:OG   | 2:2X:177:VAL:O    | 2.29                     | 0.50              |
| 2:2Y:11:GLN:HE22  | 1:3M:249:ASN:CB   | 2.25                     | 0.50              |
| 2:2Y:195:VAL:HG23 | 2:2Y:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2Z:73:GLY:HA3   | 1:3N:2:ARG:CZ     | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:394:GLN:OE1  | 1:3N:349:THR:CG2  | 2.60                     | 0.50              |
| 1:3A:138:PHE:HZ   | 1:3A:235:VAL:HG11 | 1.75                     | 0.50              |
| 1:3D:103:TYR:HD2  | 1:3D:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3J:27:GLU:OE1   | 1:3J:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:3L:103:TYR:HB2  | 1:3L:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:3H:69:ASP:OD2   | 2:3H:74:THR:OG1   | 2.20                     | 0.50              |
| 2:3Q:195:VAL:HG23 | 2:3Q:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:3S:31:ASP:OD1   | 2:3S:35:SER:N     | 2.43                     | 0.50              |
| 2:3S:69:ASP:OD2   | 2:3S:74:THR:OG1   | 2.20                     | 0.50              |
| 2:3U:306:ASP:HB3  | 2:3U:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:3W:154:ILE:HG12 | 2:3W:166:MET:HE2  | 1.94                     | 0.50              |
| 2:3Y:195:VAL:HG23 | 2:3Y:196:GLU:HG2  | 1.93                     | 0.50              |
| 1:4A:103:TYR:HD2  | 1:4A:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4C:224:TYR:O    | 1:4C:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:4D:103:TYR:HD2  | 1:4D:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4M:103:TYR:HB2  | 1:4M:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4N:224:TYR:O    | 1:4N:228:ASN:ND2  | 2.44                     | 0.50              |
| 2:4Q:283:TYR:OH   | 2:4R:85:GLN:O     | 2.18                     | 0.50              |
| 2:4S:69:ASP:OD2   | 2:4S:74:THR:OG1   | 2.20                     | 0.50              |
| 2:4T:352:LYS:NZ   | 2:4T:353:THR:O    | 2.44                     | 0.50              |
| 2:4U:306:ASP:HB3  | 2:4U:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:4W:154:ILE:HG12 | 2:4W:166:MET:HE2  | 1.94                     | 0.50              |
| 1:1A:103:TYR:HD2  | 1:1A:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1B:260:VAL:HG12 | 2:4O:406:HIS:CE1  | 2.47                     | 0.50              |
| 1:1C:103:TYR:HB2  | 1:1C:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1C:349:THR:O    | 2:4P:181:VAL:HA   | 2.12                     | 0.50              |
| 1:1D:2:ARG:HH11   | 2:4Q:71:GLU:CG    | 2.24                     | 0.50              |
| 1:1F:103:TYR:HB2  | 1:1F:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:1F:248:LEU:HA   | 2:4S:11:GLN:CD    | 2.35                     | 0.50              |
| 1:1G:326:LYS:CE   | 2:4T:210:TYR:O    | 2.59                     | 0.50              |
| 1:1I:435:VAL:CA   | 2:4U:401:ARG:NH2  | 2.74                     | 0.50              |
| 1:1J:27:GLU:OE1   | 1:1J:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:1J:248:LEU:CD1  | 5:4V:501:GDP:H8   | 2.25                     | 0.50              |
| 1:1L:346:TRP:CB   | 2:4X:398:MET:HA   | 2.27                     | 0.50              |
| 2:1O:394:GLN:HG2  | 1:2B:348:PRO:HG3  | 1.93                     | 0.50              |
| 2:1Q:195:VAL:HG23 | 2:1Q:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1S:195:VAL:HG23 | 2:1S:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1S:214:PHE:CG   | 1:2F:326:LYS:HE3  | 2.46                     | 0.50              |
| 2:1T:69:ASP:OD2   | 2:1T:74:THR:OG1   | 2.20                     | 0.50              |
| 2:1U:404:PHE:CG   | 1:2I:261:PRO:HA   | 2.47                     | 0.50              |
| 2:1W:180:THR:HA   | 1:2K:352:LYS:HD3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2C:224:TYR:O    | 1:2C:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:2D:103:TYR:HD2  | 1:2D:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2F:103:TYR:HB2  | 1:2F:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2J:27:GLU:OE1   | 1:2J:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:2L:103:TYR:HB2  | 1:2L:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:2O:401:ARG:HH22 | 1:3B:435:VAL:C    | 2.17                     | 0.50              |
| 2:2Q:101:ASN:HB2  | 1:3D:254:GLU:CB   | 2.41                     | 0.50              |
| 2:2Q:154:ILE:HG12 | 2:2Q:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2S:154:ILE:HG12 | 2:2S:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2S:195:VAL:HG23 | 2:2S:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2U:181:VAL:HG21 | 1:3I:314:ALA:CB   | 2.33                     | 0.50              |
| 2:2U:407:TRP:HE1  | 1:3I:260:VAL:CB   | 2.24                     | 0.50              |
| 2:2V:407:TRP:HE1  | 1:3J:260:VAL:CG1  | 2.25                     | 0.50              |
| 2:2W:157:ILE:O    | 2:2W:161:TYR:N    | 2.45                     | 0.50              |
| 2:2W:404:PHE:HE1  | 1:3K:260:VAL:C    | 2.14                     | 0.50              |
| 2:2Y:401:ARG:NH2  | 1:3M:435:VAL:CA   | 2.50                     | 0.50              |
| 2:2Z:154:ILE:HG12 | 2:2Z:166:MET:HE2  | 1.94                     | 0.50              |
| 1:3A:103:TYR:HD2  | 1:3A:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3C:224:TYR:O    | 1:3C:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:3J:103:TYR:HD2  | 1:3J:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3K:27:GLU:OE1   | 1:3K:243:ARG:NH1  | 2.44                     | 0.50              |
| 2:3O:195:VAL:HG23 | 2:3O:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:3S:154:ILE:HG12 | 2:3S:166:MET:HE2  | 1.94                     | 0.50              |
| 2:3T:69:ASP:OD2   | 2:3T:74:THR:OG1   | 2.20                     | 0.50              |
| 2:3W:157:ILE:O    | 2:3W:161:TYR:N    | 2.45                     | 0.50              |
| 2:3Z:154:ILE:HG12 | 2:3Z:166:MET:HE2  | 1.94                     | 0.50              |
| 1:4J:27:GLU:OE1   | 1:4J:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:4J:103:TYR:HD2  | 1:4J:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4K:27:GLU:OE1   | 1:4K:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:4L:103:TYR:HB2  | 1:4L:186:ASN:HD22 | 1.76                     | 0.50              |
| 2:4H:195:VAL:HG23 | 2:4H:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:4Q:154:ILE:HG12 | 2:4Q:166:MET:HE2  | 1.94                     | 0.50              |
| 2:4Q:195:VAL:HG23 | 2:4Q:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:4R:283:TYR:OH   | 2:4S:85:GLN:O     | 2.18                     | 0.50              |
| 2:4S:154:ILE:HG12 | 2:4S:166:MET:HE2  | 1.94                     | 0.50              |
| 2:4U:69:ASP:OD2   | 2:4U:74:THR:OG1   | 2.20                     | 0.50              |
| 2:4W:157:ILE:O    | 2:4W:161:TYR:N    | 2.45                     | 0.50              |
| 2:4X:174:SER:OG   | 2:4X:177:VAL:O    | 2.29                     | 0.50              |
| 2:4Y:195:VAL:HG23 | 2:4Y:196:GLU:HG2  | 1.93                     | 0.50              |
| 1:1A:326:LYS:CE   | 2:4H:214:PHE:CB   | 2.82                     | 0.50              |
| 1:1D:283:HIS:HB3  | 1:1E:88:HIS:CG    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:351:PHE:O    | 2:4Q:181:VAL:N    | 2.44                     | 0.50              |
| 1:1E:346:TRP:CD1  | 2:4R:401:ARG:CB   | 2.95                     | 0.50              |
| 1:1F:103:TYR:HD2  | 1:1F:413:MET:HE1  | 1.77                     | 0.50              |
| 1:1F:329:ASN:ND2  | 2:4S:210:TYR:HD2  | 2.09                     | 0.50              |
| 1:1G:261:PRO:C    | 2:4T:404:PHE:HA   | 2.36                     | 0.50              |
| 1:1J:351:PHE:N    | 2:4V:181:VAL:HG22 | 2.27                     | 0.50              |
| 1:1L:346:TRP:CH2  | 2:4X:404:PHE:CE2  | 2.99                     | 0.50              |
| 1:1N:240:ALA:HB1  | 1:1N:356:ASN:HD22 | 1.77                     | 0.50              |
| 2:1H:69:ASP:OD2   | 2:1H:74:THR:OG1   | 2.20                     | 0.50              |
| 2:1Q:154:ILE:HG12 | 2:1Q:166:MET:HE2  | 1.94                     | 0.50              |
| 2:1U:306:ASP:HB3  | 2:1U:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:1W:157:ILE:O    | 2:1W:161:TYR:N    | 2.45                     | 0.50              |
| 2:1Z:154:ILE:HG12 | 2:1Z:166:MET:HE2  | 1.94                     | 0.50              |
| 1:2D:103:TYR:HB2  | 1:2D:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:2F:103:TYR:HD2  | 1:2F:413:MET:HE1  | 1.77                     | 0.50              |
| 1:2N:224:TYR:O    | 1:2N:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:2N:240:ALA:HB1  | 1:2N:356:ASN:HD22 | 1.77                     | 0.50              |
| 2:2P:174:SER:OG   | 2:2P:177:VAL:O    | 2.29                     | 0.50              |
| 2:2P:195:VAL:HG23 | 2:2P:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2Q:195:VAL:HG23 | 2:2Q:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:2T:69:ASP:OD2   | 2:2T:74:THR:OG1   | 2.19                     | 0.50              |
| 2:2U:69:ASP:OD2   | 2:2U:74:THR:OG1   | 2.20                     | 0.50              |
| 2:2X:306:ASP:HB3  | 2:2X:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:3F:103:TYR:HB2  | 1:3F:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3F:103:TYR:HD2  | 1:3F:413:MET:HE1  | 1.77                     | 0.50              |
| 1:3G:27:GLU:OE1   | 1:3G:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:3N:224:TYR:O    | 1:3N:228:ASN:ND2  | 2.44                     | 0.50              |
| 2:3P:174:SER:OG   | 2:3P:177:VAL:O    | 2.29                     | 0.50              |
| 2:3Q:154:ILE:HG12 | 2:3Q:166:MET:HE2  | 1.94                     | 0.50              |
| 1:4A:71:GLU:HB3   | 1:4A:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:4D:103:TYR:HB2  | 1:4D:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:4G:27:GLU:OE1   | 1:4G:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:4M:240:ALA:HB1  | 1:4M:356:ASN:HD22 | 1.77                     | 0.50              |
| 1:4N:240:ALA:HB1  | 1:4N:356:ASN:HD22 | 1.77                     | 0.50              |
| 2:4H:31:ASP:OD1   | 2:4H:35:SER:N     | 2.43                     | 0.50              |
| 2:4R:174:SER:OG   | 2:4R:177:VAL:O    | 2.29                     | 0.50              |
| 2:4S:306:ASP:HB3  | 2:4S:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:4U:154:ILE:HG12 | 2:4U:166:MET:HE2  | 1.94                     | 0.50              |
| 2:4Z:154:ILE:HG12 | 2:4Z:166:MET:HE2  | 1.94                     | 0.50              |
| 1:1A:71:GLU:HB3   | 1:1A:98:ASP:HB3   | 1.93                     | 0.50              |
| 1:1A:240:ALA:HB1  | 1:1A:356:ASN:HD22 | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:261:PRO:HB2  | 2:4T:404:PHE:H    | 1.76                     | 0.50              |
| 1:1I:351:PHE:N    | 2:4U:181:VAL:HG22 | 2.27                     | 0.50              |
| 1:1J:2:ARG:HG3    | 2:4V:72:PRO:CG    | 2.42                     | 0.50              |
| 1:1L:347:CYS:SG   | 2:4X:181:VAL:HG13 | 2.51                     | 0.50              |
| 1:1M:240:ALA:HB1  | 1:1M:356:ASN:HD22 | 1.77                     | 0.50              |
| 1:1N:224:TYR:O    | 1:1N:228:ASN:ND2  | 2.44                     | 0.50              |
| 1:1N:253:THR:C    | 2:4Z:100:GLY:CA   | 2.85                     | 0.50              |
| 2:1O:174:SER:OG   | 2:1O:177:VAL:O    | 2.29                     | 0.50              |
| 2:1O:181:VAL:CG2  | 1:2B:258:ASN:O    | 2.60                     | 0.50              |
| 2:1P:174:SER:OG   | 2:1P:177:VAL:O    | 2.29                     | 0.50              |
| 2:1P:195:VAL:HG23 | 2:1P:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:1U:11:GLN:HE22  | 1:2I:249:ASN:CB   | 2.24                     | 0.50              |
| 2:1V:352:LYS:NZ   | 2:1V:353:THR:O    | 2.44                     | 0.50              |
| 2:1W:394:GLN:CD   | 1:2K:349:THR:HG23 | 2.37                     | 0.50              |
| 1:2G:27:GLU:OE1   | 1:2G:243:ARG:NH1  | 2.44                     | 0.50              |
| 1:2M:240:ALA:HB1  | 1:2M:356:ASN:HD22 | 1.77                     | 0.50              |
| 2:2H:31:ASP:OD1   | 2:2H:35:SER:N     | 2.42                     | 0.50              |
| 2:2P:100:GLY:HA2  | 1:3C:253:THR:C    | 2.36                     | 0.50              |
| 2:2Q:223:THR:HA   | 1:3D:325:PRO:CD   | 2.41                     | 0.50              |
| 2:2Q:406:HIS:CE1  | 1:3D:263:PRO:N    | 2.80                     | 0.50              |
| 2:2R:174:SER:OG   | 2:2R:177:VAL:O    | 2.29                     | 0.50              |
| 2:2R:283:TYR:OH   | 2:2S:85:GLN:O     | 2.18                     | 0.50              |
| 2:2S:101:ASN:C    | 1:3F:257:THR:HG21 | 2.36                     | 0.50              |
| 2:2S:306:ASP:HB3  | 2:2S:309:HIS:HD2  | 1.77                     | 0.50              |
| 2:2T:101:ASN:N    | 1:3G:254:GLU:HG2  | 2.27                     | 0.50              |
| 2:2T:157:ILE:O    | 2:2T:161:TYR:N    | 2.45                     | 0.50              |
| 2:2U:154:ILE:HG12 | 2:2U:166:MET:HE2  | 1.94                     | 0.50              |
| 2:2U:180:THR:N    | 1:3I:351:PHE:O    | 2.45                     | 0.50              |
| 2:2W:11:GLN:NE2   | 1:3K:249:ASN:HB2  | 2.27                     | 0.50              |
| 1:3D:103:TYR:HB2  | 1:3D:186:ASN:HD22 | 1.76                     | 0.50              |
| 1:3M:240:ALA:HB1  | 1:3M:356:ASN:HD22 | 1.77                     | 0.50              |
| 1:3N:240:ALA:HB1  | 1:3N:356:ASN:HD22 | 1.77                     | 0.50              |
| 2:3H:31:ASP:OD1   | 2:3H:35:SER:N     | 2.42                     | 0.50              |
| 2:3O:154:ILE:HG12 | 2:3O:166:MET:HE2  | 1.94                     | 0.50              |
| 2:3P:195:VAL:HG23 | 2:3P:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:3R:174:SER:OG   | 2:3R:177:VAL:O    | 2.29                     | 0.50              |
| 2:3U:69:ASP:OD2   | 2:3U:74:THR:OG1   | 2.20                     | 0.50              |
| 2:3U:154:ILE:HG12 | 2:3U:166:MET:HE2  | 1.94                     | 0.50              |
| 2:3X:306:ASP:HB3  | 2:3X:309:HIS:HD2  | 1.77                     | 0.50              |
| 1:4F:100:ALA:N    | 3:4F:501:GTP:O2G  | 2.41                     | 0.50              |
| 1:4F:103:TYR:HB2  | 1:4F:186:ASN:HD22 | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4F:103:TYR:HD2  | 1:4F:413:MET:HE1  | 1.77                     | 0.50              |
| 1:4M:100:ALA:N    | 3:4M:501:GTP:O2G  | 2.41                     | 0.50              |
| 2:4P:195:VAL:HG23 | 2:4P:196:GLU:HG2  | 1.93                     | 0.50              |
| 2:4T:69:ASP:OD2   | 2:4T:74:THR:OG1   | 2.20                     | 0.50              |
| 1:1C:2:ARG:CZ     | 2:4P:73:GLY:HA3   | 2.42                     | 0.49              |
| 1:1F:352:LYS:HA   | 2:4S:180:THR:HA   | 1.93                     | 0.49              |
| 1:1G:27:GLU:OE1   | 1:1G:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:1G:260:VAL:HG12 | 2:4T:407:TRP:NE1  | 2.26                     | 0.49              |
| 1:1L:352:LYS:CE   | 2:4U:101:ASN:ND2  | 2.74                     | 0.49              |
| 1:1K:253:THR:C    | 2:4W:100:GLY:HA2  | 2.37                     | 0.49              |
| 1:1L:71:GLU:HB3   | 1:1L:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:1L:240:ALA:HB1  | 1:1L:356:ASN:HD22 | 1.77                     | 0.49              |
| 2:1H:195:VAL:HG23 | 2:1H:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:1O:154:ILE:HG12 | 2:1O:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1P:394:GLN:HG2  | 1:2C:348:PRO:HG3  | 1.93                     | 0.49              |
| 2:1R:174:SER:OG   | 2:1R:177:VAL:O    | 2.29                     | 0.49              |
| 2:1R:404:PHE:CD1  | 1:2E:260:VAL:O    | 2.65                     | 0.49              |
| 2:1U:69:ASP:OD2   | 2:1U:74:THR:OG1   | 2.20                     | 0.49              |
| 2:1X:352:LYS:NZ   | 2:1X:353:THR:O    | 2.44                     | 0.49              |
| 2:1X:404:PHE:CZ   | 1:2L:261:PRO:CA   | 2.95                     | 0.49              |
| 2:1Z:195:VAL:HG23 | 2:1Z:196:GLU:HG2  | 1.93                     | 0.49              |
| 1:2A:71:GLU:HB3   | 1:2A:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:2A:240:ALA:HB1  | 1:2A:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2F:100:ALA:N    | 3:2F:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:2L:71:GLU:HB3   | 1:2L:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:2H:195:VAL:HG23 | 2:2H:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:2O:154:ILE:HG12 | 2:2O:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2O:174:SER:OG   | 2:2O:177:VAL:O    | 2.29                     | 0.49              |
| 2:2S:181:VAL:CB   | 1:3F:258:ASN:O    | 2.59                     | 0.49              |
| 2:2U:404:PHE:CE2  | 1:3I:261:PRO:CB   | 2.82                     | 0.49              |
| 2:2V:174:SER:OG   | 2:2V:177:VAL:O    | 2.29                     | 0.49              |
| 1:3A:71:GLU:HB3   | 1:3A:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:3F:100:ALA:N    | 3:3F:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:3N:71:GLU:HB3   | 1:3N:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:3H:195:VAL:HG23 | 2:3H:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:3S:306:ASP:HB3  | 2:3S:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:3T:157:ILE:O    | 2:3T:161:TYR:N    | 2.45                     | 0.49              |
| 2:3V:174:SER:OG   | 2:3V:177:VAL:O    | 2.29                     | 0.49              |
| 1:4K:71:GLU:HB3   | 1:4K:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:4L:71:GLU:HB3   | 1:4L:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:4N:71:GLU:HB3   | 1:4N:98:ASP:HB3   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4H:306:ASP:HB3  | 2:4H:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:4O:154:ILE:HG12 | 2:4O:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4O:174:SER:OG   | 2:4O:177:VAL:O    | 2.29                     | 0.49              |
| 2:4T:157:ILE:O    | 2:4T:161:TYR:N    | 2.45                     | 0.49              |
| 2:4X:306:ASP:HB3  | 2:4X:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:1A:326:LYS:HE2  | 2:4H:210:TYR:O    | 2.12                     | 0.49              |
| 1:1C:262:TYR:OH   | 2:4P:402:LYS:C    | 2.55                     | 0.49              |
| 1:1C:333:ALA:HB1  | 2:4P:176:LYS:CE   | 2.23                     | 0.49              |
| 1:1D:103:TYR:HB2  | 1:1D:186:ASN:HD22 | 1.76                     | 0.49              |
| 1:1E:352:LYS:CD   | 2:4R:101:ASN:HD22 | 2.21                     | 0.49              |
| 1:1F:261:PRO:O    | 2:4S:404:PHE:HA   | 2.11                     | 0.49              |
| 1:1F:435:VAL:CA   | 2:4S:401:ARG:HH21 | 2.01                     | 0.49              |
| 1:1I:247:ALA:C    | 2:4U:15:GLN:HE22  | 2.19                     | 0.49              |
| 1:1I:325:PRO:O    | 2:4U:210:TYR:CZ   | 2.64                     | 0.49              |
| 1:1J:253:THR:C    | 2:4V:100:GLY:CA   | 2.86                     | 0.49              |
| 1:1K:71:GLU:HB3   | 1:1K:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:1L:262:TYR:CZ   | 2:4X:403:ALA:HA   | 2.46                     | 0.49              |
| 1:1M:100:ALA:N    | 3:1M:501:GTP:O2G  | 2.41                     | 0.49              |
| 2:1H:31:ASP:OD1   | 2:1H:35:SER:N     | 2.42                     | 0.49              |
| 2:1P:141:LEU:HD12 | 2:1P:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1S:306:ASP:HB3  | 2:1S:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:1U:11:GLN:HE22  | 1:2I:249:ASN:H    | 1.59                     | 0.49              |
| 2:1U:154:ILE:HG12 | 2:1U:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1X:176:LYS:HE2  | 1:2L:333:ALA:CB   | 2.42                     | 0.49              |
| 5:1Y:501:GDP:C8   | 1:2M:248:LEU:CD1  | 2.95                     | 0.49              |
| 1:2K:71:GLU:HB3   | 1:2K:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:2L:240:ALA:HB1  | 1:2L:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2M:100:ALA:N    | 3:2M:501:GTP:O2G  | 2.41                     | 0.49              |
| 2:2H:306:ASP:HB3  | 2:2H:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:2O:406:HIS:CD2  | 1:3B:262:TYR:HA   | 2.47                     | 0.49              |
| 2:2P:223:THR:HA   | 1:3C:325:PRO:HD2  | 1.94                     | 0.49              |
| 2:2P:224:TYR:CD2  | 1:3C:247:ALA:O    | 2.64                     | 0.49              |
| 2:2S:179:ASP:O    | 1:3F:352:LYS:CD   | 2.52                     | 0.49              |
| 2:2V:352:LYS:NZ   | 2:2V:353:THR:O    | 2.44                     | 0.49              |
| 2:2W:174:SER:OG   | 2:2W:177:VAL:O    | 2.29                     | 0.49              |
| 2:2W:404:PHE:HA   | 1:3K:261:PRO:O    | 2.12                     | 0.49              |
| 1:3A:240:ALA:HB1  | 1:3A:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3L:71:GLU:HB3   | 1:3L:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:3L:240:ALA:HB1  | 1:3L:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3M:100:ALA:N    | 3:3M:501:GTP:O2G  | 2.41                     | 0.49              |
| 2:3O:174:SER:OG   | 2:3O:177:VAL:O    | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3V:141:LEU:HD12 | 2:3V:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3V:352:LYS:NZ   | 2:3V:353:THR:O    | 2.44                     | 0.49              |
| 2:3X:352:LYS:NZ   | 2:3X:353:THR:O    | 2.44                     | 0.49              |
| 1:4A:240:ALA:HB1  | 1:4A:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4L:240:ALA:HB1  | 1:4L:356:ASN:HD22 | 1.77                     | 0.49              |
| 2:4P:141:LEU:HD12 | 2:4P:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:4V:174:SER:OG   | 2:4V:177:VAL:O    | 2.29                     | 0.49              |
| 2:4W:174:SER:OG   | 2:4W:177:VAL:O    | 2.29                     | 0.49              |
| 1:1A:349:THR:OG1  | 2:4H:184:PRO:CD   | 2.60                     | 0.49              |
| 1:1E:435:VAL:O    | 2:4R:401:ARG:CZ   | 2.60                     | 0.49              |
| 1:1N:71:GLU:HB3   | 1:1N:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:1H:174:SER:OG   | 2:1H:177:VAL:O    | 2.29                     | 0.49              |
| 2:1H:222:PRO:O    | 1:2A:325:PRO:HD2  | 2.12                     | 0.49              |
| 2:1H:306:ASP:HB3  | 2:1H:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:1U:141:LEU:HD12 | 2:1U:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1V:154:ILE:HG12 | 2:1V:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1V:181:VAL:CB   | 1:2J:258:ASN:C    | 2.83                     | 0.49              |
| 1:2B:103:TYR:HD2  | 1:2B:413:MET:HE1  | 1.77                     | 0.49              |
| 1:2N:71:GLU:HB3   | 1:2N:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:2H:100:GLY:CA   | 1:3A:253:THR:HG22 | 2.13                     | 0.49              |
| 2:2O:141:LEU:HD12 | 2:2O:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2P:141:LEU:HD12 | 2:2P:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2R:69:ASP:OD2   | 2:2R:74:THR:OG1   | 2.19                     | 0.49              |
| 2:2T:210:TYR:CD2  | 1:3G:329:ASN:CB   | 2.96                     | 0.49              |
| 2:2U:141:LEU:HD12 | 2:2U:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2V:141:LEU:HD12 | 2:2V:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2Z:195:VAL:HG23 | 2:2Z:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:3H:174:SER:OG   | 2:3H:177:VAL:O    | 2.29                     | 0.49              |
| 2:3H:306:ASP:HB3  | 2:3H:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:3P:141:LEU:HD12 | 2:3P:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3R:69:ASP:OD2   | 2:3R:74:THR:OG1   | 2.20                     | 0.49              |
| 2:3R:283:TYR:OH   | 2:3S:85:GLN:O     | 2.18                     | 0.49              |
| 2:3U:141:LEU:HD12 | 2:3U:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3W:174:SER:OG   | 2:3W:177:VAL:O    | 2.29                     | 0.49              |
| 2:3Z:195:VAL:HG23 | 2:3Z:196:GLU:HG2  | 1.93                     | 0.49              |
| 1:4B:103:TYR:HD2  | 1:4B:413:MET:HE1  | 1.77                     | 0.49              |
| 2:4U:141:LEU:HD12 | 2:4U:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:4V:141:LEU:HD12 | 2:4V:172:VAL:HG22 | 1.94                     | 0.49              |
| 1:1B:103:TYR:HD2  | 1:1B:413:MET:HE1  | 1.77                     | 0.49              |
| 1:1C:257:THR:HG21 | 2:4P:101:ASN:C    | 2.36                     | 0.49              |
| 1:1F:100:ALA:N    | 3:1F:501:GTP:O2G  | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:326:LYS:HB2  | 2:4S:222:PRO:HG2  | 1.94                     | 0.49              |
| 1:1G:2:ARG:HH22   | 2:4T:73:GLY:HA3   | 1.77                     | 0.49              |
| 1:1J:348:PRO:CD   | 2:4V:398:MET:CG   | 2.87                     | 0.49              |
| 1:1K:435:VAL:HA   | 2:4W:401:ARG:NH2  | 2.27                     | 0.49              |
| 1:1N:324:VAL:HG11 | 2:4Z:221:THR:C    | 2.37                     | 0.49              |
| 2:1H:141:LEU:HD12 | 2:1H:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1O:141:LEU:HD12 | 2:1O:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1Q:141:LEU:HD12 | 2:1Q:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1Q:181:VAL:N    | 1:2D:258:ASN:ND2  | 2.52                     | 0.49              |
| 2:1U:401:ARG:CB   | 1:2I:262:TYR:OH   | 2.54                     | 0.49              |
| 2:1V:69:ASP:OD2   | 2:1V:74:THR:OG1   | 2.20                     | 0.49              |
| 2:1V:174:SER:OG   | 2:1V:177:VAL:O    | 2.29                     | 0.49              |
| 2:1W:174:SER:OG   | 2:1W:177:VAL:O    | 2.29                     | 0.49              |
| 1:2E:103:TYR:HD2  | 1:2E:413:MET:HE1  | 1.77                     | 0.49              |
| 1:2K:240:ALA:HB1  | 1:2K:356:ASN:HD22 | 1.77                     | 0.49              |
| 2:2H:141:LEU:HD12 | 2:2H:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2H:154:ILE:HG12 | 2:2H:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2H:174:SER:OG   | 2:2H:177:VAL:O    | 2.29                     | 0.49              |
| 2:2H:394:GLN:HB3  | 1:3A:348:PRO:HG2  | 1.93                     | 0.49              |
| 2:2P:101:ASN:CB   | 1:3C:254:GLU:HG2  | 2.39                     | 0.49              |
| 2:2Q:141:LEU:HD12 | 2:2Q:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:2R:394:GLN:OE1  | 1:3E:349:THR:HG23 | 2.13                     | 0.49              |
| 2:2U:397:ALA:O    | 1:3I:346:TRP:HB3  | 2.11                     | 0.49              |
| 2:2V:154:ILE:HG12 | 2:2V:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2X:72:PRO:HG2   | 1:3L:2:ARG:HG3    | 1.93                     | 0.49              |
| 2:2Z:214:PHE:CG   | 1:3N:326:LYS:HE3  | 2.47                     | 0.49              |
| 1:3E:103:TYR:HD2  | 1:3E:413:MET:HE1  | 1.77                     | 0.49              |
| 1:3K:71:GLU:HB3   | 1:3K:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:3H:141:LEU:HD12 | 2:3H:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3O:141:LEU:HD12 | 2:3O:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3V:154:ILE:HG12 | 2:3V:166:MET:HE2  | 1.94                     | 0.49              |
| 1:4E:103:TYR:HD2  | 1:4E:413:MET:HE1  | 1.77                     | 0.49              |
| 2:4H:141:LEU:HD12 | 2:4H:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:4H:154:ILE:HG12 | 2:4H:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4H:174:SER:OG   | 2:4H:177:VAL:O    | 2.29                     | 0.49              |
| 2:4O:141:LEU:HD12 | 2:4O:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:4Q:141:LEU:HD12 | 2:4Q:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:4V:69:ASP:OD2   | 2:4V:74:THR:OG1   | 2.19                     | 0.49              |
| 2:4V:154:ILE:HG12 | 2:4V:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4V:352:LYS:NZ   | 2:4V:353:THR:O    | 2.44                     | 0.49              |
| 2:4Z:195:VAL:HG23 | 2:4Z:196:GLU:HG2  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:324:VAL:HG11 | 2:4H:221:THR:C    | 2.37                     | 0.49              |
| 1:1A:324:VAL:CG1  | 2:4H:222:PRO:O    | 2.60                     | 0.49              |
| 1:1B:261:PRO:HA   | 2:4O:404:PHE:N    | 2.27                     | 0.49              |
| 1:1B:346:TRP:O    | 2:4O:398:MET:N    | 2.45                     | 0.49              |
| 1:1G:326:LYS:NZ   | 2:4T:210:TYR:HB3  | 2.27                     | 0.49              |
| 1:1I:346:TRP:CZ3  | 2:4U:404:PHE:HE2  | 2.27                     | 0.49              |
| 1:1J:347:CYS:SG   | 2:4V:181:VAL:HG13 | 2.52                     | 0.49              |
| 1:1J:348:PRO:HB2  | 2:4V:394:GLN:CG   | 2.43                     | 0.49              |
| 2:1H:154:ILE:HG12 | 2:1H:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1P:401:ARG:NH2  | 1:2C:435:VAL:HA   | 2.23                     | 0.49              |
| 2:1P:404:PHE:CE1  | 1:2C:260:VAL:C    | 2.90                     | 0.49              |
| 2:1R:69:ASP:OD2   | 2:1R:74:THR:OG1   | 2.20                     | 0.49              |
| 2:1R:195:VAL:HG23 | 2:1R:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:1S:221:THR:CA   | 1:2F:324:VAL:CG1  | 2.74                     | 0.49              |
| 2:1V:141:LEU:HD12 | 2:1V:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:1X:154:ILE:HG12 | 2:1X:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1Y:176:LYS:HE2  | 1:2M:333:ALA:HB2  | 1.95                     | 0.49              |
| 2:1Z:177:VAL:HG23 | 1:2N:332:ILE:HG21 | 1.94                     | 0.49              |
| 2:2R:403:ALA:HA   | 1:3E:262:TYR:CZ   | 2.47                     | 0.49              |
| 2:2R:404:PHE:HD1  | 1:3E:260:VAL:O    | 1.94                     | 0.49              |
| 2:2T:207:GLU:CD   | 1:3G:329:ASN:ND2  | 2.53                     | 0.49              |
| 2:2T:394:GLN:NE2  | 1:3G:348:PRO:HB2  | 2.28                     | 0.49              |
| 2:2U:222:PRO:C    | 1:3I:324:VAL:HG13 | 2.37                     | 0.49              |
| 2:2U:407:TRP:HE1  | 1:3I:260:VAL:HG12 | 1.78                     | 0.49              |
| 2:2V:69:ASP:OD2   | 2:2V:74:THR:OG1   | 2.20                     | 0.49              |
| 2:2V:394:GLN:CG   | 1:3J:348:PRO:HG2  | 2.40                     | 0.49              |
| 2:2W:398:MET:CG   | 1:3K:346:TRP:O    | 2.61                     | 0.49              |
| 2:2X:154:ILE:HG12 | 2:2X:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2Y:154:ILE:HG12 | 2:2Y:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2Z:141:LEU:HD12 | 2:2Z:172:VAL:HG22 | 1.94                     | 0.49              |
| 1:3B:103:TYR:HD2  | 1:3B:413:MET:HE1  | 1.77                     | 0.49              |
| 2:3H:154:ILE:HG12 | 2:3H:166:MET:HE2  | 1.94                     | 0.49              |
| 2:3Q:141:LEU:HD12 | 2:3Q:172:VAL:HG22 | 1.94                     | 0.49              |
| 2:3R:195:VAL:HG23 | 2:3R:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:3Y:154:ILE:HG12 | 2:3Y:166:MET:HE2  | 1.94                     | 0.49              |
| 2:3Z:141:LEU:HD12 | 2:3Z:172:VAL:HG22 | 1.94                     | 0.49              |
| 1:4E:103:TYR:HB2  | 1:4E:186:ASN:HD22 | 1.76                     | 0.49              |
| 1:4F:27:GLU:OE1   | 1:4F:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:4I:103:TYR:HD2  | 1:4I:413:MET:HE1  | 1.77                     | 0.49              |
| 2:4R:69:ASP:OD2   | 2:4R:74:THR:OG1   | 2.20                     | 0.49              |
| 2:4T:306:ASP:HB3  | 2:4T:309:HIS:HD2  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4X:154:ILE:HG12 | 2:4X:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4Y:154:ILE:HG12 | 2:4Y:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4Z:141:LEU:HD12 | 2:4Z:172:VAL:HG22 | 1.94                     | 0.49              |
| 1:1B:240:ALA:HB1  | 1:1B:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1B:254:GLU:CG   | 2:4O:101:ASN:HB2  | 2.43                     | 0.49              |
| 1:1B:260:VAL:O    | 2:4O:404:PHE:HD1  | 1.96                     | 0.49              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:HA   | 2.11                     | 0.49              |
| 1:1D:262:TYR:CZ   | 2:4Q:402:LYS:O    | 2.65                     | 0.49              |
| 1:1E:103:TYR:HD2  | 1:1E:413:MET:HE1  | 1.77                     | 0.49              |
| 1:1F:259:LEU:C    | 2:4S:404:PHE:HE1  | 2.21                     | 0.49              |
| 1:1F:353:VAL:CA   | 2:4S:179:ASP:OD1  | 2.57                     | 0.49              |
| 1:1G:261:PRO:CA   | 2:4T:404:PHE:H    | 2.26                     | 0.49              |
| 1:1I:27:GLU:OE1   | 1:1I:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:1I:103:TYR:HD2  | 1:1I:413:MET:HE1  | 1.77                     | 0.49              |
| 1:1I:349:THR:O    | 2:4U:181:VAL:O    | 2.30                     | 0.49              |
| 1:1K:240:ALA:HB1  | 1:1K:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1M:71:GLU:HB3   | 1:1M:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:1S:404:PHE:CE2  | 1:2F:261:PRO:HA   | 2.47                     | 0.49              |
| 2:1Y:154:ILE:HG12 | 2:1Y:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1Y:306:ASP:HB3  | 2:1Y:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:1Z:141:LEU:HD12 | 2:1Z:172:VAL:HG22 | 1.94                     | 0.49              |
| 1:2B:240:ALA:HB1  | 1:2B:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2F:27:GLU:OE1   | 1:2F:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:2I:27:GLU:OE1   | 1:2I:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:2I:100:ALA:N    | 3:2I:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:2I:103:TYR:HD2  | 1:2I:413:MET:HE1  | 1.77                     | 0.49              |
| 1:2L:334:THR:O    | 1:2L:337:THR:OG1  | 2.30                     | 0.49              |
| 2:2R:401:ARG:HG3  | 1:3E:346:TRP:CD1  | 2.47                     | 0.49              |
| 2:2R:404:PHE:CA   | 1:3E:261:PRO:HA   | 2.43                     | 0.49              |
| 2:2S:222:PRO:O    | 1:3F:324:VAL:HG13 | 2.13                     | 0.49              |
| 2:2T:174:SER:OG   | 2:2T:177:VAL:O    | 2.29                     | 0.49              |
| 2:2T:210:TYR:CD2  | 1:3G:329:ASN:HB2  | 2.47                     | 0.49              |
| 2:2Y:306:ASP:HB3  | 2:2Y:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:3F:27:GLU:OE1   | 1:3F:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:3I:27:GLU:OE1   | 1:3I:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:3I:103:TYR:HD2  | 1:3I:413:MET:HE1  | 1.77                     | 0.49              |
| 1:3K:240:ALA:HB1  | 1:3K:356:ASN:HD22 | 1.77                     | 0.49              |
| 2:3T:174:SER:OG   | 2:3T:177:VAL:O    | 2.29                     | 0.49              |
| 2:3V:69:ASP:OD2   | 2:3V:74:THR:OG1   | 2.20                     | 0.49              |
| 2:3X:154:ILE:HG12 | 2:3X:166:MET:HE2  | 1.94                     | 0.49              |
| 1:4B:240:ALA:HB1  | 1:4B:356:ASN:HD22 | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4I:100:ALA:N    | 3:4I:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:4K:240:ALA:HB1  | 1:4K:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4L:334:THR:O    | 1:4L:337:THR:OG1  | 2.30                     | 0.49              |
| 1:4M:71:GLU:HB3   | 1:4M:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:4R:195:VAL:HG23 | 2:4R:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:4T:174:SER:OG   | 2:4T:177:VAL:O    | 2.29                     | 0.49              |
| 2:4Y:306:ASP:HB3  | 2:4Y:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:1B:263:PRO:HD3  | 2:4O:406:HIS:CB   | 2.39                     | 0.49              |
| 1:1F:240:ALA:HB1  | 1:1F:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1F:260:VAL:CB   | 2:4S:407:TRP:HZ2  | 2.25                     | 0.49              |
| 1:1G:348:PRO:CG   | 2:4T:394:GLN:CG   | 2.91                     | 0.49              |
| 1:1I:260:VAL:CG1  | 2:4U:407:TRP:CE2  | 2.95                     | 0.49              |
| 1:1I:329:ASN:ND2  | 2:4U:210:TYR:CD2  | 2.72                     | 0.49              |
| 1:1M:252:LEU:HA   | 1:1M:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:1R:154:ILE:HG12 | 2:1R:166:MET:HE2  | 1.94                     | 0.49              |
| 2:1R:283:TYR:OH   | 2:1S:85:GLN:O     | 2.18                     | 0.49              |
| 2:1U:404:PHE:CE1  | 1:2I:261:PRO:CA   | 2.94                     | 0.49              |
| 2:1Y:214:PHE:HB2  | 1:2M:326:LYS:CE   | 2.31                     | 0.49              |
| 1:2G:252:LEU:HA   | 1:2G:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:2Q:406:HIS:CE1  | 1:3D:263:PRO:HA   | 2.48                     | 0.49              |
| 2:2R:195:VAL:HG23 | 2:2R:196:GLU:HG2  | 1.93                     | 0.49              |
| 2:2R:406:HIS:CG   | 1:3E:263:PRO:CD   | 2.87                     | 0.49              |
| 2:2T:306:ASP:HB3  | 2:2T:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:2W:394:GLN:CG   | 1:3K:348:PRO:HG2  | 2.38                     | 0.49              |
| 2:2Z:223:THR:HA   | 1:3N:325:PRO:CD   | 2.42                     | 0.49              |
| 1:3B:240:ALA:HB1  | 1:3B:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3E:103:TYR:HB2  | 1:3E:186:ASN:HD22 | 1.76                     | 0.49              |
| 1:3I:100:ALA:N    | 3:3I:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:3M:71:GLU:HB3   | 1:3M:98:ASP:HB3   | 1.93                     | 0.49              |
| 2:3Y:306:ASP:HB3  | 2:3Y:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:4G:252:LEU:HA   | 1:4G:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:4I:27:GLU:OE1   | 1:4I:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:4M:252:LEU:HA   | 1:4M:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:1F:27:GLU:OE1   | 1:1F:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:1I:346:TRP:CH2  | 2:4U:403:ALA:CB   | 2.81                     | 0.49              |
| 1:1J:240:ALA:HB1  | 1:1J:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1J:251:ASP:OD2  | 2:4V:71:GLU:HB3   | 2.12                     | 0.49              |
| 1:1J:329:ASN:OD1  | 2:4V:177:VAL:HG11 | 2.13                     | 0.49              |
| 1:1K:325:PRO:HB3  | 2:4W:224:TYR:CZ   | 2.48                     | 0.49              |
| 1:1M:324:VAL:HG13 | 2:4Y:222:PRO:C    | 2.38                     | 0.49              |
| 1:1M:348:PRO:HB2  | 2:4Y:394:GLN:HG2  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:352:LYS:HD3  | 2:4Y:101:ASN:ND2  | 2.28                     | 0.49              |
| 2:1T:174:SER:OG   | 2:1T:177:VAL:O    | 2.29                     | 0.49              |
| 2:1T:306:ASP:HB3  | 2:1T:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:1V:157:ILE:O    | 2:1V:161:TYR:N    | 2.45                     | 0.49              |
| 2:1X:10:GLY:O     | 2:1X:14:ASN:ND2   | 2.46                     | 0.49              |
| 1:2E:103:TYR:HB2  | 1:2E:186:ASN:HD22 | 1.76                     | 0.49              |
| 1:2J:240:ALA:HB1  | 1:2J:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2M:71:GLU:HB3   | 1:2M:98:ASP:HB3   | 1.93                     | 0.49              |
| 1:2M:252:LEU:HA   | 1:2M:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:2H:407:TRP:NE1  | 1:3A:260:VAL:HB   | 2.27                     | 0.49              |
| 2:2R:401:ARG:C    | 1:3E:262:TYR:OH   | 2.49                     | 0.49              |
| 2:2S:71:GLU:HG3   | 1:3F:2:ARG:NH1    | 2.28                     | 0.49              |
| 2:2S:406:HIS:CG   | 1:3F:263:PRO:CD   | 2.80                     | 0.49              |
| 2:2U:181:VAL:CG2  | 1:3I:258:ASN:O    | 2.61                     | 0.49              |
| 2:2V:157:ILE:O    | 2:2V:161:TYR:N    | 2.45                     | 0.49              |
| 2:2X:10:GLY:O     | 2:2X:14:ASN:ND2   | 2.46                     | 0.49              |
| 2:2Z:394:GLN:OE1  | 1:3N:349:THR:HG23 | 2.12                     | 0.49              |
| 1:3F:240:ALA:HB1  | 1:3F:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3J:240:ALA:HB1  | 1:3J:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3M:252:LEU:HA   | 1:3M:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:3T:306:ASP:HB3  | 2:3T:309:HIS:HD2  | 1.77                     | 0.49              |
| 2:3V:157:ILE:O    | 2:3V:161:TYR:N    | 2.45                     | 0.49              |
| 1:4J:240:ALA:HB1  | 1:4J:356:ASN:HD22 | 1.77                     | 0.49              |
| 2:4P:174:SER:OG   | 2:4P:177:VAL:O    | 2.29                     | 0.49              |
| 2:4X:10:GLY:O     | 2:4X:14:ASN:ND2   | 2.46                     | 0.49              |
| 1:1B:435:VAL:C    | 2:4O:401:ARG:NH2  | 2.52                     | 0.49              |
| 1:1D:261:PRO:HD3  | 2:4Q:404:PHE:CE1  | 2.48                     | 0.49              |
| 1:1E:240:ALA:HB1  | 1:1E:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1E:353:VAL:N    | 2:4R:179:ASP:O    | 2.45                     | 0.49              |
| 1:1F:324:VAL:HG12 | 2:4S:222:PRO:O    | 2.10                     | 0.49              |
| 1:1G:240:ALA:HB1  | 1:1G:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1G:252:LEU:HA   | 1:1G:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:1G:253:THR:O    | 2:4T:100:GLY:HA3  | 2.13                     | 0.49              |
| 1:1I:240:ALA:HB1  | 1:1I:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:1I:252:LEU:HA   | 1:1I:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:1J:248:LEU:HD12 | 2:4V:11:GLN:OE1   | 2.13                     | 0.49              |
| 1:1L:27:GLU:OE1   | 1:1L:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:1N:252:LEU:HA   | 1:1N:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:1N:254:GLU:N    | 2:4Z:100:GLY:HA2  | 2.27                     | 0.49              |
| 2:1W:404:PHE:CG   | 1:2K:261:PRO:HA   | 2.47                     | 0.49              |
| 1:2F:240:ALA:HB1  | 1:2F:356:ASN:HD22 | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2I:240:ALA:HB1  | 1:2I:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2L:252:LEU:HA   | 1:2L:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:2N:252:LEU:HA   | 1:2N:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:2O:101:ASN:CB   | 1:3B:254:GLU:HG2  | 2.35                     | 0.49              |
| 2:2Q:178:SER:OG   | 1:3D:351:PHE:HB2  | 2.13                     | 0.49              |
| 2:2Q:224:TYR:HD2  | 1:3D:247:ALA:O    | 1.96                     | 0.49              |
| 2:2S:221:THR:C    | 1:3F:324:VAL:HG11 | 2.38                     | 0.49              |
| 2:2S:221:THR:CA   | 1:3F:324:VAL:HG11 | 2.42                     | 0.49              |
| 2:2T:101:ASN:HB2  | 1:3G:254:GLU:HG2  | 1.93                     | 0.49              |
| 2:2U:174:SER:OG   | 2:2U:177:VAL:O    | 2.29                     | 0.49              |
| 2:2V:181:VAL:H    | 1:3J:258:ASN:HD22 | 1.60                     | 0.49              |
| 2:2Z:11:GLN:HE22  | 1:3N:249:ASN:CB   | 2.26                     | 0.49              |
| 1:3G:240:ALA:HB1  | 1:3G:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3G:252:LEU:HA   | 1:3G:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:3I:252:LEU:HA   | 1:3I:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:3K:252:LEU:HA   | 1:3K:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:3R:154:ILE:HG12 | 2:3R:166:MET:HE2  | 1.94                     | 0.49              |
| 2:3X:10:GLY:O     | 2:3X:14:ASN:ND2   | 2.46                     | 0.49              |
| 1:4F:240:ALA:HB1  | 1:4F:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4G:240:ALA:HB1  | 1:4G:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4I:240:ALA:HB1  | 1:4I:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4I:252:LEU:HA   | 1:4I:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:4L:252:LEU:HA   | 1:4L:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:4N:252:LEU:HA   | 1:4N:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:4U:174:SER:OG   | 2:4U:177:VAL:O    | 2.29                     | 0.49              |
| 2:4V:157:ILE:O    | 2:4V:161:TYR:N    | 2.45                     | 0.49              |
| 1:1B:348:PRO:HB2  | 2:4O:394:GLN:NE2  | 2.28                     | 0.49              |
| 1:1C:257:THR:CG2  | 2:4P:101:ASN:O    | 2.61                     | 0.49              |
| 1:1C:260:VAL:HG12 | 2:4P:407:TRP:NE1  | 2.24                     | 0.49              |
| 1:1C:329:ASN:ND2  | 2:4P:210:TYR:HD2  | 2.06                     | 0.49              |
| 1:1C:351:PHE:N    | 2:4P:178:SER:OG   | 2.46                     | 0.49              |
| 1:1C:439:SER:CB   | 2:4P:400:ARG:CD   | 2.90                     | 0.49              |
| 1:1D:2:ARG:HD3    | 2:4Q:71:GLU:CB    | 2.32                     | 0.49              |
| 1:1D:260:VAL:CG1  | 2:4Q:407:TRP:CE2  | 2.96                     | 0.49              |
| 1:1E:103:TYR:HB2  | 1:1E:186:ASN:HD22 | 1.76                     | 0.49              |
| 1:1G:2:ARG:HD3    | 2:4T:71:GLU:HB2   | 1.95                     | 0.49              |
| 1:1G:329:ASN:CG   | 2:4T:207:GLU:OE1  | 2.54                     | 0.49              |
| 1:1I:100:ALA:N    | 3:1I:501:GTP:O2G  | 2.41                     | 0.49              |
| 1:1J:252:LEU:HA   | 1:1J:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:1J:326:LYS:HA   | 2:4V:210:TYR:CZ   | 2.47                     | 0.49              |
| 1:1J:326:LYS:HB3  | 2:4V:222:PRO:HG2  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:346:TRP:CE2  | 2:4V:403:ALA:HB2  | 2.47                     | 0.49              |
| 1:1J:435:VAL:O    | 2:4V:401:ARG:NH2  | 2.46                     | 0.49              |
| 1:1J:439:SER:OG   | 2:4V:401:ARG:CG   | 2.61                     | 0.49              |
| 1:1L:247:ALA:O    | 2:4X:15:GLN:NE2   | 2.44                     | 0.49              |
| 1:1M:27:GLU:OE1   | 1:1M:243:ARG:NH1  | 2.44                     | 0.49              |
| 2:1H:180:THR:HA   | 1:2A:352:LYS:HD3  | 1.95                     | 0.49              |
| 2:1O:352:LYS:NZ   | 2:1O:353:THR:O    | 2.44                     | 0.49              |
| 2:1W:224:TYR:HE2  | 1:2K:248:LEU:CB   | 2.17                     | 0.49              |
| 1:2E:240:ALA:HB1  | 1:2E:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2G:240:ALA:HB1  | 1:2G:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:2I:252:LEU:HA   | 1:2I:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:2K:252:LEU:HA   | 1:2K:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:2H:394:GLN:CB   | 1:3A:348:PRO:HG2  | 2.43                     | 0.49              |
| 2:2Q:406:HIS:CD2  | 1:3D:262:TYR:CA   | 2.96                     | 0.49              |
| 2:2R:154:ILE:HG12 | 2:2R:166:MET:HE2  | 1.94                     | 0.49              |
| 2:2T:404:PHE:CD1  | 1:3G:261:PRO:N    | 2.81                     | 0.49              |
| 2:2W:10:GLY:O     | 2:2W:14:ASN:ND2   | 2.46                     | 0.49              |
| 2:2W:101:ASN:HB2  | 1:3K:254:GLU:CG   | 2.42                     | 0.49              |
| 2:2Y:222:PRO:CG   | 1:3M:326:LYS:CB   | 2.91                     | 0.49              |
| 2:2Z:306:ASP:HB3  | 2:2Z:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:3I:240:ALA:HB1  | 1:3I:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:3L:27:GLU:OE1   | 1:3L:243:ARG:NH1  | 2.44                     | 0.49              |
| 1:3L:252:LEU:HA   | 1:3L:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:3N:252:LEU:HA   | 1:3N:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:3O:352:LYS:NZ   | 2:3O:353:THR:O    | 2.44                     | 0.49              |
| 2:3U:174:SER:OG   | 2:3U:177:VAL:O    | 2.29                     | 0.49              |
| 2:3W:10:GLY:O     | 2:3W:14:ASN:ND2   | 2.46                     | 0.49              |
| 1:4E:240:ALA:HB1  | 1:4E:356:ASN:HD22 | 1.77                     | 0.49              |
| 1:4J:252:LEU:HA   | 1:4J:255:PHE:HD2  | 1.78                     | 0.49              |
| 1:4K:252:LEU:HA   | 1:4K:255:PHE:HD2  | 1.78                     | 0.49              |
| 2:4R:154:ILE:HG12 | 2:4R:166:MET:HE2  | 1.94                     | 0.49              |
| 2:4W:10:GLY:O     | 2:4W:14:ASN:ND2   | 2.46                     | 0.49              |
| 2:4Z:306:ASP:HB3  | 2:4Z:309:HIS:HD2  | 1.77                     | 0.49              |
| 1:1A:329:ASN:HB2  | 2:4H:210:TYR:HE2  | 1.68                     | 0.48              |
| 1:1A:352:LYS:HA   | 2:4H:179:ASP:C    | 2.38                     | 0.48              |
| 1:1C:353:VAL:N    | 2:4P:179:ASP:OD1  | 2.46                     | 0.48              |
| 1:1E:261:PRO:C    | 2:4R:404:PHE:CA   | 2.83                     | 0.48              |
| 1:1K:252:LEU:HA   | 1:1K:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1L:252:LEU:HA   | 1:1L:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1M:258:ASN:OD1  | 2:4Y:101:ASN:ND2  | 2.46                     | 0.48              |
| 1:1M:349:THR:HG21 | 2:4Y:183:GLU:HG3  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1R:141:LEU:HD12 | 2:1R:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1S:157:ILE:O    | 2:1S:161:TYR:N    | 2.45                     | 0.48              |
| 2:1T:406:HIS:CE1  | 1:2G:263:PRO:HB3  | 2.48                     | 0.48              |
| 2:1U:174:SER:OG   | 2:1U:177:VAL:O    | 2.29                     | 0.48              |
| 2:1V:100:GLY:O    | 1:2J:253:THR:HG22 | 2.13                     | 0.48              |
| 2:1V:404:PHE:CE1  | 1:2J:261:PRO:HA   | 2.47                     | 0.48              |
| 2:1V:404:PHE:HE1  | 1:2J:260:VAL:N    | 2.11                     | 0.48              |
| 2:1W:10:GLY:O     | 2:1W:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:2C:103:TYR:HD2  | 1:2C:413:MET:HE1  | 1.77                     | 0.48              |
| 1:2J:252:LEU:HA   | 1:2J:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:2L:27:GLU:OE1   | 1:2L:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:2M:27:GLU:OE1   | 1:2M:243:ARG:NH1  | 2.44                     | 0.48              |
| 2:2H:404:PHE:CD2  | 1:3A:261:PRO:HA   | 2.48                     | 0.48              |
| 2:2Q:179:ASP:O    | 1:3D:352:LYS:CD   | 2.46                     | 0.48              |
| 2:2R:214:PHE:HB2  | 1:3E:326:LYS:HE3  | 1.93                     | 0.48              |
| 2:2U:210:TYR:CD2  | 1:3I:329:ASN:HB2  | 2.47                     | 0.48              |
| 2:2U:407:TRP:CD1  | 1:3I:260:VAL:O    | 2.66                     | 0.48              |
| 2:2V:10:GLY:O     | 2:2V:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2Y:141:LEU:HD12 | 2:2Y:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:2Y:407:TRP:HE1  | 1:3M:260:VAL:HB   | 1.78                     | 0.48              |
| 1:3E:240:ALA:HB1  | 1:3E:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:3J:252:LEU:HA   | 1:3J:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3M:27:GLU:OE1   | 1:3M:243:ARG:NH1  | 2.44                     | 0.48              |
| 2:3S:157:ILE:O    | 2:3S:161:TYR:N    | 2.45                     | 0.48              |
| 2:3Y:141:LEU:HD12 | 2:3Y:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:3Z:306:ASP:HB3  | 2:3Z:309:HIS:HD2  | 1.77                     | 0.48              |
| 1:4C:103:TYR:HD2  | 1:4C:413:MET:HE1  | 1.77                     | 0.48              |
| 1:4M:27:GLU:OE1   | 1:4M:243:ARG:NH1  | 2.44                     | 0.48              |
| 2:4V:10:GLY:O     | 2:4V:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:1C:253:THR:O    | 2:4P:100:GLY:O    | 2.29                     | 0.48              |
| 1:1E:248:LEU:HD11 | 5:4R:501:GDP:O1A  | 2.13                     | 0.48              |
| 2:1H:10:GLY:O     | 2:1H:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1O:179:ASP:O    | 1:2B:352:LYS:CD   | 2.60                     | 0.48              |
| 2:1R:394:GLN:HG2  | 1:2E:348:PRO:CG   | 2.43                     | 0.48              |
| 2:1V:10:GLY:O     | 2:1V:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1V:100:GLY:C    | 1:2J:253:THR:HG22 | 2.38                     | 0.48              |
| 2:1Z:157:ILE:O    | 2:1Z:161:TYR:N    | 2.45                     | 0.48              |
| 1:2A:252:LEU:HA   | 1:2A:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:2G:228:ASN:OD1  | 3:2G:501:GTP:N1   | 2.46                     | 0.48              |
| 2:2Q:210:TYR:CZ   | 1:3D:325:PRO:O    | 2.66                     | 0.48              |
| 2:2R:141:LEU:HD12 | 2:2R:172:VAL:HG22 | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2S:157:ILE:O    | 2:2S:161:TYR:N    | 2.45                     | 0.48              |
| 2:2W:406:HIS:CE1  | 1:3K:263:PRO:HA   | 2.48                     | 0.48              |
| 1:3C:103:TYR:HD2  | 1:3C:413:MET:HE1  | 1.77                     | 0.48              |
| 1:3G:228:ASN:OD1  | 3:3G:501:GTP:N1   | 2.47                     | 0.48              |
| 2:3R:141:LEU:HD12 | 2:3R:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:3V:10:GLY:O     | 2:3V:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:4A:252:LEU:HA   | 1:4A:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:4C:240:ALA:HB1  | 1:4C:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:4C:252:LEU:HA   | 1:4C:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:4L:27:GLU:OE1   | 1:4L:243:ARG:NH1  | 2.44                     | 0.48              |
| 2:4H:10:GLY:O     | 2:4H:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4R:141:LEU:HD12 | 2:4R:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:4S:157:ILE:O    | 2:4S:161:TYR:N    | 2.45                     | 0.48              |
| 2:4Y:141:LEU:HD12 | 2:4Y:172:VAL:HG22 | 1.94                     | 0.48              |
| 1:1A:252:LEU:HA   | 1:1A:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1B:324:VAL:HG11 | 2:4O:222:PRO:N    | 2.28                     | 0.48              |
| 1:1C:103:TYR:HD2  | 1:1C:413:MET:HE1  | 1.77                     | 0.48              |
| 1:1C:240:ALA:HB1  | 1:1C:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:1C:252:LEU:HA   | 1:1C:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1D:326:LYS:HA   | 2:4Q:210:TYR:CZ   | 2.47                     | 0.48              |
| 1:1E:349:THR:O    | 2:4R:181:VAL:O    | 2.31                     | 0.48              |
| 1:1F:261:PRO:HB3  | 2:4S:404:PHE:CE2  | 2.47                     | 0.48              |
| 1:1F:326:LYS:NZ   | 2:4S:210:TYR:HB3  | 2.29                     | 0.48              |
| 1:1G:228:ASN:OD1  | 3:1G:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1I:332:ILE:CB   | 2:4U:177:VAL:CG2  | 2.91                     | 0.48              |
| 1:1J:346:TRP:HZ3  | 2:4V:404:PHE:CD2  | 2.31                     | 0.48              |
| 1:1M:2:ARG:HG3    | 2:4Y:72:PRO:CG    | 2.43                     | 0.48              |
| 2:1H:157:ILE:O    | 2:1H:161:TYR:N    | 2.45                     | 0.48              |
| 2:1H:306:ASP:HB3  | 2:1H:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1U:182:VAL:HG21 | 1:2I:257:THR:HG22 | 1.94                     | 0.48              |
| 2:1U:404:PHE:CD1  | 1:2I:261:PRO:HA   | 2.48                     | 0.48              |
| 2:1X:141:LEU:HD12 | 2:1X:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1X:179:ASP:O    | 1:2L:352:LYS:HE2  | 2.12                     | 0.48              |
| 2:1Y:141:LEU:HD12 | 2:1Y:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1Z:306:ASP:HB3  | 2:1Z:309:HIS:HD2  | 1.77                     | 0.48              |
| 1:2C:240:ALA:HB1  | 1:2C:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:2C:252:LEU:HA   | 1:2C:255:PHE:HD2  | 1.78                     | 0.48              |
| 2:2H:10:GLY:O     | 2:2H:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2Q:179:ASP:O    | 1:3D:352:LYS:HA   | 2.13                     | 0.48              |
| 2:2Q:404:PHE:CA   | 1:3D:261:PRO:O    | 2.61                     | 0.48              |
| 2:2S:72:PRO:CG    | 1:3F:2:ARG:HG3    | 2.41                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:407:TRP:HE1  | 1:3J:260:VAL:HB   | 1.78                     | 0.48              |
| 2:2X:11:GLN:HE22  | 1:3L:249:ASN:H    | 0.61                     | 0.48              |
| 1:3A:252:LEU:HA   | 1:3A:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3C:240:ALA:HB1  | 1:3C:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:3F:228:ASN:OD1  | 3:3F:501:GTP:N1   | 2.46                     | 0.48              |
| 2:3H:10:GLY:O     | 2:3H:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3Z:157:ILE:O    | 2:3Z:161:TYR:N    | 2.45                     | 0.48              |
| 1:4D:203:MET:HG3  | 1:4D:384:ILE:HD11 | 1.95                     | 0.48              |
| 1:4E:154:MET:HE1  | 1:4E:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:4F:154:MET:HE1  | 1:4F:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:4G:228:ASN:OD1  | 3:4G:501:GTP:N1   | 2.47                     | 0.48              |
| 2:4P:283:TYR:OH   | 2:4Q:85:GLN:O     | 2.18                     | 0.48              |
| 2:4W:141:LEU:HD12 | 2:4W:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:4Y:10:GLY:O     | 2:4Y:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:1A:228:ASN:OD1  | 3:1A:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1A:248:LEU:HA   | 2:4H:11:GLN:NE2   | 2.27                     | 0.48              |
| 1:1A:253:THR:HB   | 2:4H:100:GLY:HA2  | 1.95                     | 0.48              |
| 1:1A:346:TRP:CD1  | 2:4H:401:ARG:HG3  | 2.49                     | 0.48              |
| 1:1D:203:MET:HG3  | 1:1D:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:1D:248:LEU:CD2  | 2:4Q:179:ASP:OD2  | 2.61                     | 0.48              |
| 1:1D:253:THR:O    | 2:4Q:100:GLY:HA3  | 2.11                     | 0.48              |
| 1:1D:254:GLU:CA   | 2:4Q:100:GLY:CA   | 2.90                     | 0.48              |
| 1:1E:247:ALA:O    | 2:4R:15:GLN:NE2   | 2.46                     | 0.48              |
| 1:1E:258:ASN:OD1  | 2:4R:101:ASN:CG   | 2.57                     | 0.48              |
| 1:1E:261:PRO:C    | 2:4R:404:PHE:N    | 2.61                     | 0.48              |
| 1:1F:228:ASN:OD1  | 3:1F:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1F:257:THR:CG2  | 2:4S:102:ASN:CB   | 2.79                     | 0.48              |
| 1:1I:262:TYR:C    | 2:4U:406:HIS:CD2  | 2.78                     | 0.48              |
| 1:1K:325:PRO:HB2  | 2:4W:224:TYR:CE1  | 2.47                     | 0.48              |
| 2:1O:172:VAL:HG11 | 2:1O:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1O:224:TYR:CD2  | 1:2B:247:ALA:O    | 2.67                     | 0.48              |
| 2:1R:214:PHE:CG   | 1:2E:326:LYS:CE   | 2.96                     | 0.48              |
| 2:1R:224:TYR:CD2  | 1:2E:247:ALA:O    | 2.67                     | 0.48              |
| 2:1Z:101:ASN:HB2  | 1:2N:254:GLU:CD   | 2.38                     | 0.48              |
| 1:2D:203:MET:HG3  | 1:2D:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:2D:240:ALA:HB1  | 1:2D:356:ASN:HD22 | 1.77                     | 0.48              |
| 2:2H:71:GLU:HB2   | 1:3A:2:ARG:CD     | 2.33                     | 0.48              |
| 2:2H:157:ILE:O    | 2:2H:161:TYR:N    | 2.45                     | 0.48              |
| 2:2H:306:ASP:HB3  | 2:2H:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:2T:222:PRO:HG2  | 1:3G:326:LYS:HB3  | 1.91                     | 0.48              |
| 2:2W:178:SER:CB   | 1:3K:349:THR:HB   | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Z:101:ASN:ND2  | 1:3N:258:ASN:OD1  | 2.46                     | 0.48              |
| 2:2Z:157:ILE:O    | 2:2Z:161:TYR:N    | 2.45                     | 0.48              |
| 2:2Z:306:ASP:HB3  | 2:2Z:309:HIS:CD2  | 2.49                     | 0.48              |
| 1:3A:228:ASN:OD1  | 3:3A:501:GTP:N1   | 2.47                     | 0.48              |
| 1:3C:252:LEU:HA   | 1:3C:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3D:240:ALA:HB1  | 1:3D:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:3E:154:MET:HE1  | 1:3E:166:LYS:HB3  | 1.95                     | 0.48              |
| 2:3H:157:ILE:O    | 2:3H:161:TYR:N    | 2.45                     | 0.48              |
| 2:3H:306:ASP:HB3  | 2:3H:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3T:141:LEU:HD12 | 2:3T:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:3X:141:LEU:HD12 | 2:3X:172:VAL:HG22 | 1.94                     | 0.48              |
| 1:4A:228:ASN:OD1  | 3:4A:501:GTP:N1   | 2.47                     | 0.48              |
| 2:4H:157:ILE:O    | 2:4H:161:TYR:N    | 2.45                     | 0.48              |
| 2:4T:306:ASP:HB3  | 2:4T:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4Z:157:ILE:O    | 2:4Z:161:TYR:N    | 2.45                     | 0.48              |
| 1:1A:262:TYR:CE1  | 2:4H:402:LYS:O    | 2.66                     | 0.48              |
| 1:1C:260:VAL:O    | 2:4P:404:PHE:CD1  | 2.66                     | 0.48              |
| 1:1D:240:ALA:HB1  | 1:1D:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:1D:252:LEU:HA   | 1:1D:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1D:260:VAL:N    | 2:4Q:404:PHE:CE1  | 2.81                     | 0.48              |
| 1:1E:258:ASN:OD1  | 2:4R:101:ASN:CB   | 2.61                     | 0.48              |
| 1:1E:324:VAL:HG12 | 2:4R:222:PRO:O    | 2.08                     | 0.48              |
| 1:1F:2:ARG:HG3    | 2:4S:72:PRO:HG2   | 1.94                     | 0.48              |
| 1:1F:203:MET:HG3  | 1:1F:384:ILE:HD11 | 1.95                     | 0.48              |
| 1:1F:263:PRO:HA   | 2:4S:406:HIS:CE1  | 2.49                     | 0.48              |
| 1:1I:248:LEU:HA   | 2:4U:11:GLN:CD    | 2.32                     | 0.48              |
| 1:1I:326:LYS:CA   | 2:4U:210:TYR:CE1  | 2.90                     | 0.48              |
| 1:1L:228:ASN:OD1  | 3:1L:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1L:439:SER:OG   | 2:4X:401:ARG:CD   | 2.61                     | 0.48              |
| 2:1S:10:GLY:O     | 2:1S:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1T:141:LEU:HD12 | 2:1T:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1T:306:ASP:HB3  | 2:1T:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1Y:157:ILE:O    | 2:1Y:161:TYR:N    | 2.45                     | 0.48              |
| 2:1Z:306:ASP:HB3  | 2:1Z:309:HIS:CD2  | 2.49                     | 0.48              |
| 1:2A:228:ASN:OD1  | 3:2A:501:GTP:N1   | 2.47                     | 0.48              |
| 1:2E:154:MET:HE1  | 1:2E:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:2F:154:MET:HE1  | 1:2F:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:2F:228:ASN:OD1  | 3:2F:501:GTP:N1   | 2.47                     | 0.48              |
| 1:2G:154:MET:HE1  | 1:2G:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:2L:228:ASN:OD1  | 3:2L:501:GTP:N1   | 2.47                     | 0.48              |
| 2:2O:172:VAL:HG11 | 2:2O:387:LEU:HD21 | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2O:401:ARG:HG3  | 1:3B:346:TRP:CD1  | 2.48                     | 0.48              |
| 2:2P:283:TYR:OH   | 2:2Q:85:GLN:O     | 2.18                     | 0.48              |
| 2:2P:406:HIS:CE1  | 1:3C:263:PRO:CA   | 2.96                     | 0.48              |
| 2:2R:394:GLN:CG   | 1:3E:348:PRO:HB2  | 2.42                     | 0.48              |
| 5:2R:501:GDP:H8   | 1:3E:248:LEU:HD11 | 1.68                     | 0.48              |
| 2:2T:141:LEU:HD12 | 2:2T:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:2T:306:ASP:HB3  | 2:2T:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:2U:179:ASP:OD1  | 1:3I:353:VAL:CB   | 2.61                     | 0.48              |
| 2:2W:141:LEU:HD12 | 2:2W:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:2X:141:LEU:HD12 | 2:2X:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:2Y:10:GLY:O     | 2:2Y:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:3D:203:MET:HG3  | 1:3D:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:3F:154:MET:HE1  | 1:3F:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:3G:154:MET:HE1  | 1:3G:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:3L:228:ASN:OD1  | 3:3L:501:GTP:N1   | 2.46                     | 0.48              |
| 2:3O:172:VAL:HG11 | 2:3O:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:3T:306:ASP:HB3  | 2:3T:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3U:306:ASP:HB3  | 2:3U:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3X:288:VAL:HB   | 2:3X:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:3Y:10:GLY:O     | 2:3Y:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3Z:306:ASP:HB3  | 2:3Z:309:HIS:CD2  | 2.49                     | 0.48              |
| 1:4D:240:ALA:HB1  | 1:4D:356:ASN:HD22 | 1.77                     | 0.48              |
| 1:4F:228:ASN:OD1  | 3:4F:501:GTP:N1   | 2.47                     | 0.48              |
| 1:4F:252:LEU:HA   | 1:4F:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:4G:154:MET:HE1  | 1:4G:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:4L:228:ASN:OD1  | 3:4L:501:GTP:N1   | 2.47                     | 0.48              |
| 2:4H:306:ASP:HB3  | 2:4H:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4O:172:VAL:HG11 | 2:4O:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:4T:141:LEU:HD12 | 2:4T:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:4X:141:LEU:HD12 | 2:4X:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:4X:288:VAL:HB   | 2:4X:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:4Z:306:ASP:HB3  | 2:4Z:309:HIS:CD2  | 2.49                     | 0.48              |
| 1:1B:2:ARG:HG3    | 2:4O:72:PRO:CD    | 2.44                     | 0.48              |
| 1:1C:247:ALA:O    | 2:4P:15:GLN:OE1   | 2.32                     | 0.48              |
| 1:1E:154:MET:HE1  | 1:1E:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:1E:203:MET:HG3  | 1:1E:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:1E:228:ASN:OD1  | 3:1E:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1E:326:LYS:CG   | 2:4R:210:TYR:CD1  | 2.97                     | 0.48              |
| 1:1F:154:MET:HE1  | 1:1F:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:1G:154:MET:HE1  | 1:1G:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:1G:332:ILE:CB   | 2:4T:177:VAL:HG23 | 2.38                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:348:PRO:HG3  | 2:4U:394:GLN:C    | 2.39                     | 0.48              |
| 2:1O:306:ASP:HB3  | 2:1O:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1P:172:VAL:HG11 | 2:1P:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1U:306:ASP:HB3  | 2:1U:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1W:141:LEU:HD12 | 2:1W:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1Y:10:GLY:O     | 2:1Y:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:2E:203:MET:HG3  | 1:2E:384:ILE:HD11 | 1.95                     | 0.48              |
| 1:2F:203:MET:HG3  | 1:2F:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:2F:252:LEU:HA   | 1:2F:255:PHE:HD2  | 1.78                     | 0.48              |
| 2:2H:172:VAL:HG11 | 2:2H:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:2P:172:VAL:HG11 | 2:2P:387:LEU:HD21 | 1.96                     | 0.48              |
| 5:2P:501:GDP:H8   | 1:3C:248:LEU:HD11 | 1.74                     | 0.48              |
| 2:2U:181:VAL:HG21 | 1:3I:258:ASN:O    | 2.13                     | 0.48              |
| 2:2U:306:ASP:HB3  | 2:2U:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:2X:288:VAL:HB   | 2:2X:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:2Y:157:ILE:O    | 2:2Y:161:TYR:N    | 2.45                     | 0.48              |
| 2:2Z:406:HIS:NE2  | 1:3N:263:PRO:CD   | 2.69                     | 0.48              |
| 1:3E:203:MET:HG3  | 1:3E:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:3F:203:MET:HG3  | 1:3F:384:ILE:HD11 | 1.96                     | 0.48              |
| 2:3H:172:VAL:HG11 | 2:3H:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:3O:306:ASP:HB3  | 2:3O:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3P:172:VAL:HG11 | 2:3P:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:3S:10:GLY:O     | 2:3S:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3V:288:VAL:HB   | 2:3V:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:3W:141:LEU:HD12 | 2:3W:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:3Y:157:ILE:O    | 2:3Y:161:TYR:N    | 2.45                     | 0.48              |
| 1:4A:215:ARG:NH2  | 1:4A:299:ALA:O    | 2.47                     | 0.48              |
| 1:4B:252:LEU:HA   | 1:4B:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:4D:154:MET:HE1  | 1:4D:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:4F:203:MET:HG3  | 1:4F:384:ILE:HD11 | 1.96                     | 0.48              |
| 2:4H:172:VAL:HG11 | 2:4H:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:4P:172:VAL:HG11 | 2:4P:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:4S:10:GLY:O     | 2:4S:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4U:306:ASP:HB3  | 2:4U:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4V:288:VAL:HB   | 2:4V:327:GLU:HG2  | 1.96                     | 0.48              |
| 1:1A:215:ARG:NH2  | 1:1A:299:ALA:O    | 2.47                     | 0.48              |
| 1:1B:326:LYS:HG2  | 2:4O:210:TYR:CB   | 2.44                     | 0.48              |
| 1:1D:154:MET:HE1  | 1:1D:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:1D:352:LYS:HA   | 2:4Q:180:THR:HA   | 1.94                     | 0.48              |
| 1:1E:326:LYS:HE3  | 2:4R:214:PHE:HB2  | 1.96                     | 0.48              |
| 1:1F:252:LEU:HA   | 1:1F:255:PHE:HD2  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1G:439:SER:CB   | 2:4T:400:ARG:CD   | 2.92                     | 0.48              |
| 1:1I:258:ASN:OD1  | 2:4U:101:ASN:ND2  | 2.46                     | 0.48              |
| 1:1I:346:TRP:CH2  | 2:4U:404:PHE:CE2  | 3.02                     | 0.48              |
| 1:1J:261:PRO:O    | 2:4V:406:HIS:HD2  | 1.91                     | 0.48              |
| 1:1K:228:ASN:OD1  | 3:1K:501:GTP:N1   | 2.47                     | 0.48              |
| 1:1K:332:ILE:HB   | 2:4W:177:VAL:HG21 | 1.94                     | 0.48              |
| 1:1L:349:THR:HG21 | 2:4X:183:GLU:CG   | 2.44                     | 0.48              |
| 2:1H:172:VAL:HG11 | 2:1H:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1H:181:VAL:CB   | 1:2A:258:ASN:O    | 2.62                     | 0.48              |
| 2:1H:222:PRO:HG2  | 1:2A:326:LYS:HB2  | 1.96                     | 0.48              |
| 2:1O:157:ILE:O    | 2:1O:161:TYR:N    | 2.45                     | 0.48              |
| 2:1R:157:ILE:O    | 2:1R:161:TYR:N    | 2.45                     | 0.48              |
| 2:1R:214:PHE:CD1  | 1:2E:326:LYS:HE3  | 2.49                     | 0.48              |
| 2:1U:172:VAL:HG11 | 2:1U:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1U:181:VAL:CG2  | 1:2I:258:ASN:CA   | 2.91                     | 0.48              |
| 2:1V:180:THR:HG23 | 1:2J:258:ASN:ND2  | 2.28                     | 0.48              |
| 2:1X:205:ASP:OD2  | 2:1X:304:ALA:N    | 2.35                     | 0.48              |
| 2:1X:288:VAL:HB   | 2:1X:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:1Z:10:GLY:O     | 2:1Z:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:2A:215:ARG:NH2  | 1:2A:299:ALA:O    | 2.47                     | 0.48              |
| 1:2D:154:MET:HE1  | 1:2D:166:LYS:HB3  | 1.95                     | 0.48              |
| 5:2H:501:GDP:H8   | 1:3A:248:LEU:HD11 | 1.76                     | 0.48              |
| 2:2O:157:ILE:O    | 2:2O:161:TYR:N    | 2.45                     | 0.48              |
| 2:2O:306:ASP:HB3  | 2:2O:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:2Q:10:GLY:O     | 2:2Q:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2S:10:GLY:O     | 2:2S:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2S:141:LEU:HD12 | 2:2S:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:2W:100:GLY:O    | 1:3K:257:THR:CB   | 2.62                     | 0.48              |
| 2:2Y:404:PHE:CZ   | 1:3M:261:PRO:HB3  | 2.47                     | 0.48              |
| 1:3D:154:MET:HE1  | 1:3D:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:3D:252:LEU:HA   | 1:3D:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3F:252:LEU:HA   | 1:3F:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3G:203:MET:HG3  | 1:3G:384:ILE:HD11 | 1.96                     | 0.48              |
| 2:3Q:10:GLY:O     | 2:3Q:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3U:10:GLY:O     | 2:3U:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3U:172:VAL:HG11 | 2:3U:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:3Z:10:GLY:O     | 2:3Z:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:4E:203:MET:HG3  | 1:4E:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:4G:203:MET:HG3  | 1:4G:384:ILE:HD11 | 1.96                     | 0.48              |
| 2:4O:306:ASP:HB3  | 2:4O:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4Q:10:GLY:O     | 2:4Q:14:ASN:ND2   | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4S:141:LEU:HD12 | 2:4S:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:4S:306:ASP:HB3  | 2:4S:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4Y:157:ILE:O    | 2:4Y:161:TYR:N    | 2.45                     | 0.48              |
| 1:1B:252:LEU:HA   | 1:1B:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:1B:349:THR:CG2  | 2:4O:394:GLN:OE1  | 2.61                     | 0.48              |
| 1:1C:215:ARG:NH2  | 1:1C:299:ALA:O    | 2.47                     | 0.48              |
| 1:1C:257:THR:HG21 | 2:4P:102:ASN:HB2  | 1.96                     | 0.48              |
| 1:1E:260:VAL:HG21 | 2:4R:407:TRP:CZ2  | 2.48                     | 0.48              |
| 1:1G:203:MET:HG3  | 1:1G:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:1G:346:TRP:CZ2  | 2:4T:403:ALA:CB   | 2.97                     | 0.48              |
| 1:1I:154:MET:HE1  | 1:1I:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:1I:349:THR:CG2  | 2:4U:184:PRO:HG3  | 2.43                     | 0.48              |
| 1:1M:332:ILE:HB   | 2:4Y:177:VAL:HG21 | 1.96                     | 0.48              |
| 1:1N:346:TRP:HB2  | 2:4Z:397:ALA:O    | 2.12                     | 0.48              |
| 2:1O:10:GLY:O     | 2:1O:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1P:157:ILE:O    | 2:1P:161:TYR:N    | 2.45                     | 0.48              |
| 2:1Q:10:GLY:O     | 2:1Q:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1R:207:GLU:OE1  | 1:2E:329:ASN:ND2  | 2.43                     | 0.48              |
| 2:1T:172:VAL:HG11 | 2:1T:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1T:404:PHE:CE2  | 1:2G:261:PRO:CA   | 2.95                     | 0.48              |
| 2:1U:10:GLY:O     | 2:1U:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:1V:406:HIS:CD2  | 1:2J:263:PRO:CD   | 2.85                     | 0.48              |
| 1:2B:252:LEU:HA   | 1:2B:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:2D:252:LEU:HA   | 1:2D:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:2E:228:ASN:OD1  | 3:2E:501:GTP:N1   | 2.47                     | 0.48              |
| 1:2G:203:MET:HG3  | 1:2G:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:2I:154:MET:HE1  | 1:2I:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:2K:228:ASN:OD1  | 3:2K:501:GTP:N1   | 2.47                     | 0.48              |
| 2:2H:406:HIS:CE1  | 1:3A:263:PRO:CA   | 2.97                     | 0.48              |
| 2:2O:10:GLY:O     | 2:2O:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2P:72:PRO:HD2   | 1:3C:2:ARG:HD3    | 1.95                     | 0.48              |
| 2:2P:100:GLY:CA   | 1:3C:253:THR:C    | 2.86                     | 0.48              |
| 5:2Q:501:GDP:H8   | 1:3D:248:LEU:HD11 | 1.72                     | 0.48              |
| 2:2S:210:TYR:CD2  | 1:3F:329:ASN:HB2  | 2.49                     | 0.48              |
| 2:2S:306:ASP:HB3  | 2:2S:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:2T:172:VAL:HG11 | 2:2T:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:2U:10:GLY:O     | 2:2U:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2U:172:VAL:HG11 | 2:2U:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:2V:288:VAL:HB   | 2:2V:327:GLU:HG2  | 1.96                     | 0.48              |
| 2:2X:406:HIS:CD2  | 1:3L:262:TYR:HA   | 2.49                     | 0.48              |
| 2:2Z:10:GLY:O     | 2:2Z:14:ASN:ND2   | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3A:215:ARG:NH2  | 1:3A:299:ALA:O    | 2.47                     | 0.48              |
| 1:3B:252:LEU:HA   | 1:3B:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:3C:215:ARG:NH2  | 1:3C:299:ALA:O    | 2.47                     | 0.48              |
| 1:3E:228:ASN:OD1  | 3:3E:501:GTP:N1   | 2.47                     | 0.48              |
| 1:3I:154:MET:HE1  | 1:3I:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:3K:228:ASN:OD1  | 3:3K:501:GTP:N1   | 2.47                     | 0.48              |
| 2:3O:10:GLY:O     | 2:3O:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3O:157:ILE:O    | 2:3O:161:TYR:N    | 2.45                     | 0.48              |
| 2:3P:283:TYR:OH   | 2:3Q:85:GLN:O     | 2.18                     | 0.48              |
| 2:3S:306:ASP:HB3  | 2:3S:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3T:172:VAL:HG11 | 2:3T:387:LEU:HD21 | 1.96                     | 0.48              |
| 1:4C:100:ALA:N    | 3:4C:501:GTP:O2G  | 2.41                     | 0.48              |
| 1:4I:154:MET:HE1  | 1:4I:166:LYS:HB3  | 1.95                     | 0.48              |
| 2:4O:10:GLY:O     | 2:4O:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4O:157:ILE:O    | 2:4O:161:TYR:N    | 2.45                     | 0.48              |
| 2:4Y:306:ASP:HB3  | 2:4Y:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:4Z:10:GLY:O     | 2:4Z:14:ASN:ND2   | 2.46                     | 0.48              |
| 1:1B:329:ASN:CB   | 2:4O:210:TYR:CE2  | 2.89                     | 0.48              |
| 1:1B:346:TRP:HA   | 2:4O:397:ALA:CB   | 2.42                     | 0.48              |
| 1:1C:2:ARG:HH22   | 2:4P:73:GLY:HA3   | 1.72                     | 0.48              |
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:HA   | 2.24                     | 0.48              |
| 1:1I:329:ASN:OD1  | 2:4U:177:VAL:HG11 | 2.12                     | 0.48              |
| 1:1K:346:TRP:CA   | 2:4W:397:ALA:O    | 2.62                     | 0.48              |
| 1:1K:350:GLY:C    | 2:4W:181:VAL:HG22 | 2.39                     | 0.48              |
| 1:1M:261:PRO:HA   | 2:4Y:404:PHE:CA   | 2.44                     | 0.48              |
| 1:1N:27:GLU:OE1   | 1:1N:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:1N:215:ARG:NH2  | 1:1N:299:ALA:O    | 2.47                     | 0.48              |
| 2:1Q:174:SER:OG   | 2:1Q:177:VAL:O    | 2.29                     | 0.48              |
| 2:1S:141:LEU:HD12 | 2:1S:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:1S:306:ASP:HB3  | 2:1S:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1V:288:VAL:HB   | 2:1V:327:GLU:HG2  | 1.96                     | 0.48              |
| 1:2B:203:MET:HG3  | 1:2B:384:ILE:HD11 | 1.95                     | 0.48              |
| 1:2C:154:MET:HE1  | 1:2C:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:2C:203:MET:HG3  | 1:2C:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:2D:27:GLU:OE1   | 1:2D:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:2L:215:ARG:NH2  | 1:2L:299:ALA:O    | 2.47                     | 0.48              |
| 2:2P:10:GLY:O     | 2:2P:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2Q:404:PHE:HD1  | 1:3D:260:VAL:O    | 1.95                     | 0.48              |
| 2:2R:157:ILE:O    | 2:2R:161:TYR:N    | 2.45                     | 0.48              |
| 2:2S:100:GLY:HA2  | 1:3F:254:GLU:N    | 2.29                     | 0.48              |
| 2:2T:407:TRP:HE1  | 1:3G:260:VAL:HG12 | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:72:PRO:CG    | 1:3J:2:ARG:HG3    | 2.44                     | 0.48              |
| 2:2Y:306:ASP:HB3  | 2:2Y:309:HIS:CD2  | 2.49                     | 0.48              |
| 5:2Z:501:GDP:H8   | 1:3N:248:LEU:HD11 | 1.74                     | 0.48              |
| 1:3L:215:ARG:NH2  | 1:3L:299:ALA:O    | 2.47                     | 0.48              |
| 2:3P:10:GLY:O     | 2:3P:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:3R:157:ILE:O    | 2:3R:161:TYR:N    | 2.45                     | 0.48              |
| 2:3S:141:LEU:HD12 | 2:3S:172:VAL:HG22 | 1.94                     | 0.48              |
| 2:3Z:172:VAL:HG11 | 2:3Z:387:LEU:HD21 | 1.96                     | 0.48              |
| 1:4C:203:MET:HG3  | 1:4C:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:4C:215:ARG:NH2  | 1:4C:299:ALA:O    | 2.47                     | 0.48              |
| 1:4D:215:ARG:NH2  | 1:4D:299:ALA:O    | 2.47                     | 0.48              |
| 1:4E:228:ASN:OD1  | 3:4E:501:GTP:N1   | 2.47                     | 0.48              |
| 1:4K:228:ASN:OD1  | 3:4K:501:GTP:N1   | 2.47                     | 0.48              |
| 1:4L:215:ARG:NH2  | 1:4L:299:ALA:O    | 2.47                     | 0.48              |
| 2:4Q:174:SER:OG   | 2:4Q:177:VAL:O    | 2.29                     | 0.48              |
| 2:4T:172:VAL:HG11 | 2:4T:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:4U:10:GLY:O     | 2:4U:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4U:172:VAL:HG11 | 2:4U:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:4Z:288:VAL:HB   | 2:4Z:327:GLU:HG2  | 1.96                     | 0.48              |
| 1:1A:260:VAL:HG11 | 2:4H:407:TRP:HZ2  | 1.78                     | 0.48              |
| 1:1B:203:MET:HG3  | 1:1B:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:1B:215:ARG:NH2  | 1:1B:299:ALA:O    | 2.47                     | 0.48              |
| 1:1D:215:ARG:NH2  | 1:1D:299:ALA:O    | 2.47                     | 0.48              |
| 1:1D:253:THR:O    | 2:4Q:100:GLY:O    | 2.32                     | 0.48              |
| 1:1E:27:GLU:OE1   | 1:1E:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:1E:216:ASN:HD21 | 1:1E:300:ASN:HD22 | 1.61                     | 0.48              |
| 1:1G:216:ASN:HD21 | 1:1G:300:ASN:HD22 | 1.61                     | 0.48              |
| 1:1G:253:THR:HG22 | 2:4T:100:GLY:HA3  | 1.96                     | 0.48              |
| 1:1G:257:THR:CG2  | 2:4T:102:ASN:CB   | 2.79                     | 0.48              |
| 1:1J:348:PRO:CB   | 2:4V:394:GLN:CG   | 2.92                     | 0.48              |
| 1:1L:215:ARG:NH2  | 1:1L:299:ALA:O    | 2.47                     | 0.48              |
| 1:1M:349:THR:HG21 | 2:4Y:183:GLU:CG   | 2.44                     | 0.48              |
| 2:1O:221:THR:OG1  | 1:2B:324:VAL:HG21 | 2.13                     | 0.48              |
| 2:1P:100:GLY:CA   | 1:2C:253:THR:CG2  | 2.90                     | 0.48              |
| 2:1P:283:TYR:OH   | 2:1Q:85:GLN:O     | 2.18                     | 0.48              |
| 2:1T:207:GLU:OE1  | 1:2G:329:ASN:ND2  | 2.46                     | 0.48              |
| 2:1V:172:VAL:HG11 | 2:1V:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1Y:176:LYS:HE2  | 1:2M:333:ALA:CB   | 2.43                     | 0.48              |
| 2:1Y:306:ASP:HB3  | 2:1Y:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:1Z:172:VAL:HG11 | 2:1Z:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:1Z:288:VAL:HB   | 2:1Z:327:GLU:HG2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2C:100:ALA:N    | 3:2C:501:GTP:O2G  | 2.41                     | 0.48              |
| 1:2C:215:ARG:NH2  | 1:2C:299:ALA:O    | 2.47                     | 0.48              |
| 1:2D:215:ARG:NH2  | 1:2D:299:ALA:O    | 2.47                     | 0.48              |
| 1:2E:27:GLU:OE1   | 1:2E:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:2E:216:ASN:HD21 | 1:2E:300:ASN:HD22 | 1.61                     | 0.48              |
| 1:2G:216:ASN:HD21 | 1:2G:300:ASN:HD22 | 1.61                     | 0.48              |
| 1:2N:215:ARG:NH2  | 1:2N:299:ALA:O    | 2.47                     | 0.48              |
| 2:2O:11:GLN:CD    | 1:3B:249:ASN:H    | 2.15                     | 0.48              |
| 2:2P:157:ILE:O    | 2:2P:161:TYR:N    | 2.45                     | 0.48              |
| 2:2R:10:GLY:O     | 2:2R:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:2R:210:TYR:CZ   | 1:3E:325:PRO:O    | 2.66                     | 0.48              |
| 2:2W:394:GLN:NE2  | 1:3K:348:PRO:HB2  | 2.29                     | 0.48              |
| 2:2Z:172:VAL:HG11 | 2:2Z:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:2Z:221:THR:OG1  | 1:3N:324:VAL:HG22 | 2.13                     | 0.48              |
| 2:2Z:288:VAL:HB   | 2:2Z:327:GLU:HG2  | 1.96                     | 0.48              |
| 1:3B:215:ARG:NH2  | 1:3B:299:ALA:O    | 2.47                     | 0.48              |
| 1:3C:154:MET:HE1  | 1:3C:166:LYS:HB3  | 1.95                     | 0.48              |
| 1:3C:203:MET:HG3  | 1:3C:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:3D:27:GLU:OE1   | 1:3D:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:3D:215:ARG:NH2  | 1:3D:299:ALA:O    | 2.47                     | 0.48              |
| 1:3E:27:GLU:OE1   | 1:3E:243:ARG:NH1  | 2.44                     | 0.48              |
| 2:3P:157:ILE:O    | 2:3P:161:TYR:N    | 2.45                     | 0.48              |
| 2:3V:172:VAL:HG11 | 2:3V:387:LEU:HD21 | 1.96                     | 0.48              |
| 2:3X:205:ASP:OD2  | 2:3X:304:ALA:N    | 2.35                     | 0.48              |
| 2:3Y:306:ASP:HB3  | 2:3Y:309:HIS:CD2  | 2.49                     | 0.48              |
| 2:3Z:288:VAL:HB   | 2:3Z:327:GLU:HG2  | 1.96                     | 0.48              |
| 1:4B:203:MET:HG3  | 1:4B:384:ILE:HD11 | 1.96                     | 0.48              |
| 1:4D:27:GLU:OE1   | 1:4D:243:ARG:NH1  | 2.44                     | 0.48              |
| 1:4D:252:LEU:HA   | 1:4D:255:PHE:HD2  | 1.78                     | 0.48              |
| 1:4N:100:ALA:N    | 3:4N:501:GTP:O2G  | 2.41                     | 0.48              |
| 2:4P:10:GLY:O     | 2:4P:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4R:10:GLY:O     | 2:4R:14:ASN:ND2   | 2.46                     | 0.48              |
| 2:4R:157:ILE:O    | 2:4R:161:TYR:N    | 2.45                     | 0.48              |
| 2:4V:172:VAL:HG11 | 2:4V:387:LEU:HD21 | 1.96                     | 0.48              |
| 1:1A:260:VAL:O    | 2:4H:407:TRP:HD1  | 1.90                     | 0.47              |
| 1:1A:346:TRP:HB2  | 2:4H:398:MET:CA   | 2.29                     | 0.47              |
| 1:1B:248:LEU:HA   | 2:4O:11:GLN:NE2   | 2.28                     | 0.47              |
| 1:1B:257:THR:HG21 | 2:4O:102:ASN:CA   | 2.44                     | 0.47              |
| 1:1B:314:ALA:HB1  | 2:4O:181:VAL:CG2  | 2.25                     | 0.47              |
| 1:1C:100:ALA:N    | 3:1C:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:1C:154:MET:HE1  | 1:1C:166:LYS:HB3  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1C:203:MET:HG3  | 1:1C:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1C:257:THR:CG2  | 2:4P:102:ASN:HB2  | 2.44                     | 0.47              |
| 1:1C:349:THR:OG1  | 2:4P:184:PRO:HD2  | 2.10                     | 0.47              |
| 1:1D:27:GLU:OE1   | 1:1D:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:1N:154:MET:HE1  | 1:1N:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1N:261:PRO:HA   | 2:4Z:404:PHE:HA   | 1.96                     | 0.47              |
| 2:1O:404:PHE:CD1  | 1:2B:260:VAL:O    | 2.67                     | 0.47              |
| 2:1P:306:ASP:HB3  | 2:1P:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:1Q:172:VAL:HG11 | 2:1Q:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:1V:306:ASP:HB3  | 2:1V:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:1W:172:VAL:HG11 | 2:1W:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:2B:215:ARG:NH2  | 1:2B:299:ALA:O    | 2.47                     | 0.47              |
| 1:2N:27:GLU:OE1   | 1:2N:243:ARG:NH1  | 2.44                     | 0.47              |
| 2:2H:11:GLN:NE2   | 1:3A:249:ASN:HB2  | 2.29                     | 0.47              |
| 2:2R:179:ASP:C    | 1:3E:352:LYS:HA   | 2.39                     | 0.47              |
| 2:2T:179:ASP:O    | 1:3G:352:LYS:CD   | 2.51                     | 0.47              |
| 2:2U:210:TYR:CD2  | 1:3I:329:ASN:CB   | 2.97                     | 0.47              |
| 2:2V:172:VAL:HG11 | 2:2V:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:2V:306:ASP:HB3  | 2:2V:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:2V:406:HIS:CG   | 1:3J:263:PRO:CD   | 2.81                     | 0.47              |
| 2:2X:11:GLN:HE22  | 1:3L:249:ASN:CB   | 2.27                     | 0.47              |
| 2:2X:205:ASP:OD2  | 2:2X:304:ALA:N    | 2.35                     | 0.47              |
| 1:3B:203:MET:HG3  | 1:3B:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:3C:100:ALA:N    | 3:3C:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:3E:216:ASN:HD21 | 1:3E:300:ASN:HD22 | 1.62                     | 0.47              |
| 1:3G:216:ASN:HD21 | 1:3G:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3N:27:GLU:OE1   | 1:3N:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:3N:215:ARG:NH2  | 1:3N:299:ALA:O    | 2.47                     | 0.47              |
| 2:3R:10:GLY:O     | 2:3R:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:3V:306:ASP:HB3  | 2:3V:309:HIS:CD2  | 2.49                     | 0.47              |
| 1:4B:215:ARG:NH2  | 1:4B:299:ALA:O    | 2.47                     | 0.47              |
| 1:4C:154:MET:HE1  | 1:4C:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4E:27:GLU:OE1   | 1:4E:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:4E:216:ASN:HD21 | 1:4E:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:4I:203:MET:HG3  | 1:4I:384:ILE:HD11 | 1.95                     | 0.47              |
| 1:4N:215:ARG:NH2  | 1:4N:299:ALA:O    | 2.47                     | 0.47              |
| 2:4P:157:ILE:O    | 2:4P:161:TYR:N    | 2.45                     | 0.47              |
| 2:4V:306:ASP:HB3  | 2:4V:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:4Z:172:VAL:HG11 | 2:4Z:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:1D:228:ASN:OD1  | 3:1D:501:GTP:N1   | 2.47                     | 0.47              |
| 1:1G:260:VAL:CG2  | 2:4T:407:TRP:HZ2  | 2.27                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:439:SER:HB2  | 2:4U:400:ARG:HD2  | 1.96                     | 0.47              |
| 1:1M:262:TYR:HA   | 2:4Y:406:HIS:HD2  | 1.55                     | 0.47              |
| 1:1N:2:ARG:CZ     | 2:4Z:73:GLY:HA3   | 2.44                     | 0.47              |
| 1:1N:263:PRO:CD   | 2:4Z:406:HIS:CE1  | 2.96                     | 0.47              |
| 2:1O:401:ARG:HB3  | 1:2B:262:TYR:OH   | 2.14                     | 0.47              |
| 2:1P:10:GLY:O     | 2:1P:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:1Q:70:LEU:HD12  | 2:1Q:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1R:10:GLY:O     | 2:1R:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:1R:70:LEU:HD12  | 2:1R:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1R:178:SER:HB3  | 1:2E:349:THR:CB   | 2.43                     | 0.47              |
| 2:1S:76:ASP:HA    | 2:1S:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:1Y:172:VAL:HG11 | 2:1Y:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:2M:154:MET:HE1  | 1:2M:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2N:100:ALA:N    | 3:2N:501:GTP:O2G  | 2.41                     | 0.47              |
| 2:2O:101:ASN:ND2  | 1:3B:258:ASN:OD1  | 2.46                     | 0.47              |
| 2:2O:181:VAL:N    | 1:3B:258:ASN:ND2  | 2.62                     | 0.47              |
| 2:2P:306:ASP:HB3  | 2:2P:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:2Q:404:PHE:CD2  | 1:3D:261:PRO:HB3  | 2.49                     | 0.47              |
| 2:2R:180:THR:N    | 1:3E:351:PHE:O    | 2.47                     | 0.47              |
| 2:2S:210:TYR:CD2  | 1:3F:329:ASN:CB   | 2.97                     | 0.47              |
| 2:2X:179:ASP:OD2  | 1:3L:248:LEU:CD2  | 2.59                     | 0.47              |
| 2:2Y:172:VAL:HG11 | 2:2Y:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:3I:203:MET:HG3  | 1:3I:384:ILE:HD11 | 1.95                     | 0.47              |
| 2:3P:306:ASP:HB3  | 2:3P:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:3R:70:LEU:HD12  | 2:3R:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3R:76:ASP:HA    | 2:3R:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3T:288:VAL:HB   | 2:3T:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:3W:172:VAL:HG11 | 2:3W:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:3Y:172:VAL:HG11 | 2:3Y:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:4G:100:ALA:N    | 3:4G:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:4G:216:ASN:HD21 | 1:4G:300:ASN:HD22 | 1.62                     | 0.47              |
| 1:4N:27:GLU:OE1   | 1:4N:243:ARG:NH1  | 2.44                     | 0.47              |
| 2:4Q:70:LEU:HD12  | 2:4Q:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4Q:172:VAL:HG11 | 2:4Q:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:4R:76:ASP:HA    | 2:4R:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:4T:288:VAL:HB   | 2:4T:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:4Y:172:VAL:HG11 | 2:4Y:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:1A:329:ASN:ND2  | 2:4H:210:TYR:CD2  | 2.69                     | 0.47              |
| 1:1E:2:ARG:HH11   | 2:4R:71:GLU:CG    | 2.27                     | 0.47              |
| 1:1E:245:ASP:CB   | 2:4R:77:SER:HB3   | 2.31                     | 0.47              |
| 1:1E:252:LEU:HA   | 1:1E:255:PHE:HD2  | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:351:PHE:O    | 2:4S:180:THR:HA   | 2.07                     | 0.47              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:HB3  | 1.57                     | 0.47              |
| 1:1I:203:MET:HG3  | 1:1I:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1I:215:ARG:NH2  | 1:1I:299:ALA:O    | 2.47                     | 0.47              |
| 1:1J:351:PHE:O    | 2:4V:181:VAL:N    | 2.46                     | 0.47              |
| 1:1L:348:PRO:HG3  | 2:4X:394:GLN:HA   | 1.94                     | 0.47              |
| 1:1N:100:ALA:N    | 3:1N:501:GTP:O2G  | 2.41                     | 0.47              |
| 2:1Q:306:ASP:HB3  | 2:1Q:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:1R:76:ASP:HA    | 2:1R:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:1T:288:VAL:HB   | 2:1T:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:1X:172:VAL:HG11 | 2:1X:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:1X:406:HIS:CD2  | 1:2L:263:PRO:CD   | 2.92                     | 0.47              |
| 1:2G:100:ALA:N    | 3:2G:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:2I:203:MET:HG3  | 1:2I:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:2I:215:ARG:NH2  | 1:2I:299:ALA:O    | 2.47                     | 0.47              |
| 1:2J:154:MET:HE1  | 1:2J:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2N:154:MET:HE1  | 1:2N:166:LYS:HB3  | 1.95                     | 0.47              |
| 2:2Q:70:LEU:HD12  | 2:2Q:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2Q:172:VAL:HG11 | 2:2Q:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:2R:70:LEU:HD12  | 2:2R:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2R:76:ASP:HA    | 2:2R:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2S:172:VAL:HG11 | 2:2S:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:2S:179:ASP:C    | 1:3F:352:LYS:HA   | 2.39                     | 0.47              |
| 2:2W:172:VAL:HG11 | 2:2W:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:3D:228:ASN:OD1  | 3:3D:501:GTP:N1   | 2.47                     | 0.47              |
| 1:3I:215:ARG:NH2  | 1:3I:299:ALA:O    | 2.47                     | 0.47              |
| 1:3N:100:ALA:N    | 3:3N:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:3N:154:MET:HE1  | 1:3N:166:LYS:HB3  | 1.95                     | 0.47              |
| 2:3Q:70:LEU:HD12  | 2:3Q:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3Q:172:VAL:HG11 | 2:3Q:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:3S:76:ASP:HA    | 2:3S:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3S:172:VAL:HG11 | 2:3S:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:3X:172:VAL:HG11 | 2:3X:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:4F:216:ASN:HD21 | 1:4F:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:4I:215:ARG:NH2  | 1:4I:299:ALA:O    | 2.47                     | 0.47              |
| 1:4J:154:MET:HE1  | 1:4J:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4M:154:MET:HE1  | 1:4M:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4N:154:MET:HE1  | 1:4N:166:LYS:HB3  | 1.95                     | 0.47              |
| 2:4P:306:ASP:HB3  | 2:4P:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:4R:70:LEU:HD12  | 2:4R:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4R:306:ASP:HB3  | 2:4R:309:HIS:CD2  | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4S:76:ASP:HA    | 2:4S:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:4W:172:VAL:HG11 | 2:4W:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:4X:172:VAL:HG11 | 2:4X:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:1E:260:VAL:C    | 2:4R:407:TRP:NE1  | 2.69                     | 0.47              |
| 1:1F:215:ARG:NH2  | 1:1F:299:ALA:O    | 2.47                     | 0.47              |
| 1:1I:326:LYS:CG   | 2:4U:210:TYR:CD1  | 2.97                     | 0.47              |
| 1:1J:154:MET:HE1  | 1:1J:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1L:439:SER:OG   | 2:4X:401:ARG:CG   | 2.62                     | 0.47              |
| 1:1M:154:MET:HE1  | 1:1M:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1M:203:MET:HG3  | 1:1M:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1N:346:TRP:HZ3  | 2:4Z:404:PHE:HE2  | 1.61                     | 0.47              |
| 2:1P:70:LEU:HD12  | 2:1P:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1S:70:LEU:HD12  | 2:1S:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1U:182:VAL:CG2  | 1:2I:257:THR:CG2  | 2.92                     | 0.47              |
| 2:1W:222:PRO:HG2  | 1:2K:326:LYS:HB2  | 1.95                     | 0.47              |
| 2:1Y:179:ASP:OD1  | 1:2M:353:VAL:O    | 2.32                     | 0.47              |
| 1:2B:154:MET:HE1  | 1:2B:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2D:228:ASN:OD1  | 3:2D:501:GTP:N1   | 2.47                     | 0.47              |
| 1:2F:215:ARG:NH2  | 1:2F:299:ALA:O    | 2.47                     | 0.47              |
| 1:2F:216:ASN:HD21 | 1:2F:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:2M:203:MET:HG3  | 1:2M:384:ILE:HD11 | 1.96                     | 0.47              |
| 2:2P:70:LEU:HD12  | 2:2P:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2Q:306:ASP:HB3  | 2:2Q:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:2R:72:PRO:HG2   | 1:3E:2:ARG:HG3    | 1.96                     | 0.47              |
| 2:2R:101:ASN:HB2  | 1:3E:254:GLU:CB   | 2.45                     | 0.47              |
| 2:2S:76:ASP:HA    | 2:2S:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2S:394:GLN:CG   | 1:3F:348:PRO:HB2  | 2.44                     | 0.47              |
| 2:2T:288:VAL:HB   | 2:2T:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:2V:214:PHE:CG   | 1:3J:326:LYS:HE3  | 2.48                     | 0.47              |
| 1:3E:252:LEU:HA   | 1:3E:255:PHE:HD2  | 1.78                     | 0.47              |
| 1:3F:216:ASN:HD21 | 1:3F:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3G:100:ALA:N    | 3:3G:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:3J:154:MET:HE1  | 1:3J:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3M:154:MET:HE1  | 1:3M:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3M:203:MET:HG3  | 1:3M:384:ILE:HD11 | 1.96                     | 0.47              |
| 2:3Q:306:ASP:HB3  | 2:3Q:309:HIS:CD2  | 2.49                     | 0.47              |
| 1:4B:154:MET:HE1  | 1:4B:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4M:203:MET:HG3  | 1:4M:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:4M:215:ARG:NH2  | 1:4M:299:ALA:O    | 2.47                     | 0.47              |
| 2:4S:172:VAL:HG11 | 2:4S:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:4X:205:ASP:OD2  | 2:4X:304:ALA:N    | 2.35                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:154:MET:HE1  | 1:1A:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1A:399:TYR:OH   | 1:1A:415:GLU:OE2  | 2.27                     | 0.47              |
| 1:1B:329:ASN:HB3  | 2:4O:210:TYR:CD2  | 2.50                     | 0.47              |
| 1:1C:348:PRO:HD2  | 2:4P:398:MET:HG3  | 1.97                     | 0.47              |
| 1:1D:216:ASN:HD21 | 1:1D:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:1F:216:ASN:HD21 | 1:1F:300:ASN:HD22 | 1.62                     | 0.47              |
| 1:1G:100:ALA:N    | 3:1G:501:GTP:O2G  | 2.41                     | 0.47              |
| 1:1G:261:PRO:O    | 2:4T:404:PHE:HA   | 2.15                     | 0.47              |
| 1:1L:254:GLU:CA   | 2:4X:100:GLY:HA2  | 2.45                     | 0.47              |
| 1:1L:260:VAL:HG12 | 2:4X:406:HIS:HE1  | 1.80                     | 0.47              |
| 1:1L:265:ILE:HG22 | 1:1L:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:1N:228:ASN:OD1  | 3:1N:501:GTP:N1   | 2.47                     | 0.47              |
| 1:1N:435:VAL:C    | 2:4Z:401:ARG:HH22 | 2.23                     | 0.47              |
| 2:1O:224:TYR:HD2  | 1:2B:247:ALA:O    | 1.96                     | 0.47              |
| 2:1Q:11:GLN:HB3   | 5:1Q:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1Q:76:ASP:HA    | 2:1Q:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:1R:221:THR:CB   | 1:2E:324:VAL:HG21 | 2.45                     | 0.47              |
| 2:1S:172:VAL:HG11 | 2:1S:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:1T:404:PHE:CE1  | 1:2G:261:PRO:N    | 2.80                     | 0.47              |
| 2:1V:222:PRO:HD2  | 1:2J:324:VAL:CG1  | 2.45                     | 0.47              |
| 2:1X:11:GLN:NE2   | 1:2L:249:ASN:HD22 | 2.13                     | 0.47              |
| 1:2D:216:ASN:HD21 | 1:2D:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:2E:252:LEU:HA   | 1:2E:255:PHE:HD2  | 1.78                     | 0.47              |
| 1:2M:215:ARG:NH2  | 1:2M:299:ALA:O    | 2.47                     | 0.47              |
| 2:2O:11:GLN:HB3   | 5:2O:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:2Q:11:GLN:HB3   | 5:2Q:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:2R:306:ASP:HB3  | 2:2R:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:2S:70:LEU:HD12  | 2:2S:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2T:401:ARG:HH22 | 1:3G:435:VAL:C    | 2.21                     | 0.47              |
| 2:2X:172:VAL:HG11 | 2:2X:387:LEU:HD21 | 1.96                     | 0.47              |
| 1:3B:154:MET:HE1  | 1:3B:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3F:215:ARG:NH2  | 1:3F:299:ALA:O    | 2.47                     | 0.47              |
| 1:3M:215:ARG:NH2  | 1:3M:299:ALA:O    | 2.47                     | 0.47              |
| 1:3N:228:ASN:OD1  | 3:3N:501:GTP:N1   | 2.47                     | 0.47              |
| 2:3O:11:GLN:HB3   | 5:3O:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:3P:70:LEU:HD12  | 2:3P:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3Q:11:GLN:HB3   | 5:3Q:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:3R:306:ASP:HB3  | 2:3R:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:3S:70:LEU:HD12  | 2:3S:99:ALA:HB2   | 1.96                     | 0.47              |
| 1:4A:154:MET:HE1  | 1:4A:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4D:216:ASN:HD21 | 1:4D:300:ASN:HD22 | 1.61                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4D:228:ASN:OD1  | 3:4D:501:GTP:N1   | 2.47                     | 0.47              |
| 2:4P:70:LEU:HD12  | 2:4P:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4Q:11:GLN:HB3   | 5:4Q:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4Q:76:ASP:HA    | 2:4Q:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:4Q:306:ASP:HB3  | 2:4Q:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:4S:70:LEU:HD12  | 2:4S:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4T:10:GLY:O     | 2:4T:14:ASN:ND2   | 2.46                     | 0.47              |
| 1:1B:154:MET:HE1  | 1:1B:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1B:325:PRO:HD2  | 2:4O:222:PRO:O    | 2.15                     | 0.47              |
| 1:1B:353:VAL:HB   | 2:4O:179:ASP:CG   | 2.28                     | 0.47              |
| 1:1C:2:ARG:NH1    | 2:4P:71:GLU:CG    | 2.74                     | 0.47              |
| 1:1C:346:TRP:O    | 2:4P:398:MET:CB   | 2.62                     | 0.47              |
| 1:1E:258:ASN:O    | 2:4R:181:VAL:HB   | 2.15                     | 0.47              |
| 1:1F:262:TYR:CZ   | 2:4S:402:LYS:C    | 2.93                     | 0.47              |
| 1:1J:203:MET:HG3  | 1:1J:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1M:215:ARG:NH2  | 1:1M:299:ALA:O    | 2.47                     | 0.47              |
| 2:1O:11:GLN:HB3   | 5:1O:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1O:76:ASP:HA    | 2:1O:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:1R:306:ASP:HB3  | 2:1R:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:1T:10:GLY:O     | 2:1T:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:1U:76:ASP:HA    | 2:1U:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:1W:288:VAL:HB   | 2:1W:327:GLU:HG2  | 1.96                     | 0.47              |
| 1:2A:154:MET:HE1  | 1:2A:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2J:203:MET:HG3  | 1:2J:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:2L:203:MET:HG3  | 1:2L:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:2N:228:ASN:OD1  | 3:2N:501:GTP:N1   | 2.47                     | 0.47              |
| 2:2P:11:GLN:HB3   | 5:2P:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:2P:76:ASP:HA    | 2:2P:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2Q:76:ASP:HA    | 2:2Q:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2R:176:LYS:CE   | 1:3E:333:ALA:HB1  | 2.34                     | 0.47              |
| 2:2U:6:HIS:CD2    | 2:2U:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:2U:73:GLY:CA    | 1:3I:2:ARG:NH2    | 2.77                     | 0.47              |
| 2:2V:404:PHE:HE1  | 1:3J:260:VAL:C    | 2.18                     | 0.47              |
| 2:2W:394:GLN:HB3  | 1:3K:348:PRO:HG2  | 1.97                     | 0.47              |
| 1:3A:154:MET:HE1  | 1:3A:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3D:216:ASN:HD21 | 1:3D:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3J:203:MET:HG3  | 1:3J:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:3L:154:MET:HE1  | 1:3L:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3L:265:ILE:HG22 | 1:3L:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:3P:76:ASP:HA    | 2:3P:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3Q:76:ASP:HA    | 2:3Q:79:ARG:HG2   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4A:203:MET:HG3  | 1:4A:384:ILE:HD11 | 1.95                     | 0.47              |
| 1:4E:252:LEU:HA   | 1:4E:255:PHE:HD2  | 1.78                     | 0.47              |
| 1:4F:215:ARG:NH2  | 1:4F:299:ALA:O    | 2.47                     | 0.47              |
| 1:4L:154:MET:HE1  | 1:4L:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4L:203:MET:HG3  | 1:4L:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:4L:265:ILE:HG22 | 1:4L:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:4N:228:ASN:OD1  | 3:4N:501:GTP:N1   | 2.47                     | 0.47              |
| 2:4O:11:GLN:HB3   | 5:4O:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4P:76:ASP:HA    | 2:4P:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:4W:288:VAL:HB   | 2:4W:327:GLU:HG2  | 1.96                     | 0.47              |
| 1:1A:27:GLU:OE1   | 1:1A:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:1A:348:PRO:HB2  | 2:4H:394:GLN:NE2  | 2.29                     | 0.47              |
| 1:1A:351:PHE:HB2  | 2:4H:178:SER:OG   | 2.14                     | 0.47              |
| 1:1B:27:GLU:OE1   | 1:1B:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:1C:2:ARG:HG2    | 2:4P:72:PRO:HD2   | 1.90                     | 0.47              |
| 1:1C:216:ASN:HD21 | 1:1C:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:1C:265:ILE:HG22 | 1:1C:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:1C:349:THR:CG2  | 2:4P:184:PRO:CD   | 2.90                     | 0.47              |
| 1:1D:324:VAL:HG11 | 2:4Q:222:PRO:N    | 2.30                     | 0.47              |
| 1:1D:353:VAL:N    | 2:4Q:179:ASP:O    | 2.47                     | 0.47              |
| 1:1E:261:PRO:O    | 2:4R:406:HIS:CD2  | 2.67                     | 0.47              |
| 1:1E:314:ALA:HB2  | 2:4R:404:PHE:HZ   | 1.80                     | 0.47              |
| 1:1E:439:SER:OG   | 2:4R:400:ARG:HG3  | 2.14                     | 0.47              |
| 1:1F:261:PRO:HB3  | 2:4S:404:PHE:CG   | 2.49                     | 0.47              |
| 1:1I:216:ASN:HD21 | 1:1I:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:1I:261:PRO:HB3  | 2:4U:404:PHE:CD2  | 2.50                     | 0.47              |
| 1:1I:346:TRP:C    | 2:4U:398:MET:HA   | 2.39                     | 0.47              |
| 1:1J:228:ASN:OD1  | 3:1J:501:GTP:N1   | 2.46                     | 0.47              |
| 1:1K:215:ARG:NH2  | 1:1K:299:ALA:O    | 2.47                     | 0.47              |
| 1:1L:154:MET:HE1  | 1:1L:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:1L:203:MET:HG3  | 1:1L:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1M:324:VAL:CG1  | 2:4Y:222:PRO:O    | 2.63                     | 0.47              |
| 1:1M:348:PRO:HB2  | 2:4Y:394:GLN:CG   | 2.45                     | 0.47              |
| 1:1N:265:ILE:HG22 | 1:1N:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:1O:70:LEU:HD12  | 2:1O:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1P:11:GLN:HB3   | 5:1P:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1P:76:ASP:HA    | 2:1P:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:1S:11:GLN:HB3   | 5:1S:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1S:174:SER:OG   | 2:1S:177:VAL:O    | 2.29                     | 0.47              |
| 2:1T:70:LEU:HD12  | 2:1T:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1T:76:ASP:HA    | 2:1T:79:ARG:HG2   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1U:6:HIS:CD2    | 2:1U:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:1U:288:VAL:HB   | 2:1U:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:1W:180:THR:HG23 | 1:2K:258:ASN:ND2  | 2.27                     | 0.47              |
| 2:1W:306:ASP:HB3  | 2:1W:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:1W:404:PHE:CE2  | 1:2K:261:PRO:HB3  | 2.50                     | 0.47              |
| 2:1Y:11:GLN:NE2   | 1:2M:249:ASN:HD22 | 2.12                     | 0.47              |
| 1:2A:203:MET:HG3  | 1:2A:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:2C:265:ILE:HG22 | 1:2C:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:2E:265:ILE:HG22 | 1:2E:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:2I:216:ASN:HD21 | 1:2I:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:2I:265:ILE:HG22 | 1:2I:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:2K:215:ARG:NH2  | 1:2K:299:ALA:O    | 2.47                     | 0.47              |
| 1:2L:154:MET:HE1  | 1:2L:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2L:265:ILE:HG22 | 1:2L:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:2H:77:SER:CB    | 1:3A:245:ASP:CG   | 2.88                     | 0.47              |
| 2:2H:221:THR:CA   | 1:3A:324:VAL:HG11 | 2.38                     | 0.47              |
| 2:2O:70:LEU:HD12  | 2:2O:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2O:76:ASP:HA    | 2:2O:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2O:406:HIS:CE1  | 1:3B:263:PRO:CA   | 2.98                     | 0.47              |
| 2:2P:222:PRO:C    | 1:3C:324:VAL:HG13 | 2.40                     | 0.47              |
| 2:2S:11:GLN:HB3   | 5:2S:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:2T:10:GLY:O     | 2:2T:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:2T:11:GLN:HB3   | 5:2T:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:2T:70:LEU:HD12  | 2:2T:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2T:76:ASP:HA    | 2:2T:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2U:76:ASP:HA    | 2:2U:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:2U:288:VAL:HB   | 2:2U:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:2W:288:VAL:HB   | 2:2W:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:2W:394:GLN:CA   | 1:3K:348:PRO:HG3  | 2.44                     | 0.47              |
| 1:3A:27:GLU:OE1   | 1:3A:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:3A:203:MET:HG3  | 1:3A:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:3B:27:GLU:OE1   | 1:3B:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:3B:259:LEU:HD11 | 1:3B:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:3C:265:ILE:HG22 | 1:3C:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:3I:265:ILE:HG22 | 1:3I:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:3K:215:ARG:NH2  | 1:3K:299:ALA:O    | 2.47                     | 0.47              |
| 1:3L:203:MET:HG3  | 1:3L:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:3L:334:THR:O    | 1:3L:337:THR:OG1  | 2.30                     | 0.47              |
| 1:3N:265:ILE:HG22 | 1:3N:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:3O:70:LEU:HD12  | 2:3O:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3O:76:ASP:HA    | 2:3O:79:ARG:HG2   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3P:11:GLN:HB3   | 5:3P:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:3S:11:GLN:HB3   | 5:3S:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:3T:10:GLY:O     | 2:3T:14:ASN:ND2   | 2.46                     | 0.47              |
| 2:3T:11:GLN:HB3   | 5:3T:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:3U:6:HIS:CD2    | 2:3U:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:3U:76:ASP:HA    | 2:3U:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3U:288:VAL:HB   | 2:3U:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:3W:288:VAL:HB   | 2:3W:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:3W:306:ASP:HB3  | 2:3W:309:HIS:CD2  | 2.49                     | 0.47              |
| 1:4B:259:LEU:HD11 | 1:4B:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:4C:216:ASN:HD21 | 1:4C:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:4C:265:ILE:HG22 | 1:4C:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:4I:216:ASN:HD21 | 1:4I:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:4I:265:ILE:HG22 | 1:4I:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:4J:203:MET:HG3  | 1:4J:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:4K:215:ARG:NH2  | 1:4K:299:ALA:O    | 2.47                     | 0.47              |
| 1:4N:265:ILE:HG22 | 1:4N:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:4O:70:LEU:HD12  | 2:4O:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4O:76:ASP:HA    | 2:4O:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:4P:11:GLN:HB3   | 5:4P:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4T:11:GLN:HB3   | 5:4T:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4T:76:ASP:HA    | 2:4T:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:4U:6:HIS:CD2    | 2:4U:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:4U:76:ASP:HA    | 2:4U:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:4U:288:VAL:HB   | 2:4U:327:GLU:HG2  | 1.96                     | 0.47              |
| 1:1B:253:THR:C    | 2:4O:100:GLY:HA3  | 2.35                     | 0.47              |
| 1:1B:259:LEU:HD11 | 1:1B:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1B:260:VAL:HG11 | 2:4O:407:TRP:CZ2  | 2.50                     | 0.47              |
| 1:1C:347:CYS:HA   | 2:4P:398:MET:CG   | 2.44                     | 0.47              |
| 1:1E:215:ARG:NH2  | 1:1E:299:ALA:O    | 2.47                     | 0.47              |
| 1:1E:265:ILE:HG22 | 1:1E:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:1G:254:GLU:HB3  | 2:4T:101:ASN:HB2  | 1.96                     | 0.47              |
| 1:1I:262:TYR:CZ   | 2:4U:403:ALA:HA   | 2.50                     | 0.47              |
| 1:1I:265:ILE:HG22 | 1:1I:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:1K:248:LEU:HD12 | 2:4W:11:GLN:OE1   | 2.15                     | 0.47              |
| 2:1P:394:GLN:HG2  | 1:2C:348:PRO:CG   | 2.45                     | 0.47              |
| 2:1R:288:VAL:HB   | 2:1R:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:1T:11:GLN:HB3   | 5:1T:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1V:224:TYR:HE2  | 1:2J:248:LEU:CB   | 2.18                     | 0.47              |
| 2:1Y:214:PHE:HB3  | 1:2M:326:LYS:HE2  | 1.88                     | 0.47              |
| 2:1Y:224:TYR:HE2  | 1:2M:247:ALA:O    | 1.89                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Z:394:GLN:OE1  | 1:2N:349:THR:CG2  | 2.63                     | 0.47              |
| 1:2A:27:GLU:OE1   | 1:2A:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:2B:27:GLU:OE1   | 1:2B:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:2B:259:LEU:HD11 | 1:2B:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:2C:216:ASN:HD21 | 1:2C:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:2J:228:ASN:OD1  | 3:2J:501:GTP:N1   | 2.47                     | 0.47              |
| 1:2N:265:ILE:HG22 | 1:2N:380:ASN:HD21 | 1.80                     | 0.47              |
| 2:2H:101:ASN:ND2  | 1:3A:258:ASN:OD1  | 2.48                     | 0.47              |
| 2:2H:404:PHE:HD1  | 1:3A:260:VAL:O    | 1.90                     | 0.47              |
| 2:2P:178:SER:OG   | 1:3C:351:PHE:HB2  | 2.15                     | 0.47              |
| 2:2P:210:TYR:CE2  | 1:3C:329:ASN:HB2  | 2.50                     | 0.47              |
| 2:2Q:179:ASP:C    | 1:3D:352:LYS:HA   | 2.40                     | 0.47              |
| 2:2Q:404:PHE:CA   | 1:3D:261:PRO:HA   | 2.45                     | 0.47              |
| 2:2U:157:ILE:O    | 2:2U:161:TYR:N    | 2.45                     | 0.47              |
| 2:2W:306:ASP:HB3  | 2:2W:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:2W:406:HIS:NE2  | 1:3K:262:TYR:HA   | 2.28                     | 0.47              |
| 1:3C:216:ASN:HD21 | 1:3C:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3C:259:LEU:HD11 | 1:3C:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:3E:265:ILE:HG22 | 1:3E:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:3I:216:ASN:HD21 | 1:3I:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3J:216:ASN:HD21 | 1:3J:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:3J:228:ASN:OD1  | 3:3J:501:GTP:N1   | 2.47                     | 0.47              |
| 2:3S:174:SER:OG   | 2:3S:177:VAL:O    | 2.29                     | 0.47              |
| 2:3T:70:LEU:HD12  | 2:3T:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3T:76:ASP:HA    | 2:3T:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3U:157:ILE:O    | 2:3U:161:TYR:N    | 2.45                     | 0.47              |
| 1:4A:27:GLU:OE1   | 1:4A:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:4E:265:ILE:HG22 | 1:4E:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:4J:228:ASN:OD1  | 3:4J:501:GTP:N1   | 2.46                     | 0.47              |
| 2:4R:6:HIS:CD2    | 2:4R:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:4S:11:GLN:HB3   | 5:4S:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4T:70:LEU:HD12  | 2:4T:99:ALA:HB2   | 1.96                     | 0.47              |
| 1:1A:203:MET:HG3  | 1:1A:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1C:259:LEU:HD11 | 1:1C:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1D:399:TYR:OH   | 1:1D:415:GLU:OE2  | 2.27                     | 0.47              |
| 1:1E:121:ARG:NH1  | 1:1E:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:1E:325:PRO:CD   | 2:4R:223:THR:HA   | 2.45                     | 0.47              |
| 1:1F:261:PRO:CA   | 2:4S:404:PHE:CG   | 2.97                     | 0.47              |
| 1:1J:216:ASN:HD21 | 1:1J:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:1J:249:ASN:N    | 2:4V:11:GLN:CD    | 2.66                     | 0.47              |
| 1:1J:324:VAL:HG13 | 2:4V:222:PRO:O    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1K:121:ARG:NH1  | 1:1K:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:1M:346:TRP:CD2  | 2:4Y:403:ALA:HB2  | 2.50                     | 0.47              |
| 1:1N:259:LEU:HD11 | 1:1N:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1N:351:PHE:O    | 2:4Z:180:THR:CA   | 2.63                     | 0.47              |
| 2:1T:6:HIS:CD2    | 2:1T:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:1U:157:ILE:O    | 2:1U:161:TYR:N    | 2.45                     | 0.47              |
| 2:1X:100:GLY:C    | 1:2L:253:THR:HG22 | 2.40                     | 0.47              |
| 2:1Y:69:ASP:OD2   | 2:1Y:74:THR:OG1   | 2.20                     | 0.47              |
| 2:1Y:288:VAL:HB   | 2:1Y:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:1Y:411:GLU:OE2  | 1:2M:163:LYS:NZ   | 2.47                     | 0.47              |
| 1:2D:399:TYR:OH   | 1:2D:415:GLU:OE2  | 2.27                     | 0.47              |
| 1:2E:121:ARG:NH1  | 1:2E:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:2K:121:ARG:NH1  | 1:2K:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:2K:154:MET:HE1  | 1:2K:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:2N:259:LEU:HD11 | 1:2N:316:CYS:HB2  | 1.97                     | 0.47              |
| 2:2Q:71:GLU:HG3   | 1:3D:2:ARG:HH11   | 1.80                     | 0.47              |
| 2:2R:6:HIS:CD2    | 2:2R:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:2R:288:VAL:HB   | 2:2R:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:2S:174:SER:OG   | 2:2S:177:VAL:O    | 2.29                     | 0.47              |
| 2:2S:404:PHE:CA   | 1:3F:261:PRO:HA   | 2.45                     | 0.47              |
| 2:2T:73:GLY:CA    | 1:3G:2:ARG:NH2    | 2.76                     | 0.47              |
| 2:2T:179:ASP:C    | 1:3G:352:LYS:HA   | 2.40                     | 0.47              |
| 2:2U:398:MET:HG3  | 1:3I:346:TRP:O    | 2.12                     | 0.47              |
| 2:2Y:394:GLN:OE1  | 1:3M:349:THR:HG23 | 2.14                     | 0.47              |
| 2:2Z:222:PRO:CG   | 1:3N:326:LYS:HB2  | 2.38                     | 0.47              |
| 1:3D:399:TYR:OH   | 1:3D:415:GLU:OE2  | 2.27                     | 0.47              |
| 1:3E:121:ARG:NH1  | 1:3E:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:3N:259:LEU:HD11 | 1:3N:316:CYS:HB2  | 1.97                     | 0.47              |
| 2:3H:70:LEU:HD12  | 2:3H:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3Q:6:HIS:CD2    | 2:3Q:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:3R:6:HIS:CD2    | 2:3R:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:3R:288:VAL:HB   | 2:3R:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:3T:6:HIS:CD2    | 2:3T:8:GLN:HE21   | 2.33                     | 0.47              |
| 1:4B:27:GLU:OE1   | 1:4B:243:ARG:NH1  | 2.44                     | 0.47              |
| 1:4D:259:LEU:HD11 | 1:4D:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:4J:215:ARG:NH2  | 1:4J:299:ALA:O    | 2.47                     | 0.47              |
| 1:4J:216:ASN:HD21 | 1:4J:300:ASN:HD22 | 1.61                     | 0.47              |
| 1:4K:121:ARG:NH1  | 1:4K:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:4N:259:LEU:HD11 | 1:4N:316:CYS:HB2  | 1.97                     | 0.47              |
| 2:4H:70:LEU:HD12  | 2:4H:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:4Q:6:HIS:CD2    | 2:4Q:8:GLN:HE21   | 2.33                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4R:11:GLN:HB3   | 5:4R:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4R:172:VAL:HG11 | 2:4R:387:LEU:HD21 | 1.96                     | 0.47              |
| 2:4R:288:VAL:HB   | 2:4R:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:4X:70:LEU:HD12  | 2:4X:99:ALA:HB2   | 1.96                     | 0.47              |
| 1:1A:2:ARG:HD3    | 2:4H:72:PRO:CD    | 2.36                     | 0.47              |
| 1:1A:259:LEU:HD11 | 1:1A:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1A:261:PRO:C    | 2:4H:404:PHE:HA   | 2.40                     | 0.47              |
| 1:1B:265:ILE:HG22 | 1:1B:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:1C:346:TRP:CE3  | 2:4P:403:ALA:HB3  | 2.50                     | 0.47              |
| 1:1D:259:LEU:HD11 | 1:1D:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1D:434:GLU:C    | 2:4Q:401:ARG:NH2  | 2.72                     | 0.47              |
| 1:1E:259:LEU:HD11 | 1:1E:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:1F:2:ARG:NH1    | 2:4S:71:GLU:HB2   | 2.28                     | 0.47              |
| 1:1G:215:ARG:NH2  | 1:1G:299:ALA:O    | 2.47                     | 0.47              |
| 1:1G:261:PRO:O    | 2:4T:406:HIS:HD2  | 1.93                     | 0.47              |
| 1:1I:439:SER:OG   | 2:4U:401:ARG:HD3  | 2.14                     | 0.47              |
| 1:1J:215:ARG:NH2  | 1:1J:299:ALA:O    | 2.47                     | 0.47              |
| 1:1J:258:ASN:OD1  | 2:4V:101:ASN:HB3  | 2.15                     | 0.47              |
| 1:1J:349:THR:OG1  | 2:4V:184:PRO:HD2  | 2.15                     | 0.47              |
| 1:1L:334:THR:O    | 1:1L:337:THR:OG1  | 2.30                     | 0.47              |
| 1:1L:348:PRO:HD2  | 2:4X:398:MET:HG3  | 1.96                     | 0.47              |
| 1:1M:261:PRO:HB3  | 2:4Y:404:PHE:CD2  | 2.50                     | 0.47              |
| 1:1M:435:VAL:C    | 2:4Y:401:ARG:HH22 | 2.22                     | 0.47              |
| 1:1N:203:MET:HG3  | 1:1N:384:ILE:HD11 | 1.96                     | 0.47              |
| 1:1N:348:PRO:HB2  | 2:4Z:394:GLN:HG2  | 1.89                     | 0.47              |
| 2:1O:288:VAL:HB   | 2:1O:327:GLU:HG2  | 1.96                     | 0.47              |
| 2:1Q:6:HIS:CD2    | 2:1Q:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:1R:6:HIS:CD2    | 2:1R:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:1U:11:GLN:HB3   | 5:1U:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:1V:76:ASP:HA    | 2:1V:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:1X:70:LEU:HD12  | 2:1X:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:1Z:6:HIS:CD2    | 2:1Z:8:GLN:HE21   | 2.33                     | 0.47              |
| 1:2C:259:LEU:HD11 | 1:2C:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:2D:259:LEU:HD11 | 1:2D:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:2J:215:ARG:NH2  | 1:2J:299:ALA:O    | 2.47                     | 0.47              |
| 1:2J:216:ASN:HD21 | 1:2J:300:ASN:HD22 | 1.62                     | 0.47              |
| 1:2J:265:ILE:HG22 | 1:2J:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:2N:203:MET:HG3  | 1:2N:384:ILE:HD11 | 1.96                     | 0.47              |
| 2:2H:70:LEU:HD12  | 2:2H:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:2H:101:ASN:HB2  | 1:3A:254:GLU:CB   | 2.45                     | 0.47              |
| 2:2Q:6:HIS:CD2    | 2:2Q:8:GLN:HE21   | 2.33                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Q:404:PHE:CE1  | 1:3D:260:VAL:N    | 2.78                     | 0.47              |
| 2:2V:76:ASP:HA    | 2:2V:79:ARG:HG2   | 1.96                     | 0.47              |
| 2:2W:182:VAL:HG21 | 1:3K:257:THR:HG22 | 1.97                     | 0.47              |
| 2:2X:70:LEU:HD12  | 2:2X:99:ALA:HB2   | 1.96                     | 0.47              |
| 1:3D:259:LEU:HD11 | 1:3D:316:CYS:HB2  | 1.97                     | 0.47              |
| 1:3G:215:ARG:NH2  | 1:3G:299:ALA:O    | 2.47                     | 0.47              |
| 1:3J:215:ARG:NH2  | 1:3J:299:ALA:O    | 2.47                     | 0.47              |
| 1:3K:121:ARG:NH1  | 1:3K:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:3K:154:MET:HE1  | 1:3K:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:3N:203:MET:HG3  | 1:3N:384:ILE:HD11 | 1.96                     | 0.47              |
| 2:3V:76:ASP:HA    | 2:3V:79:ARG:HG2   | 1.97                     | 0.47              |
| 2:3X:70:LEU:HD12  | 2:3X:99:ALA:HB2   | 1.96                     | 0.47              |
| 2:3Z:6:HIS:CD2    | 2:3Z:8:GLN:HE21   | 2.33                     | 0.47              |
| 2:3Z:11:GLN:HB3   | 5:3Z:501:GDP:O1A  | 2.15                     | 0.47              |
| 1:4E:121:ARG:NH1  | 1:4E:124:LYS:HD2  | 2.30                     | 0.47              |
| 1:4J:265:ILE:HG22 | 1:4J:380:ASN:HD21 | 1.80                     | 0.47              |
| 1:4K:154:MET:HE1  | 1:4K:166:LYS:HB3  | 1.95                     | 0.47              |
| 1:4N:203:MET:HG3  | 1:4N:384:ILE:HD11 | 1.96                     | 0.47              |
| 2:4U:157:ILE:O    | 2:4U:161:TYR:N    | 2.45                     | 0.47              |
| 2:4V:11:GLN:HB3   | 5:4V:501:GDP:O1A  | 2.15                     | 0.47              |
| 2:4W:306:ASP:HB3  | 2:4W:309:HIS:CD2  | 2.49                     | 0.47              |
| 2:4X:283:TYR:OH   | 2:4Y:85:GLN:O     | 2.18                     | 0.47              |
| 1:1D:329:ASN:CB   | 2:4Q:210:TYR:HD2  | 2.25                     | 0.46              |
| 1:1J:265:ILE:HG22 | 1:1J:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:1M:260:VAL:O    | 2:4Y:407:TRP:HD1  | 1.84                     | 0.46              |
| 2:1H:70:LEU:HD12  | 2:1H:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1R:172:VAL:HG11 | 2:1R:387:LEU:HD21 | 1.96                     | 0.46              |
| 2:1R:224:TYR:HE2  | 1:2E:248:LEU:HB2  | 1.80                     | 0.46              |
| 2:1S:222:PRO:HD2  | 1:2F:326:LYS:CB   | 2.45                     | 0.46              |
| 2:1V:6:HIS:CD2    | 2:1V:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1V:11:GLN:HB3   | 5:1V:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1X:157:ILE:O    | 2:1X:161:TYR:N    | 2.45                     | 0.46              |
| 2:1Y:70:LEU:HD12  | 2:1Y:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1Z:11:GLN:HB3   | 5:1Z:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1Z:180:THR:HG23 | 1:2N:258:ASN:ND2  | 2.19                     | 0.46              |
| 1:2A:265:ILE:HG22 | 1:2A:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:2B:265:ILE:HG22 | 1:2B:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:2E:209:ILE:HG23 | 1:2E:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2E:215:ARG:NH2  | 1:2E:299:ALA:O    | 2.47                     | 0.46              |
| 1:2E:259:LEU:HD11 | 1:2E:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:2G:215:ARG:NH2  | 1:2G:299:ALA:O    | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2H:6:HIS:CD2    | 2:2H:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2O:404:PHE:CD1  | 1:3B:261:PRO:CA   | 2.95                     | 0.46              |
| 5:2O:501:GDP:H8   | 1:3B:248:LEU:HD11 | 1.76                     | 0.46              |
| 2:2R:11:GLN:HB3   | 5:2R:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2R:172:VAL:HG11 | 2:2R:387:LEU:HD21 | 1.96                     | 0.46              |
| 2:2S:394:GLN:OE1  | 1:3F:349:THR:HG23 | 2.15                     | 0.46              |
| 2:2T:6:HIS:CD2    | 2:2T:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2V:11:GLN:HB3   | 5:2V:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2V:176:LYS:CE   | 1:3J:333:ALA:HB1  | 2.35                     | 0.46              |
| 2:2X:306:ASP:HB3  | 2:2X:309:HIS:CD2  | 2.49                     | 0.46              |
| 2:2X:401:ARG:C    | 1:3L:262:TYR:HH   | 2.13                     | 0.46              |
| 2:2Y:6:HIS:CD2    | 2:2Y:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2Y:70:LEU:HD12  | 2:2Y:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:2Y:394:GLN:CA   | 1:3M:348:PRO:HG3  | 2.45                     | 0.46              |
| 2:2Z:6:HIS:CD2    | 2:2Z:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2Z:11:GLN:HB3   | 5:2Z:501:GDP:O1A  | 2.15                     | 0.46              |
| 1:3A:259:LEU:HD11 | 1:3A:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:3B:265:ILE:HG22 | 1:3B:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:3E:209:ILE:HG23 | 1:3E:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3E:215:ARG:NH2  | 1:3E:299:ALA:O    | 2.47                     | 0.46              |
| 2:3H:6:HIS:CD2    | 2:3H:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3O:288:VAL:HB   | 2:3O:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:3R:11:GLN:HB3   | 5:3R:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:3X:6:HIS:CD2    | 2:3X:8:GLN:HE21   | 2.33                     | 0.46              |
| 1:4A:265:ILE:HG22 | 1:4A:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:4C:259:LEU:HD11 | 1:4C:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4D:399:TYR:OH   | 1:4D:415:GLU:OE2  | 2.27                     | 0.46              |
| 1:4E:209:ILE:HG23 | 1:4E:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4F:265:ILE:HG22 | 1:4F:380:ASN:HD21 | 1.80                     | 0.46              |
| 2:4H:6:HIS:CD2    | 2:4H:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4S:174:SER:OG   | 2:4S:177:VAL:O    | 2.29                     | 0.46              |
| 2:4T:6:HIS:CD2    | 2:4T:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4V:6:HIS:CD2    | 2:4V:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4V:76:ASP:HA    | 2:4V:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:4Z:6:HIS:CD2    | 2:4Z:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4Z:11:GLN:HB3   | 5:4Z:501:GDP:O1A  | 2.15                     | 0.46              |
| 1:1A:121:ARG:NH1  | 1:1A:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1A:265:ILE:HG22 | 1:1A:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:1B:121:ARG:NH1  | 1:1B:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1B:325:PRO:HG2  | 2:4O:224:TYR:CD1  | 2.50                     | 0.46              |
| 1:1C:228:ASN:OD1  | 3:1C:501:GTP:N1   | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:435:VAL:O    | 2:4Q:401:ARG:CZ   | 2.62                     | 0.46              |
| 1:1E:209:ILE:HG23 | 1:1E:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1E:261:PRO:HB3  | 2:4R:404:PHE:CG   | 2.50                     | 0.46              |
| 1:1E:261:PRO:HD3  | 2:4R:404:PHE:CE1  | 2.50                     | 0.46              |
| 1:1F:260:VAL:CG2  | 2:4S:407:TRP:CZ2  | 2.98                     | 0.46              |
| 1:1F:265:ILE:HG22 | 1:1F:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:1I:439:SER:CB   | 2:4U:400:ARG:HD2  | 2.45                     | 0.46              |
| 1:1J:254:GLU:CG   | 2:4V:100:GLY:HA2  | 2.45                     | 0.46              |
| 1:1K:154:MET:HE1  | 1:1K:166:LYS:HB3  | 1.95                     | 0.46              |
| 1:1K:349:THR:HG21 | 2:4W:183:GLU:CG   | 2.45                     | 0.46              |
| 1:1M:121:ARG:NH1  | 1:1M:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1M:260:VAL:CB   | 2:4Y:407:TRP:HZ2  | 2.25                     | 0.46              |
| 2:1H:6:HIS:CD2    | 2:1H:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1R:11:GLN:HB3   | 5:1R:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1X:269:MET:HE1  | 2:1X:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:2A:121:ARG:NH1  | 1:2A:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2B:121:ARG:NH1  | 1:2B:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2F:265:ILE:HG22 | 1:2F:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:2M:121:ARG:NH1  | 1:2M:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:2O:288:VAL:HB   | 2:2O:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:2R:73:GLY:HA3   | 1:3E:2:ARG:CZ     | 2.45                     | 0.46              |
| 2:2R:100:GLY:HA2  | 1:3E:254:GLU:N    | 2.30                     | 0.46              |
| 2:2U:11:GLN:HB3   | 5:2U:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2V:6:HIS:CD2    | 2:2V:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2V:11:GLN:NE2   | 1:3J:249:ASN:N    | 2.08                     | 0.46              |
| 2:2V:100:GLY:CA   | 1:3J:253:THR:C    | 2.87                     | 0.46              |
| 2:2V:404:PHE:CD2  | 1:3J:261:PRO:HA   | 2.46                     | 0.46              |
| 2:2W:6:HIS:CD2    | 2:2W:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2W:70:LEU:HD12  | 2:2W:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:2W:181:VAL:H    | 1:3K:258:ASN:ND2  | 2.14                     | 0.46              |
| 2:2X:6:HIS:CD2    | 2:2X:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2X:11:GLN:NE2   | 1:3L:249:ASN:N    | 2.22                     | 0.46              |
| 2:2X:269:MET:HE1  | 2:2X:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:2X:283:TYR:OH   | 2:2Y:85:GLN:O     | 2.18                     | 0.46              |
| 2:2X:406:HIS:CE1  | 1:3L:263:PRO:HA   | 2.51                     | 0.46              |
| 1:3A:121:ARG:NH1  | 1:3A:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3A:265:ILE:HG22 | 1:3A:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:3E:259:LEU:HD11 | 1:3E:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:3F:265:ILE:HG22 | 1:3F:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:3J:209:ILE:HG23 | 1:3J:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3J:265:ILE:HG22 | 1:3J:380:ASN:HD21 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3M:121:ARG:NH1  | 1:3M:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:3R:172:VAL:HG11 | 2:3R:387:LEU:HD21 | 1.96                     | 0.46              |
| 2:3U:11:GLN:HB3   | 5:3U:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:3V:6:HIS:CD2    | 2:3V:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3V:11:GLN:HB3   | 5:3V:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:3W:70:LEU:HD12  | 2:3W:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:3X:157:ILE:O    | 2:3X:161:TYR:N    | 2.45                     | 0.46              |
| 2:3X:269:MET:HE1  | 2:3X:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:3Y:6:HIS:CD2    | 2:3Y:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3Y:70:LEU:HD12  | 2:3Y:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:3Y:288:VAL:HB   | 2:3Y:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:3Z:269:MET:HE1  | 2:3Z:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:4A:259:LEU:HD11 | 1:4A:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4B:121:ARG:NH1  | 1:4B:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4B:265:ILE:HG22 | 1:4B:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:4C:27:GLU:OE1   | 1:4C:243:ARG:NH1  | 2.44                     | 0.46              |
| 1:4E:215:ARG:NH2  | 1:4E:299:ALA:O    | 2.47                     | 0.46              |
| 1:4E:259:LEU:HD11 | 1:4E:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4G:215:ARG:NH2  | 1:4G:299:ALA:O    | 2.47                     | 0.46              |
| 1:4J:209:ILE:HG23 | 1:4J:230:LEU:HD22 | 1.98                     | 0.46              |
| 2:4O:6:HIS:CD2    | 2:4O:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4O:288:VAL:HB   | 2:4O:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:4U:11:GLN:HB3   | 5:4U:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:4W:6:HIS:CD2    | 2:4W:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4W:70:LEU:HD12  | 2:4W:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:4X:6:HIS:CD2    | 2:4X:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4X:306:ASP:HB3  | 2:4X:309:HIS:CD2  | 2.49                     | 0.46              |
| 2:4Y:6:HIS:CD2    | 2:4Y:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4Y:70:LEU:HD12  | 2:4Y:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:4Y:288:VAL:HB   | 2:4Y:327:GLU:HG2  | 1.96                     | 0.46              |
| 1:1C:260:VAL:O    | 2:4P:404:PHE:HD1  | 1.99                     | 0.46              |
| 1:1D:346:TRP:HA   | 2:4Q:397:ALA:CA   | 2.46                     | 0.46              |
| 1:1E:325:PRO:CG   | 2:4R:224:TYR:CD1  | 2.95                     | 0.46              |
| 1:1G:121:ARG:NH1  | 1:1G:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1G:254:GLU:CG   | 2:4T:100:GLY:CA   | 2.93                     | 0.46              |
| 1:1I:211:ASP:CG   | 1:1I:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1I:353:VAL:HG23 | 2:4U:179:ASP:HA   | 1.98                     | 0.46              |
| 1:1J:209:ILE:HG23 | 1:1J:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1K:265:ILE:HG22 | 1:1K:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:1L:249:ASN:H    | 2:4X:11:GLN:CD    | 2.10                     | 0.46              |
| 2:1O:6:HIS:CD2    | 2:1O:8:GLN:HE21   | 2.33                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1R:404:PHE:CZ   | 1:2E:261:PRO:CA   | 2.98                     | 0.46              |
| 2:1V:406:HIS:NE2  | 1:2J:263:PRO:CD   | 2.79                     | 0.46              |
| 2:1W:6:HIS:CD2    | 2:1W:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1W:70:LEU:HD12  | 2:1W:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1X:6:HIS:CD2    | 2:1X:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1X:306:ASP:HB3  | 2:1X:309:HIS:CD2  | 2.49                     | 0.46              |
| 2:1Y:6:HIS:CD2    | 2:1Y:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1Z:269:MET:HE1  | 2:1Z:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:2A:259:LEU:HD11 | 1:2A:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:2C:27:GLU:OE1   | 1:2C:243:ARG:NH1  | 2.44                     | 0.46              |
| 1:2C:121:ARG:NH1  | 1:2C:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2I:209:ILE:HG23 | 1:2I:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2J:209:ILE:HG23 | 1:2J:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2K:265:ILE:HG22 | 1:2K:380:ASN:HD21 | 1.80                     | 0.46              |
| 2:2H:223:THR:HA   | 1:3A:325:PRO:HD2  | 1.97                     | 0.46              |
| 2:2O:6:HIS:CD2    | 2:2O:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2P:69:ASP:OD2   | 2:2P:74:THR:OG1   | 2.20                     | 0.46              |
| 2:2S:404:PHE:CG   | 1:3F:261:PRO:CA   | 2.86                     | 0.46              |
| 2:2S:404:PHE:CE1  | 1:3F:261:PRO:CA   | 2.98                     | 0.46              |
| 2:2W:404:PHE:CD2  | 1:3K:261:PRO:HB3  | 2.46                     | 0.46              |
| 2:2X:157:ILE:O    | 2:2X:161:TYR:N    | 2.45                     | 0.46              |
| 2:2Y:288:VAL:HB   | 2:2Y:327:GLU:HG2  | 1.96                     | 0.46              |
| 1:3B:121:ARG:NH1  | 1:3B:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3C:27:GLU:OE1   | 1:3C:243:ARG:NH1  | 2.44                     | 0.46              |
| 1:3C:228:ASN:OD1  | 3:3C:501:GTP:N1   | 2.47                     | 0.46              |
| 1:3I:121:ARG:NH1  | 1:3I:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:3O:6:HIS:CD2    | 2:3O:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3P:69:ASP:OD2   | 2:3P:74:THR:OG1   | 2.19                     | 0.46              |
| 2:3X:306:ASP:HB3  | 2:3X:309:HIS:CD2  | 2.49                     | 0.46              |
| 2:3Z:70:LEU:HD12  | 2:3Z:99:ALA:HB2   | 1.96                     | 0.46              |
| 1:4A:121:ARG:NH1  | 1:4A:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4I:121:ARG:NH1  | 1:4I:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4K:265:ILE:HG22 | 1:4K:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:4M:121:ARG:NH1  | 1:4M:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:4X:157:ILE:O    | 2:4X:161:TYR:N    | 2.45                     | 0.46              |
| 2:4X:269:MET:HE1  | 2:4X:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:4Z:70:LEU:HD12  | 2:4Z:99:ALA:HB2   | 1.96                     | 0.46              |
| 1:1A:329:ASN:ND2  | 2:4H:207:GLU:CD   | 2.56                     | 0.46              |
| 1:1C:27:GLU:OE1   | 1:1C:243:ARG:NH1  | 2.44                     | 0.46              |
| 1:1C:352:LYS:CE   | 2:4P:101:ASN:HD22 | 2.28                     | 0.46              |
| 1:1D:209:ILE:HG23 | 1:1D:230:LEU:HD22 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:2:ARG:HH11   | 2:4S:71:GLU:CB    | 2.25                     | 0.46              |
| 1:1I:121:ARG:NH1  | 1:1I:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1I:209:ILE:HG23 | 1:1I:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1I:242:LEU:HD11 | 1:1I:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1K:203:MET:HG3  | 1:1K:384:ILE:HD11 | 1.96                     | 0.46              |
| 1:1M:346:TRP:CD2  | 2:4Y:403:ALA:CB   | 2.98                     | 0.46              |
| 1:1N:121:ARG:NH1  | 1:1N:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1N:260:VAL:HB   | 2:4Z:407:TRP:CE2  | 2.51                     | 0.46              |
| 1:1N:346:TRP:CZ3  | 2:4Z:404:PHE:CE2  | 3.03                     | 0.46              |
| 2:1H:224:TYR:HE2  | 1:2A:248:LEU:HB2  | 1.81                     | 0.46              |
| 2:1Q:178:SER:HB3  | 1:2D:349:THR:HB   | 1.96                     | 0.46              |
| 2:1Q:288:VAL:HB   | 2:1Q:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:1S:404:PHE:HE1  | 1:2F:260:VAL:C    | 2.20                     | 0.46              |
| 2:1U:394:GLN:HG2  | 1:2I:348:PRO:HG2  | 1.92                     | 0.46              |
| 5:1V:501:GDP:C8   | 1:2J:248:LEU:CD1  | 2.98                     | 0.46              |
| 2:1X:214:PHE:HB3  | 1:2L:326:LYS:HE2  | 1.79                     | 0.46              |
| 2:1Y:242:LEU:HD12 | 2:1Y:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1Z:70:LEU:HD12  | 2:1Z:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1Z:76:ASP:HA    | 2:1Z:79:ARG:HG2   | 1.96                     | 0.46              |
| 1:2C:228:ASN:OD1  | 3:2C:501:GTP:N1   | 2.47                     | 0.46              |
| 1:2G:121:ARG:NH1  | 1:2G:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2I:121:ARG:NH1  | 1:2I:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2K:203:MET:HG3  | 1:2K:384:ILE:HD11 | 1.96                     | 0.46              |
| 1:2M:259:LEU:HD11 | 1:2M:316:CYS:HB2  | 1.97                     | 0.46              |
| 2:2Q:288:VAL:HB   | 2:2Q:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:2T:101:ASN:HB2  | 1:3G:254:GLU:CG   | 2.45                     | 0.46              |
| 2:2V:178:SER:CB   | 1:3J:349:THR:HB   | 2.46                     | 0.46              |
| 2:2Z:70:LEU:HD12  | 2:2Z:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:2Z:269:MET:HE1  | 2:2Z:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:3C:121:ARG:NH1  | 1:3C:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3D:209:ILE:HG23 | 1:3D:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3G:121:ARG:NH1  | 1:3G:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3I:209:ILE:HG23 | 1:3I:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3I:211:ASP:CG   | 1:3I:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3K:203:MET:HG3  | 1:3K:384:ILE:HD11 | 1.96                     | 0.46              |
| 1:3K:265:ILE:HG22 | 1:3K:380:ASN:HD21 | 1.80                     | 0.46              |
| 2:3P:288:VAL:HB   | 2:3P:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:3Q:288:VAL:HB   | 2:3Q:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:3U:70:LEU:HD12  | 2:3U:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:3W:6:HIS:CD2    | 2:3W:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3Y:242:LEU:HD12 | 2:3Y:251:ASP:HB2  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3Y:269:MET:HE1  | 2:3Y:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:4C:121:ARG:NH1  | 1:4C:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4C:228:ASN:OD1  | 3:4C:501:GTP:N1   | 2.47                     | 0.46              |
| 1:4D:334:THR:O    | 1:4D:337:THR:OG1  | 2.30                     | 0.46              |
| 1:4I:209:ILE:HG23 | 1:4I:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4I:211:ASP:CG   | 1:4I:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:4K:203:MET:HG3  | 1:4K:384:ILE:HD11 | 1.96                     | 0.46              |
| 2:4P:69:ASP:OD2   | 2:4P:74:THR:OG1   | 2.20                     | 0.46              |
| 2:4Y:269:MET:HE1  | 2:4Y:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:4Z:76:ASP:HA    | 2:4Z:79:ARG:HG2   | 1.97                     | 0.46              |
| 1:1A:242:LEU:HD11 | 1:1A:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1B:209:ILE:HG23 | 1:1B:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1B:242:LEU:HD11 | 1:1B:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1B:332:ILE:HB   | 2:4O:177:VAL:CG2  | 2.44                     | 0.46              |
| 1:1C:121:ARG:NH1  | 1:1C:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1G:242:LEU:HD11 | 1:1G:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1G:262:TYR:CZ   | 2:4T:402:LYS:O    | 2.69                     | 0.46              |
| 1:1J:260:VAL:HG12 | 2:4V:406:HIS:CE1  | 2.44                     | 0.46              |
| 1:1K:349:THR:CB   | 2:4W:184:PRO:HD3  | 2.41                     | 0.46              |
| 1:1M:347:CYS:SG   | 2:4Y:181:VAL:HG13 | 2.56                     | 0.46              |
| 2:1H:76:ASP:HA    | 2:1H:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:1P:242:LEU:HD12 | 2:1P:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1P:288:VAL:HB   | 2:1P:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:1U:70:LEU:HD12  | 2:1U:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1V:242:LEU:HD12 | 2:1V:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1X:179:ASP:OD1  | 1:2L:353:VAL:O    | 2.34                     | 0.46              |
| 2:1Z:242:LEU:HD12 | 2:1Z:251:ASP:HB2  | 1.98                     | 0.46              |
| 1:2A:242:LEU:HD11 | 1:2A:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:2B:209:ILE:HG23 | 1:2B:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2B:242:LEU:HD11 | 1:2B:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:2D:209:ILE:HG23 | 1:2D:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2G:242:LEU:HD11 | 1:2G:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:2I:211:ASP:CG   | 1:2I:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:2N:121:ARG:NH1  | 1:2N:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:2H:11:GLN:HE22  | 1:3A:249:ASN:CB   | 2.28                     | 0.46              |
| 2:2H:76:ASP:HA    | 2:2H:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:2P:242:LEU:HD12 | 2:2P:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2P:288:VAL:HB   | 2:2P:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:2T:224:TYR:HD2  | 1:3G:247:ALA:O    | 1.98                     | 0.46              |
| 2:2T:404:PHE:CG   | 1:3G:261:PRO:CA   | 2.82                     | 0.46              |
| 2:2U:70:LEU:HD12  | 2:2U:99:ALA:HB2   | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2V:210:TYR:CD2  | 1:3J:329:ASN:HB2  | 2.50                     | 0.46              |
| 2:2V:242:LEU:HD12 | 2:2V:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2Y:242:LEU:HD12 | 2:2Y:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2Y:269:MET:HE1  | 2:2Y:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:2Z:76:ASP:HA    | 2:2Z:79:ARG:HG2   | 1.97                     | 0.46              |
| 1:3A:242:LEU:HD11 | 1:3A:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3B:242:LEU:HD11 | 1:3B:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3G:242:LEU:HD11 | 1:3G:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3N:121:ARG:NH1  | 1:3N:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:3H:76:ASP:HA    | 2:3H:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:3P:242:LEU:HD12 | 2:3P:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:3Q:200:GLU:HA   | 2:3Q:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:3V:242:LEU:HD12 | 2:3V:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:3Z:76:ASP:HA    | 2:3Z:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:3Z:242:LEU:HD12 | 2:3Z:251:ASP:HB2  | 1.98                     | 0.46              |
| 1:4B:209:ILE:HG23 | 1:4B:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4D:209:ILE:HG23 | 1:4D:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4G:121:ARG:NH1  | 1:4G:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4G:242:LEU:HD11 | 1:4G:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:4M:259:LEU:HD11 | 1:4M:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4N:121:ARG:NH1  | 1:4N:124:LYS:HD2  | 2.30                     | 0.46              |
| 2:4H:76:ASP:HA    | 2:4H:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:4P:242:LEU:HD12 | 2:4P:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4Q:288:VAL:HB   | 2:4Q:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:4U:70:LEU:HD12  | 2:4U:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:4V:242:LEU:HD12 | 2:4V:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4W:269:MET:HE1  | 2:4W:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:4X:11:GLN:HB3   | 5:4X:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:4Y:242:LEU:HD12 | 2:4Y:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4Z:242:LEU:HD12 | 2:4Z:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4Z:269:MET:HE1  | 2:4Z:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:1A:260:VAL:O    | 2:4H:404:PHE:CD1  | 2.68                     | 0.46              |
| 1:1F:259:LEU:HD11 | 1:1F:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:1I:346:TRP:HZ3  | 2:4U:404:PHE:CD2  | 2.34                     | 0.46              |
| 1:1M:259:LEU:HD11 | 1:1M:316:CYS:HB2  | 1.97                     | 0.46              |
| 2:1H:288:VAL:HB   | 2:1H:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:1P:69:ASP:OD2   | 2:1P:74:THR:OG1   | 2.20                     | 0.46              |
| 2:1T:69:ASP:HB2   | 2:1T:75:MET:HE2   | 1.98                     | 0.46              |
| 2:1V:269:MET:HE1  | 2:1V:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:1W:76:ASP:HA    | 2:1W:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:1W:176:LYS:HE2  | 1:2K:333:ALA:HB2  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1X:11:GLN:HB3   | 5:1X:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1Y:269:MET:HE1  | 2:1Y:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:2F:121:ARG:NH1  | 1:2F:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2I:242:LEU:HD11 | 1:2I:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:2L:259:LEU:HD11 | 1:2L:316:CYS:HB2  | 1.97                     | 0.46              |
| 2:2P:404:PHE:HD1  | 1:3C:260:VAL:O    | 1.95                     | 0.46              |
| 2:2P:407:TRP:HE1  | 1:3C:260:VAL:CG1  | 2.28                     | 0.46              |
| 2:2Q:69:ASP:HB2   | 2:2Q:75:MET:HE2   | 1.98                     | 0.46              |
| 2:2R:394:GLN:OE1  | 1:3E:349:THR:CG2  | 2.64                     | 0.46              |
| 2:2S:394:GLN:CB   | 1:3F:348:PRO:HG2  | 2.34                     | 0.46              |
| 2:2T:137:LEU:HG   | 2:2T:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:2U:69:ASP:HB2   | 2:2U:75:MET:HE2   | 1.98                     | 0.46              |
| 2:2V:269:MET:HE1  | 2:2V:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:2W:76:ASP:HA    | 2:2W:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:2W:269:MET:HE1  | 2:2W:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:2Z:242:LEU:HD12 | 2:2Z:251:ASP:HB2  | 1.98                     | 0.46              |
| 1:3B:209:ILE:HG23 | 1:3B:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3F:121:ARG:NH1  | 1:3F:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3I:242:LEU:HD11 | 1:3I:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3L:259:LEU:HD11 | 1:3L:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:3M:209:ILE:HG23 | 1:3M:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3M:259:LEU:HD11 | 1:3M:316:CYS:HB2  | 1.97                     | 0.46              |
| 2:3Q:69:ASP:HB2   | 2:3Q:75:MET:HE2   | 1.98                     | 0.46              |
| 2:3T:137:LEU:HG   | 2:3T:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:3U:69:ASP:HB2   | 2:3U:75:MET:HE2   | 1.98                     | 0.46              |
| 2:3V:269:MET:HE1  | 2:3V:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:3W:76:ASP:HA    | 2:3W:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:3Z:137:LEU:HG   | 2:3Z:139:HIS:HD2  | 1.81                     | 0.46              |
| 1:4A:242:LEU:HD11 | 1:4A:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:4B:242:LEU:HD11 | 1:4B:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:4F:121:ARG:NH1  | 1:4F:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4I:242:LEU:HD11 | 1:4I:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:4K:334:THR:O    | 1:4K:337:THR:OG1  | 2.30                     | 0.46              |
| 1:4L:259:LEU:HD11 | 1:4L:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4M:209:ILE:HG23 | 1:4M:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4N:242:LEU:HD11 | 1:4N:252:LEU:HD13 | 1.98                     | 0.46              |
| 2:4P:288:VAL:HB   | 2:4P:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:4Q:69:ASP:HB2   | 2:4Q:75:MET:HE2   | 1.98                     | 0.46              |
| 2:4U:69:ASP:HB2   | 2:4U:75:MET:HE2   | 1.98                     | 0.46              |
| 1:1A:346:TRP:CA   | 2:4H:397:ALA:O    | 2.63                     | 0.46              |
| 1:1B:253:THR:CG2  | 2:4O:100:GLY:CA   | 2.87                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:324:VAL:CG1  | 2:4O:222:PRO:C    | 2.87                     | 0.46              |
| 1:1B:332:ILE:CB   | 2:4O:177:VAL:HG21 | 2.46                     | 0.46              |
| 1:1C:2:ARG:HD3    | 2:4P:71:GLU:CB    | 2.34                     | 0.46              |
| 1:1C:261:PRO:HD3  | 2:4P:404:PHE:CE1  | 2.51                     | 0.46              |
| 1:1F:121:ARG:NH1  | 1:1F:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1J:121:ARG:NH1  | 1:1J:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1L:259:LEU:HD11 | 1:1L:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:1M:209:ILE:HG23 | 1:1M:230:LEU:HD22 | 1.98                     | 0.46              |
| 2:1H:3:GLU:HA     | 2:1H:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:1P:192:HIS:HD2  | 2:1P:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:1Q:69:ASP:HB2   | 2:1Q:75:MET:HE2   | 1.98                     | 0.46              |
| 2:1Q:200:GLU:HA   | 2:1Q:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:1S:137:LEU:HG   | 2:1S:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:1U:69:ASP:HB2   | 2:1U:75:MET:HE2   | 1.98                     | 0.46              |
| 2:1V:137:LEU:HG   | 2:1V:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:1W:269:MET:HE1  | 2:1W:383:ALA:HB3  | 1.97                     | 0.46              |
| 1:2F:259:LEU:HD11 | 1:2F:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:2G:211:ASP:CG   | 1:2G:215:ARG:HH12 | 2.24                     | 0.46              |
| 2:2H:288:VAL:HB   | 2:2H:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:2O:223:THR:HA   | 1:3B:325:PRO:HD2  | 1.98                     | 0.46              |
| 2:2P:6:HIS:CD2    | 2:2P:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:2P:192:HIS:HD2  | 2:2P:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:2P:210:TYR:CZ   | 1:3C:325:PRO:O    | 2.69                     | 0.46              |
| 2:2Q:200:GLU:HA   | 2:2Q:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:2R:200:GLU:HA   | 2:2R:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:2T:69:ASP:HB2   | 2:2T:75:MET:HE2   | 1.98                     | 0.46              |
| 2:2U:137:LEU:HG   | 2:2U:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:2V:72:PRO:HD2   | 1:3J:2:ARG:HG2    | 1.97                     | 0.46              |
| 2:2W:179:ASP:O    | 1:3K:352:LYS:HA   | 2.15                     | 0.46              |
| 2:2W:404:PHE:H    | 1:3K:261:PRO:C    | 2.09                     | 0.46              |
| 2:2X:11:GLN:HB3   | 5:2X:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2X:222:PRO:HD2  | 1:3L:326:LYS:HB3  | 1.98                     | 0.46              |
| 1:3J:121:ARG:NH1  | 1:3J:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3N:242:LEU:HD11 | 1:3N:252:LEU:HD13 | 1.98                     | 0.46              |
| 2:3H:137:LEU:HG   | 2:3H:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:3H:288:VAL:HB   | 2:3H:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:3P:192:HIS:HD2  | 2:3P:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:3P:200:GLU:HA   | 2:3P:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:3T:69:ASP:HB2   | 2:3T:75:MET:HE2   | 1.98                     | 0.46              |
| 2:3W:269:MET:HE1  | 2:3W:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:3X:11:GLN:HB3   | 5:3X:501:GDP:O1A  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3X:76:ASP:HA    | 2:3X:79:ARG:HG2   | 1.96                     | 0.46              |
| 1:4G:211:ASP:CG   | 1:4G:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:4N:216:ASN:HD21 | 1:4N:300:ASN:HD22 | 1.61                     | 0.46              |
| 2:4H:11:GLN:HB3   | 5:4H:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:4P:200:GLU:HA   | 2:4P:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:4Q:200:GLU:HA   | 2:4Q:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:4T:69:ASP:HB2   | 2:4T:75:MET:HE2   | 1.98                     | 0.46              |
| 2:4T:137:LEU:HG   | 2:4T:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:4V:269:MET:HE1  | 2:4V:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:4W:76:ASP:HA    | 2:4W:79:ARG:HG2   | 1.97                     | 0.46              |
| 1:1A:325:PRO:HD2  | 2:4H:222:PRO:O    | 2.15                     | 0.46              |
| 1:1B:216:ASN:HD21 | 1:1B:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:1B:260:VAL:HG12 | 2:4O:407:TRP:NE1  | 2.30                     | 0.46              |
| 1:1D:121:ARG:NH1  | 1:1D:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:1F:334:THR:O    | 1:1F:337:THR:OG1  | 2.30                     | 0.46              |
| 1:1G:211:ASP:CG   | 1:1G:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1G:259:LEU:HD11 | 1:1G:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:1G:348:PRO:HG3  | 2:4T:394:GLN:O    | 2.16                     | 0.46              |
| 1:1I:2:ARG:NH2    | 2:4U:73:GLY:CA    | 2.78                     | 0.46              |
| 1:1I:262:TYR:OH   | 2:4U:402:LYS:C    | 2.58                     | 0.46              |
| 1:1J:352:LYS:HA   | 2:4V:179:ASP:O    | 2.16                     | 0.46              |
| 1:1K:254:GLU:HG2  | 2:4W:101:ASN:N    | 2.30                     | 0.46              |
| 1:1K:346:TRP:HA   | 2:4W:397:ALA:C    | 2.40                     | 0.46              |
| 1:1L:209:ILE:HG23 | 1:1L:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1M:439:SER:OG   | 2:4Y:401:ARG:HD3  | 2.16                     | 0.46              |
| 1:1N:242:LEU:HD11 | 1:1N:252:LEU:HD13 | 1.98                     | 0.46              |
| 2:1H:11:GLN:HE22  | 1:2A:249:ASN:N    | 2.03                     | 0.46              |
| 2:1H:11:GLN:HB3   | 5:1H:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1P:6:HIS:CD2    | 2:1P:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:1Q:157:ILE:O    | 2:1Q:161:TYR:N    | 2.45                     | 0.46              |
| 2:1R:3:GLU:HA     | 2:1R:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:1R:200:GLU:HA   | 2:1R:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:1T:137:LEU:HG   | 2:1T:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:1U:137:LEU:HG   | 2:1U:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:1X:76:ASP:HA    | 2:1X:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:1X:242:LEU:HD12 | 2:1X:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1Y:76:ASP:HA    | 2:1Y:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:1Z:137:LEU:HG   | 2:1Z:139:HIS:HD2  | 1.81                     | 0.46              |
| 1:2B:211:ASP:CG   | 1:2B:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:2D:121:ARG:NH1  | 1:2D:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:2F:209:ILE:HG23 | 1:2F:230:LEU:HD22 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2I:30:ILE:HG13  | 1:2I:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:2K:334:THR:O    | 1:2K:337:THR:OG1  | 2.30                     | 0.46              |
| 1:2M:209:ILE:HG23 | 1:2M:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2N:216:ASN:HD21 | 1:2N:300:ASN:HD22 | 1.62                     | 0.46              |
| 1:2N:242:LEU:HD11 | 1:2N:252:LEU:HD13 | 1.98                     | 0.46              |
| 2:2H:3:GLU:HA     | 2:2H:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:2H:11:GLN:HB3   | 5:2H:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2H:137:LEU:HG   | 2:2H:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:2P:200:GLU:HA   | 2:2P:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:2R:3:GLU:HA     | 2:2R:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:2R:71:GLU:HG3   | 1:3E:2:ARG:HH11   | 1.81                     | 0.46              |
| 2:2U:404:PHE:CG   | 1:3I:261:PRO:CA   | 2.81                     | 0.46              |
| 2:2V:70:LEU:HD12  | 2:2V:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:2V:137:LEU:HG   | 2:2V:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:2W:221:THR:C    | 1:3K:324:VAL:CG1  | 2.88                     | 0.46              |
| 2:2X:76:ASP:HA    | 2:2X:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:2Y:3:GLU:HA     | 2:2Y:51:VAL:HG23  | 1.98                     | 0.46              |
| 1:3B:216:ASN:HD21 | 1:3B:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:3D:121:ARG:NH1  | 1:3D:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:3F:242:LEU:HD11 | 1:3F:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3G:211:ASP:CG   | 1:3G:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3L:209:ILE:HG23 | 1:3L:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3N:216:ASN:HD21 | 1:3N:300:ASN:HD22 | 1.61                     | 0.46              |
| 2:3H:3:GLU:HA     | 2:3H:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:3H:11:GLN:HB3   | 5:3H:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:3P:6:HIS:CD2    | 2:3P:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:3R:3:GLU:HA     | 2:3R:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:3U:242:LEU:HD12 | 2:3U:251:ASP:HB2  | 1.98                     | 0.46              |
| 1:4B:211:ASP:CG   | 1:4B:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:4D:121:ARG:NH1  | 1:4D:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4E:30:ILE:HG13  | 1:4E:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:4F:242:LEU:HD11 | 1:4F:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:4F:259:LEU:HD11 | 1:4F:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4K:216:ASN:HD21 | 1:4K:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:4L:211:ASP:CG   | 1:4L:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:4M:211:ASP:CG   | 1:4M:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:4M:216:ASN:HD21 | 1:4M:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:4M:265:ILE:HG22 | 1:4M:380:ASN:HD21 | 1.80                     | 0.46              |
| 2:4H:3:GLU:HA     | 2:4H:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:4H:137:LEU:HG   | 2:4H:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:4H:288:VAL:HB   | 2:4H:327:GLU:HG2  | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4P:6:HIS:CD2    | 2:4P:8:GLN:HE21   | 2.33                     | 0.46              |
| 2:4U:137:LEU:HG   | 2:4U:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:4U:242:LEU:HD12 | 2:4U:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4V:70:LEU:HD12  | 2:4V:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:4X:76:ASP:HA    | 2:4X:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:4Y:76:ASP:HA    | 2:4Y:79:ARG:HG2   | 1.96                     | 0.46              |
| 2:4Z:137:LEU:HG   | 2:4Z:139:HIS:HD2  | 1.81                     | 0.46              |
| 1:1A:209:ILE:HG23 | 1:1A:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1B:211:ASP:CG   | 1:1B:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1B:351:PHE:N    | 2:4O:178:SER:OG   | 2.49                     | 0.46              |
| 1:1D:211:ASP:CG   | 1:1D:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1D:261:PRO:N    | 2:4Q:404:PHE:CE1  | 2.83                     | 0.46              |
| 1:1E:30:ILE:HG13  | 1:1E:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:1E:329:ASN:OD1  | 2:4R:207:GLU:OE1  | 2.33                     | 0.46              |
| 1:1F:242:LEU:HD11 | 1:1F:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1G:314:ALA:CB   | 2:4T:181:VAL:HG11 | 2.45                     | 0.46              |
| 1:1G:324:VAL:CG1  | 2:4T:222:PRO:C    | 2.83                     | 0.46              |
| 1:1I:30:ILE:HG13  | 1:1I:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:1J:211:ASP:CG   | 1:1J:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1K:216:ASN:HD21 | 1:1K:300:ASN:HD22 | 1.62                     | 0.46              |
| 1:1M:211:ASP:CG   | 1:1M:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1M:349:THR:CB   | 2:4Y:184:PRO:HD3  | 2.46                     | 0.46              |
| 1:1N:260:VAL:HG11 | 2:4Z:407:TRP:CZ2  | 2.50                     | 0.46              |
| 2:1H:137:LEU:HG   | 2:1H:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:1P:3:GLU:HA     | 2:1P:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:1P:200:GLU:HA   | 2:1P:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:1R:404:PHE:CE2  | 1:2E:261:PRO:HB3  | 2.51                     | 0.46              |
| 2:1S:288:VAL:HB   | 2:1S:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:1U:242:LEU:HD12 | 2:1U:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1V:70:LEU:HD12  | 2:1V:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:1W:11:GLN:HB3   | 5:1W:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:1W:178:SER:CB   | 1:2K:349:THR:HB   | 2.43                     | 0.46              |
| 2:1X:404:PHE:CZ   | 1:2L:261:PRO:HA   | 2.50                     | 0.46              |
| 2:1Y:3:GLU:HA     | 2:1Y:51:VAL:HG23  | 1.98                     | 0.46              |
| 1:2E:30:ILE:HG13  | 1:2E:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:2F:132:LEU:HD23 | 1:2F:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:2F:242:LEU:HD11 | 1:2F:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:2F:334:THR:O    | 1:2F:337:THR:OG1  | 2.30                     | 0.46              |
| 1:2G:259:LEU:HD11 | 1:2G:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:2J:30:ILE:HG13  | 1:2J:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:2J:121:ARG:NH1  | 1:2J:124:LYS:HD2  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2K:216:ASN:HD21 | 1:2K:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:2L:211:ASP:CG   | 1:2L:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:2M:30:ILE:HG13  | 1:2M:53:PHE:HE2   | 1.81                     | 0.46              |
| 2:2H:269:MET:HE1  | 2:2H:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:2O:221:THR:CB   | 1:3B:324:VAL:HG21 | 2.46                     | 0.46              |
| 2:2P:3:GLU:HA     | 2:2P:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:2P:72:PRO:HD2   | 1:3C:2:ARG:CD     | 2.46                     | 0.46              |
| 2:2Q:176:LYS:CE   | 1:3D:333:ALA:HB1  | 2.33                     | 0.46              |
| 2:2S:207:GLU:OE1  | 1:3F:329:ASN:CG   | 2.52                     | 0.46              |
| 2:2U:242:LEU:HD12 | 2:2U:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2V:221:THR:OG1  | 1:3J:324:VAL:HG22 | 2.10                     | 0.46              |
| 2:2Y:76:ASP:HA    | 2:2Y:79:ARG:HG2   | 1.97                     | 0.46              |
| 2:2Y:77:SER:CB    | 1:3M:245:ASP:CG   | 2.89                     | 0.46              |
| 2:2Y:100:GLY:HA2  | 1:3M:253:THR:C    | 2.41                     | 0.46              |
| 2:2Y:406:HIS:CE1  | 1:3M:263:PRO:N    | 2.83                     | 0.46              |
| 2:2Z:137:LEU:HG   | 2:2Z:139:HIS:HD2  | 1.81                     | 0.46              |
| 1:3B:211:ASP:CG   | 1:3B:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3E:30:ILE:HG13  | 1:3E:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:3F:209:ILE:HG23 | 1:3F:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3F:259:LEU:HD11 | 1:3F:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:3F:334:THR:O    | 1:3F:337:THR:OG1  | 2.30                     | 0.46              |
| 1:3G:259:LEU:HD11 | 1:3G:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:3I:30:ILE:HG13  | 1:3I:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:3J:30:ILE:HG13  | 1:3J:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:3K:216:ASN:HD21 | 1:3K:300:ASN:HD22 | 1.62                     | 0.46              |
| 1:3K:334:THR:O    | 1:3K:337:THR:OG1  | 2.30                     | 0.46              |
| 1:3L:211:ASP:CG   | 1:3L:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3M:211:ASP:CG   | 1:3M:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3M:228:ASN:OD1  | 3:3M:501:GTP:N1   | 2.47                     | 0.46              |
| 2:3P:3:GLU:HA     | 2:3P:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:3Q:157:ILE:O    | 2:3Q:161:TYR:N    | 2.45                     | 0.46              |
| 2:3R:200:GLU:HA   | 2:3R:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:3S:137:LEU:HG   | 2:3S:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:3U:137:LEU:HG   | 2:3U:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:3V:70:LEU:HD12  | 2:3V:99:ALA:HB2   | 1.96                     | 0.46              |
| 2:3V:137:LEU:HG   | 2:3V:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:3W:11:GLN:HB3   | 5:3W:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:3Y:76:ASP:HA    | 2:3Y:79:ARG:HG2   | 1.97                     | 0.46              |
| 1:4F:132:LEU:HD23 | 1:4F:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:4F:209:ILE:HG23 | 1:4F:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4F:334:THR:O    | 1:4F:337:THR:OG1  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4G:259:LEU:HD11 | 1:4G:316:CYS:HB2  | 1.97                     | 0.46              |
| 1:4I:30:ILE:HG13  | 1:4I:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:4J:30:ILE:HG13  | 1:4J:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:4L:216:ASN:HD21 | 1:4L:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:4L:241:SER:OG   | 1:4L:250:VAL:O    | 2.27                     | 0.46              |
| 2:4P:3:GLU:HA     | 2:4P:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:4P:192:HIS:HD2  | 2:4P:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:4Q:192:HIS:HD2  | 2:4Q:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:4R:3:GLU:HA     | 2:4R:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:4R:200:GLU:HA   | 2:4R:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:4S:242:LEU:HD12 | 2:4S:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:4T:74:THR:O     | 2:4T:77:SER:OG    | 2.31                     | 0.46              |
| 2:4V:137:LEU:HG   | 2:4V:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:4Y:3:GLU:HA     | 2:4Y:51:VAL:HG23  | 1.98                     | 0.46              |
| 1:1A:253:THR:CG2  | 2:4H:100:GLY:CA   | 2.90                     | 0.46              |
| 1:1B:326:LYS:CE   | 2:4O:210:TYR:O    | 2.62                     | 0.46              |
| 1:1C:30:ILE:HG13  | 1:1C:53:PHE:HE2   | 1.81                     | 0.46              |
| 1:1C:132:LEU:HD23 | 1:1C:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:1C:242:LEU:HD11 | 1:1C:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1D:132:LEU:HD23 | 1:1D:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:1F:132:LEU:HD23 | 1:1F:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:1F:209:ILE:HG23 | 1:1F:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:1G:265:ILE:HG22 | 1:1G:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:1J:30:ILE:HG13  | 1:1J:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:1J:242:LEU:HD11 | 1:1J:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:1K:262:TYR:CZ   | 2:4W:403:ALA:HA   | 2.51                     | 0.46              |
| 1:1L:211:ASP:CG   | 1:1L:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:1M:30:ILE:HG13  | 1:1M:53:PHE:HE2   | 1.82                     | 0.46              |
| 1:1M:228:ASN:OD1  | 3:1M:501:GTP:N1   | 2.47                     | 0.46              |
| 1:1N:216:ASN:HD21 | 1:1N:300:ASN:HD22 | 1.62                     | 0.46              |
| 2:1H:269:MET:HE1  | 2:1H:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:1O:242:LEU:HD12 | 2:1O:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1P:404:PHE:CD1  | 1:2C:261:PRO:HA   | 2.51                     | 0.46              |
| 2:1S:3:GLU:HA     | 2:1S:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:1S:242:LEU:HD12 | 2:1S:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:1T:3:GLU:HA     | 2:1T:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:1T:404:PHE:CZ   | 1:2G:261:PRO:N    | 2.83                     | 0.46              |
| 2:1W:401:ARG:O    | 1:2K:262:TYR:CE1  | 2.69                     | 0.46              |
| 1:2A:209:ILE:HG23 | 1:2A:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2B:216:ASN:HD21 | 1:2B:300:ASN:HD22 | 1.61                     | 0.46              |
| 1:2D:132:LEU:HD23 | 1:2D:164:LYS:NZ   | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2J:132:LEU:HD23 | 1:2J:164:LYS:NZ   | 2.31                     | 0.46              |
| 1:2J:211:ASP:CG   | 1:2J:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:2K:30:ILE:HG13  | 1:2K:53:PHE:CE2   | 2.51                     | 0.46              |
| 1:2L:209:ILE:HG23 | 1:2L:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:2L:216:ASN:HD21 | 1:2L:300:ASN:HD22 | 1.62                     | 0.46              |
| 1:2M:211:ASP:CG   | 1:2M:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:2M:216:ASN:HD21 | 1:2M:300:ASN:HD22 | 1.62                     | 0.46              |
| 1:2M:265:ILE:HG22 | 1:2M:380:ASN:HD21 | 1.80                     | 0.46              |
| 2:2H:406:HIS:NE2  | 1:3A:263:PRO:CD   | 2.77                     | 0.46              |
| 2:2O:242:LEU:HD12 | 2:2O:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2Q:3:GLU:HA     | 2:2Q:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:2Q:157:ILE:O    | 2:2Q:161:TYR:N    | 2.45                     | 0.46              |
| 2:2Q:192:HIS:HD2  | 2:2Q:424:ASN:HD22 | 1.64                     | 0.46              |
| 2:2S:137:LEU:HG   | 2:2S:139:HIS:HD2  | 1.81                     | 0.46              |
| 2:2S:242:LEU:HD12 | 2:2S:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2S:288:VAL:HB   | 2:2S:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:2U:179:ASP:C    | 1:3I:352:LYS:HA   | 2.41                     | 0.46              |
| 2:2W:11:GLN:HB3   | 5:2W:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:2W:398:MET:HA   | 1:3K:346:TRP:HB2  | 1.98                     | 0.46              |
| 2:2X:101:ASN:C    | 1:3L:257:THR:HG21 | 2.36                     | 0.46              |
| 2:2X:214:PHE:CG   | 1:3L:326:LYS:CE   | 2.99                     | 0.46              |
| 2:2X:242:LEU:HD12 | 2:2X:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:2X:394:GLN:CA   | 1:3L:348:PRO:HG3  | 2.46                     | 0.46              |
| 2:2Y:221:THR:C    | 1:3M:324:VAL:HG11 | 2.41                     | 0.46              |
| 2:2Y:394:GLN:OE1  | 1:3M:349:THR:CG2  | 2.64                     | 0.46              |
| 2:2Z:3:GLU:HA     | 2:2Z:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:2Z:404:PHE:CE1  | 1:3N:261:PRO:CA   | 2.99                     | 0.46              |
| 1:3A:209:ILE:HG23 | 1:3A:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:3D:211:ASP:CG   | 1:3D:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3G:265:ILE:HG22 | 1:3G:380:ASN:HD21 | 1.80                     | 0.46              |
| 1:3J:211:ASP:CG   | 1:3J:215:ARG:HH12 | 2.24                     | 0.46              |
| 1:3J:242:LEU:HD11 | 1:3J:252:LEU:HD13 | 1.98                     | 0.46              |
| 1:3M:30:ILE:HG13  | 1:3M:53:PHE:HE2   | 1.81                     | 0.46              |
| 1:3M:216:ASN:HD21 | 1:3M:300:ASN:HD22 | 1.61                     | 0.46              |
| 2:3H:269:MET:HE1  | 2:3H:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:3S:3:GLU:HA     | 2:3S:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:3S:242:LEU:HD12 | 2:3S:251:ASP:HB2  | 1.98                     | 0.46              |
| 2:3T:74:THR:O     | 2:3T:77:SER:OG    | 2.31                     | 0.46              |
| 2:3Y:3:GLU:HA     | 2:3Y:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:3Y:137:LEU:HG   | 2:3Y:139:HIS:HD2  | 1.81                     | 0.46              |
| 1:4B:216:ASN:HD21 | 1:4B:300:ASN:HD22 | 1.62                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4J:121:ARG:NH1  | 1:4J:124:LYS:HD2  | 2.30                     | 0.46              |
| 1:4L:30:ILE:HG13  | 1:4L:53:PHE:HE2   | 1.81                     | 0.46              |
| 1:4L:209:ILE:HG23 | 1:4L:230:LEU:HD22 | 1.98                     | 0.46              |
| 1:4M:30:ILE:HG13  | 1:4M:53:PHE:HE2   | 1.81                     | 0.46              |
| 2:4H:269:MET:HE1  | 2:4H:383:ALA:HB3  | 1.97                     | 0.46              |
| 2:4O:200:GLU:HA   | 2:4O:266:HIS:HB2  | 1.98                     | 0.46              |
| 2:4S:3:GLU:HA     | 2:4S:51:VAL:HG23  | 1.98                     | 0.46              |
| 2:4S:288:VAL:HB   | 2:4S:327:GLU:HG2  | 1.96                     | 0.46              |
| 2:4W:11:GLN:HB3   | 5:4W:501:GDP:O1A  | 2.15                     | 0.46              |
| 2:4Z:3:GLU:HA     | 2:4Z:51:VAL:HG23  | 1.98                     | 0.46              |
| 1:1B:346:TRP:CZ3  | 2:4O:403:ALA:HB1  | 2.51                     | 0.45              |
| 1:1D:30:ILE:HG13  | 1:1D:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1D:265:ILE:HG22 | 1:1D:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:1E:1:MET:O      | 2:4R:96:GLN:OE1   | 2.34                     | 0.45              |
| 1:1E:132:LEU:HD23 | 1:1E:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:1E:253:THR:CB   | 2:4R:100:GLY:HA3  | 2.45                     | 0.45              |
| 1:1E:257:THR:CG2  | 2:4R:102:ASN:CB   | 2.86                     | 0.45              |
| 1:1F:349:THR:HB   | 2:4S:183:GLU:HG2  | 1.98                     | 0.45              |
| 1:1I:132:LEU:HD23 | 1:1I:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:1I:228:ASN:OD1  | 3:1I:501:GTP:N1   | 2.47                     | 0.45              |
| 1:1I:439:SER:OG   | 2:4U:401:ARG:HG2  | 2.16                     | 0.45              |
| 1:1K:30:ILE:HG13  | 1:1K:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1K:334:THR:O    | 1:1K:337:THR:OG1  | 2.30                     | 0.45              |
| 1:1K:353:VAL:CG2  | 2:4W:179:ASP:OD1  | 2.63                     | 0.45              |
| 1:1L:216:ASN:HD21 | 1:1L:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:1M:216:ASN:HD21 | 1:1M:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:1M:261:PRO:O    | 2:4Y:406:HIS:NE2  | 2.45                     | 0.45              |
| 1:1M:265:ILE:HG22 | 1:1M:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:1N:30:ILE:HG13  | 1:1N:53:PHE:HE2   | 1.81                     | 0.45              |
| 2:1O:137:LEU:HG   | 2:1O:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:1O:192:HIS:HD2  | 2:1O:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1Q:192:HIS:HD2  | 2:1Q:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1Q:224:TYR:HD2  | 1:2D:247:ALA:O    | 1.99                     | 0.45              |
| 2:1Q:269:MET:HE1  | 2:1Q:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1R:179:ASP:O    | 1:2E:352:LYS:CD   | 2.64                     | 0.45              |
| 2:1S:200:GLU:HA   | 2:1S:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1U:404:PHE:CE2  | 1:2I:261:PRO:CB   | 3.00                     | 0.45              |
| 2:1W:137:LEU:HG   | 2:1W:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:1X:69:ASP:HB2   | 2:1X:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1X:132:LEU:HB3  | 2:1X:164:ARG:HE   | 1.81                     | 0.45              |
| 2:1X:401:ARG:NH2  | 1:2L:435:VAL:HG22 | 2.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Y:137:LEU:HG   | 2:1Y:139:HIS:HD2  | 1.81                     | 0.45              |
| 1:2C:242:LEU:HD11 | 1:2C:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2D:211:ASP:CG   | 1:2D:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2G:265:ILE:HG22 | 1:2G:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:2J:242:LEU:HD11 | 1:2J:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2K:30:ILE:HG13  | 1:2K:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2L:30:ILE:HG13  | 1:2L:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2L:241:SER:OG   | 1:2L:250:VAL:O    | 2.27                     | 0.45              |
| 1:2M:228:ASN:OD1  | 3:2M:501:GTP:N1   | 2.47                     | 0.45              |
| 1:2N:30:ILE:HG13  | 1:2N:53:PHE:HE2   | 1.81                     | 0.45              |
| 2:2O:192:HIS:HD2  | 2:2O:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:2P:406:HIS:CE1  | 1:3C:263:PRO:HA   | 2.50                     | 0.45              |
| 2:2Q:269:MET:HE1  | 2:2Q:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2S:3:GLU:HA     | 2:2S:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:2T:3:GLU:HA     | 2:2T:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:2T:11:GLN:NE2   | 1:3G:249:ASN:N    | 1.98                     | 0.45              |
| 2:2V:72:PRO:HD2   | 1:3J:2:ARG:CD     | 2.45                     | 0.45              |
| 2:2X:69:ASP:HB2   | 2:2X:75:MET:HE2   | 1.98                     | 0.45              |
| 5:2X:501:GDP:N7   | 1:3L:248:LEU:HD13 | 2.28                     | 0.45              |
| 2:2Y:137:LEU:HG   | 2:2Y:139:HIS:HD2  | 1.81                     | 0.45              |
| 1:3C:132:LEU:HD23 | 1:3C:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3C:242:LEU:HD11 | 1:3C:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:3D:132:LEU:HD23 | 1:3D:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3D:265:ILE:HG22 | 1:3D:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:3F:132:LEU:HD23 | 1:3F:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:3G:132:LEU:HD23 | 1:3G:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3J:132:LEU:HD23 | 1:3J:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:3K:30:ILE:HG13  | 1:3K:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3L:30:ILE:HG13  | 1:3L:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:3L:216:ASN:HD21 | 1:3L:300:ASN:HD22 | 1.62                     | 0.45              |
| 1:3M:265:ILE:HG22 | 1:3M:380:ASN:HD21 | 1.80                     | 0.45              |
| 2:3O:242:LEU:HD12 | 2:3O:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:3Q:3:GLU:HA     | 2:3Q:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:3Q:192:HIS:HD2  | 2:3Q:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3Q:269:MET:HE1  | 2:3Q:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3S:200:GLU:HA   | 2:3S:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:3S:269:MET:HE1  | 2:3S:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3S:288:VAL:HB   | 2:3S:327:GLU:HG2  | 1.96                     | 0.45              |
| 2:3T:3:GLU:HA     | 2:3T:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:3X:69:ASP:HB2   | 2:3X:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3X:132:LEU:HB3  | 2:3X:164:ARG:HE   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3X:242:LEU:HD12 | 2:3X:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:3Y:11:GLN:HB3   | 5:3Y:501:GDP:O1A  | 2.15                     | 0.45              |
| 2:3Z:3:GLU:HA     | 2:3Z:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:4A:209:ILE:HG23 | 1:4A:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:4A:216:ASN:HD21 | 1:4A:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:4C:30:ILE:HG13  | 1:4C:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4D:30:ILE:HG13  | 1:4D:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4D:211:ASP:CG   | 1:4D:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4J:132:LEU:HD23 | 1:4J:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:4K:30:ILE:HG13  | 1:4K:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4N:30:ILE:HG13  | 1:4N:53:PHE:HE2   | 1.81                     | 0.45              |
| 2:4O:192:HIS:HD2  | 2:4O:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:4O:242:LEU:HD12 | 2:4O:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4Q:269:MET:HE1  | 2:4Q:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4S:6:HIS:CD2    | 2:4S:8:GLN:HE21   | 2.33                     | 0.45              |
| 2:4S:137:LEU:HG   | 2:4S:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:4S:269:MET:HE1  | 2:4S:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4T:3:GLU:HA     | 2:4T:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:4U:269:MET:HE1  | 2:4U:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4X:69:ASP:HB2   | 2:4X:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4X:242:LEU:HD12 | 2:4X:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4Y:137:LEU:HG   | 2:4Y:139:HIS:HD2  | 1.81                     | 0.45              |
| 1:1B:248:LEU:CD2  | 2:4O:179:ASP:OD2  | 2.63                     | 0.45              |
| 1:1B:254:GLU:CA   | 2:4O:100:GLY:C    | 2.79                     | 0.45              |
| 1:1D:324:VAL:HG12 | 2:4Q:222:PRO:O    | 2.12                     | 0.45              |
| 1:1G:132:LEU:HD23 | 1:1G:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:1G:326:LYS:CB   | 2:4T:210:TYR:CD1  | 2.99                     | 0.45              |
| 1:1I:325:PRO:HG2  | 2:4U:224:TYR:CD1  | 2.49                     | 0.45              |
| 1:1J:132:LEU:HD23 | 1:1J:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:1L:30:ILE:HG13  | 1:1L:53:PHE:HE2   | 1.82                     | 0.45              |
| 1:1L:326:LYS:HB3  | 2:4X:222:PRO:HG2  | 1.92                     | 0.45              |
| 1:1L:347:CYS:HA   | 2:4X:398:MET:HG2  | 1.98                     | 0.45              |
| 1:1L:352:LYS:HD3  | 2:4X:101:ASN:HD22 | 1.79                     | 0.45              |
| 2:1O:206:ASN:ND2  | 5:1O:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1O:269:MET:HE1  | 2:1O:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1Q:3:GLU:HA     | 2:1Q:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:1R:269:MET:HE1  | 2:1R:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1S:6:HIS:CD2    | 2:1S:8:GLN:HE21   | 2.33                     | 0.45              |
| 2:1S:269:MET:HE1  | 2:1S:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1U:3:GLU:HA     | 2:1U:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:1V:181:VAL:CG2  | 1:2J:258:ASN:CB   | 2.79                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1W:132:LEU:HB3  | 2:1W:164:ARG:HE   | 1.81                     | 0.45              |
| 2:1Y:11:GLN:HB3   | 5:1Y:501:GDP:O1A  | 2.15                     | 0.45              |
| 2:1Y:206:ASN:ND2  | 5:1Y:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1Z:3:GLU:HA     | 2:1Z:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:2A:216:ASN:HD21 | 1:2A:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:2B:30:ILE:HG13  | 1:2B:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2C:132:LEU:HD23 | 1:2C:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2D:30:ILE:HG13  | 1:2D:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:2G:30:ILE:HG13  | 1:2G:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:2G:132:LEU:HD23 | 1:2G:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:2I:132:LEU:HD23 | 1:2I:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2K:211:ASP:CG   | 1:2K:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2K:259:LEU:HD11 | 1:2K:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:2M:229:ARG:NH1  | 1:2M:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:2O:200:GLU:HA   | 2:2O:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2O:206:ASN:ND2  | 5:2O:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2O:269:MET:HE1  | 2:2O:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2P:69:ASP:HB2   | 2:2P:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2Q:407:TRP:CD1  | 1:3D:260:VAL:O    | 2.69                     | 0.45              |
| 2:2R:206:ASN:ND2  | 5:2R:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2R:269:MET:HE1  | 2:2R:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2S:6:HIS:CD2    | 2:2S:8:GLN:HE21   | 2.33                     | 0.45              |
| 2:2S:269:MET:HE1  | 2:2S:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2U:3:GLU:HA     | 2:2U:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:2U:269:MET:HE1  | 2:2U:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2W:3:GLU:HA     | 2:2W:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:2W:137:LEU:HG   | 2:2W:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:2Y:11:GLN:HB3   | 5:2Y:501:GDP:O1A  | 2.15                     | 0.45              |
| 2:2Y:206:ASN:ND2  | 5:2Y:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:3A:216:ASN:HD21 | 1:3A:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:3C:30:ILE:HG13  | 1:3C:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:3D:30:ILE:HG13  | 1:3D:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3E:132:LEU:HD23 | 1:3E:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3I:70:LEU:HD22  | 1:3I:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3I:132:LEU:HD23 | 1:3I:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:3J:259:LEU:HD11 | 1:3J:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:3K:259:LEU:HD11 | 1:3K:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:3L:121:ARG:NH1  | 1:3L:124:LYS:HD2  | 2.30                     | 0.45              |
| 1:3L:241:SER:OG   | 1:3L:250:VAL:O    | 2.27                     | 0.45              |
| 1:3M:229:ARG:NH1  | 1:3M:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3N:30:ILE:HG13  | 1:3N:53:PHE:HE2   | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3O:192:HIS:HD2  | 2:3O:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3O:200:GLU:HA   | 2:3O:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:3O:269:MET:HE1  | 2:3O:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3R:269:MET:HE1  | 2:3R:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3U:3:GLU:HA     | 2:3U:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:3W:132:LEU:HB3  | 2:3W:164:ARG:HE   | 1.81                     | 0.45              |
| 2:3W:137:LEU:HG   | 2:3W:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:3W:206:ASN:ND2  | 5:3W:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3Y:206:ASN:ND2  | 5:3Y:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:4A:30:ILE:HG13  | 1:4A:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4C:132:LEU:HD23 | 1:4C:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:4C:242:LEU:HD11 | 1:4C:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:4G:132:LEU:HD23 | 1:4G:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:4G:229:ARG:NH1  | 1:4G:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4G:265:ILE:HG22 | 1:4G:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:4I:70:LEU:HD22  | 1:4I:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4I:132:LEU:HD23 | 1:4I:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:4J:211:ASP:CG   | 1:4J:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4J:242:LEU:HD11 | 1:4J:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:4K:30:ILE:HG13  | 1:4K:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4K:211:ASP:CG   | 1:4K:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4L:121:ARG:NH1  | 1:4L:124:LYS:HD2  | 2.30                     | 0.45              |
| 1:4M:228:ASN:OD1  | 3:4M:501:GTP:N1   | 2.47                     | 0.45              |
| 2:4O:137:LEU:HG   | 2:4O:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:4O:206:ASN:ND2  | 5:4O:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4O:269:MET:HE1  | 2:4O:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4Q:157:ILE:O    | 2:4Q:161:TYR:N    | 2.45                     | 0.45              |
| 2:4R:69:ASP:HB2   | 2:4R:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4R:206:ASN:ND2  | 5:4R:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4R:269:MET:HE1  | 2:4R:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4W:132:LEU:HB3  | 2:4W:164:ARG:HE   | 1.81                     | 0.45              |
| 2:4Y:11:GLN:HB3   | 5:4Y:501:GDP:O1A  | 2.15                     | 0.45              |
| 1:1B:248:LEU:HD21 | 2:4O:179:ASP:OD2  | 2.16                     | 0.45              |
| 1:1C:229:ARG:NH1  | 1:1C:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1F:30:ILE:HG13  | 1:1F:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1F:247:ALA:O    | 2:4S:15:GLN:CD    | 2.59                     | 0.45              |
| 1:1F:346:TRP:CD1  | 2:4S:401:ARG:HB2  | 2.52                     | 0.45              |
| 1:1G:30:ILE:HG13  | 1:1G:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1G:229:ARG:NH1  | 1:1G:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1G:261:PRO:O    | 2:4T:404:PHE:CA   | 2.64                     | 0.45              |
| 1:1I:70:LEU:HD22  | 1:1I:110:ILE:HG22 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:258:ASN:OD1  | 2:4U:101:ASN:CB   | 2.64                     | 0.45              |
| 1:1J:259:LEU:HD11 | 1:1J:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:1K:30:ILE:HG13  | 1:1K:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:1L:261:PRO:HB3  | 2:4X:404:PHE:CE2  | 2.51                     | 0.45              |
| 1:1M:229:ARG:NH1  | 1:1M:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1M:253:THR:C    | 2:4Y:100:GLY:CA   | 2.89                     | 0.45              |
| 2:1O:3:GLU:HA     | 2:1O:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:1O:200:GLU:HA   | 2:1O:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1Q:404:PHE:CE1  | 1:2D:260:VAL:O    | 2.70                     | 0.45              |
| 2:1R:69:ASP:HB2   | 2:1R:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1R:206:ASN:ND2  | 5:1R:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1U:206:ASN:ND2  | 5:1U:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1U:269:MET:HE1  | 2:1U:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1W:3:GLU:HA     | 2:1W:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:1W:69:ASP:HB2   | 2:1W:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1W:206:ASN:ND2  | 5:1W:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1Y:394:GLN:OE1  | 1:2M:349:THR:CG2  | 2.65                     | 0.45              |
| 5:1Y:501:GDP:C8   | 1:2M:248:LEU:HD13 | 2.51                     | 0.45              |
| 1:2A:30:ILE:HG13  | 1:2A:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2B:334:THR:O    | 1:2B:337:THR:OG1  | 2.30                     | 0.45              |
| 1:2C:30:ILE:HG13  | 1:2C:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2D:265:ILE:HG22 | 1:2D:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:2E:132:LEU:HD23 | 1:2E:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2G:229:ARG:NH1  | 1:2G:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2I:70:LEU:HD22  | 1:2I:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2J:259:LEU:HD11 | 1:2J:316:CYS:HB2  | 1.97                     | 0.45              |
| 2:2H:71:GLU:HG3   | 1:3A:2:ARG:NH1    | 2.32                     | 0.45              |
| 2:2H:73:GLY:HA3   | 1:3A:2:ARG:CZ     | 2.47                     | 0.45              |
| 2:2H:242:LEU:HD12 | 2:2H:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:2O:137:LEU:HG   | 2:2O:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:2R:69:ASP:HB2   | 2:2R:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2R:178:SER:OG   | 1:3E:351:PHE:HB2  | 2.16                     | 0.45              |
| 2:2R:242:LEU:HD12 | 2:2R:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:2S:200:GLU:HA   | 2:2S:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2U:206:ASN:ND2  | 5:2U:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2W:72:PRO:HD2   | 1:3K:2:ARG:HG2    | 1.99                     | 0.45              |
| 2:2W:132:LEU:HB3  | 2:2W:164:ARG:HE   | 1.81                     | 0.45              |
| 2:2W:206:ASN:ND2  | 5:2W:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2X:132:LEU:HB3  | 2:2X:164:ARG:HE   | 1.81                     | 0.45              |
| 1:3A:30:ILE:HG13  | 1:3A:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:3A:399:TYR:OH   | 1:3A:415:GLU:OE2  | 2.27                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3B:132:LEU:HD23 | 1:3B:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3C:229:ARG:NH1  | 1:3C:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3D:276:ILE:HG21 | 1:3D:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3F:30:ILE:HG13  | 1:3F:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3G:30:ILE:HG13  | 1:3G:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3G:229:ARG:NH1  | 1:3G:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3K:30:ILE:HG13  | 1:3K:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:3K:209:ILE:HG23 | 1:3K:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:3K:211:ASP:CG   | 1:3K:215:ARG:HH12 | 2.24                     | 0.45              |
| 2:3O:137:LEU:HG   | 2:3O:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:3O:206:ASN:ND2  | 5:3O:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3P:69:ASP:HB2   | 2:3P:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3R:206:ASN:ND2  | 5:3R:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3S:6:HIS:CD2    | 2:3S:8:GLN:HE21   | 2.33                     | 0.45              |
| 2:3U:206:ASN:ND2  | 5:3U:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3U:269:MET:HE1  | 2:3U:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3W:3:GLU:HA     | 2:3W:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:4B:30:ILE:HG13  | 1:4B:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4D:132:LEU:HD23 | 1:4D:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:4D:265:ILE:HG22 | 1:4D:380:ASN:HD21 | 1.80                     | 0.45              |
| 1:4E:132:LEU:HD23 | 1:4E:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:4G:30:ILE:HG13  | 1:4G:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4J:259:LEU:HD11 | 1:4J:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:4K:209:ILE:HG23 | 1:4K:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:4K:259:LEU:HD11 | 1:4K:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:4M:229:ARG:NH1  | 1:4M:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:4H:242:LEU:HD12 | 2:4H:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4S:200:GLU:HA   | 2:4S:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:4U:3:GLU:HA     | 2:4U:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:4W:3:GLU:HA     | 2:4W:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:4W:137:LEU:HG   | 2:4W:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:4W:206:ASN:ND2  | 5:4W:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4X:132:LEU:HB3  | 2:4X:164:ARG:HE   | 1.81                     | 0.45              |
| 2:4Y:167:ASN:OD1  | 2:4Y:167:ASN:N    | 2.48                     | 0.45              |
| 2:4Y:206:ASN:ND2  | 5:4Y:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:1A:30:ILE:HG13  | 1:1A:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:1A:216:ASN:HD21 | 1:1A:300:ASN:HD22 | 1.61                     | 0.45              |
| 1:1A:245:ASP:OD2  | 2:4H:77:SER:HB2   | 2.17                     | 0.45              |
| 1:1B:30:ILE:HG13  | 1:1B:53:PHE:HE2   | 1.82                     | 0.45              |
| 1:1B:132:LEU:HD23 | 1:1B:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:1C:325:PRO:HB3  | 2:4P:224:TYR:CE1  | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:258:ASN:HD22 | 2:4Q:182:VAL:HG22 | 1.80                     | 0.45              |
| 1:1D:276:ILE:HG21 | 1:1D:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1F:254:GLU:CG   | 2:4S:100:GLY:CA   | 2.95                     | 0.45              |
| 1:1G:346:TRP:HZ3  | 2:4T:404:PHE:CE2  | 2.35                     | 0.45              |
| 1:1I:229:ARG:NH1  | 1:1I:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1I:256:GLN:O    | 2:4U:407:TRP:CE2  | 2.70                     | 0.45              |
| 1:1I:349:THR:HG21 | 2:4U:183:GLU:HG3  | 1.99                     | 0.45              |
| 1:1J:70:LEU:HD22  | 1:1J:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1J:276:ILE:HG21 | 1:1J:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1K:132:LEU:HD23 | 1:1K:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:1K:211:ASP:CG   | 1:1K:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:1K:346:TRP:HZ3  | 2:4W:404:PHE:CD2  | 2.33                     | 0.45              |
| 1:1L:121:ARG:NH1  | 1:1L:124:LYS:HD2  | 2.30                     | 0.45              |
| 1:1L:229:ARG:NH1  | 1:1L:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1M:346:TRP:HA   | 2:4Y:397:ALA:C    | 2.41                     | 0.45              |
| 1:1N:70:LEU:HD22  | 1:1N:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1N:276:ILE:HG21 | 1:1N:284:GLU:OE2  | 2.17                     | 0.45              |
| 2:1H:69:ASP:HB2   | 2:1H:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1O:100:GLY:CA   | 1:2B:253:THR:CG2  | 2.87                     | 0.45              |
| 2:1P:69:ASP:HB2   | 2:1P:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1R:137:LEU:HG   | 2:1R:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:1R:242:LEU:HD12 | 2:1R:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:1W:176:LYS:HE2  | 1:2K:333:ALA:CB   | 2.46                     | 0.45              |
| 2:1X:3:GLU:HA     | 2:1X:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:2B:132:LEU:HD23 | 1:2B:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2C:229:ARG:NH1  | 1:2C:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2D:276:ILE:HG21 | 1:2D:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2F:30:ILE:HG13  | 1:2F:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:2F:229:ARG:NH1  | 1:2F:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2G:276:ILE:HG21 | 1:2G:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2I:228:ASN:OD1  | 3:2I:501:GTP:N1   | 2.47                     | 0.45              |
| 1:2J:70:LEU:HD22  | 1:2J:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2J:276:ILE:HG21 | 1:2J:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2K:209:ILE:HG23 | 1:2K:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:2L:121:ARG:NH1  | 1:2L:124:LYS:HD2  | 2.30                     | 0.45              |
| 1:2M:242:LEU:HD11 | 1:2M:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2N:70:LEU:HD22  | 1:2N:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2N:211:ASP:CG   | 1:2N:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2N:276:ILE:HG21 | 1:2N:284:GLU:OE2  | 2.17                     | 0.45              |
| 2:2H:69:ASP:HB2   | 2:2H:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2O:3:GLU:HA     | 2:2O:51:VAL:HG23  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:179:ASP:C    | 1:3C:352:LYS:HA   | 2.42                     | 0.45              |
| 2:2R:137:LEU:HG   | 2:2R:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:2S:179:ASP:OD2  | 1:3F:248:LEU:CD2  | 2.63                     | 0.45              |
| 2:2W:224:TYR:CE2  | 1:3K:248:LEU:HB2  | 2.35                     | 0.45              |
| 2:2X:178:SER:CB   | 1:3L:349:THR:HB   | 2.46                     | 0.45              |
| 2:2X:404:PHE:CZ   | 1:3L:261:PRO:CB   | 2.99                     | 0.45              |
| 1:3B:30:ILE:HG13  | 1:3B:53:PHE:HE2   | 1.82                     | 0.45              |
| 1:3G:70:LEU:HD22  | 1:3G:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3I:228:ASN:OD1  | 3:3I:501:GTP:N1   | 2.47                     | 0.45              |
| 1:3J:276:ILE:HG21 | 1:3J:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3N:70:LEU:HD22  | 1:3N:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3N:276:ILE:HG21 | 1:3N:284:GLU:OE2  | 2.17                     | 0.45              |
| 2:3H:69:ASP:HB2   | 2:3H:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3H:242:LEU:HD12 | 2:3H:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:3O:3:GLU:HA     | 2:3O:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:3R:69:ASP:HB2   | 2:3R:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3R:137:LEU:HG   | 2:3R:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:3R:242:LEU:HD12 | 2:3R:251:ASP:HB2  | 1.98                     | 0.45              |
| 1:4B:132:LEU:HD23 | 1:4B:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:4C:30:ILE:HG13  | 1:4C:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4C:229:ARG:NH1  | 1:4C:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4D:276:ILE:HG21 | 1:4D:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4E:242:LEU:HD11 | 1:4E:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:4F:229:ARG:NH1  | 1:4F:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4J:70:LEU:HD22  | 1:4J:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4J:276:ILE:HG21 | 1:4J:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4M:241:SER:OG   | 1:4M:250:VAL:O    | 2.27                     | 0.45              |
| 1:4N:229:ARG:NH1  | 1:4N:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4N:276:ILE:HG21 | 1:4N:284:GLU:OE2  | 2.17                     | 0.45              |
| 2:4O:3:GLU:HA     | 2:4O:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:4P:69:ASP:HB2   | 2:4P:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4Q:3:GLU:HA     | 2:4Q:51:VAL:HG23  | 1.99                     | 0.45              |
| 2:4Q:242:LEU:HD12 | 2:4Q:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4U:74:THR:O     | 2:4U:77:SER:OG    | 2.31                     | 0.45              |
| 2:4U:206:ASN:ND2  | 5:4U:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4V:3:GLU:HA     | 2:4V:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:4W:242:LEU:HD12 | 2:4W:251:ASP:HB2  | 1.98                     | 0.45              |
| 1:1B:353:VAL:N    | 2:4O:179:ASP:OD1  | 2.49                     | 0.45              |
| 1:1C:30:ILE:HG13  | 1:1C:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1E:242:LEU:HD11 | 1:1E:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:1F:70:LEU:HD22  | 1:1F:110:ILE:HG22 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:229:ARG:NH1  | 1:1F:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1G:70:LEU:HD22  | 1:1G:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1G:209:ILE:HG23 | 1:1G:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:1G:258:ASN:ND2  | 2:4T:180:THR:CG2  | 2.68                     | 0.45              |
| 1:1G:260:VAL:CG2  | 2:4T:407:TRP:CZ2  | 2.98                     | 0.45              |
| 1:1G:276:ILE:HG21 | 1:1G:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1I:351:PHE:HB2  | 2:4U:178:SER:OG   | 2.17                     | 0.45              |
| 1:1J:346:TRP:CZ3  | 2:4V:404:PHE:CD2  | 3.04                     | 0.45              |
| 1:1K:254:GLU:HG2  | 2:4W:100:GLY:CA   | 2.46                     | 0.45              |
| 1:1K:259:LEU:HD11 | 1:1K:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:1L:241:SER:OG   | 1:1L:250:VAL:O    | 2.27                     | 0.45              |
| 1:1L:261:PRO:O    | 2:4X:404:PHE:HA   | 2.16                     | 0.45              |
| 1:1L:329:ASN:CB   | 2:4X:210:TYR:CD2  | 2.99                     | 0.45              |
| 1:1M:346:TRP:HB3  | 2:4Y:397:ALA:O    | 2.17                     | 0.45              |
| 1:1N:254:GLU:HA   | 2:4Z:100:GLY:O    | 2.16                     | 0.45              |
| 2:1H:242:LEU:HD12 | 2:1H:251:ASP:HB2  | 1.98                     | 0.45              |
| 5:1O:501:GDP:C8   | 1:2B:248:LEU:HD13 | 2.52                     | 0.45              |
| 2:1Q:100:GLY:CA   | 1:2D:253:THR:HG22 | 2.42                     | 0.45              |
| 2:1S:69:ASP:HB2   | 2:1S:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1S:206:ASN:ND2  | 5:1S:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1W:179:ASP:O    | 1:2K:352:LYS:HE2  | 2.15                     | 0.45              |
| 2:1W:200:GLU:HA   | 2:1W:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:2A:399:TYR:OH   | 1:2A:415:GLU:OE2  | 2.27                     | 0.45              |
| 1:2F:70:LEU:HD22  | 1:2F:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2G:209:ILE:HG23 | 1:2G:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:2I:229:ARG:NH1  | 1:2I:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2L:229:ARG:NH1  | 1:2L:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:2P:71:GLU:HG3   | 1:3C:2:ARG:HH11   | 1.80                     | 0.45              |
| 2:2P:181:VAL:H    | 1:3C:258:ASN:HD22 | 1.65                     | 0.45              |
| 2:2Q:242:LEU:HD12 | 2:2Q:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:2S:206:ASN:ND2  | 5:2S:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2U:72:PRO:HD2   | 1:3I:2:ARG:HG2    | 1.97                     | 0.45              |
| 2:2V:3:GLU:HA     | 2:2V:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:2W:69:ASP:HB2   | 2:2W:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2X:3:GLU:HA     | 2:2X:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:3C:30:ILE:HG13  | 1:3C:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3F:70:LEU:HD22  | 1:3F:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3F:229:ARG:NH1  | 1:3F:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3I:229:ARG:NH1  | 1:3I:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3I:259:LEU:HD11 | 1:3I:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:3J:70:LEU:HD22  | 1:3J:110:ILE:HG22 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3K:132:LEU:HD23 | 1:3K:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3L:229:ARG:NH1  | 1:3L:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3M:132:LEU:HD23 | 1:3M:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:3M:242:LEU:HD11 | 1:3M:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:3N:211:ASP:CG   | 1:3N:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:3N:229:ARG:NH1  | 1:3N:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:3P:206:ASN:ND2  | 5:3P:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3W:69:ASP:HB2   | 2:3W:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3W:200:GLU:HA   | 2:3W:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:4F:30:ILE:HG13  | 1:4F:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4F:70:LEU:HD22  | 1:4F:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4G:70:LEU:HD22  | 1:4G:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4G:209:ILE:HG23 | 1:4G:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:4G:276:ILE:HG21 | 1:4G:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4I:228:ASN:OD1  | 3:4I:501:GTP:N1   | 2.47                     | 0.45              |
| 1:4I:229:ARG:NH1  | 1:4I:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4I:259:LEU:HD11 | 1:4I:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:4L:229:ARG:NH1  | 1:4L:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4M:242:LEU:HD11 | 1:4M:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:4N:70:LEU:HD22  | 1:4N:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4N:211:ASP:CG   | 1:4N:215:ARG:HH12 | 2.24                     | 0.45              |
| 2:4H:69:ASP:HB2   | 2:4H:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4R:137:LEU:HG   | 2:4R:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:4R:242:LEU:HD12 | 2:4R:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4X:3:GLU:HA     | 2:4X:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:1A:253:THR:CB   | 2:4H:100:GLY:CA   | 2.94                     | 0.45              |
| 1:1C:248:LEU:HD21 | 2:4P:179:ASP:OD2  | 2.17                     | 0.45              |
| 1:1D:2:ARG:HH11   | 2:4Q:71:GLU:CB    | 2.29                     | 0.45              |
| 1:1F:257:THR:OG1  | 2:4S:102:ASN:HB2  | 2.17                     | 0.45              |
| 1:1F:261:PRO:N    | 2:4S:404:PHE:CD1  | 2.84                     | 0.45              |
| 1:1G:260:VAL:HG21 | 2:4T:407:TRP:CZ2  | 2.52                     | 0.45              |
| 1:1G:439:SER:OG   | 2:4T:400:ARG:HG3  | 2.17                     | 0.45              |
| 1:1J:2:ARG:CG     | 2:4V:72:PRO:HD2   | 2.44                     | 0.45              |
| 1:1J:325:PRO:CB   | 2:4V:224:TYR:CZ   | 3.00                     | 0.45              |
| 1:1K:209:ILE:HG23 | 1:1K:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:1K:254:GLU:HG2  | 2:4W:100:GLY:C    | 2.42                     | 0.45              |
| 1:1K:324:VAL:CG1  | 2:4W:222:PRO:O    | 2.65                     | 0.45              |
| 1:1M:132:LEU:HD23 | 1:1M:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:1M:242:LEU:HD11 | 1:1M:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:1N:211:ASP:CG   | 1:1N:215:ARG:HH12 | 2.24                     | 0.45              |
| 2:1P:206:ASN:ND2  | 5:1P:501:GDP:O2'  | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Q:222:PRO:CG   | 1:2D:326:LYS:HB2  | 2.43                     | 0.45              |
| 2:1Q:242:LEU:HD12 | 2:1Q:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:1T:200:GLU:HA   | 2:1T:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1T:269:MET:HE1  | 2:1T:383:ALA:HB3  | 1.97                     | 0.45              |
| 1:2C:30:ILE:HG13  | 1:2C:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:2E:242:LEU:HD11 | 1:2E:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2G:70:LEU:HD22  | 1:2G:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2J:30:ILE:HG13  | 1:2J:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2K:132:LEU:HD23 | 1:2K:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2M:132:LEU:HD23 | 1:2M:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:2M:241:SER:OG   | 1:2M:250:VAL:O    | 2.27                     | 0.45              |
| 1:2N:229:ARG:NH1  | 1:2N:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:2O:406:HIS:NE2  | 1:3B:262:TYR:CA   | 2.80                     | 0.45              |
| 2:2P:206:ASN:ND2  | 5:2P:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2P:210:TYR:HB3  | 1:3C:326:LYS:HG2  | 1.99                     | 0.45              |
| 2:2T:200:GLU:HA   | 2:2T:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2V:69:ASP:HB2   | 2:2V:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2W:200:GLU:HA   | 2:2W:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2W:242:LEU:HD12 | 2:2W:251:ASP:HB2  | 1.98                     | 0.45              |
| 1:3E:70:LEU:HD22  | 1:3E:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3E:242:LEU:HD11 | 1:3E:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:3G:209:ILE:HG23 | 1:3G:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:3G:276:ILE:HG21 | 1:3G:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3J:30:ILE:HG13  | 1:3J:53:PHE:HE2   | 1.81                     | 0.45              |
| 2:3Q:242:LEU:HD12 | 2:3Q:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:3S:206:ASN:ND2  | 5:3S:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3V:3:GLU:HA     | 2:3V:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:3V:69:ASP:HB2   | 2:3V:75:MET:HE2   | 1.98                     | 0.45              |
| 2:3W:242:LEU:HD12 | 2:3W:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:3X:3:GLU:HA     | 2:3X:51:VAL:HG23  | 1.98                     | 0.45              |
| 1:4A:132:LEU:HD23 | 1:4A:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:4A:399:TYR:OH   | 1:4A:415:GLU:OE2  | 2.27                     | 0.45              |
| 1:4E:211:ASP:CG   | 1:4E:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4J:30:ILE:HG13  | 1:4J:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4K:132:LEU:HD23 | 1:4K:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:4M:132:LEU:HD23 | 1:4M:164:LYS:NZ   | 2.31                     | 0.45              |
| 2:4P:206:ASN:ND2  | 5:4P:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4S:206:ASN:ND2  | 5:4S:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4T:206:ASN:ND2  | 5:4T:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4V:69:ASP:HB2   | 2:4V:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4V:200:GLU:HA   | 2:4V:266:HIS:HB2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4W:200:GLU:HA   | 2:4W:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:1B:229:ARG:NH1  | 1:1B:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1C:211:ASP:CG   | 1:1C:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:1C:352:LYS:HE2  | 2:4P:101:ASN:ND2  | 2.31                     | 0.45              |
| 1:1D:353:VAL:N    | 2:4Q:179:ASP:OD1  | 2.50                     | 0.45              |
| 1:1E:70:LEU:HD22  | 1:1E:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1E:251:ASP:OD2  | 2:4R:71:GLU:HB3   | 2.17                     | 0.45              |
| 1:1E:256:GLN:O    | 2:4R:407:TRP:CE2  | 2.69                     | 0.45              |
| 1:1E:276:ILE:HG21 | 1:1E:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1G:314:ALA:HB2  | 2:4T:404:PHE:HZ   | 1.80                     | 0.45              |
| 1:1G:346:TRP:CD1  | 2:4T:401:ARG:CB   | 2.99                     | 0.45              |
| 1:1I:259:LEU:HD11 | 1:1I:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:1J:30:ILE:HG13  | 1:1J:53:PHE:HE2   | 1.82                     | 0.45              |
| 1:1K:276:ILE:HG21 | 1:1K:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1N:229:ARG:NH1  | 1:1N:366:GLY:HA2  | 2.32                     | 0.45              |
| 2:1U:192:HIS:HD2  | 2:1U:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1V:3:GLU:HA     | 2:1V:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:1V:69:ASP:HB2   | 2:1V:75:MET:HE2   | 1.98                     | 0.45              |
| 2:1V:180:THR:CG2  | 1:2J:258:ASN:ND2  | 2.78                     | 0.45              |
| 2:1W:242:LEU:HD12 | 2:1W:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:1X:137:LEU:HG   | 2:1X:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:1Y:11:GLN:NE2   | 1:2M:249:ASN:ND2  | 2.65                     | 0.45              |
| 2:1Y:100:GLY:O    | 1:2M:253:THR:HG22 | 2.16                     | 0.45              |
| 1:2B:229:ARG:NH1  | 1:2B:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2C:211:ASP:CG   | 1:2C:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2E:211:ASP:CG   | 1:2E:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2E:276:ILE:HG21 | 1:2E:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2I:259:LEU:HD11 | 1:2I:316:CYS:HB2  | 1.97                     | 0.45              |
| 1:2K:276:ILE:HG21 | 1:2K:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2N:132:LEU:HD23 | 1:2N:164:LYS:NZ   | 2.31                     | 0.45              |
| 2:2O:100:GLY:HA2  | 1:3B:253:THR:C    | 2.41                     | 0.45              |
| 2:2S:69:ASP:HB2   | 2:2S:75:MET:HE2   | 1.98                     | 0.45              |
| 2:2T:206:ASN:ND2  | 5:2T:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2T:269:MET:HE1  | 2:2T:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2V:200:GLU:HA   | 2:2V:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2V:407:TRP:NE1  | 1:3J:260:VAL:HB   | 2.32                     | 0.45              |
| 1:3B:229:ARG:NH1  | 1:3B:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3E:276:ILE:HG21 | 1:3E:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3K:276:ILE:HG21 | 1:3K:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3N:132:LEU:HD23 | 1:3N:164:LYS:NZ   | 2.31                     | 0.45              |
| 2:3S:69:ASP:HB2   | 2:3S:75:MET:HE2   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3T:200:GLU:HA   | 2:3T:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:3T:269:MET:HE1  | 2:3T:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3X:200:GLU:HA   | 2:3X:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:4C:209:ILE:HG23 | 1:4C:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:4D:229:ARG:NH1  | 1:4D:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4E:70:LEU:HD22  | 1:4E:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4F:211:ASP:CG   | 1:4F:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4K:276:ILE:HG21 | 1:4K:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4N:132:LEU:HD23 | 1:4N:164:LYS:NZ   | 2.32                     | 0.45              |
| 2:4H:132:LEU:HB3  | 2:4H:164:ARG:HE   | 1.81                     | 0.45              |
| 2:4W:69:ASP:HB2   | 2:4W:75:MET:HE2   | 1.98                     | 0.45              |
| 1:1A:326:LYS:HA   | 2:4H:210:TYR:CE1  | 2.52                     | 0.45              |
| 1:1C:70:LEU:HD22  | 1:1C:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1C:325:PRO:HB3  | 2:4P:224:TYR:CZ   | 2.52                     | 0.45              |
| 1:1D:242:LEU:HD11 | 1:1D:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:1D:329:ASN:ND2  | 2:4Q:210:TYR:HD2  | 2.11                     | 0.45              |
| 1:1E:2:ARG:HH12   | 2:4R:71:GLU:HG3   | 1.77                     | 0.45              |
| 1:1E:211:ASP:CG   | 1:1E:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:1F:352:LYS:HD2  | 2:4S:179:ASP:O    | 2.17                     | 0.45              |
| 1:1G:333:ALA:HB1  | 2:4T:176:LYS:HB3  | 1.98                     | 0.45              |
| 1:1K:242:LEU:HD11 | 1:1K:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:1N:132:LEU:HD23 | 1:1N:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:1N:326:LYS:HE2  | 2:4Z:214:PHE:CB   | 2.32                     | 0.45              |
| 2:1H:206:ASN:ND2  | 5:1H:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1O:181:VAL:HG23 | 1:2B:258:ASN:HB3  | 1.98                     | 0.45              |
| 2:1P:137:LEU:HG   | 2:1P:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:1T:206:ASN:ND2  | 5:1T:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1V:200:GLU:HA   | 2:1V:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1X:200:GLU:HA   | 2:1X:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1Y:132:LEU:HB3  | 2:1Y:164:ARG:HE   | 1.82                     | 0.45              |
| 2:1Z:206:ASN:ND2  | 5:1Z:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:2A:132:LEU:HD23 | 1:2A:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:2C:209:ILE:HG23 | 1:2C:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:2D:229:ARG:NH1  | 1:2D:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2E:70:LEU:HD22  | 1:2E:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2K:241:SER:OG   | 1:2K:250:VAL:O    | 2.27                     | 0.45              |
| 1:2M:30:ILE:HG13  | 1:2M:53:PHE:CE2   | 2.51                     | 0.45              |
| 2:2H:206:ASN:ND2  | 5:2H:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2O:132:LEU:HB3  | 2:2O:164:ARG:HE   | 1.81                     | 0.45              |
| 2:2P:181:VAL:H    | 1:3C:258:ASN:ND2  | 2.14                     | 0.45              |
| 2:2Q:100:GLY:O    | 1:3D:257:THR:OG1  | 2.26                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:394:GLN:CG   | 1:3E:348:PRO:CB   | 2.80                     | 0.45              |
| 2:2R:398:MET:HG3  | 1:3E:346:TRP:O    | 2.16                     | 0.45              |
| 2:2S:73:GLY:CA    | 1:3F:2:ARG:NH2    | 2.77                     | 0.45              |
| 2:2T:192:HIS:HD2  | 2:2T:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:2V:132:LEU:HB3  | 2:2V:164:ARG:HE   | 1.81                     | 0.45              |
| 2:2V:206:ASN:ND2  | 5:2V:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2V:407:TRP:HE1  | 1:3J:260:VAL:HG12 | 1.82                     | 0.45              |
| 2:2X:137:LEU:HG   | 2:2X:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:2Z:10:GLY:HA2   | 2:2Z:145:THR:HB   | 1.99                     | 0.45              |
| 2:2Z:206:ASN:ND2  | 5:2Z:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:2Z:394:GLN:HG2  | 1:3N:348:PRO:HB2  | 1.96                     | 0.45              |
| 1:3A:132:LEU:HD23 | 1:3A:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:3A:276:ILE:HG21 | 1:3A:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3B:70:LEU:HD22  | 1:3B:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3C:209:ILE:HG23 | 1:3C:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:3C:211:ASP:CG   | 1:3C:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:3E:211:ASP:CG   | 1:3E:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:3K:242:LEU:HD11 | 1:3K:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:3M:241:SER:OG   | 1:3M:250:VAL:O    | 2.27                     | 0.45              |
| 2:3P:137:LEU:HG   | 2:3P:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:3T:192:HIS:HD2  | 2:3T:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3T:206:ASN:ND2  | 5:3T:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3U:192:HIS:HD2  | 2:3U:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3X:137:LEU:HG   | 2:3X:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:3Y:132:LEU:HB3  | 2:3Y:164:ARG:HE   | 1.81                     | 0.45              |
| 2:3Z:10:GLY:HA2   | 2:3Z:145:THR:HB   | 1.99                     | 0.45              |
| 2:3Z:206:ASN:ND2  | 5:3Z:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:4A:241:SER:OG   | 1:4A:250:VAL:O    | 2.27                     | 0.45              |
| 1:4B:229:ARG:NH1  | 1:4B:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4C:211:ASP:CG   | 1:4C:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:4E:276:ILE:HG21 | 1:4E:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4J:334:THR:O    | 1:4J:337:THR:OG1  | 2.30                     | 0.45              |
| 1:4L:276:ILE:HG21 | 1:4L:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4M:30:ILE:HG13  | 1:4M:53:PHE:CE2   | 2.51                     | 0.45              |
| 2:4H:206:ASN:ND2  | 5:4H:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4S:69:ASP:HB2   | 2:4S:75:MET:HE2   | 1.98                     | 0.45              |
| 2:4S:74:THR:O     | 2:4S:77:SER:OG    | 2.31                     | 0.45              |
| 2:4V:132:LEU:HB3  | 2:4V:164:ARG:HE   | 1.82                     | 0.45              |
| 2:4X:137:LEU:HG   | 2:4X:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:4X:200:GLU:HA   | 2:4X:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:4Y:10:GLY:HA2   | 2:4Y:145:THR:HB   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4Z:10:GLY:HA2   | 2:4Z:145:THR:HB   | 1.99                     | 0.45              |
| 1:1A:132:LEU:HD23 | 1:1A:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:1A:276:ILE:HG21 | 1:1A:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1B:70:LEU:HD22  | 1:1B:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1C:209:ILE:HG23 | 1:1C:230:LEU:HD22 | 1.98                     | 0.45              |
| 1:1D:1:MET:O      | 2:4Q:96:GLN:OE1   | 2.35                     | 0.45              |
| 1:1D:30:ILE:HG13  | 1:1D:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:1D:229:ARG:NH1  | 1:1D:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1D:254:GLU:CG   | 2:4Q:100:GLY:C    | 2.88                     | 0.45              |
| 1:1E:248:LEU:HD11 | 5:4R:501:GDP:H5'' | 1.99                     | 0.45              |
| 1:1G:261:PRO:HB3  | 2:4T:404:PHE:CG   | 2.52                     | 0.45              |
| 1:1J:248:LEU:HD11 | 5:4V:501:GDP:O1A  | 2.16                     | 0.45              |
| 1:1J:326:LYS:HG2  | 2:4V:210:TYR:CG   | 2.52                     | 0.45              |
| 1:1L:132:LEU:HD23 | 1:1L:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:1L:257:THR:HG21 | 2:4X:102:ASN:CB   | 2.39                     | 0.45              |
| 1:1L:276:ILE:HG21 | 1:1L:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1L:326:LYS:HE2  | 2:4X:214:PHE:HB2  | 1.99                     | 0.45              |
| 1:1L:352:LYS:HA   | 2:4X:179:ASP:O    | 2.17                     | 0.45              |
| 1:1M:30:ILE:HG13  | 1:1M:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1M:276:ILE:HG21 | 1:1M:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1N:209:ILE:HG23 | 1:1N:230:LEU:HD22 | 1.98                     | 0.45              |
| 2:1H:192:HIS:HD2  | 2:1H:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1O:132:LEU:HB3  | 2:1O:164:ARG:HE   | 1.81                     | 0.45              |
| 2:1P:10:GLY:HA2   | 2:1P:145:THR:HB   | 1.99                     | 0.45              |
| 2:1P:269:MET:HE1  | 2:1P:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:1T:192:HIS:HD2  | 2:1T:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1T:404:PHE:CG   | 1:2G:261:PRO:HA   | 2.51                     | 0.45              |
| 2:1V:71:GLU:HB2   | 1:2J:2:ARG:HD3    | 1.99                     | 0.45              |
| 2:1V:132:LEU:HB3  | 2:1V:164:ARG:HE   | 1.81                     | 0.45              |
| 2:1V:192:HIS:HD2  | 2:1V:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:1V:206:ASN:ND2  | 5:1V:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:1Y:200:GLU:HA   | 2:1Y:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:1Z:10:GLY:HA2   | 2:1Z:145:THR:HB   | 1.99                     | 0.45              |
| 1:2A:70:LEU:HD22  | 1:2A:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2A:241:SER:OG   | 1:2A:250:VAL:O    | 2.27                     | 0.45              |
| 1:2B:70:LEU:HD22  | 1:2B:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2C:276:ILE:HG21 | 1:2C:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2F:211:ASP:CG   | 1:2F:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:2J:334:THR:O    | 1:2J:337:THR:OG1  | 2.30                     | 0.45              |
| 1:2K:242:LEU:HD11 | 1:2K:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2L:132:LEU:HD23 | 1:2L:164:LYS:NZ   | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2L:276:ILE:HG21 | 1:2L:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2M:276:ILE:HG21 | 1:2M:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2N:209:ILE:HG23 | 1:2N:230:LEU:HD22 | 1.98                     | 0.45              |
| 2:2H:10:GLY:HA2   | 2:2H:145:THR:HB   | 1.99                     | 0.45              |
| 2:2P:137:LEU:HG   | 2:2P:139:HIS:HD2  | 1.81                     | 0.45              |
| 2:2P:269:MET:HE1  | 2:2P:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:2P:398:MET:CG   | 1:3C:346:TRP:O    | 2.65                     | 0.45              |
| 2:2R:192:HIS:HD2  | 2:2R:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:2S:74:THR:O     | 2:2S:77:SER:OG    | 2.31                     | 0.45              |
| 2:2T:394:GLN:CD   | 1:3G:348:PRO:HB2  | 2.42                     | 0.45              |
| 2:2U:192:HIS:HD2  | 2:2U:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:2V:221:THR:C    | 1:3J:324:VAL:CG1  | 2.89                     | 0.45              |
| 2:2W:382:THR:HG21 | 2:2W:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:2X:200:GLU:HA   | 2:2X:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:2Y:200:GLU:HA   | 2:2Y:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:3A:70:LEU:HD22  | 1:3A:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3C:70:LEU:HD22  | 1:3C:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:3D:229:ARG:NH1  | 1:3D:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3F:211:ASP:CG   | 1:3F:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:3I:30:ILE:HG13  | 1:3I:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:3J:334:THR:O    | 1:3J:337:THR:OG1  | 2.30                     | 0.45              |
| 1:3L:276:ILE:HG21 | 1:3L:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3M:30:ILE:HG13  | 1:3M:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3M:276:ILE:HG21 | 1:3M:284:GLU:OE2  | 2.17                     | 0.45              |
| 2:3H:10:GLY:HA2   | 2:3H:145:THR:HB   | 1.99                     | 0.45              |
| 2:3H:206:ASN:ND2  | 5:3H:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3O:132:LEU:HB3  | 2:3O:164:ARG:HE   | 1.81                     | 0.45              |
| 2:3P:269:MET:HE1  | 2:3P:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:3V:132:LEU:HB3  | 2:3V:164:ARG:HE   | 1.82                     | 0.45              |
| 2:3V:200:GLU:HA   | 2:3V:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:3V:206:ASN:ND2  | 5:3V:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:3W:382:THR:HG21 | 2:3W:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:3Y:10:GLY:HA2   | 2:3Y:145:THR:HB   | 1.99                     | 0.45              |
| 1:4A:70:LEU:HD22  | 1:4A:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4C:70:LEU:HD22  | 1:4C:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:4C:276:ILE:HG21 | 1:4C:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4E:229:ARG:NH1  | 1:4E:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:4K:399:TYR:OH   | 1:4K:415:GLU:OE2  | 2.27                     | 0.45              |
| 1:4M:276:ILE:HG21 | 1:4M:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4N:209:ILE:HG23 | 1:4N:230:LEU:HD22 | 1.98                     | 0.45              |
| 2:4H:10:GLY:HA2   | 2:4H:145:THR:HB   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4H:382:THR:HG21 | 2:4H:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:4O:132:LEU:HB3  | 2:4O:164:ARG:HE   | 1.81                     | 0.45              |
| 2:4P:269:MET:HE1  | 2:4P:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4R:192:HIS:HD2  | 2:4R:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:4T:200:GLU:HA   | 2:4T:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:4T:269:MET:HE1  | 2:4T:383:ALA:HB3  | 1.97                     | 0.45              |
| 2:4U:192:HIS:HD2  | 2:4U:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:4V:206:ASN:ND2  | 5:4V:501:GDP:O2'  | 2.50                     | 0.45              |
| 2:4Y:132:LEU:HB3  | 2:4Y:164:ARG:HE   | 1.81                     | 0.45              |
| 2:4Z:206:ASN:ND2  | 5:4Z:501:GDP:O2'  | 2.50                     | 0.45              |
| 1:1A:70:LEU:HD22  | 1:1A:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:1A:261:PRO:CA   | 2:4H:404:PHE:CE1  | 2.98                     | 0.45              |
| 1:1C:276:ILE:HG21 | 1:1C:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:1E:229:ARG:NH1  | 1:1E:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1F:211:ASP:CG   | 1:1F:215:ARG:HH12 | 2.24                     | 0.45              |
| 1:1G:260:VAL:HG12 | 2:4T:407:TRP:HE1  | 1.79                     | 0.45              |
| 1:1G:326:LYS:HZ2  | 2:4T:210:TYR:HB3  | 1.82                     | 0.45              |
| 1:1I:30:ILE:HG13  | 1:1I:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:1J:172:TYR:N    | 1:1J:204:VAL:O    | 2.44                     | 0.45              |
| 1:1J:229:ARG:NH1  | 1:1J:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:1L:30:ILE:HG13  | 1:1L:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:1L:349:THR:HG21 | 2:4X:183:GLU:HG3  | 1.98                     | 0.45              |
| 1:1N:2:ARG:HD3    | 2:4Z:72:PRO:CD    | 2.35                     | 0.45              |
| 1:1N:30:ILE:HG13  | 1:1N:53:PHE:CE2   | 2.51                     | 0.45              |
| 2:1H:10:GLY:HA2   | 2:1H:145:THR:HB   | 1.99                     | 0.45              |
| 2:1H:132:LEU:HB3  | 2:1H:164:ARG:HE   | 1.81                     | 0.45              |
| 2:1H:382:THR:HG21 | 2:1H:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:1U:382:THR:HG21 | 2:1U:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:1W:214:PHE:CD2  | 1:2K:326:LYS:CE   | 2.97                     | 0.45              |
| 2:1W:382:THR:HG21 | 2:1W:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:1Y:382:THR:HG21 | 2:1Y:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:1Z:132:LEU:HB3  | 2:1Z:164:ARG:HE   | 1.81                     | 0.45              |
| 1:2A:276:ILE:HG21 | 1:2A:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:2C:70:LEU:HD22  | 1:2C:110:ILE:HG22 | 1.98                     | 0.45              |
| 1:2D:242:LEU:HD11 | 1:2D:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:2E:229:ARG:NH1  | 1:2E:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:2I:30:ILE:HG13  | 1:2I:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:2J:172:TYR:N    | 1:2J:204:VAL:O    | 2.44                     | 0.45              |
| 2:2H:100:GLY:O    | 1:3A:254:GLU:HA   | 2.16                     | 0.45              |
| 2:2H:132:LEU:HB3  | 2:2H:164:ARG:HE   | 1.82                     | 0.45              |
| 2:2O:406:HIS:CE1  | 1:3B:263:PRO:HA   | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:10:GLY:HA2   | 2:2P:145:THR:HB   | 1.99                     | 0.45              |
| 2:2V:192:HIS:HD2  | 2:2V:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:2Y:10:GLY:HA2   | 2:2Y:145:THR:HB   | 1.99                     | 0.45              |
| 2:2Y:132:LEU:HB3  | 2:2Y:164:ARG:HE   | 1.81                     | 0.45              |
| 2:2Y:382:THR:HG21 | 2:2Y:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:2Z:132:LEU:HB3  | 2:2Z:164:ARG:HE   | 1.81                     | 0.45              |
| 1:3A:30:ILE:HG13  | 1:3A:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:3C:276:ILE:HG21 | 1:3C:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:3D:242:LEU:HD11 | 1:3D:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:3E:229:ARG:NH1  | 1:3E:366:GLY:HA2  | 2.32                     | 0.45              |
| 1:3L:132:LEU:HD23 | 1:3L:164:LYS:NZ   | 2.32                     | 0.45              |
| 1:3N:209:ILE:HG23 | 1:3N:230:LEU:HD22 | 1.98                     | 0.45              |
| 2:3H:132:LEU:HB3  | 2:3H:164:ARG:HE   | 1.81                     | 0.45              |
| 2:3H:382:THR:HG21 | 2:3H:436:GLN:HB2  | 2.00                     | 0.45              |
| 2:3R:192:HIS:HD2  | 2:3R:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3V:192:HIS:HD2  | 2:3V:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:3Y:200:GLU:HA   | 2:3Y:266:HIS:HB2  | 1.98                     | 0.45              |
| 1:4A:276:ILE:HG21 | 1:4A:284:GLU:OE2  | 2.17                     | 0.45              |
| 1:4I:30:ILE:HG13  | 1:4I:53:PHE:HE2   | 1.81                     | 0.45              |
| 1:4J:172:TYR:N    | 1:4J:204:VAL:O    | 2.44                     | 0.45              |
| 1:4K:242:LEU:HD11 | 1:4K:252:LEU:HD13 | 1.98                     | 0.45              |
| 1:4L:30:ILE:HG13  | 1:4L:53:PHE:CE2   | 2.51                     | 0.45              |
| 1:4L:132:LEU:HD23 | 1:4L:164:LYS:NZ   | 2.31                     | 0.45              |
| 1:4L:242:LEU:HD11 | 1:4L:252:LEU:HD13 | 1.98                     | 0.45              |
| 2:4T:192:HIS:HD2  | 2:4T:424:ASN:HD22 | 1.64                     | 0.45              |
| 2:4T:242:LEU:HD12 | 2:4T:251:ASP:HB2  | 1.98                     | 0.45              |
| 2:4U:200:GLU:HA   | 2:4U:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:4V:382:THR:HG21 | 2:4V:436:GLN:HB2  | 1.99                     | 0.45              |
| 2:4W:74:THR:O     | 2:4W:77:SER:OG    | 2.31                     | 0.45              |
| 2:4Y:200:GLU:HA   | 2:4Y:266:HIS:HB2  | 1.98                     | 0.45              |
| 2:4Y:382:THR:HG21 | 2:4Y:436:GLN:HB2  | 1.99                     | 0.45              |
| 1:1A:30:ILE:HG13  | 1:1A:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:1A:211:ASP:CG   | 1:1A:215:ARG:HH12 | 2.24                     | 0.44              |
| 1:1C:260:VAL:CG1  | 2:4P:406:HIS:HE1  | 2.29                     | 0.44              |
| 1:1D:260:VAL:HG11 | 2:4Q:407:TRP:HZ2  | 1.80                     | 0.44              |
| 1:1E:329:ASN:ND2  | 2:4R:210:TYR:HD2  | 2.12                     | 0.44              |
| 1:1I:276:ILE:HG21 | 1:1I:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:1J:329:ASN:CB   | 2:4V:210:TYR:CD2  | 2.99                     | 0.44              |
| 1:1J:334:THR:O    | 1:1J:337:THR:OG1  | 2.30                     | 0.44              |
| 1:1M:241:SER:OG   | 1:1M:250:VAL:O    | 2.27                     | 0.44              |
| 1:1M:247:ALA:O    | 2:4Y:15:GLN:NE2   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:314:ALA:CB   | 2:4Y:181:VAL:HG21 | 2.43                     | 0.44              |
| 2:1O:10:GLY:HA2   | 2:1O:145:THR:HB   | 1.99                     | 0.44              |
| 2:1Q:137:LEU:HG   | 2:1Q:139:HIS:HD2  | 1.81                     | 0.44              |
| 2:1R:192:HIS:HD2  | 2:1R:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:1V:382:THR:HG21 | 2:1V:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:1Y:10:GLY:HA2   | 2:1Y:145:THR:HB   | 1.99                     | 0.44              |
| 2:1Z:69:ASP:HB2   | 2:1Z:75:MET:HE2   | 1.98                     | 0.44              |
| 2:1Z:401:ARG:O    | 1:2N:262:TYR:CE1  | 2.71                     | 0.44              |
| 1:2G:30:ILE:HG13  | 1:2G:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:2J:229:ARG:NH1  | 1:2J:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:2L:242:LEU:HD11 | 1:2L:252:LEU:HD13 | 1.98                     | 0.44              |
| 1:2N:30:ILE:HG13  | 1:2N:53:PHE:CE2   | 2.51                     | 0.44              |
| 2:2H:192:HIS:HD2  | 2:2H:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:2H:200:GLU:HA   | 2:2H:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:2H:382:THR:HG21 | 2:2H:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:2P:397:ALA:O    | 1:3C:346:TRP:HB3  | 2.15                     | 0.44              |
| 2:2Q:137:LEU:HG   | 2:2Q:139:HIS:HD2  | 1.81                     | 0.44              |
| 2:2S:210:TYR:CZ   | 1:3F:325:PRO:O    | 2.70                     | 0.44              |
| 2:2T:242:LEU:HD12 | 2:2T:251:ASP:HB2  | 1.98                     | 0.44              |
| 1:3A:93:ILE:HD11  | 1:3A:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3A:241:SER:OG   | 1:3A:250:VAL:O    | 2.27                     | 0.44              |
| 1:3J:172:TYR:N    | 1:3J:204:VAL:O    | 2.44                     | 0.44              |
| 1:3L:30:ILE:HG13  | 1:3L:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:3L:242:LEU:HD11 | 1:3L:252:LEU:HD13 | 1.98                     | 0.44              |
| 1:3N:30:ILE:HG13  | 1:3N:53:PHE:CE2   | 2.51                     | 0.44              |
| 2:3H:192:HIS:HD2  | 2:3H:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:3O:10:GLY:HA2   | 2:3O:145:THR:HB   | 1.99                     | 0.44              |
| 2:3P:10:GLY:HA2   | 2:3P:145:THR:HB   | 1.99                     | 0.44              |
| 2:3Q:137:LEU:HG   | 2:3Q:139:HIS:HD2  | 1.81                     | 0.44              |
| 2:3T:242:LEU:HD12 | 2:3T:251:ASP:HB2  | 1.98                     | 0.44              |
| 2:3U:200:GLU:HA   | 2:3U:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:3W:192:HIS:HD2  | 2:3W:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:3Y:382:THR:HG21 | 2:3Y:436:GLN:HB2  | 2.00                     | 0.44              |
| 1:4A:93:ILE:HD11  | 1:4A:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4B:70:LEU:HD22  | 1:4B:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:4B:228:ASN:OD1  | 3:4B:501:GTP:N1   | 2.47                     | 0.44              |
| 1:4D:242:LEU:HD11 | 1:4D:252:LEU:HD13 | 1.98                     | 0.44              |
| 1:4I:241:SER:OG   | 1:4I:250:VAL:O    | 2.27                     | 0.44              |
| 1:4K:229:ARG:NH1  | 1:4K:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:4N:30:ILE:HG13  | 1:4N:53:PHE:CE2   | 2.51                     | 0.44              |
| 2:4H:192:HIS:HD2  | 2:4H:424:ASN:HD22 | 1.64                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4H:200:GLU:HA   | 2:4H:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:4P:137:LEU:HG   | 2:4P:139:HIS:HD2  | 1.81                     | 0.44              |
| 2:4T:382:THR:HG21 | 2:4T:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4V:192:HIS:HD2  | 2:4V:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:4W:382:THR:HG21 | 2:4W:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4Z:382:THR:HG21 | 2:4Z:436:GLN:HB2  | 1.99                     | 0.44              |
| 1:1A:93:ILE:HD11  | 1:1A:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1A:260:VAL:HG11 | 2:4H:407:TRP:CZ2  | 2.52                     | 0.44              |
| 1:1B:93:ILE:HD11  | 1:1B:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1B:228:ASN:OD1  | 3:1B:501:GTP:N1   | 2.47                     | 0.44              |
| 1:1G:30:ILE:HG13  | 1:1G:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:1G:349:THR:HB   | 2:4T:183:GLU:HG2  | 1.99                     | 0.44              |
| 1:1I:172:TYR:N    | 1:1I:204:VAL:O    | 2.44                     | 0.44              |
| 1:1I:262:TYR:CE2  | 2:4U:403:ALA:HA   | 2.52                     | 0.44              |
| 1:1I:326:LYS:NZ   | 2:4U:210:TYR:HB3  | 2.32                     | 0.44              |
| 1:1J:93:ILE:HD11  | 1:1J:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1K:70:LEU:HD22  | 1:1K:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:1K:257:THR:OG1  | 2:4W:100:GLY:O    | 2.35                     | 0.44              |
| 1:1K:349:THR:HG23 | 2:4W:184:PRO:CG   | 2.48                     | 0.44              |
| 1:1K:351:PHE:O    | 2:4W:180:THR:HA   | 2.13                     | 0.44              |
| 1:1L:242:LEU:HD11 | 1:1L:252:LEU:HD13 | 1.98                     | 0.44              |
| 1:1N:93:ILE:HD11  | 1:1N:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:1P:382:THR:HG21 | 2:1P:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:1R:404:PHE:CE1  | 1:2E:261:PRO:CA   | 2.98                     | 0.44              |
| 2:1W:192:HIS:HD2  | 2:1W:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:1X:10:GLY:HA2   | 2:1X:145:THR:HB   | 1.99                     | 0.44              |
| 2:1X:404:PHE:CG   | 1:2L:261:PRO:HA   | 2.52                     | 0.44              |
| 2:1Y:11:GLN:HE22  | 1:2M:249:ASN:H    | 1.65                     | 0.44              |
| 1:2A:30:ILE:HG13  | 1:2A:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:2A:93:ILE:HD11  | 1:2A:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2D:30:ILE:HG13  | 1:2D:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:2I:172:TYR:N    | 1:2I:204:VAL:O    | 2.44                     | 0.44              |
| 1:2I:241:SER:OG   | 1:2I:250:VAL:O    | 2.27                     | 0.44              |
| 1:2I:276:ILE:HG21 | 1:2I:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:2J:93:ILE:HD11  | 1:2J:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2L:30:ILE:HG13  | 1:2L:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:2N:93:ILE:HD11  | 1:2N:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:2O:69:ASP:HB2   | 2:2O:75:MET:HE2   | 1.98                     | 0.44              |
| 2:2P:132:LEU:HB3  | 2:2P:164:ARG:HE   | 1.81                     | 0.44              |
| 2:2P:181:VAL:HG21 | 1:3C:258:ASN:O    | 2.18                     | 0.44              |
| 2:2Q:397:ALA:O    | 1:3D:346:TRP:HB3  | 2.10                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2U:200:GLU:HA   | 2:2U:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:2U:382:THR:HG21 | 2:2U:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:2V:214:PHE:CB   | 1:3J:326:LYS:HE3  | 2.47                     | 0.44              |
| 2:2V:382:THR:HG21 | 2:2V:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:2X:394:GLN:OE1  | 1:3L:349:THR:HG23 | 2.17                     | 0.44              |
| 2:2Z:11:GLN:HE22  | 1:3N:249:ASN:CA   | 2.24                     | 0.44              |
| 2:2Z:69:ASP:HB2   | 2:2Z:75:MET:HE2   | 1.98                     | 0.44              |
| 2:2Z:77:SER:CB    | 1:3N:245:ASP:CG   | 2.89                     | 0.44              |
| 2:2Z:382:THR:HG21 | 2:2Z:436:GLN:HB2  | 1.99                     | 0.44              |
| 1:3A:211:ASP:CG   | 1:3A:215:ARG:HH12 | 2.24                     | 0.44              |
| 1:3B:228:ASN:OD1  | 3:3B:501:GTP:N1   | 2.47                     | 0.44              |
| 1:3D:30:ILE:HG13  | 1:3D:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:3I:93:ILE:HD11  | 1:3I:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3I:172:TYR:N    | 1:3I:204:VAL:O    | 2.44                     | 0.44              |
| 1:3I:241:SER:OG   | 1:3I:250:VAL:O    | 2.27                     | 0.44              |
| 1:3J:93:ILE:HD11  | 1:3J:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3J:229:ARG:NH1  | 1:3J:366:GLY:HA2  | 2.32                     | 0.44              |
| 2:3T:382:THR:HG21 | 2:3T:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3U:382:THR:HG21 | 2:3U:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3V:382:THR:HG21 | 2:3V:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3Z:69:ASP:HB2   | 2:3Z:75:MET:HE2   | 1.98                     | 0.44              |
| 2:3Z:132:LEU:HB3  | 2:3Z:164:ARG:HE   | 1.82                     | 0.44              |
| 1:4A:30:ILE:HG13  | 1:4A:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:4I:276:ILE:HG21 | 1:4I:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:4J:93:ILE:HD11  | 1:4J:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4J:229:ARG:NH1  | 1:4J:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:4N:93:ILE:HD11  | 1:4N:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:4O:69:ASP:HB2   | 2:4O:75:MET:HE2   | 1.98                     | 0.44              |
| 2:4P:10:GLY:HA2   | 2:4P:145:THR:HB   | 1.99                     | 0.44              |
| 2:4Q:206:ASN:ND2  | 5:4Q:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:4U:382:THR:HG21 | 2:4U:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4W:192:HIS:HD2  | 2:4W:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:4X:382:THR:HG21 | 2:4X:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4Z:132:LEU:HB3  | 2:4Z:164:ARG:HE   | 1.82                     | 0.44              |
| 1:1B:325:PRO:CB   | 2:4O:224:TYR:CE1  | 3.00                     | 0.44              |
| 1:1C:258:ASN:ND2  | 2:4P:182:VAL:HG22 | 2.32                     | 0.44              |
| 1:1C:333:ALA:HB1  | 2:4P:176:LYS:HB3  | 1.99                     | 0.44              |
| 1:1C:348:PRO:HB2  | 2:4P:394:GLN:NE2  | 2.31                     | 0.44              |
| 1:1E:253:THR:CB   | 2:4R:100:GLY:CA   | 2.95                     | 0.44              |
| 1:1E:329:ASN:CB   | 2:4R:210:TYR:HD2  | 2.29                     | 0.44              |
| 1:1E:346:TRP:HA   | 2:4R:397:ALA:CB   | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:248:LEU:HD12 | 2:4S:11:GLN:CD    | 2.42                     | 0.44              |
| 1:1G:260:VAL:CG1  | 2:4T:406:HIS:HE1  | 2.15                     | 0.44              |
| 1:1I:93:ILE:HD11  | 1:1I:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1I:241:SER:OG   | 1:1I:250:VAL:O    | 2.27                     | 0.44              |
| 1:1K:93:ILE:HD11  | 1:1K:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1K:229:ARG:NH1  | 1:1K:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:1K:329:ASN:OD1  | 2:4W:177:VAL:HG11 | 2.18                     | 0.44              |
| 1:1N:2:ARG:NH2    | 2:4Z:73:GLY:CA    | 2.80                     | 0.44              |
| 1:1N:439:SER:CB   | 2:4Z:400:ARG:HD2  | 2.47                     | 0.44              |
| 2:1H:200:GLU:HA   | 2:1H:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:1P:71:GLU:HB2   | 1:2C:2:ARG:HD3    | 1.99                     | 0.44              |
| 2:1P:132:LEU:HB3  | 2:1P:164:ARG:HE   | 1.81                     | 0.44              |
| 2:1Q:10:GLY:HA2   | 2:1Q:145:THR:HB   | 1.99                     | 0.44              |
| 2:1Q:206:ASN:ND2  | 5:1Q:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:1T:181:VAL:H    | 1:2G:258:ASN:HD22 | 0.60                     | 0.44              |
| 2:1T:382:THR:HG21 | 2:1T:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:1U:200:GLU:HA   | 2:1U:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:1V:11:GLN:HE22  | 1:2J:249:ASN:H    | 1.65                     | 0.44              |
| 2:1W:221:THR:C    | 1:2K:324:VAL:HG13 | 2.41                     | 0.44              |
| 1:2A:211:ASP:CG   | 1:2A:215:ARG:HH12 | 2.24                     | 0.44              |
| 1:2B:228:ASN:OD1  | 3:2B:501:GTP:N1   | 2.47                     | 0.44              |
| 1:2I:93:ILE:HD11  | 1:2I:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2K:229:ARG:NH1  | 1:2K:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:2M:93:ILE:HD11  | 1:2M:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:2O:10:GLY:HA2   | 2:2O:145:THR:HB   | 1.99                     | 0.44              |
| 2:2O:179:ASP:OD1  | 1:3B:353:VAL:CB   | 2.61                     | 0.44              |
| 2:2P:382:THR:HG21 | 2:2P:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:2Q:206:ASN:ND2  | 5:2Q:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:2R:72:PRO:CG    | 1:3E:2:ARG:HG3    | 2.47                     | 0.44              |
| 2:2S:222:PRO:HG2  | 1:3F:326:LYS:HB3  | 1.94                     | 0.44              |
| 2:2T:382:THR:HG21 | 2:2T:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:2V:101:ASN:HB2  | 1:3J:254:GLU:CG   | 2.47                     | 0.44              |
| 2:2W:192:HIS:HD2  | 2:2W:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:2X:10:GLY:HA2   | 2:2X:145:THR:HB   | 1.99                     | 0.44              |
| 2:2X:206:ASN:ND2  | 5:2X:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:2Z:404:PHE:CE1  | 1:3N:260:VAL:N    | 2.78                     | 0.44              |
| 1:3I:276:ILE:HG21 | 1:3I:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:3N:93:ILE:HD11  | 1:3N:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:3H:200:GLU:HA   | 2:3H:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:3P:382:THR:HG21 | 2:3P:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3X:10:GLY:HA2   | 2:3X:145:THR:HB   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3X:206:ASN:ND2  | 5:3X:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:3X:382:THR:HG21 | 2:3X:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3Y:69:ASP:HB2   | 2:3Y:75:MET:HE2   | 1.98                     | 0.44              |
| 2:3Z:382:THR:HG21 | 2:3Z:436:GLN:HB2  | 1.99                     | 0.44              |
| 1:4A:211:ASP:CG   | 1:4A:215:ARG:HH12 | 2.24                     | 0.44              |
| 1:4B:93:ILE:HD11  | 1:4B:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4D:30:ILE:HG13  | 1:4D:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:4G:30:ILE:HG13  | 1:4G:53:PHE:HE2   | 1.82                     | 0.44              |
| 1:4K:93:ILE:HD11  | 1:4K:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:4O:10:GLY:HA2   | 2:4O:145:THR:HB   | 1.99                     | 0.44              |
| 2:4P:132:LEU:HB3  | 2:4P:164:ARG:HE   | 1.81                     | 0.44              |
| 2:4Q:137:LEU:HG   | 2:4Q:139:HIS:HD2  | 1.81                     | 0.44              |
| 2:4X:10:GLY:HA2   | 2:4X:145:THR:HB   | 1.99                     | 0.44              |
| 2:4X:206:ASN:ND2  | 5:4X:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:4Y:69:ASP:HB2   | 2:4Y:75:MET:HE2   | 1.98                     | 0.44              |
| 1:1A:229:ARG:NH1  | 1:1A:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:1A:241:SER:OG   | 1:1A:250:VAL:O    | 2.27                     | 0.44              |
| 1:1B:30:ILE:HG13  | 1:1B:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:1D:257:THR:HG21 | 2:4Q:101:ASN:C    | 2.42                     | 0.44              |
| 1:1D:262:TYR:OH   | 2:4Q:403:ALA:N    | 2.50                     | 0.44              |
| 1:1E:346:TRP:CD2  | 2:4R:403:ALA:HB2  | 2.52                     | 0.44              |
| 1:1E:346:TRP:C    | 2:4R:398:MET:HA   | 2.42                     | 0.44              |
| 1:1G:241:SER:OG   | 1:1G:250:VAL:O    | 2.27                     | 0.44              |
| 1:1J:324:VAL:HG13 | 2:4V:222:PRO:C    | 2.42                     | 0.44              |
| 1:1L:70:LEU:HD22  | 1:1L:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:1M:93:ILE:HD11  | 1:1M:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1M:254:GLU:HG2  | 2:4Y:101:ASN:N    | 2.33                     | 0.44              |
| 2:1O:69:ASP:HB2   | 2:1O:75:MET:HE2   | 1.98                     | 0.44              |
| 2:1O:382:THR:HG21 | 2:1O:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:1S:210:TYR:HD2  | 1:2F:329:ASN:HD22 | 1.66                     | 0.44              |
| 2:1T:242:LEU:HD12 | 2:1T:251:ASP:HB2  | 1.98                     | 0.44              |
| 2:1W:222:PRO:CG   | 1:2K:326:LYS:HB2  | 2.47                     | 0.44              |
| 2:1X:206:ASN:ND2  | 5:1X:501:GDP:O2'  | 2.50                     | 0.44              |
| 2:1Z:382:THR:HG21 | 2:1Z:436:GLN:HB2  | 1.99                     | 0.44              |
| 1:2B:93:ILE:HD11  | 1:2B:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2K:70:LEU:HD22  | 1:2K:110:ILE:HG22 | 1.98                     | 0.44              |
| 2:2P:181:VAL:N    | 1:3C:258:ASN:HD22 | 2.14                     | 0.44              |
| 2:2Q:10:GLY:HA2   | 2:2Q:145:THR:HB   | 1.99                     | 0.44              |
| 2:2S:404:PHE:CD1  | 1:3F:261:PRO:N    | 2.84                     | 0.44              |
| 2:2T:100:GLY:HA2  | 1:3G:254:GLU:N    | 2.32                     | 0.44              |
| 2:2X:181:VAL:N    | 1:3L:258:ASN:ND2  | 2.65                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2X:382:THR:HG21 | 2:2X:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:2Y:69:ASP:HB2   | 2:2Y:75:MET:HE2   | 1.98                     | 0.44              |
| 1:3B:93:ILE:HD11  | 1:3B:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3G:30:ILE:HG13  | 1:3G:53:PHE:HE2   | 1.82                     | 0.44              |
| 1:3K:93:ILE:HD11  | 1:3K:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3K:229:ARG:NH1  | 1:3K:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:3M:93:ILE:HD11  | 1:3M:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:3O:69:ASP:HB2   | 2:3O:75:MET:HE2   | 1.98                     | 0.44              |
| 2:3P:132:LEU:HB3  | 2:3P:164:ARG:HE   | 1.82                     | 0.44              |
| 2:3Q:10:GLY:HA2   | 2:3Q:145:THR:HB   | 1.99                     | 0.44              |
| 2:3Q:206:ASN:ND2  | 5:3Q:501:GDP:O2'  | 2.50                     | 0.44              |
| 1:4I:172:TYR:N    | 1:4I:204:VAL:O    | 2.44                     | 0.44              |
| 1:4M:93:ILE:HD11  | 1:4M:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:4P:382:THR:HG21 | 2:4P:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4Q:10:GLY:HA2   | 2:4Q:145:THR:HB   | 1.99                     | 0.44              |
| 2:4X:192:HIS:HD2  | 2:4X:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:4Z:69:ASP:HB2   | 2:4Z:75:MET:HE2   | 1.98                     | 0.44              |
| 1:1A:314:ALA:CB   | 2:4H:181:VAL:HG21 | 2.27                     | 0.44              |
| 1:1B:245:ASP:OD2  | 2:4O:77:SER:CB    | 2.63                     | 0.44              |
| 1:1D:248:LEU:HD11 | 5:4Q:501:GDP:H5'' | 2.00                     | 0.44              |
| 1:1D:435:VAL:O    | 2:4Q:401:ARG:NH1  | 2.50                     | 0.44              |
| 1:1F:62:VAL:HA    | 1:1F:63:PRO:HD3   | 1.86                     | 0.44              |
| 1:1F:346:TRP:CG   | 2:4S:401:ARG:HB2  | 2.52                     | 0.44              |
| 1:1G:332:ILE:HG21 | 2:4T:177:VAL:HG22 | 1.96                     | 0.44              |
| 1:1K:325:PRO:CB   | 2:4W:224:TYR:CE1  | 3.00                     | 0.44              |
| 1:1K:348:PRO:CD   | 2:4W:398:MET:CG   | 2.93                     | 0.44              |
| 1:1L:348:PRO:CD   | 2:4X:398:MET:HG3  | 2.48                     | 0.44              |
| 1:1M:260:VAL:HG12 | 2:4Y:406:HIS:HE1  | 1.83                     | 0.44              |
| 1:1M:326:LYS:HE2  | 2:4Y:210:TYR:O    | 2.18                     | 0.44              |
| 1:1M:349:THR:OG1  | 2:4Y:184:PRO:CD   | 2.65                     | 0.44              |
| 1:1N:253:THR:HG22 | 2:4Z:100:GLY:CA   | 2.34                     | 0.44              |
| 2:1S:192:HIS:HD2  | 2:1S:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:1S:382:THR:HG21 | 2:1S:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:1V:404:PHE:CE2  | 1:2J:261:PRO:CB   | 3.00                     | 0.44              |
| 2:1X:382:THR:HG21 | 2:1X:436:GLN:HB2  | 2.00                     | 0.44              |
| 1:2A:229:ARG:NH1  | 1:2A:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:2B:30:ILE:HG13  | 1:2B:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:2C:93:ILE:HD11  | 1:2C:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2G:93:ILE:HD11  | 1:2G:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2K:93:ILE:HD11  | 1:2K:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2L:70:LEU:HD22  | 1:2L:110:ILE:HG22 | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2M:70:LEU:HD22  | 1:2M:110:ILE:HG22 | 1.98                     | 0.44              |
| 2:2O:222:PRO:O    | 1:3B:324:VAL:HG13 | 2.18                     | 0.44              |
| 2:2P:100:GLY:O    | 1:3C:257:THR:OG1  | 2.30                     | 0.44              |
| 2:2P:404:PHE:CA   | 1:3C:261:PRO:O    | 2.66                     | 0.44              |
| 2:2S:382:THR:HG21 | 2:2S:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:2U:404:PHE:CD1  | 1:3I:261:PRO:N    | 2.80                     | 0.44              |
| 2:2X:192:HIS:HD2  | 2:2X:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:2Z:394:GLN:HB3  | 1:3N:348:PRO:HG2  | 1.98                     | 0.44              |
| 1:3A:229:ARG:NH1  | 1:3A:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:3C:93:ILE:HD11  | 1:3C:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3K:70:LEU:HD22  | 1:3K:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:3L:70:LEU:HD22  | 1:3L:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:3M:70:LEU:HD22  | 1:3M:110:ILE:HG22 | 1.98                     | 0.44              |
| 2:3R:382:THR:HG21 | 2:3R:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3S:382:THR:HG21 | 2:3S:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3X:192:HIS:HD2  | 2:3X:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:4B:30:ILE:HG13  | 1:4B:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:4D:241:SER:OG   | 1:4D:250:VAL:O    | 2.27                     | 0.44              |
| 1:4I:93:ILE:HD11  | 1:4I:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4K:70:LEU:HD22  | 1:4K:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:4L:70:LEU:HD22  | 1:4L:110:ILE:HG22 | 1.98                     | 0.44              |
| 2:4Q:132:LEU:HB3  | 2:4Q:164:ARG:HE   | 1.81                     | 0.44              |
| 1:1A:334:THR:O    | 1:1A:337:THR:OG1  | 2.30                     | 0.44              |
| 1:1B:349:THR:CG2  | 2:4O:184:PRO:HG3  | 2.47                     | 0.44              |
| 1:1C:93:ILE:HD11  | 1:1C:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1D:325:PRO:C    | 2:4Q:210:TYR:CE1  | 2.96                     | 0.44              |
| 1:1E:439:SER:HB3  | 2:4R:400:ARG:CD   | 2.48                     | 0.44              |
| 1:1G:93:ILE:HD11  | 1:1G:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1I:261:PRO:O    | 2:4U:404:PHE:HA   | 2.18                     | 0.44              |
| 1:1J:262:TYR:CZ   | 2:4V:403:ALA:HA   | 2.52                     | 0.44              |
| 1:1J:349:THR:HG21 | 2:4V:183:GLU:HG3  | 1.99                     | 0.44              |
| 1:1L:253:THR:HG22 | 2:4X:100:GLY:HA3  | 1.99                     | 0.44              |
| 1:1M:70:LEU:HD22  | 1:1M:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:1M:346:TRP:CA   | 2:4Y:397:ALA:O    | 2.65                     | 0.44              |
| 1:1N:248:LEU:HD11 | 5:4Z:501:GDP:H8   | 1.80                     | 0.44              |
| 1:1N:324:VAL:HG11 | 2:4Z:221:THR:CA   | 2.47                     | 0.44              |
| 2:1R:382:THR:HG21 | 2:1R:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:1T:157:ILE:O    | 2:1T:161:TYR:N    | 2.45                     | 0.44              |
| 2:1T:221:THR:CB   | 1:2G:324:VAL:CG2  | 2.86                     | 0.44              |
| 2:1X:192:HIS:HD2  | 2:1X:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:1Y:69:ASP:HB2   | 2:1Y:75:MET:HE2   | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Y:401:ARG:NH2  | 1:2M:435:VAL:HG22 | 2.32                     | 0.44              |
| 2:1Z:179:ASP:OD2  | 1:2N:248:LEU:HD22 | 2.10                     | 0.44              |
| 1:2D:70:LEU:HD22  | 1:2D:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:2D:93:ILE:HD11  | 1:2D:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2D:241:SER:OG   | 1:2D:250:VAL:O    | 2.27                     | 0.44              |
| 2:2H:223:THR:HA   | 1:3A:325:PRO:CD   | 2.47                     | 0.44              |
| 2:2O:382:THR:HG21 | 2:2O:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:2Q:69:ASP:OD2   | 2:2Q:74:THR:OG1   | 2.20                     | 0.44              |
| 2:2S:192:HIS:HD2  | 2:2S:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:2S:224:TYR:HD2  | 1:3F:247:ALA:O    | 2.01                     | 0.44              |
| 2:2V:222:PRO:C    | 1:3J:324:VAL:HG13 | 2.42                     | 0.44              |
| 2:2X:407:TRP:HE1  | 1:3L:260:VAL:HB   | 1.82                     | 0.44              |
| 1:3A:334:THR:O    | 1:3A:337:THR:OG1  | 2.30                     | 0.44              |
| 1:3B:30:ILE:HG13  | 1:3B:53:PHE:CE2   | 2.51                     | 0.44              |
| 1:3D:70:LEU:HD22  | 1:3D:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:3F:93:ILE:HD11  | 1:3F:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3G:93:ILE:HD11  | 1:3G:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:3O:382:THR:HG21 | 2:3O:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:3S:192:HIS:HD2  | 2:3S:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:4A:229:ARG:NH1  | 1:4A:366:GLY:HA2  | 2.32                     | 0.44              |
| 1:4A:334:THR:O    | 1:4A:337:THR:OG1  | 2.30                     | 0.44              |
| 1:4C:93:ILE:HD11  | 1:4C:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4D:70:LEU:HD22  | 1:4D:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:4E:93:ILE:HD11  | 1:4E:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4F:276:ILE:HG21 | 1:4F:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:4G:93:ILE:HD11  | 1:4G:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4L:93:ILE:HD11  | 1:4L:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:4O:382:THR:HG21 | 2:4O:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:4R:382:THR:HG21 | 2:4R:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:4Y:192:HIS:HD2  | 2:4Y:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:1B:346:TRP:HE3  | 2:4O:398:MET:HG2  | 1.83                     | 0.44              |
| 1:1B:349:THR:HG21 | 2:4O:184:PRO:CD   | 2.44                     | 0.44              |
| 1:1D:93:ILE:HD11  | 1:1D:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1E:93:ILE:HD11  | 1:1E:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1F:276:ILE:HG21 | 1:1F:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:1G:245:ASP:OD1  | 2:4T:73:GLY:O     | 2.36                     | 0.44              |
| 1:1G:247:ALA:O    | 2:4T:15:GLN:OE1   | 2.35                     | 0.44              |
| 1:1J:256:GLN:HB2  | 2:4V:407:TRP:CH2  | 2.53                     | 0.44              |
| 1:1J:263:PRO:HD3  | 2:4V:406:HIS:CB   | 2.46                     | 0.44              |
| 1:1K:351:PHE:N    | 2:4W:181:VAL:HG22 | 2.33                     | 0.44              |
| 1:1L:93:ILE:HD11  | 1:1L:121:ARG:HG3  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1N:260:VAL:C    | 2:4Z:404:PHE:CE1  | 2.95                     | 0.44              |
| 2:1Q:382:THR:HG21 | 2:1Q:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:1T:224:TYR:OH   | 1:2G:248:LEU:HD22 | 2.17                     | 0.44              |
| 2:1W:158:ARG:HD3  | 2:1W:162:PRO:HA   | 2.00                     | 0.44              |
| 2:1X:180:THR:HG23 | 1:2L:258:ASN:ND2  | 2.28                     | 0.44              |
| 2:1Y:101:ASN:O    | 1:2M:257:THR:HG21 | 2.18                     | 0.44              |
| 2:1Y:214:PHE:CD1  | 1:2M:326:LYS:HE3  | 2.53                     | 0.44              |
| 1:2A:334:THR:O    | 1:2A:337:THR:OG1  | 2.30                     | 0.44              |
| 1:2E:93:ILE:HD11  | 1:2E:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2F:93:ILE:HD11  | 1:2F:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:2F:276:ILE:HG21 | 1:2F:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:2I:334:THR:O    | 1:2I:337:THR:OG1  | 2.30                     | 0.44              |
| 1:2L:93:ILE:HD11  | 1:2L:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:2O:100:GLY:O    | 1:3B:257:THR:OG1  | 2.30                     | 0.44              |
| 2:2Q:132:LEU:HB3  | 2:2Q:164:ARG:HE   | 1.81                     | 0.44              |
| 2:2R:382:THR:HG21 | 2:2R:436:GLN:HB2  | 2.00                     | 0.44              |
| 2:2S:394:GLN:CD   | 1:3F:348:PRO:HB2  | 2.43                     | 0.44              |
| 2:2U:101:ASN:HB2  | 1:3I:254:GLU:CG   | 2.48                     | 0.44              |
| 2:2V:11:GLN:NE2   | 1:3J:249:ASN:HB2  | 2.32                     | 0.44              |
| 2:2Y:404:PHE:CE2  | 1:3M:261:PRO:CB   | 2.89                     | 0.44              |
| 1:3E:93:ILE:HD11  | 1:3E:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3F:276:ILE:HG21 | 1:3F:284:GLU:OE2  | 2.17                     | 0.44              |
| 1:3L:93:ILE:HD11  | 1:3L:121:ARG:HG3  | 2.00                     | 0.44              |
| 2:3Q:69:ASP:OD2   | 2:3Q:74:THR:OG1   | 2.20                     | 0.44              |
| 2:3Q:132:LEU:HB3  | 2:3Q:164:ARG:HE   | 1.81                     | 0.44              |
| 2:3U:132:LEU:HB3  | 2:3U:164:ARG:HE   | 1.81                     | 0.44              |
| 2:3W:158:ARG:HD3  | 2:3W:162:PRO:HA   | 2.00                     | 0.44              |
| 2:3Y:192:HIS:HD2  | 2:3Y:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:4D:93:ILE:HD11  | 1:4D:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4F:93:ILE:HD11  | 1:4F:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:4I:334:THR:O    | 1:4I:337:THR:OG1  | 2.30                     | 0.44              |
| 1:4M:70:LEU:HD22  | 1:4M:110:ILE:HG22 | 1.98                     | 0.44              |
| 2:4R:132:LEU:HB3  | 2:4R:164:ARG:HE   | 1.81                     | 0.44              |
| 2:4S:192:HIS:HD2  | 2:4S:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:4S:382:THR:HG21 | 2:4S:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:4W:158:ARG:HD3  | 2:4W:162:PRO:HA   | 2.00                     | 0.44              |
| 1:1D:2:ARG:CD     | 2:4Q:72:PRO:CD    | 2.69                     | 0.44              |
| 1:1D:70:LEU:HD22  | 1:1D:110:ILE:HG22 | 1.98                     | 0.44              |
| 1:1D:241:SER:OG   | 1:1D:250:VAL:O    | 2.27                     | 0.44              |
| 1:1K:172:TYR:N    | 1:1K:204:VAL:O    | 2.44                     | 0.44              |
| 1:1L:2:ARG:HG3    | 2:4X:72:PRO:CG    | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1H:224:TYR:CE2  | 1:2A:247:ALA:O    | 2.71                     | 0.44              |
| 2:1Q:77:SER:HB3   | 1:2D:245:ASP:OD1  | 2.18                     | 0.44              |
| 2:1T:222:PRO:HD2  | 1:2G:326:LYS:CB   | 2.48                     | 0.44              |
| 2:1U:207:GLU:OE2  | 1:2I:329:ASN:ND2  | 2.44                     | 0.44              |
| 2:1V:181:VAL:HB   | 1:2J:258:ASN:C    | 2.42                     | 0.44              |
| 2:1Y:192:HIS:HD2  | 2:1Y:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:1Y:394:GLN:CD   | 1:2M:349:THR:CG2  | 2.90                     | 0.44              |
| 2:1Z:179:ASP:CG   | 1:2N:248:LEU:CD2  | 2.78                     | 0.44              |
| 1:2N:60:LYS:NZ    | 2:3Y:283:TYR:CE1  | 2.85                     | 0.44              |
| 2:2H:406:HIS:CE1  | 1:3A:263:PRO:HA   | 2.53                     | 0.44              |
| 2:2Q:72:PRO:HD2   | 1:3D:2:ARG:HG3    | 1.97                     | 0.44              |
| 2:2Q:382:THR:HG21 | 2:2Q:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:2R:132:LEU:HB3  | 2:2R:164:ARG:HE   | 1.81                     | 0.44              |
| 2:2W:158:ARG:HD3  | 2:2W:162:PRO:HA   | 2.00                     | 0.44              |
| 2:2Y:192:HIS:HD2  | 2:2Y:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:2Z:192:HIS:HD2  | 2:2Z:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:3D:93:ILE:HD11  | 1:3D:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:3D:241:SER:OG   | 1:3D:250:VAL:O    | 2.27                     | 0.44              |
| 1:3I:334:THR:O    | 1:3I:337:THR:OG1  | 2.30                     | 0.44              |
| 2:3Z:200:GLU:HA   | 2:3Z:266:HIS:HB2  | 1.98                     | 0.44              |
| 2:4U:132:LEU:HB3  | 2:4U:164:ARG:HE   | 1.81                     | 0.44              |
| 2:4Z:192:HIS:HD2  | 2:4Z:424:ASN:HD22 | 1.64                     | 0.44              |
| 1:1C:311:LYS:H    | 1:1C:382:THR:HB   | 1.83                     | 0.44              |
| 1:1D:257:THR:OG1  | 2:4Q:100:GLY:O    | 2.32                     | 0.44              |
| 1:1D:258:ASN:OD1  | 2:4Q:101:ASN:CG   | 2.59                     | 0.44              |
| 1:1D:346:TRP:CE2  | 2:4Q:403:ALA:HB2  | 2.53                     | 0.44              |
| 1:1F:93:ILE:HD11  | 1:1F:121:ARG:HG3  | 2.00                     | 0.44              |
| 1:1G:261:PRO:CA   | 2:4T:404:PHE:N    | 2.81                     | 0.44              |
| 1:1G:351:PHE:N    | 2:4T:181:VAL:HG22 | 2.33                     | 0.44              |
| 1:1J:352:LYS:CD   | 2:4V:101:ASN:HD22 | 2.29                     | 0.44              |
| 1:1L:261:PRO:HB3  | 2:4X:404:PHE:CZ   | 2.53                     | 0.44              |
| 2:1Q:132:LEU:HB3  | 2:1Q:164:ARG:HE   | 1.81                     | 0.44              |
| 2:1Q:222:PRO:HD2  | 1:2D:326:LYS:HB3  | 1.99                     | 0.44              |
| 2:1S:401:ARG:HB3  | 1:2F:262:TYR:OH   | 2.18                     | 0.44              |
| 2:1V:221:THR:CA   | 1:2J:324:VAL:HG13 | 2.46                     | 0.44              |
| 2:1W:10:GLY:HA2   | 2:1W:145:THR:HB   | 1.99                     | 0.44              |
| 2:1Z:200:GLU:HA   | 2:1Z:266:HIS:HB2  | 1.98                     | 0.44              |
| 1:2F:30:ILE:HG13  | 1:2F:53:PHE:HE2   | 1.81                     | 0.44              |
| 1:2K:172:TYR:N    | 1:2K:204:VAL:O    | 2.44                     | 0.44              |
| 2:2H:100:GLY:HA2  | 1:3A:253:THR:C    | 2.43                     | 0.44              |
| 2:2H:406:HIS:CD2  | 1:3A:262:TYR:HA   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2P:72:PRO:HD2   | 1:3C:2:ARG:HG3    | 1.98                     | 0.44              |
| 2:2R:224:TYR:HD2  | 1:3E:247:ALA:O    | 2.00                     | 0.44              |
| 2:2U:158:ARG:HD3  | 2:2U:162:PRO:HA   | 2.00                     | 0.44              |
| 2:2W:10:GLY:HA2   | 2:2W:145:THR:HB   | 1.99                     | 0.44              |
| 2:2Z:100:GLY:HA2  | 1:3N:253:THR:C    | 2.43                     | 0.44              |
| 1:3F:62:VAL:HA    | 1:3F:63:PRO:HD3   | 1.86                     | 0.44              |
| 1:3K:172:TYR:N    | 1:3K:204:VAL:O    | 2.44                     | 0.44              |
| 2:3Q:382:THR:HG21 | 2:3Q:436:GLN:HB2  | 1.99                     | 0.44              |
| 2:3R:132:LEU:HB3  | 2:3R:164:ARG:HE   | 1.81                     | 0.44              |
| 2:3T:154:ILE:HG23 | 2:3T:166:MET:HG2  | 2.00                     | 0.44              |
| 2:3W:10:GLY:HA2   | 2:3W:145:THR:HB   | 1.99                     | 0.44              |
| 2:3Z:192:HIS:HD2  | 2:3Z:424:ASN:HD22 | 1.64                     | 0.44              |
| 2:4S:154:ILE:HG23 | 2:4S:166:MET:HG2  | 2.00                     | 0.44              |
| 2:4U:154:ILE:HG23 | 2:4U:166:MET:HG2  | 2.00                     | 0.44              |
| 1:1B:276:ILE:HG21 | 1:1B:284:GLU:OE2  | 2.17                     | 0.43              |
| 1:1B:435:VAL:O    | 2:4O:401:ARG:NH2  | 2.49                     | 0.43              |
| 1:1C:325:PRO:C    | 2:4P:210:TYR:CZ   | 2.93                     | 0.43              |
| 1:1D:346:TRP:CZ2  | 2:4Q:403:ALA:CB   | 3.01                     | 0.43              |
| 1:1E:326:LYS:HE2  | 2:4R:214:PHE:HB2  | 1.99                     | 0.43              |
| 1:1F:30:ILE:HG13  | 1:1F:53:PHE:HE2   | 1.81                     | 0.43              |
| 1:1I:261:PRO:HA   | 2:4U:404:PHE:CG   | 2.53                     | 0.43              |
| 1:1I:334:THR:O    | 1:1I:337:THR:OG1  | 2.30                     | 0.43              |
| 1:1L:260:VAL:CA   | 2:4X:407:TRP:HE1  | 2.30                     | 0.43              |
| 1:1L:332:ILE:HB   | 2:4X:177:VAL:HG21 | 1.98                     | 0.43              |
| 1:1M:2:ARG:HG3    | 2:4Y:72:PRO:HG2   | 1.98                     | 0.43              |
| 1:1M:347:CYS:HA   | 2:4Y:398:MET:HG2  | 2.00                     | 0.43              |
| 1:1N:348:PRO:HB2  | 2:4Z:394:GLN:CG   | 2.45                     | 0.43              |
| 2:1P:181:VAL:CG2  | 1:2C:258:ASN:O    | 2.59                     | 0.43              |
| 2:1R:10:GLY:HA2   | 2:1R:145:THR:HB   | 1.99                     | 0.43              |
| 2:1R:132:LEU:HB3  | 2:1R:164:ARG:HE   | 1.82                     | 0.43              |
| 2:1S:180:THR:CG2  | 1:2F:258:ASN:HD21 | 2.30                     | 0.43              |
| 2:1T:132:LEU:HB3  | 2:1T:164:ARG:HE   | 1.81                     | 0.43              |
| 2:1T:154:ILE:HG23 | 2:1T:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1U:154:ILE:HG23 | 2:1U:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1U:180:THR:HG23 | 1:2I:258:ASN:ND2  | 2.31                     | 0.43              |
| 2:1V:411:GLU:OE2  | 1:2J:163:LYS:NZ   | 2.51                     | 0.43              |
| 2:1W:401:ARG:HH22 | 1:2K:435:VAL:CA   | 2.14                     | 0.43              |
| 1:2F:62:VAL:HA    | 1:2F:63:PRO:HD3   | 1.86                     | 0.43              |
| 2:2O:401:ARG:O    | 1:3B:262:TYR:CZ   | 2.66                     | 0.43              |
| 2:2P:401:ARG:O    | 1:3C:262:TYR:CZ   | 2.65                     | 0.43              |
| 2:2R:10:GLY:HA2   | 2:2R:145:THR:HB   | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:154:ILE:HG23 | 2:2R:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2S:154:ILE:HG23 | 2:2S:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2T:71:GLU:HB2   | 1:3G:2:ARG:CD     | 2.45                     | 0.43              |
| 2:2T:154:ILE:HG23 | 2:2T:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2U:132:LEU:HB3  | 2:2U:164:ARG:HE   | 1.82                     | 0.43              |
| 2:2U:154:ILE:HG23 | 2:2U:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2Y:406:HIS:CE1  | 1:3M:263:PRO:HA   | 2.53                     | 0.43              |
| 2:2Z:200:GLU:HA   | 2:2Z:266:HIS:HB2  | 1.98                     | 0.43              |
| 1:3C:311:LYS:H    | 1:3C:382:THR:HB   | 1.83                     | 0.43              |
| 1:3F:30:ILE:HG13  | 1:3F:53:PHE:HE2   | 1.81                     | 0.43              |
| 1:3F:172:TYR:N    | 1:3F:204:VAL:O    | 2.44                     | 0.43              |
| 2:3R:154:ILE:HG23 | 2:3R:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3S:154:ILE:HG23 | 2:3S:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3U:154:ILE:HG23 | 2:3U:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3U:158:ARG:HD3  | 2:3U:162:PRO:HA   | 2.00                     | 0.43              |
| 1:4B:276:ILE:HG21 | 1:4B:284:GLU:OE2  | 2.17                     | 0.43              |
| 1:4C:311:LYS:H    | 1:4C:382:THR:HB   | 1.83                     | 0.43              |
| 1:4F:30:ILE:HG13  | 1:4F:53:PHE:HE2   | 1.82                     | 0.43              |
| 1:4F:172:TYR:N    | 1:4F:204:VAL:O    | 2.44                     | 0.43              |
| 1:4K:172:TYR:N    | 1:4K:204:VAL:O    | 2.44                     | 0.43              |
| 2:4Q:382:THR:HG21 | 2:4Q:436:GLN:HB2  | 1.99                     | 0.43              |
| 2:4R:10:GLY:HA2   | 2:4R:145:THR:HB   | 1.99                     | 0.43              |
| 2:4R:154:ILE:HG23 | 2:4R:166:MET:HG2  | 2.00                     | 0.43              |
| 2:4T:154:ILE:HG23 | 2:4T:166:MET:HG2  | 2.00                     | 0.43              |
| 2:4U:158:ARG:HD3  | 2:4U:162:PRO:HA   | 2.00                     | 0.43              |
| 1:1B:324:VAL:HG11 | 2:4O:221:THR:C    | 2.42                     | 0.43              |
| 1:1C:257:THR:HG21 | 2:4P:102:ASN:CB   | 2.48                     | 0.43              |
| 1:1D:260:VAL:CB   | 2:4Q:407:TRP:CZ2  | 3.01                     | 0.43              |
| 1:1E:253:THR:O    | 2:4R:100:GLY:CA   | 2.63                     | 0.43              |
| 1:1E:260:VAL:N    | 2:4R:404:PHE:HE1  | 2.17                     | 0.43              |
| 1:1F:352:LYS:HA   | 2:4S:179:ASP:C    | 2.42                     | 0.43              |
| 1:1I:248:LEU:HD12 | 2:4U:11:GLN:OE1   | 2.17                     | 0.43              |
| 1:1I:329:ASN:CG   | 2:4U:177:VAL:HG11 | 2.43                     | 0.43              |
| 1:1J:349:THR:HG21 | 2:4V:183:GLU:CG   | 2.48                     | 0.43              |
| 1:1J:435:VAL:HA   | 2:4V:401:ARG:HH21 | 1.83                     | 0.43              |
| 1:1K:349:THR:HG21 | 2:4W:183:GLU:HG3  | 1.99                     | 0.43              |
| 1:1M:2:ARG:NH2    | 2:4Y:73:GLY:HA3   | 2.33                     | 0.43              |
| 1:1M:254:GLU:CA   | 2:4Y:100:GLY:HA2  | 2.48                     | 0.43              |
| 1:1N:399:TYR:OH   | 1:1N:415:GLU:OE2  | 2.27                     | 0.43              |
| 2:1R:154:ILE:HG23 | 2:1R:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1S:132:LEU:HB3  | 2:1S:164:ARG:HE   | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1S:154:ILE:HG23 | 2:1S:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1Z:192:HIS:HD2  | 2:1Z:424:ASN:HD22 | 1.64                     | 0.43              |
| 1:2B:276:ILE:HG21 | 1:2B:284:GLU:OE2  | 2.17                     | 0.43              |
| 1:2C:311:LYS:H    | 1:2C:382:THR:HB   | 1.84                     | 0.43              |
| 1:2F:172:TYR:N    | 1:2F:204:VAL:O    | 2.44                     | 0.43              |
| 1:2G:172:TYR:N    | 1:2G:204:VAL:O    | 2.44                     | 0.43              |
| 2:2O:100:GLY:CA   | 1:3B:253:THR:C    | 2.92                     | 0.43              |
| 2:2P:100:GLY:C    | 1:3C:254:GLU:HA   | 2.43                     | 0.43              |
| 2:2S:132:LEU:HB3  | 2:2S:164:ARG:HE   | 1.81                     | 0.43              |
| 2:2S:394:GLN:NE2  | 1:3F:348:PRO:HB2  | 2.33                     | 0.43              |
| 2:2V:51:VAL:HG11  | 2:2V:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:3B:276:ILE:HG21 | 1:3B:284:GLU:OE2  | 2.17                     | 0.43              |
| 2:3Q:154:ILE:HG23 | 2:3Q:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3R:10:GLY:HA2   | 2:3R:145:THR:HB   | 1.99                     | 0.43              |
| 2:3S:132:LEU:HB3  | 2:3S:164:ARG:HE   | 1.81                     | 0.43              |
| 1:4G:172:TYR:N    | 1:4G:204:VAL:O    | 2.44                     | 0.43              |
| 2:4V:51:VAL:HG11  | 2:4V:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:4V:154:ILE:HG23 | 2:4V:166:MET:HG2  | 2.00                     | 0.43              |
| 2:4W:10:GLY:HA2   | 2:4W:145:THR:HB   | 1.99                     | 0.43              |
| 1:1A:311:LYS:H    | 1:1A:382:THR:HB   | 1.83                     | 0.43              |
| 1:1C:241:SER:OG   | 1:1C:250:VAL:O    | 2.27                     | 0.43              |
| 1:1C:263:PRO:N    | 2:4P:406:HIS:CG   | 2.83                     | 0.43              |
| 1:1C:346:TRP:HE3  | 2:4P:398:MET:HG2  | 1.83                     | 0.43              |
| 1:1D:254:GLU:HB3  | 2:4Q:101:ASN:CB   | 2.40                     | 0.43              |
| 1:1D:346:TRP:CZ2  | 2:4Q:403:ALA:HB2  | 2.54                     | 0.43              |
| 1:1E:30:ILE:HG13  | 1:1E:53:PHE:HE2   | 1.81                     | 0.43              |
| 1:1E:311:LYS:H    | 1:1E:382:THR:HB   | 1.83                     | 0.43              |
| 1:1E:329:ASN:OD1  | 2:4R:177:VAL:CG1  | 2.65                     | 0.43              |
| 1:1F:325:PRO:CD   | 2:4S:223:THR:HA   | 2.47                     | 0.43              |
| 1:1G:311:LYS:H    | 1:1G:382:THR:HB   | 1.83                     | 0.43              |
| 1:1G:325:PRO:CD   | 2:4T:223:THR:HA   | 2.48                     | 0.43              |
| 1:1G:352:LYS:HD3  | 2:4T:101:ASN:HD21 | 1.72                     | 0.43              |
| 1:1K:2:ARG:HG3    | 2:4W:72:PRO:CG    | 2.48                     | 0.43              |
| 1:1L:254:GLU:HA   | 2:4X:100:GLY:CA   | 2.48                     | 0.43              |
| 2:1Q:222:PRO:O    | 1:2D:325:PRO:HD2  | 2.19                     | 0.43              |
| 2:1S:44:LEU:HA    | 2:1S:49:ILE:HB    | 2.01                     | 0.43              |
| 2:1U:132:LEU:HB3  | 2:1U:164:ARG:HE   | 1.82                     | 0.43              |
| 2:1U:158:ARG:HD3  | 2:1U:162:PRO:HA   | 2.00                     | 0.43              |
| 2:1V:44:LEU:HA    | 2:1V:49:ILE:HB    | 2.01                     | 0.43              |
| 2:1V:51:VAL:HG11  | 2:1V:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1V:154:ILE:HG23 | 2:1V:166:MET:HG2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2G:311:LYS:H    | 1:2G:382:THR:HB   | 1.83                     | 0.43              |
| 1:2N:399:TYR:OH   | 1:2N:415:GLU:OE2  | 2.27                     | 0.43              |
| 2:2Q:210:TYR:HB3  | 1:3D:326:LYS:HG2  | 1.99                     | 0.43              |
| 2:2V:154:ILE:HG23 | 2:2V:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2W:407:TRP:HE1  | 1:3K:260:VAL:HB   | 1.82                     | 0.43              |
| 2:2X:221:THR:C    | 1:3L:324:VAL:CG1  | 2.92                     | 0.43              |
| 2:2Y:406:HIS:NE2  | 1:3M:262:TYR:CA   | 2.82                     | 0.43              |
| 2:2Z:406:HIS:CE1  | 1:3N:263:PRO:HA   | 2.53                     | 0.43              |
| 1:3G:172:TYR:N    | 1:3G:204:VAL:O    | 2.44                     | 0.43              |
| 1:3G:311:LYS:H    | 1:3G:382:THR:HB   | 1.83                     | 0.43              |
| 1:3N:399:TYR:OH   | 1:3N:415:GLU:OE2  | 2.27                     | 0.43              |
| 2:3T:132:LEU:HB3  | 2:3T:164:ARG:HE   | 1.81                     | 0.43              |
| 2:3V:51:VAL:HG11  | 2:3V:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:3V:154:ILE:HG23 | 2:3V:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3W:51:VAL:HG11  | 2:3W:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:4G:311:LYS:H    | 1:4G:382:THR:HB   | 1.83                     | 0.43              |
| 2:4Q:154:ILE:HG23 | 2:4Q:166:MET:HG2  | 2.00                     | 0.43              |
| 2:4Z:200:GLU:HA   | 2:4Z:266:HIS:HB2  | 1.98                     | 0.43              |
| 1:1B:248:LEU:C    | 2:4O:11:GLN:NE2   | 2.66                     | 0.43              |
| 1:1C:261:PRO:CB   | 2:4P:404:PHE:H    | 2.30                     | 0.43              |
| 1:1C:346:TRP:CE3  | 2:4P:403:ALA:CB   | 3.01                     | 0.43              |
| 1:1E:325:PRO:CG   | 2:4R:224:TYR:CE1  | 3.00                     | 0.43              |
| 1:1F:172:TYR:N    | 1:1F:204:VAL:O    | 2.44                     | 0.43              |
| 1:1G:324:VAL:HG12 | 2:4T:222:PRO:O    | 2.17                     | 0.43              |
| 1:1I:245:ASP:OD1  | 2:4U:73:GLY:O     | 2.37                     | 0.43              |
| 1:1I:333:ALA:HB1  | 2:4U:176:LYS:HE2  | 1.98                     | 0.43              |
| 1:1M:260:VAL:CG1  | 2:4Y:407:TRP:HE1  | 2.31                     | 0.43              |
| 1:1N:311:LYS:H    | 1:1N:382:THR:HB   | 1.83                     | 0.43              |
| 2:1Q:154:ILE:HG23 | 2:1Q:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1T:10:GLY:HA2   | 2:1T:145:THR:HB   | 1.99                     | 0.43              |
| 2:1U:51:VAL:HG11  | 2:1U:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1W:51:VAL:HG11  | 2:1W:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1X:158:ARG:HD3  | 2:1X:162:PRO:HA   | 2.00                     | 0.43              |
| 2:1Z:11:GLN:HE22  | 1:2N:249:ASN:N    | 2.10                     | 0.43              |
| 1:2A:311:LYS:H    | 1:2A:382:THR:HB   | 1.83                     | 0.43              |
| 2:2P:223:THR:HA   | 1:3C:325:PRO:CD   | 2.47                     | 0.43              |
| 2:2P:398:MET:HA   | 1:3C:346:TRP:HB2  | 2.00                     | 0.43              |
| 2:2Q:154:ILE:HG23 | 2:2Q:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2R:182:VAL:HG21 | 1:3E:257:THR:HG22 | 1.98                     | 0.43              |
| 2:2S:44:LEU:HA    | 2:2S:49:ILE:HB    | 2.01                     | 0.43              |
| 2:2S:407:TRP:HE1  | 1:3F:260:VAL:HG12 | 1.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2T:51:VAL:HG11 | 2:2T:243:ARG:HG2 | 2.00                     | 0.43              |
| 2:2T:77:SER:HB2  | 1:3G:245:ASP:CG  | 2.43                     | 0.43              |
| 2:2U:51:VAL:HG11 | 2:2U:243:ARG:HG2 | 2.00                     | 0.43              |
| 2:2U:394:GLN:CG  | 1:3I:348:PRO:CB  | 2.86                     | 0.43              |
| 2:2V:44:LEU:HA   | 2:2V:49:ILE:HB   | 2.01                     | 0.43              |
| 2:2V:179:ASP:C   | 1:3J:352:LYS:HA  | 2.43                     | 0.43              |
| 2:2W:51:VAL:HG11 | 2:2W:243:ARG:HG2 | 2.00                     | 0.43              |
| 2:2X:158:ARG:HD3 | 2:2X:162:PRO:HA  | 2.00                     | 0.43              |
| 2:2Y:404:PHE:CA  | 1:3M:261:PRO:O   | 2.62                     | 0.43              |
| 1:3A:311:LYS:H   | 1:3A:382:THR:HB  | 1.84                     | 0.43              |
| 2:3R:44:LEU:HA   | 2:3R:49:ILE:HB   | 2.01                     | 0.43              |
| 2:3S:44:LEU:HA   | 2:3S:49:ILE:HB   | 2.01                     | 0.43              |
| 2:3U:51:VAL:HG11 | 2:3U:243:ARG:HG2 | 2.00                     | 0.43              |
| 2:3V:10:GLY:HA2  | 2:3V:145:THR:HB  | 1.99                     | 0.43              |
| 1:4A:311:LYS:H   | 1:4A:382:THR:HB  | 1.84                     | 0.43              |
| 1:4I:311:LYS:H   | 1:4I:382:THR:HB  | 1.83                     | 0.43              |
| 2:4R:44:LEU:HA   | 2:4R:49:ILE:HB   | 2.01                     | 0.43              |
| 2:4S:44:LEU:HA   | 2:4S:49:ILE:HB   | 2.01                     | 0.43              |
| 2:4S:132:LEU:HB3 | 2:4S:164:ARG:HE  | 1.81                     | 0.43              |
| 2:4U:10:GLY:HA2  | 2:4U:145:THR:HB  | 1.99                     | 0.43              |
| 2:4U:51:VAL:HG11 | 2:4U:243:ARG:HG2 | 2.00                     | 0.43              |
| 2:4V:10:GLY:HA2  | 2:4V:145:THR:HB  | 1.99                     | 0.43              |
| 2:4X:158:ARG:HD3 | 2:4X:162:PRO:HA  | 2.00                     | 0.43              |
| 1:1G:172:TYR:N   | 1:1G:204:VAL:O   | 2.44                     | 0.43              |
| 1:1J:348:PRO:HB2 | 2:4V:394:GLN:CD  | 2.43                     | 0.43              |
| 1:1M:2:ARG:CG    | 2:4Y:72:PRO:HD2  | 2.46                     | 0.43              |
| 1:1N:261:PRO:CA  | 2:4Z:404:PHE:CG  | 2.93                     | 0.43              |
| 2:1O:221:THR:OG1 | 1:2B:324:VAL:CG2 | 2.66                     | 0.43              |
| 2:1Q:394:GLN:HG2 | 1:2D:348:PRO:CG  | 2.47                     | 0.43              |
| 2:1R:44:LEU:HA   | 2:1R:49:ILE:HB   | 2.01                     | 0.43              |
| 2:1T:158:ARG:HD3 | 2:1T:162:PRO:HA  | 2.00                     | 0.43              |
| 2:1U:10:GLY:HA2  | 2:1U:145:THR:HB  | 1.99                     | 0.43              |
| 2:1V:145:THR:O   | 2:1V:149:MET:N   | 2.52                     | 0.43              |
| 2:1X:394:GLN:CD  | 1:2L:349:THR:CG2 | 2.91                     | 0.43              |
| 1:2E:311:LYS:H   | 1:2E:382:THR:HB  | 1.83                     | 0.43              |
| 1:2I:311:LYS:H   | 1:2I:382:THR:HB  | 1.83                     | 0.43              |
| 2:2H:214:PHE:CG  | 1:3A:326:LYS:HE3 | 2.53                     | 0.43              |
| 2:2R:222:PRO:CG  | 1:3E:326:LYS:CB  | 2.92                     | 0.43              |
| 2:2T:10:GLY:HA2  | 2:2T:145:THR:HB  | 1.99                     | 0.43              |
| 2:2T:132:LEU:HB3 | 2:2T:164:ARG:HE  | 1.82                     | 0.43              |
| 2:2W:44:LEU:HA   | 2:2W:49:ILE:HB   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2W:72:PRO:HD2   | 1:3K:2:ARG:HD3    | 1.99                     | 0.43              |
| 2:2W:214:PHE:HB2  | 1:3K:326:LYS:HE3  | 1.91                     | 0.43              |
| 2:2W:394:GLN:HB3  | 1:3K:348:PRO:CG   | 2.49                     | 0.43              |
| 1:3I:311:LYS:H    | 1:3I:382:THR:HB   | 1.83                     | 0.43              |
| 1:3N:311:LYS:H    | 1:3N:382:THR:HB   | 1.83                     | 0.43              |
| 2:3T:10:GLY:HA2   | 2:3T:145:THR:HB   | 1.99                     | 0.43              |
| 2:3T:51:VAL:HG11  | 2:3T:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:3V:44:LEU:HA    | 2:3V:49:ILE:HB    | 2.01                     | 0.43              |
| 2:3V:145:THR:O    | 2:3V:149:MET:N    | 2.52                     | 0.43              |
| 2:3W:44:LEU:HA    | 2:3W:49:ILE:HB    | 2.01                     | 0.43              |
| 2:3X:158:ARG:HD3  | 2:3X:162:PRO:HA   | 2.00                     | 0.43              |
| 1:4E:311:LYS:H    | 1:4E:382:THR:HB   | 1.83                     | 0.43              |
| 1:4F:62:VAL:HA    | 1:4F:63:PRO:HD3   | 1.86                     | 0.43              |
| 2:4R:74:THR:O     | 2:4R:77:SER:OG    | 2.31                     | 0.43              |
| 2:4S:10:GLY:HA2   | 2:4S:145:THR:HB   | 1.99                     | 0.43              |
| 2:4T:10:GLY:HA2   | 2:4T:145:THR:HB   | 1.99                     | 0.43              |
| 2:4T:51:VAL:HG11  | 2:4T:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:4T:158:ARG:HD3  | 2:4T:162:PRO:HA   | 2.00                     | 0.43              |
| 2:4V:44:LEU:HA    | 2:4V:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4W:44:LEU:HA    | 2:4W:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4W:51:VAL:HG11  | 2:4W:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:1A:260:VAL:N    | 2:4H:404:PHE:HE1  | 2.17                     | 0.43              |
| 1:1B:260:VAL:HG12 | 2:4O:406:HIS:HE1  | 1.84                     | 0.43              |
| 1:1D:351:PHE:N    | 2:4Q:178:SER:OG   | 2.51                     | 0.43              |
| 1:1F:326:LYS:CE   | 2:4S:214:PHE:HB2  | 2.48                     | 0.43              |
| 1:1G:326:LYS:CA   | 2:4T:210:TYR:CD1  | 2.99                     | 0.43              |
| 1:1I:2:ARG:CG     | 2:4U:72:PRO:CD    | 2.96                     | 0.43              |
| 1:1K:251:ASP:OD2  | 2:4W:71:GLU:HB3   | 2.19                     | 0.43              |
| 1:1L:248:LEU:CD1  | 5:4X:501:GDP:H8   | 2.30                     | 0.43              |
| 1:1N:245:ASP:OD2  | 2:4Z:77:SER:HB2   | 2.19                     | 0.43              |
| 2:1H:221:THR:OG1  | 1:2A:324:VAL:HG21 | 2.19                     | 0.43              |
| 2:1S:207:GLU:OE1  | 1:2F:329:ASN:ND2  | 2.47                     | 0.43              |
| 2:1T:51:VAL:HG11  | 2:1T:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1T:181:VAL:HG23 | 1:2G:258:ASN:CB   | 2.44                     | 0.43              |
| 2:1W:44:LEU:HA    | 2:1W:49:ILE:HB    | 2.01                     | 0.43              |
| 1:2L:311:LYS:H    | 1:2L:382:THR:HB   | 1.83                     | 0.43              |
| 1:2N:311:LYS:H    | 1:2N:382:THR:HB   | 1.83                     | 0.43              |
| 2:2P:398:MET:HG2  | 1:3C:346:TRP:O    | 2.18                     | 0.43              |
| 2:2S:394:GLN:CG   | 1:3F:348:PRO:HG2  | 2.42                     | 0.43              |
| 2:2T:72:PRO:HD2   | 1:3G:2:ARG:HG2    | 1.98                     | 0.43              |
| 2:2T:222:PRO:HD2  | 1:3G:326:LYS:HB3  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2U:10:GLY:HA2   | 2:2U:145:THR:HB   | 1.99                     | 0.43              |
| 2:2V:10:GLY:HA2   | 2:2V:145:THR:HB   | 1.99                     | 0.43              |
| 2:2V:145:THR:O    | 2:2V:149:MET:N    | 2.52                     | 0.43              |
| 2:2V:165:ILE:H    | 2:2V:165:ILE:HG13 | 1.71                     | 0.43              |
| 2:2W:11:GLN:HE22  | 1:3K:249:ASN:CB   | 2.31                     | 0.43              |
| 2:2W:154:ILE:HG23 | 2:2W:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2Y:74:THR:O     | 2:2Y:77:SER:OG    | 2.31                     | 0.43              |
| 1:3E:30:ILE:HG13  | 1:3E:53:PHE:HE2   | 1.82                     | 0.43              |
| 1:3E:311:LYS:H    | 1:3E:382:THR:HB   | 1.84                     | 0.43              |
| 1:3L:311:LYS:H    | 1:3L:382:THR:HB   | 1.83                     | 0.43              |
| 2:3T:158:ARG:HD3  | 2:3T:162:PRO:HA   | 2.00                     | 0.43              |
| 2:3U:10:GLY:HA2   | 2:3U:145:THR:HB   | 1.99                     | 0.43              |
| 2:3Y:74:THR:O     | 2:3Y:77:SER:OG    | 2.31                     | 0.43              |
| 1:4E:30:ILE:HG13  | 1:4E:53:PHE:HE2   | 1.81                     | 0.43              |
| 2:4P:154:ILE:HG23 | 2:4P:166:MET:HG2  | 2.00                     | 0.43              |
| 2:4T:132:LEU:HB3  | 2:4T:164:ARG:HE   | 1.82                     | 0.43              |
| 2:4W:154:ILE:HG23 | 2:4W:166:MET:HG2  | 2.00                     | 0.43              |
| 1:1E:439:SER:HB3  | 2:4R:400:ARG:HD3  | 2.00                     | 0.43              |
| 1:1F:254:GLU:CG   | 2:4S:100:GLY:HA2  | 2.49                     | 0.43              |
| 1:1F:258:ASN:OD1  | 2:4S:101:ASN:CG   | 2.62                     | 0.43              |
| 1:1F:346:TRP:CE2  | 2:4S:403:ALA:CB   | 3.01                     | 0.43              |
| 1:1G:346:TRP:CE2  | 2:4T:403:ALA:CB   | 2.99                     | 0.43              |
| 1:1I:311:LYS:H    | 1:1I:382:THR:HB   | 1.83                     | 0.43              |
| 1:1K:349:THR:OG1  | 2:4W:184:PRO:CD   | 2.67                     | 0.43              |
| 1:1L:311:LYS:H    | 1:1L:382:THR:HB   | 1.83                     | 0.43              |
| 1:1M:439:SER:OG   | 2:4Y:401:ARG:HG2  | 2.19                     | 0.43              |
| 1:1N:326:LYS:HB3  | 2:4Z:222:PRO:HD2  | 2.01                     | 0.43              |
| 2:1P:36:TYR:OH    | 2:1P:40:SER:O     | 2.35                     | 0.43              |
| 2:1S:10:GLY:HA2   | 2:1S:145:THR:HB   | 1.99                     | 0.43              |
| 2:1V:10:GLY:HA2   | 2:1V:145:THR:HB   | 1.99                     | 0.43              |
| 2:1W:154:ILE:HG23 | 2:1W:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1X:36:TYR:OH    | 2:1X:40:SER:O     | 2.35                     | 0.43              |
| 2:1Y:180:THR:HG23 | 1:2M:258:ASN:ND2  | 2.30                     | 0.43              |
| 1:2E:30:ILE:HG13  | 1:2E:53:PHE:HE2   | 1.82                     | 0.43              |
| 2:2P:154:ILE:HG23 | 2:2P:166:MET:HG2  | 2.00                     | 0.43              |
| 2:2P:158:ARG:HD3  | 2:2P:162:PRO:HA   | 2.00                     | 0.43              |
| 2:2R:44:LEU:HA    | 2:2R:49:ILE:HB    | 2.01                     | 0.43              |
| 2:2S:10:GLY:HA2   | 2:2S:145:THR:HB   | 1.99                     | 0.43              |
| 2:2T:158:ARG:HD3  | 2:2T:162:PRO:HA   | 2.00                     | 0.43              |
| 2:2V:398:MET:HG3  | 1:3J:346:TRP:O    | 2.19                     | 0.43              |
| 2:2W:407:TRP:HE1  | 1:3K:260:VAL:CG1  | 2.31                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3P:154:ILE:HG23 | 2:3P:166:MET:HG2  | 2.00                     | 0.43              |
| 2:3Q:158:ARG:HD3  | 2:3Q:162:PRO:HA   | 2.00                     | 0.43              |
| 2:3W:154:ILE:HG23 | 2:3W:166:MET:HG2  | 2.00                     | 0.43              |
| 1:4G:334:THR:O    | 1:4G:337:THR:OG1  | 2.30                     | 0.43              |
| 1:4N:311:LYS:H    | 1:4N:382:THR:HB   | 1.83                     | 0.43              |
| 2:4X:51:VAL:HG11  | 2:4X:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:4Z:158:ARG:HD3  | 2:4Z:162:PRO:HA   | 2.00                     | 0.43              |
| 1:1C:248:LEU:HB2  | 2:4P:224:TYR:HE2  | 1.84                     | 0.43              |
| 1:1C:262:TYR:OH   | 2:4P:403:ALA:N    | 2.52                     | 0.43              |
| 1:1E:346:TRP:CD1  | 2:4R:401:ARG:HB2  | 2.54                     | 0.43              |
| 1:1G:326:LYS:HG2  | 2:4T:210:TYR:HB3  | 2.00                     | 0.43              |
| 1:1G:349:THR:HG21 | 2:4T:183:GLU:HG3  | 2.01                     | 0.43              |
| 1:1I:346:TRP:CZ3  | 2:4U:404:PHE:CD2  | 3.07                     | 0.43              |
| 1:1K:311:LYS:H    | 1:1K:382:THR:HB   | 1.83                     | 0.43              |
| 2:1O:44:LEU:HA    | 2:1O:49:ILE:HB    | 2.01                     | 0.43              |
| 2:1P:154:ILE:HG23 | 2:1P:166:MET:HG2  | 2.00                     | 0.43              |
| 2:1P:158:ARG:HD3  | 2:1P:162:PRO:HA   | 2.00                     | 0.43              |
| 2:1Q:158:ARG:HD3  | 2:1Q:162:PRO:HA   | 2.00                     | 0.43              |
| 2:1X:51:VAL:HG11  | 2:1X:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:2L:62:VAL:HA    | 1:2L:63:PRO:HD3   | 1.86                     | 0.43              |
| 2:2O:44:LEU:HA    | 2:2O:49:ILE:HB    | 2.01                     | 0.43              |
| 2:2P:36:TYR:OH    | 2:2P:40:SER:O     | 2.35                     | 0.43              |
| 2:2Q:158:ARG:HD3  | 2:2Q:162:PRO:HA   | 2.00                     | 0.43              |
| 2:2R:210:TYR:CD2  | 1:3E:329:ASN:HB2  | 2.53                     | 0.43              |
| 2:2S:101:ASN:O    | 1:3F:257:THR:CG2  | 2.60                     | 0.43              |
| 2:2T:394:GLN:OE1  | 1:3G:349:THR:HG23 | 2.18                     | 0.43              |
| 2:2U:100:GLY:O    | 1:3I:254:GLU:HA   | 2.19                     | 0.43              |
| 2:2V:180:THR:N    | 1:3J:351:PHE:O    | 2.51                     | 0.43              |
| 2:2X:51:VAL:HG11  | 2:2X:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:2Y:214:PHE:CG   | 1:3M:326:LYS:CE   | 3.00                     | 0.43              |
| 2:2Z:386:GLU:HA   | 2:2Z:389:LYS:HB2  | 2.01                     | 0.43              |
| 2:3P:36:TYR:OH    | 2:3P:40:SER:O     | 2.35                     | 0.43              |
| 2:3P:158:ARG:HD3  | 2:3P:162:PRO:HA   | 2.00                     | 0.43              |
| 2:3S:10:GLY:HA2   | 2:3S:145:THR:HB   | 1.99                     | 0.43              |
| 2:3V:165:ILE:H    | 2:3V:165:ILE:HG13 | 1.71                     | 0.43              |
| 2:3X:51:VAL:HG11  | 2:3X:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:4L:311:LYS:H    | 1:4L:382:THR:HB   | 1.84                     | 0.43              |
| 2:4P:44:LEU:HA    | 2:4P:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4P:158:ARG:HD3  | 2:4P:162:PRO:HA   | 2.00                     | 0.43              |
| 2:4X:36:TYR:OH    | 2:4X:40:SER:O     | 2.35                     | 0.43              |
| 1:1A:62:VAL:HA    | 1:1A:63:PRO:HD3   | 1.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1B:346:TRP:CH2  | 2:4O:403:ALA:CB   | 3.02                     | 0.43              |
| 1:1E:262:TYR:OH   | 2:4R:403:ALA:N    | 2.52                     | 0.43              |
| 1:1F:326:LYS:HZ2  | 2:4S:210:TYR:HB3  | 1.84                     | 0.43              |
| 1:1G:247:ALA:O    | 2:4T:15:GLN:CD    | 2.62                     | 0.43              |
| 1:1G:346:TRP:CG   | 2:4T:401:ARG:HB2  | 2.54                     | 0.43              |
| 1:1K:248:LEU:CD1  | 5:4W:501:GDP:H8   | 2.31                     | 0.43              |
| 1:1K:325:PRO:HG2  | 2:4W:224:TYR:CG   | 2.54                     | 0.43              |
| 1:1K:435:VAL:C    | 2:4W:401:ARG:HH22 | 2.27                     | 0.43              |
| 1:1L:346:TRP:CA   | 2:4X:397:ALA:O    | 2.67                     | 0.43              |
| 1:1M:263:PRO:N    | 2:4Y:406:HIS:NE2  | 2.56                     | 0.43              |
| 1:1M:348:PRO:HB3  | 2:4Y:394:GLN:HG2  | 1.96                     | 0.43              |
| 2:1H:182:VAL:HG21 | 1:2A:257:THR:CG2  | 2.47                     | 0.43              |
| 2:1P:44:LEU:HA    | 2:1P:49:ILE:HB    | 2.01                     | 0.43              |
| 2:1W:36:TYR:OH    | 2:1W:40:SER:O     | 2.35                     | 0.43              |
| 2:1Y:36:TYR:OH    | 2:1Y:40:SER:O     | 2.35                     | 0.43              |
| 2:1Y:51:VAL:HG11  | 2:1Y:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1Y:394:GLN:OE1  | 1:2M:349:THR:HG21 | 2.18                     | 0.43              |
| 2:1Z:158:ARG:HD3  | 2:1Z:162:PRO:HA   | 2.00                     | 0.43              |
| 2:1Z:386:GLU:HA   | 2:1Z:389:LYS:HB2  | 2.01                     | 0.43              |
| 1:2G:334:THR:O    | 1:2G:337:THR:OG1  | 2.30                     | 0.43              |
| 2:2P:44:LEU:HA    | 2:2P:49:ILE:HB    | 2.01                     | 0.43              |
| 2:2Q:224:TYR:CD2  | 1:3D:247:ALA:O    | 2.72                     | 0.43              |
| 2:2U:100:GLY:C    | 1:3I:254:GLU:HA   | 2.44                     | 0.43              |
| 2:2W:394:GLN:OE1  | 1:3K:349:THR:HG23 | 2.19                     | 0.43              |
| 2:2X:36:TYR:OH    | 2:2X:40:SER:O     | 2.35                     | 0.43              |
| 2:2X:101:ASN:O    | 1:3L:257:THR:CG2  | 2.54                     | 0.43              |
| 2:2Y:51:VAL:HG11  | 2:2Y:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:2Z:158:ARG:HD3  | 2:2Z:162:PRO:HA   | 2.00                     | 0.43              |
| 2:2Z:401:ARG:C    | 1:3N:262:TYR:OH   | 2.60                     | 0.43              |
| 1:3E:172:TYR:N    | 1:3E:204:VAL:O    | 2.44                     | 0.43              |
| 1:3K:311:LYS:H    | 1:3K:382:THR:HB   | 1.83                     | 0.43              |
| 2:3P:44:LEU:HA    | 2:3P:49:ILE:HB    | 2.01                     | 0.43              |
| 2:3W:36:TYR:OH    | 2:3W:40:SER:O     | 2.35                     | 0.43              |
| 2:3X:36:TYR:OH    | 2:3X:40:SER:O     | 2.35                     | 0.43              |
| 2:3Y:36:TYR:OH    | 2:3Y:40:SER:O     | 2.35                     | 0.43              |
| 2:3Z:158:ARG:HD3  | 2:3Z:162:PRO:HA   | 2.00                     | 0.43              |
| 2:3Z:386:GLU:HA   | 2:3Z:389:LYS:HB2  | 2.01                     | 0.43              |
| 1:4E:172:TYR:N    | 1:4E:204:VAL:O    | 2.44                     | 0.43              |
| 2:4P:36:TYR:OH    | 2:4P:40:SER:O     | 2.35                     | 0.43              |
| 2:4P:51:VAL:HG11  | 2:4P:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:4Q:158:ARG:HD3  | 2:4Q:162:PRO:HA   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4T:44:LEU:HA    | 2:4T:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4Z:386:GLU:HA   | 2:4Z:389:LYS:HB2  | 2.01                     | 0.43              |
| 1:1B:260:VAL:HG11 | 2:4O:407:TRP:HZ2  | 1.83                     | 0.43              |
| 1:1B:311:LYS:H    | 1:1B:382:THR:HB   | 1.83                     | 0.43              |
| 1:1C:257:THR:OG1  | 2:4P:102:ASN:HB2  | 2.19                     | 0.43              |
| 1:1C:439:SER:HB2  | 2:4P:400:ARG:HD2  | 2.00                     | 0.43              |
| 1:1J:2:ARG:CD     | 2:4V:72:PRO:CD    | 2.79                     | 0.43              |
| 1:1K:349:THR:CG2  | 2:4W:184:PRO:CG   | 2.97                     | 0.43              |
| 1:1M:439:SER:CB   | 2:4Y:400:ARG:HD2  | 2.49                     | 0.43              |
| 2:1P:51:VAL:HG11  | 2:1P:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1P:77:SER:HB3   | 1:2C:245:ASP:OD1  | 2.19                     | 0.43              |
| 2:1S:51:VAL:HG11  | 2:1S:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:1X:180:THR:CG2  | 1:2L:258:ASN:ND2  | 2.73                     | 0.43              |
| 2:1X:394:GLN:OE1  | 1:2L:349:THR:HG21 | 2.19                     | 0.43              |
| 2:1X:394:GLN:OE1  | 1:2L:349:THR:CG2  | 2.66                     | 0.43              |
| 5:1X:501:GDP:C8   | 1:2L:248:LEU:HD13 | 2.53                     | 0.43              |
| 2:1Y:158:ARG:HD3  | 2:1Y:162:PRO:HA   | 2.00                     | 0.43              |
| 5:1Z:501:GDP:H8   | 1:2N:248:LEU:CD1  | 2.32                     | 0.43              |
| 1:2E:172:TYR:N    | 1:2E:204:VAL:O    | 2.44                     | 0.43              |
| 1:2K:311:LYS:H    | 1:2K:382:THR:HB   | 1.83                     | 0.43              |
| 2:2R:210:TYR:CD2  | 1:3E:329:ASN:CB   | 3.02                     | 0.43              |
| 2:2T:145:THR:O    | 2:2T:149:MET:N    | 2.52                     | 0.43              |
| 2:2V:224:TYR:CE2  | 1:3J:248:LEU:HB2  | 2.40                     | 0.43              |
| 2:2W:36:TYR:OH    | 2:2W:40:SER:O     | 2.35                     | 0.43              |
| 2:2Y:36:TYR:OH    | 2:2Y:40:SER:O     | 2.35                     | 0.43              |
| 2:2Y:44:LEU:HA    | 2:2Y:49:ILE:HB    | 2.01                     | 0.43              |
| 5:2Y:501:GDP:N7   | 1:3M:248:LEU:HD13 | 2.33                     | 0.43              |
| 2:3O:44:LEU:HA    | 2:3O:49:ILE:HB    | 2.01                     | 0.43              |
| 2:3P:51:VAL:HG11  | 2:3P:243:ARG:HG2  | 2.00                     | 0.43              |
| 2:3Y:44:LEU:HA    | 2:3Y:49:ILE:HB    | 2.01                     | 0.43              |
| 1:4K:311:LYS:H    | 1:4K:382:THR:HB   | 1.83                     | 0.43              |
| 1:4L:62:VAL:HA    | 1:4L:63:PRO:HD3   | 1.86                     | 0.43              |
| 2:4O:44:LEU:HA    | 2:4O:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4T:145:THR:O    | 2:4T:149:MET:N    | 2.52                     | 0.43              |
| 2:4Y:36:TYR:OH    | 2:4Y:40:SER:O     | 2.35                     | 0.43              |
| 2:4Y:44:LEU:HA    | 2:4Y:49:ILE:HB    | 2.01                     | 0.43              |
| 2:4Y:51:VAL:HG11  | 2:4Y:243:ARG:HG2  | 2.00                     | 0.43              |
| 1:1C:261:PRO:CD   | 2:4P:404:PHE:CE1  | 3.02                     | 0.42              |
| 1:1C:325:PRO:HG2  | 2:4P:224:TYR:CG   | 2.54                     | 0.42              |
| 1:1D:260:VAL:C    | 2:4Q:407:TRP:HE1  | 2.26                     | 0.42              |
| 1:1D:439:SER:HB3  | 2:4Q:400:ARG:CD   | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:349:THR:HG23 | 2:4R:394:GLN:OE1  | 2.19                     | 0.42              |
| 1:1F:311:LYS:H    | 1:1F:382:THR:HB   | 1.83                     | 0.42              |
| 1:1F:348:PRO:HG3  | 2:4S:394:GLN:O    | 2.19                     | 0.42              |
| 1:1G:261:PRO:HB3  | 2:4T:404:PHE:CE2  | 2.54                     | 0.42              |
| 1:1G:437:VAL:O    | 2:4T:401:ARG:CZ   | 2.55                     | 0.42              |
| 1:1J:329:ASN:CG   | 2:4V:177:VAL:HG11 | 2.44                     | 0.42              |
| 1:1J:348:PRO:HB3  | 2:4V:394:GLN:HG2  | 2.01                     | 0.42              |
| 1:1L:325:PRO:HB3  | 2:4X:224:TYR:CZ   | 2.54                     | 0.42              |
| 1:1N:248:LEU:HD13 | 5:4Z:501:GDP:N7   | 2.29                     | 0.42              |
| 2:1T:44:LEU:HA    | 2:1T:49:ILE:HB    | 2.01                     | 0.42              |
| 2:1U:44:LEU:HA    | 2:1U:49:ILE:HB    | 2.01                     | 0.42              |
| 2:1V:165:ILE:H    | 2:1V:165:ILE:HG13 | 1.71                     | 0.42              |
| 2:1X:404:PHE:CE1  | 1:2L:260:VAL:CA   | 3.00                     | 0.42              |
| 2:1Y:44:LEU:HA    | 2:1Y:49:ILE:HB    | 2.01                     | 0.42              |
| 2:2O:11:GLN:NE2   | 1:3B:249:ASN:HB2  | 2.34                     | 0.42              |
| 2:2O:71:GLU:HG3   | 1:3B:2:ARG:HH11   | 1.82                     | 0.42              |
| 2:2P:51:VAL:HG11  | 2:2P:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:2T:44:LEU:HA    | 2:2T:49:ILE:HB    | 2.01                     | 0.42              |
| 2:2V:73:GLY:CA    | 1:3J:2:ARG:NH2    | 2.80                     | 0.42              |
| 2:2V:394:GLN:OE1  | 1:3J:349:THR:HG23 | 2.19                     | 0.42              |
| 2:2Y:158:ARG:HD3  | 2:2Y:162:PRO:HA   | 2.00                     | 0.42              |
| 1:3G:334:THR:O    | 1:3G:337:THR:OG1  | 2.30                     | 0.42              |
| 2:3T:44:LEU:HA    | 2:3T:49:ILE:HB    | 2.01                     | 0.42              |
| 2:3Y:51:VAL:HG11  | 2:3Y:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3Y:158:ARG:HD3  | 2:3Y:162:PRO:HA   | 2.00                     | 0.42              |
| 2:3Z:44:LEU:HA    | 2:3Z:49:ILE:HB    | 2.01                     | 0.42              |
| 1:4A:407:TRP:CD2  | 2:4H:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:4W:36:TYR:OH    | 2:4W:40:SER:O     | 2.35                     | 0.42              |
| 2:4Z:44:LEU:HA    | 2:4Z:49:ILE:HB    | 2.01                     | 0.42              |
| 1:1B:253:THR:O    | 2:4O:100:GLY:O    | 2.37                     | 0.42              |
| 1:1E:172:TYR:N    | 1:1E:204:VAL:O    | 2.44                     | 0.42              |
| 1:1G:334:THR:O    | 1:1G:337:THR:OG1  | 2.30                     | 0.42              |
| 1:1L:324:VAL:CG1  | 2:4X:222:PRO:O    | 2.67                     | 0.42              |
| 1:1M:258:ASN:HD21 | 2:4Y:101:ASN:ND2  | 2.16                     | 0.42              |
| 2:1H:51:VAL:HG11  | 2:1H:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:1O:36:TYR:OH    | 2:1O:40:SER:O     | 2.35                     | 0.42              |
| 2:1O:51:VAL:HG11  | 2:1O:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:1O:154:ILE:HG23 | 2:1O:166:MET:HG2  | 2.00                     | 0.42              |
| 2:1T:145:THR:O    | 2:1T:149:MET:N    | 2.52                     | 0.42              |
| 2:1X:283:TYR:OH   | 2:1Y:85:GLN:O     | 2.18                     | 0.42              |
| 2:1Z:44:LEU:HA    | 2:1Z:49:ILE:HB    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2B:311:LYS:H    | 1:2B:382:THR:HB   | 1.83                     | 0.42              |
| 2:2H:51:VAL:HG11  | 2:2H:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:2H:158:ARG:HD3  | 2:2H:162:PRO:HA   | 2.00                     | 0.42              |
| 2:2O:154:ILE:HG23 | 2:2O:166:MET:HG2  | 2.00                     | 0.42              |
| 2:2O:179:ASP:C    | 1:3B:352:LYS:HA   | 2.44                     | 0.42              |
| 2:2S:71:GLU:HB2   | 1:3F:2:ARG:CD     | 2.39                     | 0.42              |
| 2:2S:71:GLU:HG3   | 1:3F:2:ARG:HH11   | 1.84                     | 0.42              |
| 2:2T:11:GLN:HE22  | 1:3G:249:ASN:CA   | 2.14                     | 0.42              |
| 2:2Y:72:PRO:HG2   | 1:3M:2:ARG:HG3    | 2.01                     | 0.42              |
| 2:2Z:44:LEU:HA    | 2:2Z:49:ILE:HB    | 2.01                     | 0.42              |
| 1:3A:62:VAL:HA    | 1:3A:63:PRO:HD3   | 1.86                     | 0.42              |
| 1:3B:311:LYS:H    | 1:3B:382:THR:HB   | 1.84                     | 0.42              |
| 1:3F:311:LYS:H    | 1:3F:382:THR:HB   | 1.83                     | 0.42              |
| 2:3H:51:VAL:HG11  | 2:3H:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3O:36:TYR:OH    | 2:3O:40:SER:O     | 2.35                     | 0.42              |
| 2:3O:51:VAL:HG11  | 2:3O:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3O:154:ILE:HG23 | 2:3O:166:MET:HG2  | 2.00                     | 0.42              |
| 2:3S:51:VAL:HG11  | 2:3S:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3T:145:THR:O    | 2:3T:149:MET:N    | 2.52                     | 0.42              |
| 2:3X:283:TYR:OH   | 2:3Y:85:GLN:O     | 2.18                     | 0.42              |
| 1:4B:311:LYS:H    | 1:4B:382:THR:HB   | 1.83                     | 0.42              |
| 1:4F:311:LYS:H    | 1:4F:382:THR:HB   | 1.83                     | 0.42              |
| 1:4F:407:TRP:CD2  | 2:4S:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:4M:311:LYS:H    | 1:4M:382:THR:HB   | 1.83                     | 0.42              |
| 1:4N:407:TRP:CD2  | 2:4Z:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:4H:51:VAL:HG11  | 2:4H:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:4H:158:ARG:HD3  | 2:4H:162:PRO:HA   | 2.00                     | 0.42              |
| 2:4O:51:VAL:HG11  | 2:4O:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:4O:154:ILE:HG23 | 2:4O:166:MET:HG2  | 2.00                     | 0.42              |
| 2:4Y:158:ARG:HD3  | 2:4Y:162:PRO:HA   | 2.00                     | 0.42              |
| 1:1B:352:LYS:CE   | 2:4O:101:ASN:ND2  | 2.83                     | 0.42              |
| 1:1D:247:ALA:HB1  | 2:4Q:224:TYR:HD2  | 1.83                     | 0.42              |
| 1:1D:260:VAL:CG1  | 2:4Q:407:TRP:CZ2  | 3.02                     | 0.42              |
| 1:1I:345:ASP:O    | 2:4U:397:ALA:HB1  | 2.19                     | 0.42              |
| 1:1N:257:THR:CG2  | 2:4Z:101:ASN:O    | 2.65                     | 0.42              |
| 2:1O:386:GLU:HA   | 2:1O:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:1T:11:GLN:NE2   | 1:2G:249:ASN:HB2  | 2.32                     | 0.42              |
| 2:1T:221:THR:C    | 1:2G:324:VAL:HG13 | 2.44                     | 0.42              |
| 2:1V:158:ARG:HD3  | 2:1V:162:PRO:HA   | 2.00                     | 0.42              |
| 1:2F:311:LYS:H    | 1:2F:382:THR:HB   | 1.83                     | 0.42              |
| 2:2O:51:VAL:HG11  | 2:2O:243:ARG:HG2  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2O:158:ARG:HD3  | 2:2O:162:PRO:HA   | 2.00                     | 0.42              |
| 2:2O:386:GLU:HA   | 2:2O:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:2P:181:VAL:CG2  | 1:3C:258:ASN:O    | 2.68                     | 0.42              |
| 2:2P:386:GLU:HA   | 2:2P:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:2S:51:VAL:HG11  | 2:2S:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:2U:394:GLN:OE1  | 1:3I:349:THR:HG23 | 2.19                     | 0.42              |
| 2:2V:158:ARG:HD3  | 2:2V:162:PRO:HA   | 2.00                     | 0.42              |
| 2:2W:386:GLU:HA   | 2:2W:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:3O:386:GLU:HA   | 2:3O:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:3R:51:VAL:HG11  | 2:3R:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3V:158:ARG:HD3  | 2:3V:162:PRO:HA   | 2.00                     | 0.42              |
| 1:4E:407:TRP:CD2  | 2:4R:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:4S:51:VAL:HG11  | 2:4S:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:4W:386:GLU:HA   | 2:4W:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:4X:154:ILE:HG23 | 2:4X:166:MET:HG2  | 2.00                     | 0.42              |
| 1:1C:352:LYS:HD3  | 2:4P:101:ASN:HD21 | 1.83                     | 0.42              |
| 1:1D:257:THR:CG2  | 2:4Q:101:ASN:O    | 2.68                     | 0.42              |
| 1:1D:346:TRP:O    | 2:4Q:397:ALA:C    | 2.63                     | 0.42              |
| 1:1F:349:THR:HG21 | 2:4S:184:PRO:HG3  | 1.86                     | 0.42              |
| 1:1F:407:TRP:CD2  | 2:1S:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:1I:349:THR:O    | 2:4U:181:VAL:C    | 2.62                     | 0.42              |
| 2:1H:36:TYR:OH    | 2:1H:40:SER:O     | 2.35                     | 0.42              |
| 2:1H:397:ALA:O    | 1:2A:346:TRP:HB2  | 2.20                     | 0.42              |
| 2:1O:100:GLY:HA3  | 1:2B:253:THR:HG21 | 1.95                     | 0.42              |
| 2:1O:158:ARG:HD3  | 2:1O:162:PRO:HA   | 2.00                     | 0.42              |
| 2:1P:224:TYR:HD2  | 1:2C:247:ALA:O    | 2.01                     | 0.42              |
| 2:1P:386:GLU:HA   | 2:1P:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:1Q:74:THR:O     | 2:1Q:77:SER:OG    | 2.31                     | 0.42              |
| 2:1W:386:GLU:HA   | 2:1W:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:1W:394:GLN:CG   | 1:2K:348:PRO:HG2  | 2.42                     | 0.42              |
| 2:1Y:178:SER:HB3  | 1:2M:349:THR:HB   | 2.01                     | 0.42              |
| 2:1Z:36:TYR:OH    | 2:1Z:40:SER:O     | 2.35                     | 0.42              |
| 2:1Z:179:ASP:OD1  | 1:2N:353:VAL:O    | 2.38                     | 0.42              |
| 1:2E:407:TRP:CD2  | 2:2R:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2F:407:TRP:CD2  | 2:2S:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2G:407:TRP:CD2  | 2:2T:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2M:311:LYS:H    | 1:2M:382:THR:HB   | 1.83                     | 0.42              |
| 2:2H:401:ARG:HB3  | 1:3A:262:TYR:OH   | 2.19                     | 0.42              |
| 2:2O:36:TYR:OH    | 2:2O:40:SER:O     | 2.35                     | 0.42              |
| 2:2P:406:HIS:CE1  | 1:3C:263:PRO:N    | 2.87                     | 0.42              |
| 2:2Q:73:GLY:HA3   | 1:3D:2:ARG:CZ     | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2R:51:VAL:HG11  | 2:2R:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:2R:158:ARG:HD3  | 2:2R:162:PRO:HA   | 2.00                     | 0.42              |
| 2:2R:210:TYR:CD1  | 1:3E:326:LYS:HA   | 2.54                     | 0.42              |
| 2:2S:101:ASN:HB2  | 1:3F:254:GLU:CB   | 2.49                     | 0.42              |
| 2:2S:221:THR:CB   | 1:3F:324:VAL:HG21 | 2.47                     | 0.42              |
| 2:2T:176:LYS:CE   | 1:3G:333:ALA:HB1  | 2.35                     | 0.42              |
| 2:2U:44:LEU:HA    | 2:2U:49:ILE:HB    | 2.01                     | 0.42              |
| 2:2V:224:TYR:CD2  | 1:3J:247:ALA:O    | 2.68                     | 0.42              |
| 2:2Y:394:GLN:HB3  | 1:3M:348:PRO:HG2  | 2.02                     | 0.42              |
| 2:2Z:401:ARG:HB3  | 1:3N:262:TYR:OH   | 2.20                     | 0.42              |
| 1:3B:399:TYR:OH   | 1:3B:415:GLU:OE2  | 2.27                     | 0.42              |
| 1:3E:407:TRP:CD2  | 2:3R:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3F:283:HIS:CG   | 1:3G:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3F:407:TRP:CD2  | 2:3S:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:3H:158:ARG:HD3  | 2:3H:162:PRO:HA   | 2.00                     | 0.42              |
| 2:3O:158:ARG:HD3  | 2:3O:162:PRO:HA   | 2.00                     | 0.42              |
| 2:3P:386:GLU:HA   | 2:3P:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:3U:44:LEU:HA    | 2:3U:49:ILE:HB    | 2.01                     | 0.42              |
| 2:3W:386:GLU:HA   | 2:3W:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:3X:154:ILE:HG23 | 2:3X:166:MET:HG2  | 2.00                     | 0.42              |
| 2:3Y:386:GLU:HA   | 2:3Y:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:4B:407:TRP:CD2  | 2:4O:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:4G:407:TRP:CD2  | 2:4T:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:4O:158:ARG:HD3  | 2:4O:162:PRO:HA   | 2.00                     | 0.42              |
| 2:4O:386:GLU:HA   | 2:4O:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:4P:386:GLU:HA   | 2:4P:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:4R:51:VAL:HG11  | 2:4R:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:4R:158:ARG:HD3  | 2:4R:162:PRO:HA   | 2.00                     | 0.42              |
| 2:4V:158:ARG:HD3  | 2:4V:162:PRO:HA   | 2.00                     | 0.42              |
| 1:1C:326:LYS:HE3  | 2:4P:214:PHE:CB   | 2.49                     | 0.42              |
| 1:1C:329:ASN:CB   | 2:4P:210:TYR:HD2  | 2.26                     | 0.42              |
| 1:1C:333:ALA:CB   | 2:4P:176:LYS:HB3  | 2.49                     | 0.42              |
| 1:1C:346:TRP:CD1  | 2:4P:401:ARG:CG   | 2.94                     | 0.42              |
| 1:1D:7:ILE:HD13   | 1:1D:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1D:352:LYS:CA   | 2:4Q:179:ASP:O    | 2.59                     | 0.42              |
| 1:1D:407:TRP:CD2  | 2:1Q:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:1E:7:ILE:HD13   | 1:1E:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1E:283:HIS:CG   | 1:1F:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1E:407:TRP:CD2  | 2:1R:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:1F:326:LYS:HA   | 2:4S:210:TYR:CG   | 2.54                     | 0.42              |
| 1:1G:407:TRP:CD2  | 2:1T:257:VAL:HG22 | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1I:260:VAL:CG2  | 2:4U:407:TRP:HZ2  | 2.33                     | 0.42              |
| 1:1L:7:ILE:HD13   | 1:1L:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1L:261:PRO:HA   | 2:4X:404:PHE:CG   | 2.53                     | 0.42              |
| 1:1M:348:PRO:HD2  | 2:4Y:398:MET:HG3  | 2.01                     | 0.42              |
| 1:1M:353:VAL:CG2  | 2:4Y:179:ASP:OD1  | 2.67                     | 0.42              |
| 2:1H:158:ARG:HD3  | 2:1H:162:PRO:HA   | 2.00                     | 0.42              |
| 2:1O:100:GLY:CA   | 1:2B:253:THR:CB   | 2.98                     | 0.42              |
| 2:1O:283:TYR:OH   | 2:1P:85:GLN:O     | 2.18                     | 0.42              |
| 2:1R:51:VAL:HG11  | 2:1R:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:1S:180:THR:CA   | 1:2F:258:ASN:HD21 | 2.32                     | 0.42              |
| 2:1U:180:THR:CB   | 1:2I:258:ASN:HD21 | 2.32                     | 0.42              |
| 2:1Y:386:GLU:HA   | 2:1Y:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:2A:62:VAL:HA    | 1:2A:63:PRO:HD3   | 1.86                     | 0.42              |
| 1:2B:407:TRP:CD2  | 2:2O:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2D:311:LYS:H    | 1:2D:382:THR:HB   | 1.83                     | 0.42              |
| 1:2D:407:TRP:CD2  | 2:2Q:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2E:7:ILE:HD13   | 1:2E:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2E:283:HIS:CG   | 1:2F:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2L:7:ILE:HD13   | 1:2L:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:2Q:394:GLN:CG   | 1:3D:348:PRO:HB2  | 2.44                     | 0.42              |
| 2:2W:214:PHE:CG   | 1:3K:326:LYS:CE   | 3.02                     | 0.42              |
| 2:2X:154:ILE:HG23 | 2:2X:166:MET:HG2  | 2.00                     | 0.42              |
| 2:2X:398:MET:HG2  | 1:3L:346:TRP:O    | 2.20                     | 0.42              |
| 2:2Y:386:GLU:HA   | 2:2Y:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:3D:7:ILE:HD13   | 1:3D:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3D:311:LYS:H    | 1:3D:382:THR:HB   | 1.83                     | 0.42              |
| 1:3D:407:TRP:CD2  | 2:3Q:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3E:7:ILE:HD13   | 1:3E:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3E:283:HIS:CG   | 1:3F:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3G:407:TRP:CD2  | 2:3T:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3L:7:ILE:HD13   | 1:3L:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3M:311:LYS:H    | 1:3M:382:THR:HB   | 1.83                     | 0.42              |
| 1:3N:407:TRP:CD2  | 2:3Z:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:3R:158:ARG:HD3  | 2:3R:162:PRO:HA   | 2.00                     | 0.42              |
| 1:4E:283:HIS:CG   | 1:4F:88:HIS:HA    | 2.55                     | 0.42              |
| 1:4M:334:THR:O    | 1:4M:337:THR:OG1  | 2.30                     | 0.42              |
| 2:4O:36:TYR:OH    | 2:4O:40:SER:O     | 2.35                     | 0.42              |
| 2:4Y:386:GLU:HA   | 2:4Y:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:1A:260:VAL:CG1  | 2:4H:407:TRP:NE1  | 2.77                     | 0.42              |
| 1:1A:346:TRP:CZ3  | 2:4H:403:ALA:CB   | 3.03                     | 0.42              |
| 1:1F:283:HIS:CG   | 1:1G:88:HIS:HA    | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1J:329:ASN:HB3  | 2:4V:210:TYR:CD2  | 2.55                     | 0.42              |
| 1:1J:332:ILE:HG21 | 2:4V:177:VAL:CG2  | 2.47                     | 0.42              |
| 1:1K:261:PRO:HA   | 2:4W:404:PHE:CA   | 2.45                     | 0.42              |
| 1:1K:326:LYS:HB3  | 2:4W:222:PRO:HG2  | 1.95                     | 0.42              |
| 1:1L:325:PRO:HB2  | 2:4X:224:TYR:CE1  | 2.53                     | 0.42              |
| 1:1L:346:TRP:HA   | 2:4X:397:ALA:C    | 2.44                     | 0.42              |
| 1:1L:348:PRO:HB2  | 2:4X:394:GLN:CD   | 2.44                     | 0.42              |
| 2:1R:158:ARG:HD3  | 2:1R:162:PRO:HA   | 2.00                     | 0.42              |
| 2:1S:36:TYR:OH    | 2:1S:40:SER:O     | 2.35                     | 0.42              |
| 2:1T:36:TYR:OH    | 2:1T:40:SER:O     | 2.35                     | 0.42              |
| 2:1T:181:VAL:CG2  | 1:2G:258:ASN:C    | 2.82                     | 0.42              |
| 2:1X:154:ILE:HG23 | 2:1X:166:MET:HG2  | 2.00                     | 0.42              |
| 2:1Y:179:ASP:O    | 1:2M:352:LYS:HE2  | 2.17                     | 0.42              |
| 2:1Z:51:VAL:HG11  | 2:1Z:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:1Z:181:VAL:CB   | 1:2N:258:ASN:HD22 | 2.32                     | 0.42              |
| 1:2F:283:HIS:CG   | 1:2G:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2J:7:ILE:HD13   | 1:2J:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2N:407:TRP:CD2  | 2:2Z:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:2H:36:TYR:OH    | 2:2H:40:SER:O     | 2.35                     | 0.42              |
| 2:2O:404:PHE:CD2  | 1:3B:261:PRO:HA   | 2.53                     | 0.42              |
| 2:2R:101:ASN:C    | 1:3E:257:THR:HG21 | 2.44                     | 0.42              |
| 2:2T:36:TYR:OH    | 2:2T:40:SER:O     | 2.35                     | 0.42              |
| 2:2V:210:TYR:CD2  | 1:3J:329:ASN:CB   | 3.03                     | 0.42              |
| 2:2Z:36:TYR:OH    | 2:2Z:40:SER:O     | 2.35                     | 0.42              |
| 2:2Z:51:VAL:HG11  | 2:2Z:243:ARG:HG2  | 2.00                     | 0.42              |
| 1:3J:7:ILE:HD13   | 1:3J:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:3H:36:TYR:OH    | 2:3H:40:SER:O     | 2.35                     | 0.42              |
| 2:3Q:74:THR:O     | 2:3Q:77:SER:OG    | 2.31                     | 0.42              |
| 2:3T:36:TYR:OH    | 2:3T:40:SER:O     | 2.35                     | 0.42              |
| 2:3Z:36:TYR:OH    | 2:3Z:40:SER:O     | 2.35                     | 0.42              |
| 1:4C:7:ILE:HD13   | 1:4C:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4D:7:ILE:HD13   | 1:4D:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4D:311:LYS:H    | 1:4D:382:THR:HB   | 1.83                     | 0.42              |
| 1:4D:407:TRP:CD2  | 2:4Q:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:4E:7:ILE:HD13   | 1:4E:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4G:241:SER:OG   | 1:4G:250:VAL:O    | 2.27                     | 0.42              |
| 1:4J:7:ILE:HD13   | 1:4J:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4K:283:HIS:CG   | 1:4L:88:HIS:HA    | 2.55                     | 0.42              |
| 1:4L:7:ILE:HD13   | 1:4L:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4L:283:HIS:CG   | 1:4M:88:HIS:HA    | 2.55                     | 0.42              |
| 2:4S:36:TYR:OH    | 2:4S:40:SER:O     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4T:36:TYR:OH    | 2:4T:40:SER:O     | 2.35                     | 0.42              |
| 2:4U:44:LEU:HA    | 2:4U:49:ILE:HB    | 2.01                     | 0.42              |
| 2:4Z:36:TYR:OH    | 2:4Z:40:SER:O     | 2.35                     | 0.42              |
| 2:4Z:51:VAL:HG11  | 2:4Z:243:ARG:HG2  | 2.00                     | 0.42              |
| 1:1A:245:ASP:CG   | 2:4H:77:SER:HB2   | 2.38                     | 0.42              |
| 1:1A:407:TRP:CD2  | 2:1H:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:1B:132:LEU:HD23 | 1:1B:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:1C:324:VAL:CG2  | 2:4P:221:THR:OG1  | 2.60                     | 0.42              |
| 1:1D:311:LYS:H    | 1:1D:382:THR:HB   | 1.84                     | 0.42              |
| 1:1E:326:LYS:HG2  | 2:4R:210:TYR:CD1  | 2.54                     | 0.42              |
| 1:1I:7:ILE:HD13   | 1:1I:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1J:7:ILE:HD13   | 1:1J:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1L:172:TYR:N    | 1:1L:204:VAL:O    | 2.44                     | 0.42              |
| 1:1L:254:GLU:HG2  | 2:4X:101:ASN:N    | 2.34                     | 0.42              |
| 1:1L:283:HIS:CG   | 1:1M:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1L:329:ASN:OD1  | 2:4X:177:VAL:CG1  | 2.67                     | 0.42              |
| 1:1M:311:LYS:H    | 1:1M:382:THR:HB   | 1.83                     | 0.42              |
| 1:1N:348:PRO:HB3  | 2:4Z:394:GLN:HG2  | 1.94                     | 0.42              |
| 1:1N:407:TRP:CD2  | 2:1Z:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:1P:221:THR:CA   | 1:2C:324:VAL:HG11 | 2.40                     | 0.42              |
| 2:1Q:51:VAL:HG11  | 2:1Q:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:1T:47:GLU:HG2   | 2:1T:48:ARG:NH1   | 2.35                     | 0.42              |
| 1:2B:7:ILE:HD13   | 1:2B:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2D:7:ILE:HD13   | 1:2D:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2D:132:LEU:HD23 | 1:2D:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:2G:241:SER:OG   | 1:2G:250:VAL:O    | 2.27                     | 0.42              |
| 1:2I:407:TRP:CD2  | 2:2U:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2L:283:HIS:CG   | 1:2M:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2M:334:THR:O    | 1:2M:337:THR:OG1  | 2.30                     | 0.42              |
| 2:2Q:51:VAL:HG11  | 2:2Q:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:2Q:74:THR:O     | 2:2Q:77:SER:OG    | 2.31                     | 0.42              |
| 2:2Q:100:GLY:HA2  | 1:3D:254:GLU:N    | 2.35                     | 0.42              |
| 2:2S:11:GLN:HE22  | 1:3F:249:ASN:CA   | 2.17                     | 0.42              |
| 2:2S:36:TYR:OH    | 2:2S:40:SER:O     | 2.35                     | 0.42              |
| 2:2S:401:ARG:C    | 1:3F:262:TYR:OH   | 2.55                     | 0.42              |
| 2:2T:47:GLU:HG2   | 2:2T:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:2Z:394:GLN:CB   | 1:3N:348:PRO:HG2  | 2.48                     | 0.42              |
| 1:3B:7:ILE:HD13   | 1:3B:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3I:7:ILE:HD13   | 1:3I:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3L:283:HIS:CG   | 1:3M:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3M:334:THR:O    | 1:3M:337:THR:OG1  | 2.30                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3Q:44:LEU:HA    | 2:3Q:49:ILE:HB    | 2.01                     | 0.42              |
| 2:3S:36:TYR:OH    | 2:3S:40:SER:O     | 2.35                     | 0.42              |
| 2:3T:47:GLU:HG2   | 2:3T:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:3Z:51:VAL:HG11  | 2:3Z:243:ARG:HG2  | 2.00                     | 0.42              |
| 1:4B:7:ILE:HD13   | 1:4B:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4B:334:THR:O    | 1:4B:337:THR:OG1  | 2.30                     | 0.42              |
| 1:4D:283:HIS:CG   | 1:4E:88:HIS:HA    | 2.55                     | 0.42              |
| 1:4E:334:THR:O    | 1:4E:337:THR:OG1  | 2.30                     | 0.42              |
| 1:4F:283:HIS:CG   | 1:4G:88:HIS:HA    | 2.55                     | 0.42              |
| 1:4I:7:ILE:HD13   | 1:4I:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4M:132:LEU:HD23 | 1:4M:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:4M:407:TRP:CD2  | 2:4Y:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:4H:36:TYR:OH    | 2:4H:40:SER:O     | 2.35                     | 0.42              |
| 2:4Q:51:VAL:HG11  | 2:4Q:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:4T:47:GLU:HG2   | 2:4T:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:4X:386:GLU:HA   | 2:4X:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:1B:7:ILE:HD13   | 1:1B:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1B:261:PRO:CB   | 2:4O:404:PHE:CD2  | 2.98                     | 0.42              |
| 1:1B:334:THR:O    | 1:1B:337:THR:OG1  | 2.30                     | 0.42              |
| 1:1D:283:HIS:CG   | 1:1E:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1G:2:ARG:HG3    | 2:4T:72:PRO:HG2   | 1.99                     | 0.42              |
| 1:1I:346:TRP:O    | 2:4U:398:MET:N    | 2.52                     | 0.42              |
| 1:1I:407:TRP:CD2  | 2:1U:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:1I:439:SER:OG   | 2:4U:401:ARG:CD   | 2.67                     | 0.42              |
| 1:1J:326:LYS:HG2  | 2:4V:210:TYR:CD1  | 2.54                     | 0.42              |
| 1:1K:7:ILE:HD13   | 1:1K:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1N:7:ILE:HD13   | 1:1N:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1N:262:TYR:CE2  | 2:4Z:403:ALA:HA   | 2.52                     | 0.42              |
| 2:1H:181:VAL:HB   | 1:2A:258:ASN:CA   | 2.49                     | 0.42              |
| 2:1H:404:PHE:CE1  | 1:2A:260:VAL:O    | 2.73                     | 0.42              |
| 2:1Q:44:LEU:HA    | 2:1Q:49:ILE:HB    | 2.01                     | 0.42              |
| 2:1Q:221:THR:OG1  | 1:2D:324:VAL:HG22 | 2.20                     | 0.42              |
| 2:1U:207:GLU:CD   | 1:2I:329:ASN:ND2  | 2.68                     | 0.42              |
| 2:1X:11:GLN:NE2   | 1:2L:249:ASN:ND2  | 2.68                     | 0.42              |
| 2:1X:386:GLU:HA   | 2:1X:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:2A:407:TRP:CD2  | 2:2H:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2C:7:ILE:HD13   | 1:2C:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2D:283:HIS:CG   | 1:2E:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2E:334:THR:O    | 1:2E:337:THR:OG1  | 2.30                     | 0.42              |
| 1:2I:7:ILE:HD13   | 1:2I:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2K:7:ILE:HD13   | 1:2K:153:LEU:HD21 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2M:132:LEU:HD23 | 1:2M:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:2N:7:ILE:HD13   | 1:2N:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:2H:11:GLN:NE2   | 1:3A:249:ASN:N    | 2.26                     | 0.42              |
| 2:2O:223:THR:HA   | 1:3B:325:PRO:CD   | 2.49                     | 0.42              |
| 2:2Q:44:LEU:HA    | 2:2Q:49:ILE:HB    | 2.01                     | 0.42              |
| 2:2U:394:GLN:CD   | 1:3I:348:PRO:HB2  | 2.45                     | 0.42              |
| 2:2X:386:GLU:HA   | 2:2X:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:2X:394:GLN:HB3  | 1:3L:348:PRO:HG2  | 2.01                     | 0.42              |
| 2:2Y:406:HIS:CD2  | 1:3M:262:TYR:HA   | 2.55                     | 0.42              |
| 1:3B:132:LEU:HD23 | 1:3B:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:3B:334:THR:O    | 1:3B:337:THR:OG1  | 2.30                     | 0.42              |
| 1:3C:7:ILE:HD13   | 1:3C:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3C:407:TRP:CD2  | 2:3P:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3D:132:LEU:HD23 | 1:3D:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:3D:283:HIS:CG   | 1:3E:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3F:7:ILE:HD13   | 1:3F:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3F:319:TYR:HE2  | 1:3F:328:VAL:HG13 | 1.84                     | 0.42              |
| 1:3G:132:LEU:HD23 | 1:3G:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:3G:241:SER:OG   | 1:3G:250:VAL:O    | 2.27                     | 0.42              |
| 1:3I:407:TRP:CD2  | 2:3U:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3J:311:LYS:H    | 1:3J:382:THR:HB   | 1.83                     | 0.42              |
| 1:3K:7:ILE:HD13   | 1:3K:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3K:283:HIS:CG   | 1:3L:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3M:132:LEU:HD23 | 1:3M:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:3M:407:TRP:CD2  | 2:3Y:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3N:7:ILE:HD13   | 1:3N:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:3H:154:ILE:HG23 | 2:3H:166:MET:HG2  | 2.00                     | 0.42              |
| 2:3U:47:GLU:HG2   | 2:3U:48:ARG:NH1   | 2.35                     | 0.42              |
| 1:4A:7:ILE:HD13   | 1:4A:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4C:334:THR:O    | 1:4C:337:THR:OG1  | 2.30                     | 0.42              |
| 1:4I:407:TRP:CD2  | 2:4U:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:4J:311:LYS:H    | 1:4J:382:THR:HB   | 1.83                     | 0.42              |
| 1:4K:7:ILE:HD13   | 1:4K:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4L:172:TYR:N    | 1:4L:204:VAL:O    | 2.44                     | 0.42              |
| 2:4H:386:GLU:HA   | 2:4H:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:1A:88:HIS:HA    | 1:1N:283:HIS:CG   | 2.55                     | 0.42              |
| 1:1A:283:HIS:CG   | 1:1B:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1B:254:GLU:HG2  | 2:4O:100:GLY:C    | 2.43                     | 0.42              |
| 1:1C:7:ILE:HD13   | 1:1C:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1C:319:TYR:HE2  | 1:1C:328:VAL:HG13 | 1.84                     | 0.42              |
| 1:1C:407:TRP:CD2  | 2:1P:257:VAL:HG22 | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1D:249:ASN:O    | 2:4Q:11:GLN:OE1   | 2.37                     | 0.42              |
| 1:1D:439:SER:HB3  | 2:4Q:400:ARG:HD3  | 2.02                     | 0.42              |
| 1:1E:132:LEU:HD23 | 1:1E:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:1E:319:TYR:HE2  | 1:1E:328:VAL:HG13 | 1.84                     | 0.42              |
| 1:1F:319:TYR:HE2  | 1:1F:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:1G:62:VAL:HA    | 1:1G:63:PRO:HD3   | 1.86                     | 0.42              |
| 1:1G:132:LEU:HD23 | 1:1G:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:1G:261:PRO:CB   | 2:4T:404:PHE:N    | 2.83                     | 0.42              |
| 1:1G:283:HIS:CG   | 1:1I:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1I:352:LYS:HE2  | 2:4U:101:ASN:ND2  | 2.34                     | 0.42              |
| 1:1I:437:VAL:O    | 2:4U:401:ARG:CZ   | 2.57                     | 0.42              |
| 1:1J:257:THR:HG21 | 2:4V:102:ASN:CA   | 2.50                     | 0.42              |
| 1:1J:311:LYS:H    | 1:1J:382:THR:HB   | 1.83                     | 0.42              |
| 1:1K:261:PRO:O    | 2:4W:404:PHE:HA   | 2.20                     | 0.42              |
| 1:1K:283:HIS:CG   | 1:1L:88:HIS:HA    | 2.55                     | 0.42              |
| 1:1N:258:ASN:ND2  | 2:4Z:180:THR:CG2  | 2.59                     | 0.42              |
| 2:1O:210:TYR:HD2  | 1:2B:329:ASN:HD22 | 1.67                     | 0.42              |
| 2:1U:47:GLU:HG2   | 2:1U:48:ARG:NH1   | 2.35                     | 0.42              |
| 1:2A:7:ILE:HD13   | 1:2A:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2A:88:HIS:HA    | 1:2N:283:HIS:CG   | 2.55                     | 0.42              |
| 1:2B:132:LEU:HD23 | 1:2B:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:2C:334:THR:O    | 1:2C:337:THR:OG1  | 2.30                     | 0.42              |
| 1:2F:7:ILE:HD13   | 1:2F:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2G:7:ILE:HD13   | 1:2G:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:2I:132:LEU:HD23 | 1:2I:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:2J:311:LYS:H    | 1:2J:382:THR:HB   | 1.83                     | 0.42              |
| 1:2K:283:HIS:CG   | 1:2L:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2L:172:TYR:N    | 1:2L:204:VAL:O    | 2.44                     | 0.42              |
| 1:2M:407:TRP:CD2  | 2:2Y:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:2H:154:ILE:HG23 | 2:2H:166:MET:HG2  | 2.00                     | 0.42              |
| 2:2H:386:GLU:HA   | 2:2H:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:2S:47:GLU:HG2   | 2:2S:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:2U:214:PHE:CG   | 1:3I:326:LYS:HE3  | 2.55                     | 0.42              |
| 2:2W:210:TYR:CD2  | 1:3K:329:ASN:HB2  | 2.54                     | 0.42              |
| 2:2X:54:ASN:OD1   | 2:2X:64:ARG:NH2   | 2.46                     | 0.42              |
| 2:2X:401:ARG:NH2  | 1:3L:435:VAL:CA   | 2.54                     | 0.42              |
| 2:2X:404:PHE:CD2  | 1:3L:261:PRO:HB3  | 2.52                     | 0.42              |
| 2:2Z:71:GLU:HB2   | 1:3N:2:ARG:CD     | 2.39                     | 0.42              |
| 2:2Z:154:ILE:HG23 | 2:2Z:166:MET:HG2  | 2.00                     | 0.42              |
| 1:3A:7:ILE:HD13   | 1:3A:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3A:88:HIS:HA    | 1:3N:283:HIS:CG   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3A:407:TRP:CD2  | 2:3H:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:3E:132:LEU:HD23 | 1:3E:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:3L:172:TYR:N    | 1:3L:204:VAL:O    | 2.44                     | 0.42              |
| 2:3Q:51:VAL:HG11  | 2:3Q:243:ARG:HG2  | 2.00                     | 0.42              |
| 2:3S:47:GLU:HG2   | 2:3S:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:3S:158:ARG:HD3  | 2:3S:162:PRO:HA   | 2.00                     | 0.42              |
| 2:3X:386:GLU:HA   | 2:3X:389:LYS:HB2  | 2.01                     | 0.42              |
| 1:4C:407:TRP:CD2  | 2:4P:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:4E:319:TYR:HE2  | 1:4E:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:4F:7:ILE:HD13   | 1:4F:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:4F:319:TYR:HE2  | 1:4F:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:4I:132:LEU:HD23 | 1:4I:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:4M:7:ILE:HD13   | 1:4M:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:4Q:44:LEU:HA    | 2:4Q:49:ILE:HB    | 2.01                     | 0.42              |
| 2:4W:165:ILE:H    | 2:4W:165:ILE:HG13 | 1.71                     | 0.42              |
| 2:4Z:154:ILE:HG23 | 2:4Z:166:MET:HG2  | 2.00                     | 0.42              |
| 1:1A:7:ILE:HD13   | 1:1A:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1A:324:VAL:HG11 | 2:4H:222:PRO:N    | 2.35                     | 0.42              |
| 1:1B:262:TYR:CZ   | 2:4O:403:ALA:CA   | 3.01                     | 0.42              |
| 1:1C:2:ARG:HH11   | 2:4P:71:GLU:CG    | 2.31                     | 0.42              |
| 1:1C:253:THR:O    | 2:4P:100:GLY:CA   | 2.67                     | 0.42              |
| 1:1D:319:TYR:HE2  | 1:1D:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:1F:7:ILE:HD13   | 1:1F:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1G:7:ILE:HD13   | 1:1G:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1G:346:TRP:CA   | 2:4T:398:MET:HA   | 2.50                     | 0.42              |
| 1:1J:348:PRO:HD3  | 2:4V:398:MET:HG3  | 2.02                     | 0.42              |
| 1:1M:7:ILE:HD13   | 1:1M:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:1M:132:LEU:HD23 | 1:1M:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:1M:260:VAL:HG12 | 2:4Y:407:TRP:HE1  | 1.84                     | 0.42              |
| 1:1M:334:THR:O    | 1:1M:337:THR:OG1  | 2.30                     | 0.42              |
| 1:1M:407:TRP:CD2  | 2:1Y:257:VAL:HG22 | 2.54                     | 0.42              |
| 2:1H:154:ILE:HG23 | 2:1H:166:MET:HG2  | 2.00                     | 0.42              |
| 2:1H:386:GLU:HA   | 2:1H:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:1O:47:GLU:HG2   | 2:1O:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:1R:101:ASN:O    | 1:2E:257:THR:HG21 | 2.19                     | 0.42              |
| 2:1S:158:ARG:HD3  | 2:1S:162:PRO:HA   | 2.00                     | 0.42              |
| 2:1Z:154:ILE:HG23 | 2:1Z:166:MET:HG2  | 2.00                     | 0.42              |
| 1:2C:407:TRP:CD2  | 2:2P:257:VAL:HG22 | 2.54                     | 0.42              |
| 1:2D:319:TYR:HE2  | 1:2D:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:2D:334:THR:O    | 1:2D:337:THR:OG1  | 2.30                     | 0.42              |
| 1:2E:132:LEU:HD23 | 1:2E:164:LYS:HZ3  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2E:319:TYR:HE2  | 1:2E:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:2F:319:TYR:HE2  | 1:2F:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:2G:283:HIS:CG   | 1:2I:88:HIS:HA    | 2.55                     | 0.42              |
| 1:2M:7:ILE:HD13   | 1:2M:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:2O:47:GLU:HG2   | 2:2O:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:2P:179:ASP:O    | 1:3C:352:LYS:HA   | 2.20                     | 0.42              |
| 2:2Q:36:TYR:OH    | 2:2Q:40:SER:O     | 2.35                     | 0.42              |
| 2:2Q:403:ALA:HA   | 1:3D:262:TYR:CZ   | 2.55                     | 0.42              |
| 2:2S:158:ARG:HD3  | 2:2S:162:PRO:HA   | 2.00                     | 0.42              |
| 2:2T:71:GLU:HG3   | 1:3G:2:ARG:NH1    | 2.35                     | 0.42              |
| 2:2U:47:GLU:HG2   | 2:2U:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:2X:210:TYR:CE2  | 1:3L:329:ASN:HB2  | 2.54                     | 0.42              |
| 2:2Y:11:GLN:NE2   | 1:3M:249:ASN:CB   | 2.83                     | 0.42              |
| 2:2Z:406:HIS:CD2  | 1:3N:262:TYR:HA   | 2.55                     | 0.42              |
| 1:3D:319:TYR:HE2  | 1:3D:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:3E:319:TYR:HE2  | 1:3E:328:VAL:HG13 | 1.85                     | 0.42              |
| 1:3E:334:THR:O    | 1:3E:337:THR:OG1  | 2.30                     | 0.42              |
| 1:3G:7:ILE:HD13   | 1:3G:153:LEU:HD21 | 2.02                     | 0.42              |
| 1:3G:283:HIS:CG   | 1:3I:88:HIS:HA    | 2.55                     | 0.42              |
| 1:3M:7:ILE:HD13   | 1:3M:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:3H:386:GLU:HA   | 2:3H:389:LYS:HB2  | 2.01                     | 0.42              |
| 2:3Z:154:ILE:HG23 | 2:3Z:166:MET:HG2  | 2.00                     | 0.42              |
| 1:4A:62:VAL:HA    | 1:4A:63:PRO:HD3   | 1.86                     | 0.42              |
| 1:4A:88:HIS:HA    | 1:4N:283:HIS:CG   | 2.55                     | 0.42              |
| 1:4B:132:LEU:HD23 | 1:4B:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:4E:132:LEU:HD23 | 1:4E:164:LYS:HZ3  | 1.85                     | 0.42              |
| 1:4N:7:ILE:HD13   | 1:4N:153:LEU:HD21 | 2.02                     | 0.42              |
| 2:4H:85:GLN:O     | 2:4Z:283:TYR:OH   | 2.18                     | 0.42              |
| 2:4H:154:ILE:HG23 | 2:4H:166:MET:HG2  | 2.00                     | 0.42              |
| 2:4O:47:GLU:HG2   | 2:4O:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:4Q:74:THR:O     | 2:4Q:77:SER:OG    | 2.31                     | 0.42              |
| 2:4S:47:GLU:HG2   | 2:4S:48:ARG:NH1   | 2.35                     | 0.42              |
| 2:4S:158:ARG:HD3  | 2:4S:162:PRO:HA   | 2.00                     | 0.42              |
| 2:4U:47:GLU:HG2   | 2:4U:48:ARG:NH1   | 2.35                     | 0.42              |
| 1:1C:434:GLU:C    | 2:4P:401:ARG:HH21 | 2.26                     | 0.41              |
| 1:1D:262:TYR:N    | 2:4Q:406:HIS:CD2  | 2.73                     | 0.41              |
| 1:1E:2:ARG:NH1    | 2:4R:71:GLU:HB2   | 2.31                     | 0.41              |
| 1:1E:247:ALA:O    | 2:4R:15:GLN:CD    | 2.62                     | 0.41              |
| 1:1E:334:THR:O    | 1:1E:337:THR:OG1  | 2.30                     | 0.41              |
| 1:1E:346:TRP:CD2  | 2:4R:403:ALA:CB   | 3.03                     | 0.41              |
| 1:1F:314:ALA:CB   | 2:4S:181:VAL:HG21 | 2.38                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1J:326:LYS:HA  | 2:4V:210:TYR:CD1  | 2.54                     | 0.41              |
| 1:1K:326:LYS:HE2 | 2:4W:210:TYR:O    | 2.20                     | 0.41              |
| 1:1K:352:LYS:HA  | 2:4W:179:ASP:O    | 2.20                     | 0.41              |
| 2:1O:17:GLY:HA2  | 2:1O:20:PHE:HB3   | 2.02                     | 0.41              |
| 2:1R:222:PRO:HD2 | 1:2E:326:LYS:CB   | 2.50                     | 0.41              |
| 2:1S:47:GLU:HG2  | 2:1S:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1S:224:TYR:CE2 | 1:2F:248:LEU:HB2  | 2.51                     | 0.41              |
| 2:1S:406:HIS:NE2 | 1:2F:263:PRO:CD   | 2.77                     | 0.41              |
| 2:1X:11:GLN:HE22 | 1:2L:249:ASN:H    | 1.68                     | 0.41              |
| 1:2A:283:HIS:CG  | 1:2B:88:HIS:HA    | 2.55                     | 0.41              |
| 1:2J:147:SER:HB2 | 1:2J:190:THR:HB   | 2.02                     | 0.41              |
| 2:2H:85:GLN:O    | 2:2Z:283:TYR:OH   | 2.18                     | 0.41              |
| 2:2X:47:GLU:HG2  | 2:2X:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2Z:406:HIS:CE1 | 1:3N:263:PRO:N    | 2.88                     | 0.41              |
| 1:3C:319:TYR:HE2 | 1:3C:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:3C:334:THR:O   | 1:3C:337:THR:OG1  | 2.30                     | 0.41              |
| 2:3O:47:GLU:HG2  | 2:3O:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3Q:36:TYR:OH   | 2:3Q:40:SER:O     | 2.35                     | 0.41              |
| 2:3X:47:GLU:HG2  | 2:3X:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3X:54:ASN:OD1  | 2:3X:64:ARG:NH2   | 2.46                     | 0.41              |
| 1:4D:319:TYR:HE2 | 1:4D:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:4E:147:SER:HB2 | 1:4E:190:THR:HB   | 2.02                     | 0.41              |
| 1:4G:7:ILE:HD13  | 1:4G:153:LEU:HD21 | 2.02                     | 0.41              |
| 1:4G:283:HIS:CG  | 1:4I:88:HIS:HA    | 2.55                     | 0.41              |
| 1:4J:407:TRP:CD2 | 2:4V:257:VAL:HG22 | 2.54                     | 0.41              |
| 2:4Q:36:TYR:OH   | 2:4Q:40:SER:O     | 2.35                     | 0.41              |
| 2:4W:145:THR:O   | 2:4W:149:MET:N    | 2.52                     | 0.41              |
| 2:4X:47:GLU:HG2  | 2:4X:48:ARG:NH1   | 2.35                     | 0.41              |
| 1:1B:258:ASN:O   | 2:4O:181:VAL:CB   | 2.67                     | 0.41              |
| 1:1B:319:TYR:HE2 | 1:1B:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1C:147:SER:HB2 | 1:1C:190:THR:HB   | 2.02                     | 0.41              |
| 1:1C:326:LYS:HG3 | 2:4P:210:TYR:HA   | 2.01                     | 0.41              |
| 1:1C:334:THR:O   | 1:1C:337:THR:OG1  | 2.30                     | 0.41              |
| 1:1D:334:THR:O   | 1:1D:337:THR:OG1  | 2.30                     | 0.41              |
| 1:1F:260:VAL:C   | 2:4S:404:PHE:CD1  | 2.98                     | 0.41              |
| 1:1F:262:TYR:O   | 2:4S:406:HIS:NE2  | 2.42                     | 0.41              |
| 1:1I:251:ASP:OD2 | 2:4U:71:GLU:CB    | 2.67                     | 0.41              |
| 1:1J:346:TRP:HB2 | 2:4V:398:MET:CA   | 2.25                     | 0.41              |
| 1:1K:260:VAL:CB  | 2:4W:407:TRP:CE2  | 2.90                     | 0.41              |
| 1:1K:329:ASN:CB  | 2:4W:210:TYR:CD2  | 3.02                     | 0.41              |
| 1:1K:346:TRP:CZ3 | 2:4W:404:PHE:CD2  | 3.06                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1M:319:TYR:HE2  | 1:1M:328:VAL:HG13 | 1.85                     | 0.41              |
| 2:1H:85:GLN:O     | 2:1Z:283:TYR:OH   | 2.18                     | 0.41              |
| 2:1P:178:SER:CB   | 1:2C:349:THR:HB   | 2.50                     | 0.41              |
| 2:1Q:36:TYR:OH    | 2:1Q:40:SER:O     | 2.35                     | 0.41              |
| 2:1S:74:THR:O     | 2:1S:77:SER:OG    | 2.31                     | 0.41              |
| 2:1V:404:PHE:CE1  | 1:2J:261:PRO:CA   | 3.03                     | 0.41              |
| 2:1X:47:GLU:HG2   | 2:1X:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1X:54:ASN:OD1   | 2:1X:64:ARG:NH2   | 2.46                     | 0.41              |
| 2:1Z:214:PHE:HB2  | 1:2N:326:LYS:CE   | 2.40                     | 0.41              |
| 1:2C:283:HIS:CG   | 1:2D:88:HIS:HA    | 2.55                     | 0.41              |
| 1:2E:147:SER:HB2  | 1:2E:190:THR:HB   | 2.03                     | 0.41              |
| 1:2G:147:SER:HB2  | 1:2G:190:THR:HB   | 2.02                     | 0.41              |
| 2:2O:17:GLY:HA2   | 2:2O:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2R:221:THR:CA   | 1:3E:324:VAL:HG11 | 2.49                     | 0.41              |
| 2:2R:404:PHE:HA   | 1:3E:261:PRO:O    | 2.19                     | 0.41              |
| 2:2W:145:THR:O    | 2:2W:149:MET:N    | 2.52                     | 0.41              |
| 1:3A:283:HIS:CG   | 1:3B:88:HIS:HA    | 2.55                     | 0.41              |
| 1:3C:147:SER:HB2  | 1:3C:190:THR:HB   | 2.03                     | 0.41              |
| 1:3C:283:HIS:CG   | 1:3D:88:HIS:HA    | 2.55                     | 0.41              |
| 1:3D:334:THR:O    | 1:3D:337:THR:OG1  | 2.30                     | 0.41              |
| 1:3E:147:SER:HB2  | 1:3E:190:THR:HB   | 2.03                     | 0.41              |
| 1:3G:62:VAL:HA    | 1:3G:63:PRO:HD3   | 1.86                     | 0.41              |
| 1:3I:132:LEU:HD23 | 1:3I:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3J:283:HIS:CG   | 1:3K:88:HIS:HA    | 2.55                     | 0.41              |
| 2:3H:85:GLN:O     | 2:3Z:283:TYR:OH   | 2.18                     | 0.41              |
| 2:3O:17:GLY:HA2   | 2:3O:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3X:44:LEU:HA    | 2:3X:49:ILE:HB    | 2.01                     | 0.41              |
| 1:4A:283:HIS:CG   | 1:4B:88:HIS:HA    | 2.55                     | 0.41              |
| 1:4C:147:SER:HB2  | 1:4C:190:THR:HB   | 2.03                     | 0.41              |
| 1:4C:283:HIS:CG   | 1:4D:88:HIS:HA    | 2.55                     | 0.41              |
| 1:4C:319:TYR:HE2  | 1:4C:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:4J:147:SER:HB2  | 1:4J:190:THR:HB   | 2.03                     | 0.41              |
| 1:4J:283:HIS:CG   | 1:4K:88:HIS:HA    | 2.55                     | 0.41              |
| 1:4N:132:LEU:HD23 | 1:4N:164:LYS:HZ3  | 1.85                     | 0.41              |
| 2:4X:44:LEU:HA    | 2:4X:49:ILE:HB    | 2.01                     | 0.41              |
| 1:1A:319:TYR:HE2  | 1:1A:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:1B:407:TRP:CD2  | 2:1O:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:1C:283:HIS:CG   | 1:1D:88:HIS:HA    | 2.55                     | 0.41              |
| 1:1D:245:ASP:CB   | 2:4Q:77:SER:HB3   | 2.35                     | 0.41              |
| 1:1D:349:THR:OG1  | 2:4Q:184:PRO:CG   | 2.67                     | 0.41              |
| 1:1E:147:SER:HB2  | 1:1E:190:THR:HB   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:325:PRO:CG   | 2:4S:224:TYR:CD1  | 2.99                     | 0.41              |
| 1:1G:147:SER:HB2  | 1:1G:190:THR:HB   | 2.03                     | 0.41              |
| 1:1G:319:TYR:HE2  | 1:1G:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:1I:348:PRO:HD3  | 2:4U:398:MET:HG3  | 1.99                     | 0.41              |
| 1:1I:349:THR:HG21 | 2:4U:184:PRO:CG   | 2.40                     | 0.41              |
| 1:1J:407:TRP:CD2  | 2:1V:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:1K:348:PRO:HB2  | 2:4W:394:GLN:HG2  | 1.99                     | 0.41              |
| 1:1L:333:ALA:HB1  | 2:4X:176:LYS:HE2  | 2.03                     | 0.41              |
| 1:1L:348:PRO:HB2  | 2:4X:394:GLN:HG2  | 2.00                     | 0.41              |
| 1:1L:353:VAL:CG2  | 2:4X:179:ASP:OD1  | 2.67                     | 0.41              |
| 2:1H:47:GLU:HG2   | 2:1H:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1O:179:ASP:CG   | 1:2B:248:LEU:HD21 | 2.43                     | 0.41              |
| 2:1V:386:GLU:HA   | 2:1V:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:1W:11:GLN:HE22  | 1:2K:249:ASN:H    | 1.69                     | 0.41              |
| 2:1W:403:ALA:HA   | 1:2K:261:PRO:O    | 2.20                     | 0.41              |
| 2:1X:44:LEU:HA    | 2:1X:49:ILE:HB    | 2.01                     | 0.41              |
| 2:1Z:17:GLY:HA2   | 2:1Z:20:PHE:HB3   | 2.03                     | 0.41              |
| 1:2C:147:SER:HB2  | 1:2C:190:THR:HB   | 2.03                     | 0.41              |
| 1:2C:319:TYR:HE2  | 1:2C:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:2G:62:VAL:HA    | 1:2G:63:PRO:HD3   | 1.86                     | 0.41              |
| 1:2G:319:TYR:HE2  | 1:2G:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:2J:132:LEU:HD23 | 1:2J:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:2J:283:HIS:CG   | 1:2K:88:HIS:HA    | 2.55                     | 0.41              |
| 1:2J:407:TRP:CD2  | 2:2V:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:2L:407:TRP:CD2  | 2:2X:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:2M:319:TYR:HE2  | 1:2M:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:2O:210:TYR:HB3  | 1:3B:326:LYS:HG2  | 2.02                     | 0.41              |
| 2:2O:222:PRO:C    | 1:3B:324:VAL:HG13 | 2.46                     | 0.41              |
| 2:2Q:11:GLN:HE22  | 1:3D:249:ASN:H    | 0.50                     | 0.41              |
| 2:2R:184:PRO:HD3  | 1:3E:349:THR:HG21 | 2.03                     | 0.41              |
| 2:2X:44:LEU:HA    | 2:2X:49:ILE:HB    | 2.01                     | 0.41              |
| 2:2Z:11:GLN:NE2   | 1:3N:249:ASN:CB   | 2.83                     | 0.41              |
| 2:2Z:17:GLY:HA2   | 2:2Z:20:PHE:HB3   | 2.03                     | 0.41              |
| 1:3G:147:SER:HB2  | 1:3G:190:THR:HB   | 2.03                     | 0.41              |
| 1:3J:147:SER:HB2  | 1:3J:190:THR:HB   | 2.03                     | 0.41              |
| 1:3J:407:TRP:CD2  | 2:3V:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:3M:319:TYR:HE2  | 1:3M:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:3S:386:GLU:HA   | 2:3S:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:3V:386:GLU:HA   | 2:3V:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:3W:145:THR:O    | 2:3W:149:MET:N    | 2.52                     | 0.41              |
| 2:3Z:17:GLY:HA2   | 2:3Z:20:PHE:HB3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4C:132:LEU:HD23 | 1:4C:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:4G:147:SER:HB2  | 1:4G:190:THR:HB   | 2.03                     | 0.41              |
| 1:4G:319:TYR:HE2  | 1:4G:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:4L:407:TRP:CD2  | 2:4X:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:4M:319:TYR:HE2  | 1:4M:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:4O:17:GLY:HA2   | 2:4O:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4Y:154:ILE:HG23 | 2:4Y:166:MET:HG2  | 2.00                     | 0.41              |
| 2:4Z:17:GLY:HA2   | 2:4Z:20:PHE:HB3   | 2.03                     | 0.41              |
| 1:1B:347:CYS:HA   | 2:4O:398:MET:HG2  | 2.03                     | 0.41              |
| 1:1B:348:PRO:CG   | 2:4O:394:GLN:CA   | 2.67                     | 0.41              |
| 1:1C:262:TYR:CZ   | 2:4P:403:ALA:CA   | 3.03                     | 0.41              |
| 1:1F:147:SER:HB2  | 1:1F:190:THR:HB   | 2.02                     | 0.41              |
| 1:1F:260:VAL:CG2  | 2:4S:407:TRP:HZ2  | 2.30                     | 0.41              |
| 1:1J:147:SER:HB2  | 1:1J:190:THR:HB   | 2.03                     | 0.41              |
| 1:1J:283:HIS:CG   | 1:1K:88:HIS:HA    | 2.55                     | 0.41              |
| 1:1L:319:TYR:HE2  | 1:1L:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1L:324:VAL:HG13 | 2:4X:222:PRO:C    | 2.45                     | 0.41              |
| 2:1O:145:THR:O    | 2:1O:149:MET:N    | 2.52                     | 0.41              |
| 2:1R:386:GLU:HA   | 2:1R:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:1S:386:GLU:HA   | 2:1S:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:1V:404:PHE:HE1  | 1:2J:260:VAL:H    | 1.69                     | 0.41              |
| 2:1W:145:THR:O    | 2:1W:149:MET:N    | 2.52                     | 0.41              |
| 1:2B:319:TYR:HE2  | 1:2B:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:2L:147:SER:HB2  | 1:2L:190:THR:HB   | 2.02                     | 0.41              |
| 1:2L:319:TYR:HE2  | 1:2L:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:2N:319:TYR:HE2  | 1:2N:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:2P:221:THR:CB   | 1:3C:324:VAL:HG21 | 2.51                     | 0.41              |
| 2:2R:36:TYR:OH    | 2:2R:40:SER:O     | 2.35                     | 0.41              |
| 2:2S:386:GLU:HA   | 2:2S:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:2V:386:GLU:HA   | 2:2V:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:2W:100:GLY:CA   | 1:3K:253:THR:C    | 2.92                     | 0.41              |
| 2:2W:165:ILE:H    | 2:2W:165:ILE:HG13 | 1.71                     | 0.41              |
| 2:2W:179:ASP:OD2  | 1:3K:248:LEU:CD2  | 2.68                     | 0.41              |
| 2:2X:17:GLY:HA2   | 2:2X:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2Y:11:GLN:NE2   | 1:3M:249:ASN:N    | 2.27                     | 0.41              |
| 2:2Z:101:ASN:HB2  | 1:3N:254:GLU:CB   | 2.49                     | 0.41              |
| 2:2Z:177:VAL:CG2  | 1:3N:332:ILE:CG2  | 2.88                     | 0.41              |
| 1:3A:319:TYR:HE2  | 1:3A:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:3B:319:TYR:HE2  | 1:3B:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:3B:407:TRP:CD2  | 2:3O:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:3G:319:TYR:HE2  | 1:3G:328:VAL:HG13 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:3L:407:TRP:CD2  | 2:3X:257:VAL:HG22 | 2.54                     | 0.41              |
| 2:3H:47:GLU:HG2   | 2:3H:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3O:145:THR:O    | 2:3O:149:MET:N    | 2.52                     | 0.41              |
| 2:3R:36:TYR:OH    | 2:3R:40:SER:O     | 2.35                     | 0.41              |
| 2:3S:74:THR:O     | 2:3S:77:SER:OG    | 2.31                     | 0.41              |
| 1:4D:132:LEU:HD23 | 1:4D:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:4L:319:TYR:HE2  | 1:4L:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:4P:47:GLU:HG2   | 2:4P:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:4R:36:TYR:OH    | 2:4R:40:SER:O     | 2.35                     | 0.41              |
| 2:4V:386:GLU:HA   | 2:4V:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:4W:47:GLU:HG2   | 2:4W:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:4X:17:GLY:HA2   | 2:4X:20:PHE:HB3   | 2.03                     | 0.41              |
| 1:1A:332:ILE:HB   | 2:4H:177:VAL:HG21 | 2.02                     | 0.41              |
| 1:1B:147:SER:HB2  | 1:1B:190:THR:HB   | 2.03                     | 0.41              |
| 1:1B:248:LEU:CA   | 2:4O:11:GLN:NE2   | 2.83                     | 0.41              |
| 1:1C:325:PRO:HB2  | 2:4P:224:TYR:CE1  | 2.54                     | 0.41              |
| 1:1G:346:TRP:CH2  | 2:4T:404:PHE:CE2  | 3.08                     | 0.41              |
| 1:1G:349:THR:O    | 2:4T:181:VAL:C    | 2.64                     | 0.41              |
| 1:1I:132:LEU:HD23 | 1:1I:164:LYS:HZ3  | 1.86                     | 0.41              |
| 1:1I:147:SER:HB2  | 1:1I:190:THR:HB   | 2.03                     | 0.41              |
| 1:1I:347:CYS:SG   | 2:4U:181:VAL:HG13 | 2.60                     | 0.41              |
| 1:1J:251:ASP:OD2  | 2:4V:71:GLU:CB    | 2.69                     | 0.41              |
| 1:1K:147:SER:HB2  | 1:1K:190:THR:HB   | 2.03                     | 0.41              |
| 1:1L:147:SER:HB2  | 1:1L:190:THR:HB   | 2.03                     | 0.41              |
| 1:1L:258:ASN:HD21 | 2:4X:101:ASN:ND2  | 2.18                     | 0.41              |
| 1:1L:332:ILE:HG21 | 2:4X:177:VAL:CG2  | 2.48                     | 0.41              |
| 1:1L:407:TRP:CD2  | 2:1X:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:1L:435:VAL:C    | 2:4X:401:ARG:HH22 | 2.28                     | 0.41              |
| 2:1H:44:LEU:HA    | 2:1H:49:ILE:HB    | 2.01                     | 0.41              |
| 2:1P:47:GLU:HG2   | 2:1P:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1Q:17:GLY:HA2   | 2:1Q:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1R:36:TYR:OH    | 2:1R:40:SER:O     | 2.35                     | 0.41              |
| 2:1S:298:ALA:HB2  | 2:1S:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1W:406:HIS:NE2  | 1:2K:263:PRO:HD3  | 2.33                     | 0.41              |
| 2:1X:17:GLY:HA2   | 2:1X:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1Y:154:ILE:HG23 | 2:1Y:166:MET:HG2  | 2.00                     | 0.41              |
| 1:2A:319:TYR:HE2  | 1:2A:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:2F:147:SER:HB2  | 1:2F:190:THR:HB   | 2.03                     | 0.41              |
| 1:2I:147:SER:HB2  | 1:2I:190:THR:HB   | 2.03                     | 0.41              |
| 1:2I:319:TYR:HE2  | 1:2I:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:2K:147:SER:HB2  | 1:2K:190:THR:HB   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2H:47:GLU:HG2   | 2:2H:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2H:145:THR:O    | 2:2H:149:MET:N    | 2.52                     | 0.41              |
| 2:2O:11:GLN:HE22  | 1:3B:249:ASN:CB   | 2.33                     | 0.41              |
| 2:2O:145:THR:O    | 2:2O:149:MET:N    | 2.52                     | 0.41              |
| 2:2O:407:TRP:HE1  | 1:3B:260:VAL:CG1  | 2.33                     | 0.41              |
| 2:2P:47:GLU:HG2   | 2:2P:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2Q:17:GLY:HA2   | 2:2Q:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2R:73:GLY:CA    | 1:3E:2:ARG:NH2    | 2.81                     | 0.41              |
| 2:2R:181:VAL:HG11 | 1:3E:314:ALA:HB2  | 2.02                     | 0.41              |
| 2:2R:298:ALA:HB2  | 2:2R:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2R:386:GLU:HA   | 2:2R:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:2T:394:GLN:CG   | 1:3G:348:PRO:HG2  | 2.43                     | 0.41              |
| 2:2T:404:PHE:CA   | 1:3G:261:PRO:HA   | 2.51                     | 0.41              |
| 2:2U:36:TYR:OH    | 2:2U:40:SER:O     | 2.35                     | 0.41              |
| 2:2W:404:PHE:CZ   | 1:3K:261:PRO:CA   | 3.03                     | 0.41              |
| 2:2Y:154:ILE:HG23 | 2:2Y:166:MET:HG2  | 2.00                     | 0.41              |
| 1:3B:147:SER:HB2  | 1:3B:190:THR:HB   | 2.03                     | 0.41              |
| 1:3F:147:SER:HB2  | 1:3F:190:THR:HB   | 2.02                     | 0.41              |
| 1:3I:147:SER:HB2  | 1:3I:190:THR:HB   | 2.03                     | 0.41              |
| 1:3L:147:SER:HB2  | 1:3L:190:THR:HB   | 2.03                     | 0.41              |
| 1:3N:319:TYR:HE2  | 1:3N:328:VAL:HG13 | 1.84                     | 0.41              |
| 2:3H:44:LEU:HA    | 2:3H:49:ILE:HB    | 2.01                     | 0.41              |
| 2:3H:145:THR:O    | 2:3H:149:MET:N    | 2.52                     | 0.41              |
| 2:3P:47:GLU:HG2   | 2:3P:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3Q:17:GLY:HA2   | 2:3Q:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3S:298:ALA:HB2  | 2:3S:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3V:298:ALA:HB2  | 2:3V:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3W:165:ILE:H    | 2:3W:165:ILE:HG13 | 1.71                     | 0.41              |
| 2:3X:17:GLY:HA2   | 2:3X:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3Y:17:GLY:HA2   | 2:3Y:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3Y:47:GLU:HG2   | 2:3Y:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3Y:154:ILE:HG23 | 2:3Y:166:MET:HG2  | 2.00                     | 0.41              |
| 2:3Z:145:THR:O    | 2:3Z:149:MET:N    | 2.52                     | 0.41              |
| 1:4A:319:TYR:HE2  | 1:4A:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:4B:147:SER:HB2  | 1:4B:190:THR:HB   | 2.03                     | 0.41              |
| 1:4B:319:TYR:HE2  | 1:4B:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:4F:132:LEU:HD23 | 1:4F:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:4F:147:SER:HB2  | 1:4F:190:THR:HB   | 2.03                     | 0.41              |
| 1:4I:147:SER:HB2  | 1:4I:190:THR:HB   | 2.03                     | 0.41              |
| 1:4J:132:LEU:HD23 | 1:4J:164:LYS:HZ3  | 1.85                     | 0.41              |
| 2:4H:47:GLU:HG2   | 2:4H:48:ARG:NH1   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:4H:145:THR:O   | 2:4H:149:MET:N    | 2.52                     | 0.41              |
| 2:4O:145:THR:O   | 2:4O:149:MET:N    | 2.52                     | 0.41              |
| 2:4R:298:ALA:HB2 | 2:4R:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:4R:386:GLU:HA  | 2:4R:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:4S:386:GLU:HA  | 2:4S:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:4T:298:ALA:HB2 | 2:4T:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:4U:384:ILE:H   | 2:4U:384:ILE:HG13 | 1.77                     | 0.41              |
| 2:4V:298:ALA:HB2 | 2:4V:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:4X:298:ALA:HB2 | 2:4X:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:4Y:47:GLU:HG2  | 2:4Y:48:ARG:NH1   | 2.35                     | 0.41              |
| 1:1A:260:VAL:O   | 2:4H:404:PHE:HD1  | 2.02                     | 0.41              |
| 1:1B:283:HIS:CG  | 1:1C:88:HIS:HA    | 2.55                     | 0.41              |
| 1:1B:326:LYS:HA  | 2:4O:210:TYR:CG   | 2.56                     | 0.41              |
| 1:1C:352:LYS:CD  | 2:4P:101:ASN:ND2  | 2.83                     | 0.41              |
| 1:1D:147:SER:HB2 | 1:1D:190:THR:HB   | 2.03                     | 0.41              |
| 1:1D:253:THR:HB  | 2:4Q:100:GLY:N    | 2.36                     | 0.41              |
| 1:1E:349:THR:CG2 | 2:4R:394:GLN:OE1  | 2.69                     | 0.41              |
| 1:1I:283:HIS:CG  | 1:1J:88:HIS:HA    | 2.55                     | 0.41              |
| 1:1J:260:VAL:CG1 | 2:4V:407:TRP:HE1  | 2.34                     | 0.41              |
| 1:1N:319:TYR:HE2 | 1:1N:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1N:348:PRO:HB2 | 2:4Z:394:GLN:NE2  | 2.36                     | 0.41              |
| 2:1H:17:GLY:HA2  | 2:1H:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1H:145:THR:O   | 2:1H:149:MET:N    | 2.52                     | 0.41              |
| 5:1H:501:GDP:C8  | 1:2A:248:LEU:CD1  | 3.03                     | 0.41              |
| 2:1P:17:GLY:HA2  | 2:1P:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1P:145:THR:O   | 2:1P:149:MET:N    | 2.52                     | 0.41              |
| 2:1U:36:TYR:OH   | 2:1U:40:SER:O     | 2.35                     | 0.41              |
| 2:1U:181:VAL:CB  | 1:2I:258:ASN:HA   | 2.35                     | 0.41              |
| 2:1V:47:GLU:HG2  | 2:1V:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1V:74:THR:O    | 2:1V:77:SER:OG    | 2.31                     | 0.41              |
| 2:1V:298:ALA:HB2 | 2:1V:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1W:47:GLU:HG2  | 2:1W:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1X:298:ALA:HB2 | 2:1X:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1Y:17:GLY:HA2  | 2:1Y:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1Y:47:GLU:HG2  | 2:1Y:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1Z:145:THR:O   | 2:1Z:149:MET:N    | 2.52                     | 0.41              |
| 1:2B:147:SER:HB2 | 1:2B:190:THR:HB   | 2.03                     | 0.41              |
| 1:2B:283:HIS:CG  | 1:2C:88:HIS:HA    | 2.55                     | 0.41              |
| 1:2D:172:TYR:N   | 1:2D:204:VAL:O    | 2.44                     | 0.41              |
| 2:2H:17:GLY:HA2  | 2:2H:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2P:145:THR:O   | 2:2P:149:MET:N    | 2.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2Q:404:PHE:H    | 1:3D:261:PRO:CA   | 2.34                     | 0.41              |
| 2:2S:298:ALA:HB2  | 2:2S:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2T:298:ALA:HB2  | 2:2T:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2T:386:GLU:HA   | 2:2T:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:2V:298:ALA:HB2  | 2:2V:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2W:11:GLN:NE2   | 1:3K:249:ASN:N    | 2.15                     | 0.41              |
| 2:2W:47:GLU:HG2   | 2:2W:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2X:298:ALA:HB2  | 2:2X:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2Y:17:GLY:HA2   | 2:2Y:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2Y:47:GLU:HG2   | 2:2Y:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2Y:403:ALA:HA   | 1:3M:262:TYR:CZ   | 2.55                     | 0.41              |
| 2:2Z:145:THR:O    | 2:2Z:149:MET:N    | 2.52                     | 0.41              |
| 2:2Z:406:HIS:NE2  | 1:3N:262:TYR:CA   | 2.84                     | 0.41              |
| 1:3B:283:HIS:CG   | 1:3C:88:HIS:HA    | 2.55                     | 0.41              |
| 1:3C:132:LEU:HD23 | 1:3C:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3D:147:SER:HB2  | 1:3D:190:THR:HB   | 2.03                     | 0.41              |
| 1:3J:132:LEU:HD23 | 1:3J:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3L:319:TYR:HE2  | 1:3L:328:VAL:HG13 | 1.85                     | 0.41              |
| 2:3H:17:GLY:HA2   | 2:3H:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3R:298:ALA:HB2  | 2:3R:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3R:386:GLU:HA   | 2:3R:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:3T:298:ALA:HB2  | 2:3T:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3U:36:TYR:OH    | 2:3U:40:SER:O     | 2.35                     | 0.41              |
| 2:3V:74:THR:O     | 2:3V:77:SER:OG    | 2.31                     | 0.41              |
| 2:3X:298:ALA:HB2  | 2:3X:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:4C:241:SER:OG   | 1:4C:250:VAL:O    | 2.27                     | 0.41              |
| 1:4D:147:SER:HB2  | 1:4D:190:THR:HB   | 2.03                     | 0.41              |
| 1:4G:62:VAL:HA    | 1:4G:63:PRO:HD3   | 1.86                     | 0.41              |
| 1:4K:147:SER:HB2  | 1:4K:190:THR:HB   | 2.03                     | 0.41              |
| 1:4L:147:SER:HB2  | 1:4L:190:THR:HB   | 2.03                     | 0.41              |
| 1:4N:319:TYR:HE2  | 1:4N:328:VAL:HG13 | 1.85                     | 0.41              |
| 2:4H:17:GLY:HA2   | 2:4H:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4P:17:GLY:HA2   | 2:4P:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4P:145:THR:O    | 2:4P:149:MET:N    | 2.52                     | 0.41              |
| 2:4Q:17:GLY:HA2   | 2:4Q:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4S:298:ALA:HB2  | 2:4S:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:1A:2:ARG:CG     | 2:4H:72:PRO:CD    | 2.95                     | 0.41              |
| 1:1A:132:LEU:HD23 | 1:1A:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:1B:254:GLU:N    | 2:4O:100:GLY:CA   | 2.76                     | 0.41              |
| 1:1C:132:LEU:HD23 | 1:1C:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:1E:314:ALA:CB   | 2:4R:181:VAL:HG21 | 2.33                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:CA   | 2.54                     | 0.41              |
| 1:1G:251:ASP:OD2  | 2:4T:71:GLU:CB    | 2.68                     | 0.41              |
| 1:1G:329:ASN:OD1  | 2:4T:177:VAL:HG11 | 2.19                     | 0.41              |
| 1:1I:314:ALA:HB2  | 2:4U:181:VAL:HG11 | 2.02                     | 0.41              |
| 1:1I:347:CYS:CA   | 2:4U:398:MET:HG2  | 2.44                     | 0.41              |
| 1:1J:132:LEU:HD23 | 1:1J:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:1J:261:PRO:O    | 2:4V:404:PHE:HA   | 2.20                     | 0.41              |
| 1:1M:147:SER:HB2  | 1:1M:190:THR:HB   | 2.03                     | 0.41              |
| 1:1N:261:PRO:HA   | 2:4Z:404:PHE:CA   | 2.50                     | 0.41              |
| 1:1N:346:TRP:HZ3  | 2:4Z:404:PHE:CE2  | 2.39                     | 0.41              |
| 2:1R:298:ALA:HB2  | 2:1R:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1T:298:ALA:HB2  | 2:1T:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1T:386:GLU:HA   | 2:1T:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:1W:74:THR:O     | 2:1W:77:SER:OG    | 2.31                     | 0.41              |
| 2:1W:165:ILE:H    | 2:1W:165:ILE:HG13 | 1.71                     | 0.41              |
| 1:2C:132:LEU:HD23 | 1:2C:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:2C:241:SER:OG   | 1:2C:250:VAL:O    | 2.27                     | 0.41              |
| 1:2D:147:SER:HB2  | 1:2D:190:THR:HB   | 2.03                     | 0.41              |
| 1:2I:283:HIS:CG   | 1:2J:88:HIS:HA    | 2.55                     | 0.41              |
| 2:2H:44:LEU:HA    | 2:2H:49:ILE:HB    | 2.01                     | 0.41              |
| 2:2H:179:ASP:C    | 1:3A:352:LYS:HA   | 2.45                     | 0.41              |
| 2:2O:11:GLN:HE22  | 1:3B:249:ASN:CA   | 2.26                     | 0.41              |
| 2:2O:73:GLY:HA3   | 1:3B:2:ARG:CZ     | 2.50                     | 0.41              |
| 2:2P:17:GLY:HA2   | 2:2P:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2P:404:PHE:CA   | 1:3C:261:PRO:HA   | 2.51                     | 0.41              |
| 2:2Q:386:GLU:HA   | 2:2Q:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:2R:100:GLY:O    | 1:3E:257:THR:CB   | 2.68                     | 0.41              |
| 2:2S:167:ASN:OD1  | 2:2S:167:ASN:N    | 2.48                     | 0.41              |
| 2:2S:401:ARG:HG3  | 1:3F:346:TRP:CD1  | 2.56                     | 0.41              |
| 2:2U:384:ILE:H    | 2:2U:384:ILE:HG13 | 1.77                     | 0.41              |
| 2:2U:394:GLN:CB   | 1:3I:348:PRO:HG2  | 2.44                     | 0.41              |
| 1:3D:172:TYR:N    | 1:3D:204:VAL:O    | 2.44                     | 0.41              |
| 1:3I:283:HIS:CG   | 1:3J:88:HIS:HA    | 2.55                     | 0.41              |
| 1:3I:319:TYR:HE2  | 1:3I:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:3K:147:SER:HB2  | 1:3K:190:THR:HB   | 2.03                     | 0.41              |
| 2:3P:145:THR:O    | 2:3P:149:MET:N    | 2.52                     | 0.41              |
| 2:3T:386:GLU:HA   | 2:3T:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:3U:384:ILE:H    | 2:3U:384:ILE:HG13 | 1.77                     | 0.41              |
| 2:3V:47:GLU:HG2   | 2:3V:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3W:47:GLU:HG2   | 2:3W:48:ARG:NH1   | 2.35                     | 0.41              |
| 1:4B:283:HIS:CG   | 1:4C:88:HIS:HA    | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:4D:172:TYR:N    | 1:4D:204:VAL:O    | 2.44                     | 0.41              |
| 1:4I:319:TYR:HE2  | 1:4I:328:VAL:HG13 | 1.85                     | 0.41              |
| 2:4H:44:LEU:HA    | 2:4H:49:ILE:HB    | 2.01                     | 0.41              |
| 2:4Q:386:GLU:HA   | 2:4Q:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:4R:47:GLU:HG2   | 2:4R:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:4S:167:ASN:OD1  | 2:4S:167:ASN:N    | 2.48                     | 0.41              |
| 2:4U:36:TYR:OH    | 2:4U:40:SER:O     | 2.35                     | 0.41              |
| 2:4V:47:GLU:HG2   | 2:4V:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:4Y:17:GLY:HA2   | 2:4Y:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4Z:145:THR:O    | 2:4Z:149:MET:N    | 2.52                     | 0.41              |
| 1:1A:326:LYS:HB3  | 2:4H:222:PRO:CG   | 2.49                     | 0.41              |
| 1:1C:260:VAL:HG11 | 2:4P:407:TRP:HZ2  | 1.84                     | 0.41              |
| 1:1D:172:TYR:N    | 1:1D:204:VAL:O    | 2.44                     | 0.41              |
| 1:1G:258:ASN:ND2  | 2:4T:182:VAL:HG22 | 2.35                     | 0.41              |
| 1:1G:329:ASN:OD1  | 2:4T:177:VAL:HG12 | 2.20                     | 0.41              |
| 1:1I:319:TYR:HE2  | 1:1I:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1J:2:ARG:NH2    | 2:4V:73:GLY:HA3   | 2.36                     | 0.41              |
| 1:1K:132:LEU:HD23 | 1:1K:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:1M:329:ASN:HB3  | 2:4Y:210:TYR:CD2  | 2.55                     | 0.41              |
| 1:1N:132:LEU:HD23 | 1:1N:164:LYS:HZ3  | 1.85                     | 0.41              |
| 2:1O:222:PRO:O    | 1:2B:325:PRO:HD2  | 2.20                     | 0.41              |
| 2:1P:404:PHE:CD1  | 1:2C:260:VAL:O    | 2.74                     | 0.41              |
| 2:1Q:298:ALA:HB2  | 2:1Q:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1R:180:THR:HA   | 1:2E:258:ASN:ND2  | 2.35                     | 0.41              |
| 2:1U:74:THR:O     | 2:1U:77:SER:OG    | 2.31                     | 0.41              |
| 1:2F:132:LEU:HD23 | 1:2F:164:LYS:HZ3  | 1.86                     | 0.41              |
| 1:2M:147:SER:HB2  | 1:2M:190:THR:HB   | 2.03                     | 0.41              |
| 2:2O:178:SER:OG   | 1:3B:351:PHE:HB2  | 2.20                     | 0.41              |
| 2:2Q:180:THR:N    | 1:3D:351:PHE:O    | 2.54                     | 0.41              |
| 2:2R:47:GLU:HG2   | 2:2R:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2R:180:THR:C    | 1:3E:351:PHE:O    | 2.63                     | 0.41              |
| 2:2R:221:THR:C    | 1:3E:324:VAL:HG11 | 2.45                     | 0.41              |
| 2:2T:222:PRO:O    | 1:3G:324:VAL:HG13 | 2.20                     | 0.41              |
| 2:2U:11:GLN:NE2   | 1:3I:249:ASN:N    | 2.02                     | 0.41              |
| 2:2V:47:GLU:HG2   | 2:2V:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2Z:101:ASN:N    | 1:3N:254:GLU:HG2  | 2.35                     | 0.41              |
| 1:3J:319:TYR:HE2  | 1:3J:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:3M:147:SER:HB2  | 1:3M:190:THR:HB   | 2.03                     | 0.41              |
| 2:3P:17:GLY:HA2   | 2:3P:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3Q:298:ALA:HB2  | 2:3Q:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3Q:386:GLU:HA   | 2:3Q:389:LYS:HB2  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3S:167:ASN:OD1  | 2:3S:167:ASN:N    | 2.48                     | 0.41              |
| 2:3W:74:THR:O     | 2:3W:77:SER:OG    | 2.31                     | 0.41              |
| 1:4A:132:LEU:HD23 | 1:4A:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:4J:319:TYR:HE2  | 1:4J:328:VAL:HG13 | 1.84                     | 0.41              |
| 1:4M:147:SER:HB2  | 1:4M:190:THR:HB   | 2.03                     | 0.41              |
| 2:4Q:298:ALA:HB2  | 2:4Q:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:4T:386:GLU:HA   | 2:4T:389:LYS:HB2  | 2.01                     | 0.41              |
| 1:1A:346:TRP:CH2  | 2:4H:403:ALA:HB1  | 2.56                     | 0.41              |
| 1:1B:261:PRO:C    | 2:4O:404:PHE:CA   | 2.92                     | 0.41              |
| 1:1B:345:ASP:O    | 2:4O:397:ALA:HB1  | 2.21                     | 0.41              |
| 1:1C:326:LYS:HG2  | 2:4P:210:TYR:CG   | 2.55                     | 0.41              |
| 1:1D:132:LEU:HD23 | 1:1D:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:1D:247:ALA:C    | 2:4Q:15:GLN:HE22  | 2.29                     | 0.41              |
| 1:1D:258:ASN:OD1  | 2:4Q:101:ASN:HB3  | 2.21                     | 0.41              |
| 1:1D:261:PRO:HB2  | 2:4Q:404:PHE:H    | 1.82                     | 0.41              |
| 1:1F:352:LYS:HE3  | 2:4S:101:ASN:HD22 | 1.82                     | 0.41              |
| 1:1G:258:ASN:HD22 | 2:4T:182:VAL:HG22 | 1.85                     | 0.41              |
| 1:1G:261:PRO:O    | 2:4T:404:PHE:N    | 2.54                     | 0.41              |
| 1:1G:435:VAL:CA   | 2:4T:401:ARG:HH21 | 2.23                     | 0.41              |
| 1:1J:319:TYR:HE2  | 1:1J:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1K:319:TYR:HE2  | 1:1K:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:1L:326:LYS:CG   | 2:4X:222:PRO:HG2  | 2.51                     | 0.41              |
| 1:1M:62:VAL:HA    | 1:1M:63:PRO:HD3   | 1.86                     | 0.41              |
| 1:1N:147:SER:HB2  | 1:1N:190:THR:HB   | 2.03                     | 0.41              |
| 1:1N:260:VAL:C    | 2:4Z:404:PHE:CD1  | 2.99                     | 0.41              |
| 2:1P:252:LEU:HD23 | 2:1P:252:LEU:HA   | 1.93                     | 0.41              |
| 2:1P:298:ALA:HB2  | 2:1P:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1Q:47:GLU:HG2   | 2:1Q:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1Q:386:GLU:HA   | 2:1Q:389:LYS:HB2  | 2.01                     | 0.41              |
| 2:1R:47:GLU:HG2   | 2:1R:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:1R:77:SER:HB3   | 1:2E:245:ASP:OD1  | 2.21                     | 0.41              |
| 2:1S:180:THR:CA   | 1:2F:258:ASN:ND2  | 2.84                     | 0.41              |
| 2:1S:404:PHE:CE1  | 1:2F:261:PRO:N    | 2.88                     | 0.41              |
| 2:1T:182:VAL:CG2  | 1:2G:257:THR:HG22 | 2.51                     | 0.41              |
| 2:1U:298:ALA:HB2  | 2:1U:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:1U:384:ILE:H    | 2:1U:384:ILE:HG13 | 1.77                     | 0.41              |
| 2:1Y:74:THR:O     | 2:1Y:77:SER:OG    | 2.31                     | 0.41              |
| 1:2A:132:LEU:HD23 | 1:2A:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:2J:319:TYR:HE2  | 1:2J:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:2K:132:LEU:HD23 | 1:2K:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:2K:319:TYR:HE2  | 1:2K:328:VAL:HG13 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2K:407:TRP:CD2  | 2:2W:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:2N:132:LEU:HD23 | 1:2N:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:2N:147:SER:HB2  | 1:2N:190:THR:HB   | 2.03                     | 0.41              |
| 2:2H:406:HIS:NE2  | 1:3A:262:TYR:CA   | 2.84                     | 0.41              |
| 2:2Q:210:TYR:CD1  | 1:3D:326:LYS:HA   | 2.56                     | 0.41              |
| 2:2Q:298:ALA:HB2  | 2:2Q:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2S:407:TRP:NE1  | 1:3F:260:VAL:O    | 2.54                     | 0.41              |
| 2:2T:407:TRP:NE1  | 1:3G:260:VAL:O    | 2.54                     | 0.41              |
| 2:2U:298:ALA:HB2  | 2:2U:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2U:394:GLN:HG2  | 1:3I:348:PRO:HB2  | 1.94                     | 0.41              |
| 2:2U:394:GLN:CG   | 1:3I:348:PRO:HG2  | 2.42                     | 0.41              |
| 2:2V:74:THR:O     | 2:2V:77:SER:OG    | 2.31                     | 0.41              |
| 2:2V:181:VAL:N    | 1:3J:258:ASN:HD22 | 2.18                     | 0.41              |
| 2:2W:17:GLY:HA2   | 2:2W:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2W:179:ASP:C    | 1:3K:352:LYS:HA   | 2.45                     | 0.41              |
| 1:3A:132:LEU:HD23 | 1:3A:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3C:241:SER:OG   | 1:3C:250:VAL:O    | 2.27                     | 0.41              |
| 1:3G:185:TYR:HE2  | 1:3G:404:PHE:HB2  | 1.86                     | 0.41              |
| 1:3K:132:LEU:HD23 | 1:3K:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3K:319:TYR:HE2  | 1:3K:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:3K:407:TRP:CD2  | 2:3W:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:3N:132:LEU:HD23 | 1:3N:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:3N:147:SER:HB2  | 1:3N:190:THR:HB   | 2.03                     | 0.41              |
| 2:3R:47:GLU:HG2   | 2:3R:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3U:74:THR:O     | 2:3U:77:SER:OG    | 2.31                     | 0.41              |
| 2:3U:298:ALA:HB2  | 2:3U:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:4A:147:SER:HB2  | 1:4A:190:THR:HB   | 2.02                     | 0.41              |
| 1:4G:185:TYR:HE2  | 1:4G:404:PHE:HB2  | 1.86                     | 0.41              |
| 1:4I:283:HIS:CG   | 1:4J:88:HIS:HA    | 2.55                     | 0.41              |
| 1:4J:324:VAL:HA   | 1:4J:325:PRO:HD3  | 1.96                     | 0.41              |
| 1:4K:132:LEU:HD23 | 1:4K:164:LYS:HZ3  | 1.85                     | 0.41              |
| 1:4K:319:TYR:HE2  | 1:4K:328:VAL:HG13 | 1.85                     | 0.41              |
| 1:4K:407:TRP:CD2  | 2:4W:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:4L:132:LEU:HD23 | 1:4L:164:LYS:HZ3  | 1.86                     | 0.41              |
| 1:4N:147:SER:HB2  | 1:4N:190:THR:HB   | 2.03                     | 0.41              |
| 2:4U:298:ALA:HB2  | 2:4U:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:1A:147:SER:HB2  | 1:1A:190:THR:HB   | 2.03                     | 0.41              |
| 1:1A:346:TRP:HA   | 2:4H:397:ALA:C    | 2.46                     | 0.41              |
| 1:1C:141:PHE:HB2  | 1:1C:173:PRO:HD3  | 2.03                     | 0.41              |
| 1:1C:352:LYS:HE3  | 2:4P:101:ASN:HD22 | 1.85                     | 0.41              |
| 1:1E:141:PHE:HB2  | 1:1E:173:PRO:HD3  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1E:249:ASN:O    | 2:4R:11:GLN:OE1   | 2.38                     | 0.41              |
| 1:1F:132:LEU:HD23 | 1:1F:164:LYS:HZ3  | 1.86                     | 0.41              |
| 1:1G:185:TYR:HE2  | 1:1G:404:PHE:HB2  | 1.86                     | 0.41              |
| 1:1I:346:TRP:CE2  | 2:4U:403:ALA:CB   | 3.03                     | 0.41              |
| 1:1J:2:ARG:HH11   | 2:4V:71:GLU:HB2   | 1.86                     | 0.41              |
| 1:1K:407:TRP:CD2  | 2:1W:257:VAL:HG22 | 2.54                     | 0.41              |
| 1:1N:261:PRO:N    | 2:4Z:404:PHE:CD1  | 2.88                     | 0.41              |
| 2:1Q:404:PHE:CD1  | 1:2D:260:VAL:O    | 2.73                     | 0.41              |
| 2:1R:17:GLY:HA2   | 2:1R:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1R:100:GLY:HA2  | 1:2E:253:THR:CB   | 2.49                     | 0.41              |
| 2:1V:394:GLN:CG   | 1:2J:348:PRO:HG2  | 2.49                     | 0.41              |
| 2:1V:404:PHE:CE1  | 1:2J:261:PRO:N    | 2.76                     | 0.41              |
| 2:1W:17:GLY:HA2   | 2:1W:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:1W:179:ASP:C    | 1:2K:352:LYS:CD   | 2.84                     | 0.41              |
| 2:1W:404:PHE:CE1  | 1:2K:260:VAL:CA   | 3.01                     | 0.41              |
| 1:2A:147:SER:HB2  | 1:2A:190:THR:HB   | 2.03                     | 0.41              |
| 1:2E:141:PHE:HB2  | 1:2E:173:PRO:HD3  | 2.03                     | 0.41              |
| 1:2G:185:TYR:HE2  | 1:2G:404:PHE:HB2  | 1.86                     | 0.41              |
| 1:2L:132:LEU:HD23 | 1:2L:164:LYS:HZ3  | 1.86                     | 0.41              |
| 2:2P:298:ALA:HB2  | 2:2P:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:2Q:47:GLU:HG2   | 2:2Q:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:2R:17:GLY:HA2   | 2:2R:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:2S:210:TYR:CD1  | 1:3F:326:LYS:HA   | 2.56                     | 0.41              |
| 2:2T:165:ILE:H    | 2:2T:165:ILE:HG13 | 1.71                     | 0.41              |
| 2:2T:181:VAL:CG2  | 1:3G:258:ASN:O    | 2.69                     | 0.41              |
| 2:2U:74:THR:O     | 2:2U:77:SER:OG    | 2.31                     | 0.41              |
| 2:2X:72:PRO:HD2   | 1:3L:2:ARG:HG2    | 2.02                     | 0.41              |
| 2:2X:394:GLN:NE2  | 1:3L:348:PRO:HB2  | 2.35                     | 0.41              |
| 2:2Z:298:ALA:HB2  | 2:2Z:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:3A:147:SER:HB2  | 1:3A:190:THR:HB   | 2.03                     | 0.41              |
| 1:3E:141:PHE:HB2  | 1:3E:173:PRO:HD3  | 2.03                     | 0.41              |
| 1:3F:132:LEU:HD23 | 1:3F:164:LYS:HZ3  | 1.86                     | 0.41              |
| 1:3M:62:VAL:HA    | 1:3M:63:PRO:HD3   | 1.86                     | 0.41              |
| 2:3P:298:ALA:HB2  | 2:3P:308:ARG:NH1  | 2.36                     | 0.41              |
| 2:3Q:47:GLU:HG2   | 2:3Q:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:3W:17:GLY:HA2   | 2:3W:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:3Z:298:ALA:HB2  | 2:3Z:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:4F:185:TYR:HE2  | 1:4F:404:PHE:HB2  | 1.86                     | 0.41              |
| 2:4Q:47:GLU:HG2   | 2:4Q:48:ARG:NH1   | 2.35                     | 0.41              |
| 2:4R:17:GLY:HA2   | 2:4R:20:PHE:HB3   | 2.03                     | 0.41              |
| 2:4V:74:THR:O     | 2:4V:77:SER:OG    | 2.31                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:4Z:298:ALA:HB2  | 2:4Z:308:ARG:NH1  | 2.36                     | 0.41              |
| 1:1B:324:VAL:HG11 | 2:4O:221:THR:HA   | 2.03                     | 0.40              |
| 1:1D:247:ALA:HB1  | 2:4Q:224:TYR:CD2  | 2.56                     | 0.40              |
| 1:1F:185:TYR:HE2  | 1:1F:404:PHE:HB2  | 1.86                     | 0.40              |
| 1:1L:326:LYS:CE   | 2:4X:214:PHE:HB2  | 2.51                     | 0.40              |
| 1:1M:324:VAL:HG13 | 2:4Y:222:PRO:O    | 2.20                     | 0.40              |
| 1:1M:326:LYS:HA   | 2:4Y:210:TYR:CD1  | 2.56                     | 0.40              |
| 2:1V:221:THR:C    | 1:2J:324:VAL:CG1  | 2.93                     | 0.40              |
| 2:1X:394:GLN:CG   | 1:2L:348:PRO:HG2  | 2.41                     | 0.40              |
| 2:1Y:404:PHE:CE2  | 1:2M:261:PRO:CA   | 3.03                     | 0.40              |
| 2:1Z:298:ALA:HB2  | 2:1Z:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:1Z:404:PHE:CD1  | 1:2N:257:THR:O    | 2.74                     | 0.40              |
| 1:2C:141:PHE:HB2  | 1:2C:173:PRO:HD3  | 2.03                     | 0.40              |
| 2:2R:72:PRO:HD2   | 1:3E:2:ARG:HG3    | 2.00                     | 0.40              |
| 2:2U:176:LYS:CE   | 1:3I:333:ALA:HB1  | 2.35                     | 0.40              |
| 2:2U:221:THR:C    | 1:3I:324:VAL:CG1  | 2.93                     | 0.40              |
| 2:2U:386:GLU:HA   | 2:2U:389:LYS:HB2  | 2.01                     | 0.40              |
| 2:2X:11:GLN:NE2   | 1:3L:249:ASN:CB   | 2.84                     | 0.40              |
| 2:2Z:404:PHE:CZ   | 1:3N:261:PRO:HB3  | 2.55                     | 0.40              |
| 1:3C:141:PHE:HB2  | 1:3C:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:3L:132:LEU:HD23 | 1:3L:164:LYS:HZ3  | 1.86                     | 0.40              |
| 2:3R:17:GLY:HA2   | 2:3R:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:3T:165:ILE:H    | 2:3T:165:ILE:HG13 | 1.71                     | 0.40              |
| 1:4D:141:PHE:HB2  | 1:4D:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:4E:141:PHE:HB2  | 1:4E:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:4J:241:SER:OG   | 1:4J:250:VAL:O    | 2.27                     | 0.40              |
| 2:4P:298:ALA:HB2  | 2:4P:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:4U:54:ASN:OD1   | 2:4U:64:ARG:NH2   | 2.46                     | 0.40              |
| 2:4V:17:GLY:HA2   | 2:4V:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:4W:17:GLY:HA2   | 2:4W:20:PHE:HB3   | 2.03                     | 0.40              |
| 1:1B:141:PHE:HB2  | 1:1B:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:1M:257:THR:HG21 | 2:4Y:101:ASN:C    | 2.46                     | 0.40              |
| 1:1M:325:PRO:HB3  | 2:4Y:224:TYR:CZ   | 2.57                     | 0.40              |
| 1:1N:262:TYR:CA   | 2:4Z:406:HIS:CD2  | 2.62                     | 0.40              |
| 2:1P:41:ASP:O     | 2:1P:47:GLU:N     | 2.55                     | 0.40              |
| 2:1S:17:GLY:HA2   | 2:1S:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:1T:180:THR:C    | 1:2G:258:ASN:ND2  | 2.76                     | 0.40              |
| 2:1U:386:GLU:HA   | 2:1U:389:LYS:HB2  | 2.01                     | 0.40              |
| 2:1X:41:ASP:O     | 2:1X:47:GLU:N     | 2.55                     | 0.40              |
| 2:1Y:298:ALA:HB2  | 2:1Y:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:1Z:221:THR:OG1  | 1:2N:324:VAL:CG2  | 2.69                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2B:141:PHE:HB2  | 1:2B:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:2D:141:PHE:HB2  | 1:2D:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:2F:185:TYR:HE2  | 1:2F:404:PHE:HB2  | 1.86                     | 0.40              |
| 1:2J:324:VAL:HA   | 1:2J:325:PRO:HD3  | 1.97                     | 0.40              |
| 1:2M:62:VAL:HA    | 1:2M:63:PRO:HD3   | 1.86                     | 0.40              |
| 2:2P:41:ASP:O     | 2:2P:47:GLU:N     | 2.55                     | 0.40              |
| 2:2P:73:GLY:HA3   | 1:3C:2:ARG:CZ     | 2.51                     | 0.40              |
| 2:2P:404:PHE:CD2  | 1:3C:261:PRO:HB3  | 2.55                     | 0.40              |
| 2:2Q:180:THR:C    | 1:3D:351:PHE:O    | 2.64                     | 0.40              |
| 2:2R:101:ASN:HB2  | 1:3E:254:GLU:HB3  | 2.04                     | 0.40              |
| 2:2R:179:ASP:O    | 1:3E:352:LYS:CD   | 2.50                     | 0.40              |
| 2:2T:394:GLN:CG   | 1:3G:348:PRO:HB2  | 2.49                     | 0.40              |
| 1:3B:141:PHE:HB2  | 1:3B:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:3D:141:PHE:HB2  | 1:3D:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:3J:324:VAL:HA   | 1:3J:325:PRO:HD3  | 1.97                     | 0.40              |
| 2:3O:298:ALA:HB2  | 2:3O:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:3U:386:GLU:HA   | 2:3U:389:LYS:HB2  | 2.01                     | 0.40              |
| 2:3V:17:GLY:HA2   | 2:3V:20:PHE:HB3   | 2.03                     | 0.40              |
| 1:4B:141:PHE:HB2  | 1:4B:173:PRO:HD3  | 2.04                     | 0.40              |
| 1:4C:141:PHE:HB2  | 1:4C:173:PRO:HD3  | 2.03                     | 0.40              |
| 2:4P:41:ASP:O     | 2:4P:47:GLU:N     | 2.55                     | 0.40              |
| 2:4U:386:GLU:HA   | 2:4U:389:LYS:HB2  | 2.01                     | 0.40              |
| 2:4W:298:ALA:HB2  | 2:4W:308:ARG:NH1  | 2.36                     | 0.40              |
| 1:1B:253:THR:CB   | 2:4O:100:GLY:HA2  | 2.48                     | 0.40              |
| 1:1B:261:PRO:CD   | 2:4O:404:PHE:CE1  | 3.04                     | 0.40              |
| 1:1D:141:PHE:HB2  | 1:1D:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:1E:254:GLU:HB3  | 2:4R:101:ASN:CB   | 2.44                     | 0.40              |
| 1:1E:346:TRP:C    | 2:4R:398:MET:HG2  | 2.39                     | 0.40              |
| 1:1E:348:PRO:HD2  | 2:4R:398:MET:SD   | 2.62                     | 0.40              |
| 1:1F:329:ASN:OD1  | 2:4S:177:VAL:HG12 | 2.20                     | 0.40              |
| 1:1I:2:ARG:HG3    | 2:4U:72:PRO:HG2   | 2.04                     | 0.40              |
| 1:1I:329:ASN:HB3  | 2:4U:210:TYR:CE2  | 2.55                     | 0.40              |
| 1:1J:324:VAL:HA   | 1:1J:325:PRO:HD3  | 1.97                     | 0.40              |
| 1:1K:348:PRO:CB   | 2:4W:394:GLN:CG   | 2.99                     | 0.40              |
| 1:1M:435:VAL:HA   | 2:4Y:401:ARG:HH21 | 1.85                     | 0.40              |
| 2:1O:298:ALA:HB2  | 2:1O:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:1Q:33:THR:HG22  | 2:1Q:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:1S:41:ASP:O     | 2:1S:47:GLU:N     | 2.55                     | 0.40              |
| 2:1V:41:ASP:O     | 2:1V:47:GLU:N     | 2.55                     | 0.40              |
| 2:1V:275:LEU:HD23 | 2:1V:275:LEU:HA   | 1.97                     | 0.40              |
| 2:1W:180:THR:CG2  | 1:2K:258:ASN:ND2  | 2.73                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1Z:47:GLU:HG2   | 2:1Z:48:ARG:NH1   | 2.35                     | 0.40              |
| 1:2J:241:SER:OG   | 1:2J:250:VAL:O    | 2.27                     | 0.40              |
| 2:2H:11:GLN:NE2   | 1:3A:249:ASN:CB   | 2.84                     | 0.40              |
| 2:2H:71:GLU:HG3   | 1:3A:2:ARG:HH11   | 1.85                     | 0.40              |
| 2:2H:207:GLU:OE1  | 1:3A:329:ASN:CG   | 2.49                     | 0.40              |
| 2:2O:298:ALA:HB2  | 2:2O:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:2S:41:ASP:O     | 2:2S:47:GLU:N     | 2.55                     | 0.40              |
| 2:2S:181:VAL:HG11 | 1:3F:314:ALA:HB2  | 2.01                     | 0.40              |
| 2:2U:54:ASN:OD1   | 2:2U:64:ARG:NH2   | 2.46                     | 0.40              |
| 2:2U:101:ASN:N    | 1:3I:254:GLU:HG2  | 2.36                     | 0.40              |
| 2:2V:17:GLY:HA2   | 2:2V:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:2V:41:ASP:O     | 2:2V:47:GLU:N     | 2.55                     | 0.40              |
| 2:2V:404:PHE:CD1  | 1:3J:261:PRO:N    | 2.82                     | 0.40              |
| 2:2W:298:ALA:HB2  | 2:2W:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:2X:41:ASP:O     | 2:2X:47:GLU:N     | 2.55                     | 0.40              |
| 1:3F:185:TYR:HE2  | 1:3F:404:PHE:HB2  | 1.86                     | 0.40              |
| 2:3P:41:ASP:O     | 2:3P:47:GLU:N     | 2.55                     | 0.40              |
| 2:3S:17:GLY:HA2   | 2:3S:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:3V:41:ASP:O     | 2:3V:47:GLU:N     | 2.55                     | 0.40              |
| 2:3W:298:ALA:HB2  | 2:3W:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:3X:41:ASP:O     | 2:3X:47:GLU:N     | 2.55                     | 0.40              |
| 2:3Y:298:ALA:HB2  | 2:3Y:308:ARG:NH1  | 2.36                     | 0.40              |
| 1:4A:141:PHE:HB2  | 1:4A:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:4C:185:TYR:HE2  | 1:4C:404:PHE:HB2  | 1.86                     | 0.40              |
| 2:4O:298:ALA:HB2  | 2:4O:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:4S:41:ASP:O     | 2:4S:47:GLU:N     | 2.55                     | 0.40              |
| 2:4U:145:THR:O    | 2:4U:149:MET:N    | 2.52                     | 0.40              |
| 2:4X:41:ASP:O     | 2:4X:47:GLU:N     | 2.55                     | 0.40              |
| 1:1A:141:PHE:HB2  | 1:1A:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:1D:326:LYS:CG   | 2:4Q:210:TYR:HA   | 2.52                     | 0.40              |
| 1:1F:141:PHE:HB2  | 1:1F:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:1F:348:PRO:CG   | 2:4S:394:GLN:O    | 2.69                     | 0.40              |
| 1:1G:2:ARG:HG3    | 2:4T:72:PRO:CD    | 2.51                     | 0.40              |
| 1:1I:260:VAL:HG12 | 2:4U:407:TRP:NE1  | 2.35                     | 0.40              |
| 1:1K:348:PRO:HB2  | 2:4W:394:GLN:CG   | 2.51                     | 0.40              |
| 2:1O:33:THR:HG22  | 2:1O:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:1P:33:THR:HG22  | 2:1P:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:1Q:41:ASP:O     | 2:1Q:47:GLU:N     | 2.55                     | 0.40              |
| 2:1Q:145:THR:O    | 2:1Q:149:MET:N    | 2.52                     | 0.40              |
| 2:1S:167:ASN:OD1  | 2:1S:167:ASN:N    | 2.48                     | 0.40              |
| 2:1T:165:ILE:H    | 2:1T:165:ILE:HG13 | 1.71                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:1U:17:GLY:HA2  | 2:1U:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:1U:221:THR:C   | 1:2I:324:VAL:CG1  | 2.91                     | 0.40              |
| 2:1V:17:GLY:HA2  | 2:1V:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:1W:298:ALA:HB2 | 2:1W:308:ARG:NH1  | 2.36                     | 0.40              |
| 1:2A:141:PHE:HB2 | 1:2A:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:2C:185:TYR:HE2 | 1:2C:404:PHE:HB2  | 1.86                     | 0.40              |
| 2:2O:210:TYR:CZ  | 1:3B:325:PRO:O    | 2.75                     | 0.40              |
| 2:2Q:33:THR:HG22 | 2:2Q:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:2Q:41:ASP:O    | 2:2Q:47:GLU:N     | 2.55                     | 0.40              |
| 2:2S:17:GLY:HA2  | 2:2S:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:2S:394:GLN:OE1 | 1:3F:349:THR:CG2  | 2.70                     | 0.40              |
| 2:2U:17:GLY:HA2  | 2:2U:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:2V:397:ALA:O   | 1:3J:346:TRP:HB3  | 2.17                     | 0.40              |
| 2:2X:404:PHE:HA  | 1:3L:261:PRO:O    | 2.21                     | 0.40              |
| 2:2Y:298:ALA:HB2 | 2:2Y:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:2Z:221:THR:C   | 1:3N:324:VAL:HG11 | 2.47                     | 0.40              |
| 1:3A:141:PHE:HB2 | 1:3A:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:3C:185:TYR:HE2 | 1:3C:404:PHE:HB2  | 1.86                     | 0.40              |
| 2:3H:33:THR:HG22 | 2:3H:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:3Q:33:THR:HG22 | 2:3Q:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:3Q:41:ASP:O    | 2:3Q:47:GLU:N     | 2.55                     | 0.40              |
| 2:3S:41:ASP:O    | 2:3S:47:GLU:N     | 2.55                     | 0.40              |
| 2:3T:17:GLY:HA2  | 2:3T:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:3U:54:ASN:OD1  | 2:3U:64:ARG:NH2   | 2.46                     | 0.40              |
| 2:3Z:47:GLU:HG2  | 2:3Z:48:ARG:NH1   | 2.35                     | 0.40              |
| 1:4M:62:VAL:HA   | 1:4M:63:PRO:HD3   | 1.86                     | 0.40              |
| 1:4N:334:THR:O   | 1:4N:337:THR:OG1  | 2.30                     | 0.40              |
| 2:4Q:33:THR:HG22 | 2:4Q:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:4S:17:GLY:HA2  | 2:4S:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:4V:41:ASP:O    | 2:4V:47:GLU:N     | 2.55                     | 0.40              |
| 2:4Y:74:THR:O    | 2:4Y:77:SER:OG    | 2.31                     | 0.40              |
| 2:4Y:298:ALA:HB2 | 2:4Y:308:ARG:NH1  | 2.36                     | 0.40              |
| 2:4Z:47:GLU:HG2  | 2:4Z:48:ARG:NH1   | 2.35                     | 0.40              |
| 1:1C:185:TYR:HE2 | 1:1C:404:PHE:HB2  | 1.86                     | 0.40              |
| 1:1D:325:PRO:CG  | 2:4Q:224:TYR:CD1  | 2.99                     | 0.40              |
| 1:1D:434:GLU:C   | 2:4Q:401:ARG:HH21 | 2.26                     | 0.40              |
| 1:1E:349:THR:HB  | 2:4R:183:GLU:HG2  | 2.02                     | 0.40              |
| 1:1G:141:PHE:HB2 | 1:1G:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:1I:348:PRO:HG3 | 2:4U:394:GLN:O    | 2.20                     | 0.40              |
| 1:1M:325:PRO:CB  | 2:4Y:224:TYR:CE1  | 3.05                     | 0.40              |
| 2:1H:33:THR:HG22 | 2:1H:60:LYS:HE3   | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1T:17:GLY:HA2   | 2:1T:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:1T:41:ASP:O     | 2:1T:47:GLU:N     | 2.55                     | 0.40              |
| 2:1T:182:VAL:HG21 | 1:2G:257:THR:CG2  | 2.51                     | 0.40              |
| 2:1U:54:ASN:OD1   | 2:1U:64:ARG:NH2   | 2.46                     | 0.40              |
| 2:1V:179:ASP:CG   | 1:2J:248:LEU:HD21 | 2.40                     | 0.40              |
| 2:1X:406:HIS:HD2  | 1:2L:263:PRO:HD3  | 1.78                     | 0.40              |
| 2:1Z:41:ASP:O     | 2:1Z:47:GLU:N     | 2.55                     | 0.40              |
| 1:2F:141:PHE:HB2  | 1:2F:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:2N:334:THR:O    | 1:2N:337:THR:OG1  | 2.30                     | 0.40              |
| 2:2H:41:ASP:O     | 2:2H:47:GLU:N     | 2.55                     | 0.40              |
| 2:2O:33:THR:HG22  | 2:2O:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:2O:180:THR:HA   | 1:3B:352:LYS:HD3  | 2.02                     | 0.40              |
| 2:2R:404:PHE:CD1  | 1:3E:261:PRO:N    | 2.88                     | 0.40              |
| 2:2T:17:GLY:HA2   | 2:2T:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:2T:404:PHE:CZ   | 1:3G:261:PRO:CB   | 3.02                     | 0.40              |
| 2:2U:145:THR:O    | 2:2U:149:MET:N    | 2.52                     | 0.40              |
| 2:2V:403:ALA:CA   | 1:3J:262:TYR:CZ   | 3.03                     | 0.40              |
| 2:2Y:202:TYR:HE1  | 2:2Y:378:ILE:HD12 | 1.87                     | 0.40              |
| 2:2Z:407:TRP:NE1  | 1:3N:260:VAL:HB   | 2.35                     | 0.40              |
| 1:3F:141:PHE:HB2  | 1:3F:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:3F:283:HIS:CE1  | 1:3G:87:PHE:O     | 2.75                     | 0.40              |
| 1:3J:241:SER:OG   | 1:3J:250:VAL:O    | 2.27                     | 0.40              |
| 2:3O:33:THR:HG22  | 2:3O:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:3P:33:THR:HG22  | 2:3P:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:3U:17:GLY:HA2   | 2:3U:20:PHE:HB3   | 2.03                     | 0.40              |
| 2:3Y:33:THR:HG22  | 2:3Y:60:LYS:HE3   | 2.04                     | 0.40              |
| 1:4F:141:PHE:HB2  | 1:4F:173:PRO:HD3  | 2.03                     | 0.40              |
| 1:4G:141:PHE:HB2  | 1:4G:173:PRO:HD3  | 2.03                     | 0.40              |
| 2:4H:33:THR:HG22  | 2:4H:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:4O:33:THR:HG22  | 2:4O:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:4P:33:THR:HG22  | 2:4P:60:LYS:HE3   | 2.04                     | 0.40              |
| 2:4Q:41:ASP:O     | 2:4Q:47:GLU:N     | 2.55                     | 0.40              |
| 2:4U:17:GLY:HA2   | 2:4U:20:PHE:HB3   | 2.03                     | 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   | 1A    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1B    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1C    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1D    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1E    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1F    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1G    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1I    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1J    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1K    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1L    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1M    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 1N    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2A    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2B    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2C    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2D    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2E    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2F    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2G    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2I    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2J    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2K    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2L    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 2M    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 2N    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3A    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3B    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3C    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3D    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3E    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3F    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3G    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3I    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3J    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3K    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3L    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3M    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 3N    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4A    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4B    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4C    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4D    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4E    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4F    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4G    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4I    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4J    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4K    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4L    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4M    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | 4N    | 433/451 (96%) | 415 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1H    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1O    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1P    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1Q    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | 1R    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1S    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1T    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1U    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1V    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1W    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1X    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1Y    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 1Z    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2H    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2O    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2P    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2Q    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2R    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2S    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2T    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2U    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2V    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2W    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2X    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2Y    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 2Z    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3H    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3O    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3P    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3Q    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3R    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3S    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3T    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3U    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |
| 2   | 3V    | 427/445 (96%) | 409 (96%) | 18 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 2   | 3W    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 3X    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 3Y    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 3Z    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4H    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4O    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4P    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4Q    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4R    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4S    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4T    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4U    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4V    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4W    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4X    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4Y    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| 2   | 4Z    | 427/445 (96%)     | 409 (96%)   | 18 (4%)   | 0        | 100         | 100 |
| All | All   | 44720/46592 (96%) | 42848 (96%) | 1872 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | 1A    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1B    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1C    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1D    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |    |
|-----|-------|---------------|------------|----------|-------------|----|
| 1   | 1E    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1F    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1G    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1I    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1J    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1K    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1L    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1M    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 1N    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2A    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2B    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2C    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2D    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2E    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2F    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2G    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2I    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2J    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2K    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2L    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2M    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 2N    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3A    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3B    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3C    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3D    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3E    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3F    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3G    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3I    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |
| 1   | 3J    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 3K    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 3L    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 3M    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 3N    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4A    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4B    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4C    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4D    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4E    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4F    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4G    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4I    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4J    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4K    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4L    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4M    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 1   | 4N    | 368/379 (97%) | 367 (100%) | 1 (0%)   | 86          | 85  |
| 2   | 1H    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1O    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1P    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1Q    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1R    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1S    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1T    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1U    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1V    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1W    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1X    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1Y    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 1Z    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2H    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2   | 2O    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2P    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2Q    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2R    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2S    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2T    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2U    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2V    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2W    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2X    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2Y    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 2Z    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3H    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3O    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3P    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3Q    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3R    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3S    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3T    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3U    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3V    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3W    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3X    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3Y    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 3Z    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4H    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4O    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4P    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4Q    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4R    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |
| 2   | 4S    | 368/381 (97%) | 368 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 2   | 4T    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4U    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4V    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4W    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4X    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4Y    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| 2   | 4Z    | 368/381 (97%)     | 368 (100%)   | 0        | 100         | 100 |
| All | All   | 38272/39520 (97%) | 38220 (100%) | 52 (0%)  | 87          | 89  |

All (52) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 375 | VAL  |
| 1   | 1B    | 375 | VAL  |
| 1   | 1C    | 375 | VAL  |
| 1   | 1D    | 375 | VAL  |
| 1   | 1E    | 375 | VAL  |
| 1   | 1F    | 375 | VAL  |
| 1   | 1G    | 375 | VAL  |
| 1   | 1I    | 375 | VAL  |
| 1   | 1J    | 375 | VAL  |
| 1   | 1K    | 375 | VAL  |
| 1   | 1L    | 375 | VAL  |
| 1   | 1M    | 375 | VAL  |
| 1   | 1N    | 375 | VAL  |
| 1   | 2A    | 375 | VAL  |
| 1   | 2B    | 375 | VAL  |
| 1   | 2C    | 375 | VAL  |
| 1   | 2D    | 375 | VAL  |
| 1   | 2E    | 375 | VAL  |
| 1   | 2F    | 375 | VAL  |
| 1   | 2G    | 375 | VAL  |
| 1   | 2I    | 375 | VAL  |
| 1   | 2J    | 375 | VAL  |
| 1   | 2K    | 375 | VAL  |
| 1   | 2L    | 375 | VAL  |
| 1   | 2M    | 375 | VAL  |
| 1   | 2N    | 375 | VAL  |
| 1   | 3A    | 375 | VAL  |
| 1   | 3B    | 375 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3C    | 375 | VAL  |
| 1   | 3D    | 375 | VAL  |
| 1   | 3E    | 375 | VAL  |
| 1   | 3F    | 375 | VAL  |
| 1   | 3G    | 375 | VAL  |
| 1   | 3I    | 375 | VAL  |
| 1   | 3J    | 375 | VAL  |
| 1   | 3K    | 375 | VAL  |
| 1   | 3L    | 375 | VAL  |
| 1   | 3M    | 375 | VAL  |
| 1   | 3N    | 375 | VAL  |
| 1   | 4A    | 375 | VAL  |
| 1   | 4B    | 375 | VAL  |
| 1   | 4C    | 375 | VAL  |
| 1   | 4D    | 375 | VAL  |
| 1   | 4E    | 375 | VAL  |
| 1   | 4F    | 375 | VAL  |
| 1   | 4G    | 375 | VAL  |
| 1   | 4I    | 375 | VAL  |
| 1   | 4J    | 375 | VAL  |
| 1   | 4K    | 375 | VAL  |
| 1   | 4L    | 375 | VAL  |
| 1   | 4M    | 375 | VAL  |
| 1   | 4N    | 375 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1167) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 8   | HIS  |
| 1   | 1A    | 107 | HIS  |
| 1   | 1A    | 139 | HIS  |
| 1   | 1A    | 186 | ASN  |
| 1   | 1A    | 192 | HIS  |
| 1   | 1A    | 216 | ASN  |
| 1   | 1A    | 258 | ASN  |
| 1   | 1A    | 293 | ASN  |
| 1   | 1A    | 356 | ASN  |
| 1   | 1A    | 380 | ASN  |
| 1   | 1A    | 393 | HIS  |
| 1   | 1B    | 8   | HIS  |
| 1   | 1B    | 107 | HIS  |
| 1   | 1B    | 139 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1B    | 186 | ASN  |
| 1   | 1B    | 192 | HIS  |
| 1   | 1B    | 216 | ASN  |
| 1   | 1B    | 258 | ASN  |
| 1   | 1B    | 356 | ASN  |
| 1   | 1B    | 380 | ASN  |
| 1   | 1B    | 393 | HIS  |
| 1   | 1C    | 8   | HIS  |
| 1   | 1C    | 107 | HIS  |
| 1   | 1C    | 139 | HIS  |
| 1   | 1C    | 186 | ASN  |
| 1   | 1C    | 192 | HIS  |
| 1   | 1C    | 216 | ASN  |
| 1   | 1C    | 256 | GLN  |
| 1   | 1C    | 258 | ASN  |
| 1   | 1C    | 356 | ASN  |
| 1   | 1C    | 380 | ASN  |
| 1   | 1C    | 393 | HIS  |
| 1   | 1D    | 8   | HIS  |
| 1   | 1D    | 107 | HIS  |
| 1   | 1D    | 139 | HIS  |
| 1   | 1D    | 186 | ASN  |
| 1   | 1D    | 216 | ASN  |
| 1   | 1D    | 256 | GLN  |
| 1   | 1D    | 356 | ASN  |
| 1   | 1D    | 380 | ASN  |
| 1   | 1D    | 393 | HIS  |
| 1   | 1E    | 8   | HIS  |
| 1   | 1E    | 28  | HIS  |
| 1   | 1E    | 107 | HIS  |
| 1   | 1E    | 139 | HIS  |
| 1   | 1E    | 186 | ASN  |
| 1   | 1E    | 216 | ASN  |
| 1   | 1E    | 256 | GLN  |
| 1   | 1E    | 356 | ASN  |
| 1   | 1E    | 380 | ASN  |
| 1   | 1E    | 393 | HIS  |
| 1   | 1F    | 8   | HIS  |
| 1   | 1F    | 28  | HIS  |
| 1   | 1F    | 107 | HIS  |
| 1   | 1F    | 139 | HIS  |
| 1   | 1F    | 186 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1F    | 216 | ASN  |
| 1   | 1F    | 256 | GLN  |
| 1   | 1F    | 356 | ASN  |
| 1   | 1F    | 380 | ASN  |
| 1   | 1F    | 393 | HIS  |
| 1   | 1G    | 8   | HIS  |
| 1   | 1G    | 107 | HIS  |
| 1   | 1G    | 139 | HIS  |
| 1   | 1G    | 186 | ASN  |
| 1   | 1G    | 216 | ASN  |
| 1   | 1G    | 356 | ASN  |
| 1   | 1G    | 380 | ASN  |
| 1   | 1G    | 393 | HIS  |
| 1   | 1I    | 8   | HIS  |
| 1   | 1I    | 107 | HIS  |
| 1   | 1I    | 139 | HIS  |
| 1   | 1I    | 186 | ASN  |
| 1   | 1I    | 216 | ASN  |
| 1   | 1I    | 356 | ASN  |
| 1   | 1I    | 380 | ASN  |
| 1   | 1I    | 393 | HIS  |
| 1   | 1J    | 8   | HIS  |
| 1   | 1J    | 107 | HIS  |
| 1   | 1J    | 139 | HIS  |
| 1   | 1J    | 186 | ASN  |
| 1   | 1J    | 216 | ASN  |
| 1   | 1J    | 356 | ASN  |
| 1   | 1J    | 380 | ASN  |
| 1   | 1J    | 393 | HIS  |
| 1   | 1K    | 8   | HIS  |
| 1   | 1K    | 107 | HIS  |
| 1   | 1K    | 139 | HIS  |
| 1   | 1K    | 186 | ASN  |
| 1   | 1K    | 216 | ASN  |
| 1   | 1K    | 356 | ASN  |
| 1   | 1K    | 380 | ASN  |
| 1   | 1K    | 393 | HIS  |
| 1   | 1L    | 8   | HIS  |
| 1   | 1L    | 28  | HIS  |
| 1   | 1L    | 107 | HIS  |
| 1   | 1L    | 186 | ASN  |
| 1   | 1L    | 216 | ASN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1L    | 258 | ASN  |
| 1   | 1L    | 356 | ASN  |
| 1   | 1L    | 380 | ASN  |
| 1   | 1L    | 393 | HIS  |
| 1   | 1M    | 8   | HIS  |
| 1   | 1M    | 107 | HIS  |
| 1   | 1M    | 139 | HIS  |
| 1   | 1M    | 186 | ASN  |
| 1   | 1M    | 192 | HIS  |
| 1   | 1M    | 216 | ASN  |
| 1   | 1M    | 258 | ASN  |
| 1   | 1M    | 356 | ASN  |
| 1   | 1M    | 380 | ASN  |
| 1   | 1M    | 393 | HIS  |
| 1   | 1N    | 8   | HIS  |
| 1   | 1N    | 107 | HIS  |
| 1   | 1N    | 139 | HIS  |
| 1   | 1N    | 186 | ASN  |
| 1   | 1N    | 192 | HIS  |
| 1   | 1N    | 216 | ASN  |
| 1   | 1N    | 258 | ASN  |
| 1   | 1N    | 356 | ASN  |
| 1   | 1N    | 380 | ASN  |
| 1   | 1N    | 393 | HIS  |
| 2   | 1H    | 11  | GLN  |
| 2   | 1H    | 14  | ASN  |
| 2   | 1H    | 37  | HIS  |
| 2   | 1H    | 85  | GLN  |
| 2   | 1H    | 101 | ASN  |
| 2   | 1H    | 133 | GLN  |
| 2   | 1H    | 192 | HIS  |
| 2   | 1H    | 197 | ASN  |
| 2   | 1H    | 228 | ASN  |
| 2   | 1H    | 300 | ASN  |
| 2   | 1H    | 309 | HIS  |
| 2   | 1H    | 336 | GLN  |
| 2   | 1H    | 385 | GLN  |
| 2   | 1H    | 433 | GLN  |
| 2   | 1O    | 11  | GLN  |
| 2   | 1O    | 14  | ASN  |
| 2   | 1O    | 37  | HIS  |
| 2   | 1O    | 85  | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1O    | 101 | ASN  |
| 2   | 1O    | 192 | HIS  |
| 2   | 1O    | 197 | ASN  |
| 2   | 1O    | 228 | ASN  |
| 2   | 1O    | 300 | ASN  |
| 2   | 1O    | 309 | HIS  |
| 2   | 1O    | 336 | GLN  |
| 2   | 1O    | 385 | GLN  |
| 2   | 1O    | 433 | GLN  |
| 2   | 1P    | 11  | GLN  |
| 2   | 1P    | 14  | ASN  |
| 2   | 1P    | 37  | HIS  |
| 2   | 1P    | 85  | GLN  |
| 2   | 1P    | 101 | ASN  |
| 2   | 1P    | 192 | HIS  |
| 2   | 1P    | 197 | ASN  |
| 2   | 1P    | 228 | ASN  |
| 2   | 1P    | 300 | ASN  |
| 2   | 1P    | 309 | HIS  |
| 2   | 1P    | 385 | GLN  |
| 2   | 1P    | 433 | GLN  |
| 2   | 1Q    | 11  | GLN  |
| 2   | 1Q    | 14  | ASN  |
| 2   | 1Q    | 37  | HIS  |
| 2   | 1Q    | 85  | GLN  |
| 2   | 1Q    | 101 | ASN  |
| 2   | 1Q    | 133 | GLN  |
| 2   | 1Q    | 192 | HIS  |
| 2   | 1Q    | 197 | ASN  |
| 2   | 1Q    | 228 | ASN  |
| 2   | 1Q    | 300 | ASN  |
| 2   | 1Q    | 309 | HIS  |
| 2   | 1Q    | 336 | GLN  |
| 2   | 1Q    | 385 | GLN  |
| 2   | 1Q    | 433 | GLN  |
| 2   | 1R    | 11  | GLN  |
| 2   | 1R    | 14  | ASN  |
| 2   | 1R    | 37  | HIS  |
| 2   | 1R    | 85  | GLN  |
| 2   | 1R    | 101 | ASN  |
| 2   | 1R    | 192 | HIS  |
| 2   | 1R    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1R    | 228 | ASN  |
| 2   | 1R    | 300 | ASN  |
| 2   | 1R    | 309 | HIS  |
| 2   | 1R    | 336 | GLN  |
| 2   | 1R    | 385 | GLN  |
| 2   | 1R    | 433 | GLN  |
| 2   | 1S    | 8   | GLN  |
| 2   | 1S    | 11  | GLN  |
| 2   | 1S    | 37  | HIS  |
| 2   | 1S    | 85  | GLN  |
| 2   | 1S    | 101 | ASN  |
| 2   | 1S    | 192 | HIS  |
| 2   | 1S    | 197 | ASN  |
| 2   | 1S    | 228 | ASN  |
| 2   | 1S    | 300 | ASN  |
| 2   | 1S    | 309 | HIS  |
| 2   | 1S    | 385 | GLN  |
| 2   | 1S    | 433 | GLN  |
| 2   | 1T    | 11  | GLN  |
| 2   | 1T    | 14  | ASN  |
| 2   | 1T    | 37  | HIS  |
| 2   | 1T    | 85  | GLN  |
| 2   | 1T    | 101 | ASN  |
| 2   | 1T    | 192 | HIS  |
| 2   | 1T    | 197 | ASN  |
| 2   | 1T    | 228 | ASN  |
| 2   | 1T    | 300 | ASN  |
| 2   | 1T    | 309 | HIS  |
| 2   | 1T    | 385 | GLN  |
| 2   | 1T    | 433 | GLN  |
| 2   | 1U    | 11  | GLN  |
| 2   | 1U    | 14  | ASN  |
| 2   | 1U    | 37  | HIS  |
| 2   | 1U    | 85  | GLN  |
| 2   | 1U    | 101 | ASN  |
| 2   | 1U    | 192 | HIS  |
| 2   | 1U    | 197 | ASN  |
| 2   | 1U    | 228 | ASN  |
| 2   | 1U    | 300 | ASN  |
| 2   | 1U    | 309 | HIS  |
| 2   | 1U    | 385 | GLN  |
| 2   | 1U    | 433 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1V    | 11  | GLN  |
| 2   | 1V    | 14  | ASN  |
| 2   | 1V    | 37  | HIS  |
| 2   | 1V    | 85  | GLN  |
| 2   | 1V    | 101 | ASN  |
| 2   | 1V    | 192 | HIS  |
| 2   | 1V    | 197 | ASN  |
| 2   | 1V    | 228 | ASN  |
| 2   | 1V    | 300 | ASN  |
| 2   | 1V    | 309 | HIS  |
| 2   | 1V    | 336 | GLN  |
| 2   | 1V    | 385 | GLN  |
| 2   | 1V    | 433 | GLN  |
| 2   | 1W    | 11  | GLN  |
| 2   | 1W    | 14  | ASN  |
| 2   | 1W    | 37  | HIS  |
| 2   | 1W    | 85  | GLN  |
| 2   | 1W    | 192 | HIS  |
| 2   | 1W    | 197 | ASN  |
| 2   | 1W    | 228 | ASN  |
| 2   | 1W    | 300 | ASN  |
| 2   | 1W    | 309 | HIS  |
| 2   | 1W    | 385 | GLN  |
| 2   | 1W    | 433 | GLN  |
| 2   | 1X    | 11  | GLN  |
| 2   | 1X    | 14  | ASN  |
| 2   | 1X    | 37  | HIS  |
| 2   | 1X    | 85  | GLN  |
| 2   | 1X    | 192 | HIS  |
| 2   | 1X    | 197 | ASN  |
| 2   | 1X    | 228 | ASN  |
| 2   | 1X    | 300 | ASN  |
| 2   | 1X    | 309 | HIS  |
| 2   | 1X    | 336 | GLN  |
| 2   | 1X    | 385 | GLN  |
| 2   | 1X    | 433 | GLN  |
| 2   | 1Y    | 11  | GLN  |
| 2   | 1Y    | 14  | ASN  |
| 2   | 1Y    | 37  | HIS  |
| 2   | 1Y    | 85  | GLN  |
| 2   | 1Y    | 192 | HIS  |
| 2   | 1Y    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1Y    | 228 | ASN  |
| 2   | 1Y    | 300 | ASN  |
| 2   | 1Y    | 309 | HIS  |
| 2   | 1Y    | 336 | GLN  |
| 2   | 1Y    | 385 | GLN  |
| 2   | 1Y    | 433 | GLN  |
| 2   | 1Z    | 11  | GLN  |
| 2   | 1Z    | 14  | ASN  |
| 2   | 1Z    | 37  | HIS  |
| 2   | 1Z    | 85  | GLN  |
| 2   | 1Z    | 101 | ASN  |
| 2   | 1Z    | 133 | GLN  |
| 2   | 1Z    | 192 | HIS  |
| 2   | 1Z    | 197 | ASN  |
| 2   | 1Z    | 228 | ASN  |
| 2   | 1Z    | 300 | ASN  |
| 2   | 1Z    | 309 | HIS  |
| 2   | 1Z    | 385 | GLN  |
| 2   | 1Z    | 433 | GLN  |
| 1   | 2A    | 8   | HIS  |
| 1   | 2A    | 107 | HIS  |
| 1   | 2A    | 139 | HIS  |
| 1   | 2A    | 186 | ASN  |
| 1   | 2A    | 192 | HIS  |
| 1   | 2A    | 216 | ASN  |
| 1   | 2A    | 258 | ASN  |
| 1   | 2A    | 329 | ASN  |
| 1   | 2A    | 356 | ASN  |
| 1   | 2A    | 380 | ASN  |
| 1   | 2A    | 393 | HIS  |
| 1   | 2B    | 8   | HIS  |
| 1   | 2B    | 107 | HIS  |
| 1   | 2B    | 139 | HIS  |
| 1   | 2B    | 186 | ASN  |
| 1   | 2B    | 192 | HIS  |
| 1   | 2B    | 216 | ASN  |
| 1   | 2B    | 258 | ASN  |
| 1   | 2B    | 329 | ASN  |
| 1   | 2B    | 356 | ASN  |
| 1   | 2B    | 380 | ASN  |
| 1   | 2B    | 393 | HIS  |
| 1   | 2C    | 8   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2C    | 107 | HIS  |
| 1   | 2C    | 139 | HIS  |
| 1   | 2C    | 186 | ASN  |
| 1   | 2C    | 192 | HIS  |
| 1   | 2C    | 216 | ASN  |
| 1   | 2C    | 258 | ASN  |
| 1   | 2C    | 356 | ASN  |
| 1   | 2C    | 380 | ASN  |
| 1   | 2C    | 393 | HIS  |
| 1   | 2D    | 8   | HIS  |
| 1   | 2D    | 107 | HIS  |
| 1   | 2D    | 139 | HIS  |
| 1   | 2D    | 186 | ASN  |
| 1   | 2D    | 192 | HIS  |
| 1   | 2D    | 216 | ASN  |
| 1   | 2D    | 258 | ASN  |
| 1   | 2D    | 356 | ASN  |
| 1   | 2D    | 380 | ASN  |
| 1   | 2D    | 393 | HIS  |
| 1   | 2E    | 8   | HIS  |
| 1   | 2E    | 28  | HIS  |
| 1   | 2E    | 107 | HIS  |
| 1   | 2E    | 139 | HIS  |
| 1   | 2E    | 186 | ASN  |
| 1   | 2E    | 216 | ASN  |
| 1   | 2E    | 258 | ASN  |
| 1   | 2E    | 356 | ASN  |
| 1   | 2E    | 380 | ASN  |
| 1   | 2E    | 393 | HIS  |
| 1   | 2F    | 8   | HIS  |
| 1   | 2F    | 28  | HIS  |
| 1   | 2F    | 107 | HIS  |
| 1   | 2F    | 139 | HIS  |
| 1   | 2F    | 186 | ASN  |
| 1   | 2F    | 216 | ASN  |
| 1   | 2F    | 258 | ASN  |
| 1   | 2F    | 293 | ASN  |
| 1   | 2F    | 329 | ASN  |
| 1   | 2F    | 356 | ASN  |
| 1   | 2F    | 380 | ASN  |
| 1   | 2F    | 393 | HIS  |
| 1   | 2G    | 8   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2G    | 107 | HIS  |
| 1   | 2G    | 139 | HIS  |
| 1   | 2G    | 186 | ASN  |
| 1   | 2G    | 216 | ASN  |
| 1   | 2G    | 258 | ASN  |
| 1   | 2G    | 329 | ASN  |
| 1   | 2G    | 356 | ASN  |
| 1   | 2G    | 380 | ASN  |
| 1   | 2G    | 393 | HIS  |
| 1   | 2I    | 8   | HIS  |
| 1   | 2I    | 107 | HIS  |
| 1   | 2I    | 139 | HIS  |
| 1   | 2I    | 186 | ASN  |
| 1   | 2I    | 216 | ASN  |
| 1   | 2I    | 258 | ASN  |
| 1   | 2I    | 356 | ASN  |
| 1   | 2I    | 380 | ASN  |
| 1   | 2I    | 393 | HIS  |
| 1   | 2J    | 8   | HIS  |
| 1   | 2J    | 107 | HIS  |
| 1   | 2J    | 139 | HIS  |
| 1   | 2J    | 186 | ASN  |
| 1   | 2J    | 216 | ASN  |
| 1   | 2J    | 258 | ASN  |
| 1   | 2J    | 329 | ASN  |
| 1   | 2J    | 356 | ASN  |
| 1   | 2J    | 380 | ASN  |
| 1   | 2J    | 393 | HIS  |
| 1   | 2K    | 8   | HIS  |
| 1   | 2K    | 107 | HIS  |
| 1   | 2K    | 139 | HIS  |
| 1   | 2K    | 186 | ASN  |
| 1   | 2K    | 216 | ASN  |
| 1   | 2K    | 329 | ASN  |
| 1   | 2K    | 356 | ASN  |
| 1   | 2K    | 380 | ASN  |
| 1   | 2K    | 393 | HIS  |
| 1   | 2L    | 8   | HIS  |
| 1   | 2L    | 28  | HIS  |
| 1   | 2L    | 107 | HIS  |
| 1   | 2L    | 139 | HIS  |
| 1   | 2L    | 186 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2L    | 216 | ASN  |
| 1   | 2L    | 329 | ASN  |
| 1   | 2L    | 356 | ASN  |
| 1   | 2L    | 380 | ASN  |
| 1   | 2L    | 393 | HIS  |
| 1   | 2M    | 8   | HIS  |
| 1   | 2M    | 107 | HIS  |
| 1   | 2M    | 139 | HIS  |
| 1   | 2M    | 186 | ASN  |
| 1   | 2M    | 192 | HIS  |
| 1   | 2M    | 216 | ASN  |
| 1   | 2M    | 329 | ASN  |
| 1   | 2M    | 356 | ASN  |
| 1   | 2M    | 380 | ASN  |
| 1   | 2M    | 393 | HIS  |
| 1   | 2N    | 8   | HIS  |
| 1   | 2N    | 107 | HIS  |
| 1   | 2N    | 139 | HIS  |
| 1   | 2N    | 186 | ASN  |
| 1   | 2N    | 192 | HIS  |
| 1   | 2N    | 216 | ASN  |
| 1   | 2N    | 258 | ASN  |
| 1   | 2N    | 329 | ASN  |
| 1   | 2N    | 356 | ASN  |
| 1   | 2N    | 380 | ASN  |
| 1   | 2N    | 393 | HIS  |
| 2   | 2H    | 11  | GLN  |
| 2   | 2H    | 14  | ASN  |
| 2   | 2H    | 37  | HIS  |
| 2   | 2H    | 85  | GLN  |
| 2   | 2H    | 101 | ASN  |
| 2   | 2H    | 133 | GLN  |
| 2   | 2H    | 192 | HIS  |
| 2   | 2H    | 197 | ASN  |
| 2   | 2H    | 228 | ASN  |
| 2   | 2H    | 300 | ASN  |
| 2   | 2H    | 309 | HIS  |
| 2   | 2H    | 385 | GLN  |
| 2   | 2H    | 433 | GLN  |
| 2   | 2O    | 11  | GLN  |
| 2   | 2O    | 14  | ASN  |
| 2   | 2O    | 37  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2O    | 85  | GLN  |
| 2   | 2O    | 101 | ASN  |
| 2   | 2O    | 192 | HIS  |
| 2   | 2O    | 197 | ASN  |
| 2   | 2O    | 228 | ASN  |
| 2   | 2O    | 300 | ASN  |
| 2   | 2O    | 309 | HIS  |
| 2   | 2O    | 336 | GLN  |
| 2   | 2O    | 385 | GLN  |
| 2   | 2O    | 433 | GLN  |
| 2   | 2P    | 11  | GLN  |
| 2   | 2P    | 14  | ASN  |
| 2   | 2P    | 37  | HIS  |
| 2   | 2P    | 85  | GLN  |
| 2   | 2P    | 101 | ASN  |
| 2   | 2P    | 192 | HIS  |
| 2   | 2P    | 197 | ASN  |
| 2   | 2P    | 228 | ASN  |
| 2   | 2P    | 300 | ASN  |
| 2   | 2P    | 309 | HIS  |
| 2   | 2P    | 385 | GLN  |
| 2   | 2P    | 433 | GLN  |
| 2   | 2Q    | 11  | GLN  |
| 2   | 2Q    | 14  | ASN  |
| 2   | 2Q    | 37  | HIS  |
| 2   | 2Q    | 85  | GLN  |
| 2   | 2Q    | 101 | ASN  |
| 2   | 2Q    | 192 | HIS  |
| 2   | 2Q    | 197 | ASN  |
| 2   | 2Q    | 228 | ASN  |
| 2   | 2Q    | 300 | ASN  |
| 2   | 2Q    | 309 | HIS  |
| 2   | 2Q    | 385 | GLN  |
| 2   | 2Q    | 433 | GLN  |
| 2   | 2R    | 11  | GLN  |
| 2   | 2R    | 14  | ASN  |
| 2   | 2R    | 37  | HIS  |
| 2   | 2R    | 85  | GLN  |
| 2   | 2R    | 101 | ASN  |
| 2   | 2R    | 192 | HIS  |
| 2   | 2R    | 197 | ASN  |
| 2   | 2R    | 228 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2R    | 300 | ASN  |
| 2   | 2R    | 309 | HIS  |
| 2   | 2R    | 336 | GLN  |
| 2   | 2R    | 385 | GLN  |
| 2   | 2R    | 433 | GLN  |
| 2   | 2S    | 8   | GLN  |
| 2   | 2S    | 11  | GLN  |
| 2   | 2S    | 37  | HIS  |
| 2   | 2S    | 85  | GLN  |
| 2   | 2S    | 101 | ASN  |
| 2   | 2S    | 192 | HIS  |
| 2   | 2S    | 197 | ASN  |
| 2   | 2S    | 228 | ASN  |
| 2   | 2S    | 300 | ASN  |
| 2   | 2S    | 309 | HIS  |
| 2   | 2S    | 385 | GLN  |
| 2   | 2S    | 433 | GLN  |
| 2   | 2T    | 11  | GLN  |
| 2   | 2T    | 14  | ASN  |
| 2   | 2T    | 37  | HIS  |
| 2   | 2T    | 85  | GLN  |
| 2   | 2T    | 101 | ASN  |
| 2   | 2T    | 192 | HIS  |
| 2   | 2T    | 197 | ASN  |
| 2   | 2T    | 228 | ASN  |
| 2   | 2T    | 300 | ASN  |
| 2   | 2T    | 309 | HIS  |
| 2   | 2T    | 385 | GLN  |
| 2   | 2T    | 433 | GLN  |
| 2   | 2U    | 11  | GLN  |
| 2   | 2U    | 14  | ASN  |
| 2   | 2U    | 37  | HIS  |
| 2   | 2U    | 85  | GLN  |
| 2   | 2U    | 101 | ASN  |
| 2   | 2U    | 192 | HIS  |
| 2   | 2U    | 197 | ASN  |
| 2   | 2U    | 228 | ASN  |
| 2   | 2U    | 300 | ASN  |
| 2   | 2U    | 309 | HIS  |
| 2   | 2U    | 385 | GLN  |
| 2   | 2U    | 433 | GLN  |
| 2   | 2V    | 11  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2V    | 14  | ASN  |
| 2   | 2V    | 37  | HIS  |
| 2   | 2V    | 85  | GLN  |
| 2   | 2V    | 101 | ASN  |
| 2   | 2V    | 192 | HIS  |
| 2   | 2V    | 197 | ASN  |
| 2   | 2V    | 228 | ASN  |
| 2   | 2V    | 300 | ASN  |
| 2   | 2V    | 309 | HIS  |
| 2   | 2V    | 336 | GLN  |
| 2   | 2V    | 385 | GLN  |
| 2   | 2V    | 433 | GLN  |
| 2   | 2W    | 11  | GLN  |
| 2   | 2W    | 14  | ASN  |
| 2   | 2W    | 37  | HIS  |
| 2   | 2W    | 85  | GLN  |
| 2   | 2W    | 101 | ASN  |
| 2   | 2W    | 192 | HIS  |
| 2   | 2W    | 197 | ASN  |
| 2   | 2W    | 228 | ASN  |
| 2   | 2W    | 300 | ASN  |
| 2   | 2W    | 309 | HIS  |
| 2   | 2W    | 385 | GLN  |
| 2   | 2W    | 433 | GLN  |
| 2   | 2X    | 11  | GLN  |
| 2   | 2X    | 14  | ASN  |
| 2   | 2X    | 15  | GLN  |
| 2   | 2X    | 37  | HIS  |
| 2   | 2X    | 85  | GLN  |
| 2   | 2X    | 101 | ASN  |
| 2   | 2X    | 192 | HIS  |
| 2   | 2X    | 197 | ASN  |
| 2   | 2X    | 228 | ASN  |
| 2   | 2X    | 300 | ASN  |
| 2   | 2X    | 309 | HIS  |
| 2   | 2X    | 336 | GLN  |
| 2   | 2X    | 385 | GLN  |
| 2   | 2X    | 433 | GLN  |
| 2   | 2Y    | 11  | GLN  |
| 2   | 2Y    | 14  | ASN  |
| 2   | 2Y    | 37  | HIS  |
| 2   | 2Y    | 85  | GLN  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2Y    | 101 | ASN  |
| 2   | 2Y    | 192 | HIS  |
| 2   | 2Y    | 197 | ASN  |
| 2   | 2Y    | 228 | ASN  |
| 2   | 2Y    | 300 | ASN  |
| 2   | 2Y    | 309 | HIS  |
| 2   | 2Y    | 336 | GLN  |
| 2   | 2Y    | 385 | GLN  |
| 2   | 2Y    | 433 | GLN  |
| 2   | 2Z    | 11  | GLN  |
| 2   | 2Z    | 14  | ASN  |
| 2   | 2Z    | 37  | HIS  |
| 2   | 2Z    | 85  | GLN  |
| 2   | 2Z    | 101 | ASN  |
| 2   | 2Z    | 133 | GLN  |
| 2   | 2Z    | 192 | HIS  |
| 2   | 2Z    | 197 | ASN  |
| 2   | 2Z    | 228 | ASN  |
| 2   | 2Z    | 300 | ASN  |
| 2   | 2Z    | 309 | HIS  |
| 2   | 2Z    | 385 | GLN  |
| 2   | 2Z    | 433 | GLN  |
| 1   | 3A    | 8   | HIS  |
| 1   | 3A    | 28  | HIS  |
| 1   | 3A    | 107 | HIS  |
| 1   | 3A    | 139 | HIS  |
| 1   | 3A    | 186 | ASN  |
| 1   | 3A    | 192 | HIS  |
| 1   | 3A    | 216 | ASN  |
| 1   | 3A    | 258 | ASN  |
| 1   | 3A    | 293 | ASN  |
| 1   | 3A    | 356 | ASN  |
| 1   | 3A    | 380 | ASN  |
| 1   | 3A    | 393 | HIS  |
| 1   | 3B    | 8   | HIS  |
| 1   | 3B    | 107 | HIS  |
| 1   | 3B    | 139 | HIS  |
| 1   | 3B    | 186 | ASN  |
| 1   | 3B    | 192 | HIS  |
| 1   | 3B    | 216 | ASN  |
| 1   | 3B    | 258 | ASN  |
| 1   | 3B    | 356 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3B    | 380 | ASN  |
| 1   | 3B    | 393 | HIS  |
| 1   | 3C    | 8   | HIS  |
| 1   | 3C    | 107 | HIS  |
| 1   | 3C    | 139 | HIS  |
| 1   | 3C    | 186 | ASN  |
| 1   | 3C    | 192 | HIS  |
| 1   | 3C    | 216 | ASN  |
| 1   | 3C    | 258 | ASN  |
| 1   | 3C    | 356 | ASN  |
| 1   | 3C    | 380 | ASN  |
| 1   | 3C    | 393 | HIS  |
| 1   | 3D    | 8   | HIS  |
| 1   | 3D    | 107 | HIS  |
| 1   | 3D    | 139 | HIS  |
| 1   | 3D    | 186 | ASN  |
| 1   | 3D    | 192 | HIS  |
| 1   | 3D    | 216 | ASN  |
| 1   | 3D    | 258 | ASN  |
| 1   | 3D    | 356 | ASN  |
| 1   | 3D    | 380 | ASN  |
| 1   | 3D    | 393 | HIS  |
| 1   | 3E    | 8   | HIS  |
| 1   | 3E    | 28  | HIS  |
| 1   | 3E    | 107 | HIS  |
| 1   | 3E    | 139 | HIS  |
| 1   | 3E    | 186 | ASN  |
| 1   | 3E    | 216 | ASN  |
| 1   | 3E    | 258 | ASN  |
| 1   | 3E    | 356 | ASN  |
| 1   | 3E    | 380 | ASN  |
| 1   | 3E    | 393 | HIS  |
| 1   | 3F    | 8   | HIS  |
| 1   | 3F    | 28  | HIS  |
| 1   | 3F    | 107 | HIS  |
| 1   | 3F    | 139 | HIS  |
| 1   | 3F    | 186 | ASN  |
| 1   | 3F    | 216 | ASN  |
| 1   | 3F    | 258 | ASN  |
| 1   | 3F    | 356 | ASN  |
| 1   | 3F    | 380 | ASN  |
| 1   | 3F    | 393 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3G    | 8   | HIS  |
| 1   | 3G    | 107 | HIS  |
| 1   | 3G    | 139 | HIS  |
| 1   | 3G    | 186 | ASN  |
| 1   | 3G    | 216 | ASN  |
| 1   | 3G    | 258 | ASN  |
| 1   | 3G    | 356 | ASN  |
| 1   | 3G    | 380 | ASN  |
| 1   | 3G    | 393 | HIS  |
| 1   | 3I    | 8   | HIS  |
| 1   | 3I    | 107 | HIS  |
| 1   | 3I    | 139 | HIS  |
| 1   | 3I    | 186 | ASN  |
| 1   | 3I    | 216 | ASN  |
| 1   | 3I    | 258 | ASN  |
| 1   | 3I    | 356 | ASN  |
| 1   | 3I    | 380 | ASN  |
| 1   | 3I    | 393 | HIS  |
| 1   | 3J    | 8   | HIS  |
| 1   | 3J    | 107 | HIS  |
| 1   | 3J    | 139 | HIS  |
| 1   | 3J    | 186 | ASN  |
| 1   | 3J    | 216 | ASN  |
| 1   | 3J    | 258 | ASN  |
| 1   | 3J    | 356 | ASN  |
| 1   | 3J    | 380 | ASN  |
| 1   | 3J    | 393 | HIS  |
| 1   | 3K    | 8   | HIS  |
| 1   | 3K    | 107 | HIS  |
| 1   | 3K    | 139 | HIS  |
| 1   | 3K    | 186 | ASN  |
| 1   | 3K    | 216 | ASN  |
| 1   | 3K    | 258 | ASN  |
| 1   | 3K    | 356 | ASN  |
| 1   | 3K    | 380 | ASN  |
| 1   | 3K    | 393 | HIS  |
| 1   | 3L    | 8   | HIS  |
| 1   | 3L    | 28  | HIS  |
| 1   | 3L    | 107 | HIS  |
| 1   | 3L    | 139 | HIS  |
| 1   | 3L    | 186 | ASN  |
| 1   | 3L    | 216 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3L    | 258 | ASN  |
| 1   | 3L    | 329 | ASN  |
| 1   | 3L    | 356 | ASN  |
| 1   | 3L    | 380 | ASN  |
| 1   | 3L    | 393 | HIS  |
| 1   | 3M    | 8   | HIS  |
| 1   | 3M    | 107 | HIS  |
| 1   | 3M    | 139 | HIS  |
| 1   | 3M    | 186 | ASN  |
| 1   | 3M    | 192 | HIS  |
| 1   | 3M    | 216 | ASN  |
| 1   | 3M    | 258 | ASN  |
| 1   | 3M    | 329 | ASN  |
| 1   | 3M    | 356 | ASN  |
| 1   | 3M    | 380 | ASN  |
| 1   | 3M    | 393 | HIS  |
| 1   | 3N    | 8   | HIS  |
| 1   | 3N    | 107 | HIS  |
| 1   | 3N    | 139 | HIS  |
| 1   | 3N    | 186 | ASN  |
| 1   | 3N    | 192 | HIS  |
| 1   | 3N    | 216 | ASN  |
| 1   | 3N    | 258 | ASN  |
| 1   | 3N    | 329 | ASN  |
| 1   | 3N    | 356 | ASN  |
| 1   | 3N    | 380 | ASN  |
| 1   | 3N    | 393 | HIS  |
| 2   | 3H    | 14  | ASN  |
| 2   | 3H    | 15  | GLN  |
| 2   | 3H    | 37  | HIS  |
| 2   | 3H    | 85  | GLN  |
| 2   | 3H    | 101 | ASN  |
| 2   | 3H    | 133 | GLN  |
| 2   | 3H    | 192 | HIS  |
| 2   | 3H    | 197 | ASN  |
| 2   | 3H    | 228 | ASN  |
| 2   | 3H    | 300 | ASN  |
| 2   | 3H    | 309 | HIS  |
| 2   | 3H    | 385 | GLN  |
| 2   | 3H    | 433 | GLN  |
| 2   | 3O    | 14  | ASN  |
| 2   | 3O    | 15  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3O    | 37  | HIS  |
| 2   | 3O    | 85  | GLN  |
| 2   | 3O    | 101 | ASN  |
| 2   | 3O    | 192 | HIS  |
| 2   | 3O    | 197 | ASN  |
| 2   | 3O    | 228 | ASN  |
| 2   | 3O    | 300 | ASN  |
| 2   | 3O    | 309 | HIS  |
| 2   | 3O    | 336 | GLN  |
| 2   | 3O    | 385 | GLN  |
| 2   | 3O    | 433 | GLN  |
| 2   | 3P    | 14  | ASN  |
| 2   | 3P    | 15  | GLN  |
| 2   | 3P    | 37  | HIS  |
| 2   | 3P    | 85  | GLN  |
| 2   | 3P    | 101 | ASN  |
| 2   | 3P    | 192 | HIS  |
| 2   | 3P    | 228 | ASN  |
| 2   | 3P    | 300 | ASN  |
| 2   | 3P    | 309 | HIS  |
| 2   | 3P    | 385 | GLN  |
| 2   | 3P    | 433 | GLN  |
| 2   | 3Q    | 14  | ASN  |
| 2   | 3Q    | 15  | GLN  |
| 2   | 3Q    | 37  | HIS  |
| 2   | 3Q    | 85  | GLN  |
| 2   | 3Q    | 101 | ASN  |
| 2   | 3Q    | 192 | HIS  |
| 2   | 3Q    | 197 | ASN  |
| 2   | 3Q    | 228 | ASN  |
| 2   | 3Q    | 300 | ASN  |
| 2   | 3Q    | 309 | HIS  |
| 2   | 3Q    | 385 | GLN  |
| 2   | 3Q    | 433 | GLN  |
| 2   | 3R    | 14  | ASN  |
| 2   | 3R    | 15  | GLN  |
| 2   | 3R    | 37  | HIS  |
| 2   | 3R    | 85  | GLN  |
| 2   | 3R    | 101 | ASN  |
| 2   | 3R    | 192 | HIS  |
| 2   | 3R    | 197 | ASN  |
| 2   | 3R    | 228 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3R    | 300 | ASN  |
| 2   | 3R    | 309 | HIS  |
| 2   | 3R    | 336 | GLN  |
| 2   | 3R    | 385 | GLN  |
| 2   | 3R    | 433 | GLN  |
| 2   | 3S    | 8   | GLN  |
| 2   | 3S    | 15  | GLN  |
| 2   | 3S    | 37  | HIS  |
| 2   | 3S    | 85  | GLN  |
| 2   | 3S    | 101 | ASN  |
| 2   | 3S    | 192 | HIS  |
| 2   | 3S    | 197 | ASN  |
| 2   | 3S    | 228 | ASN  |
| 2   | 3S    | 300 | ASN  |
| 2   | 3S    | 309 | HIS  |
| 2   | 3S    | 385 | GLN  |
| 2   | 3S    | 433 | GLN  |
| 2   | 3T    | 14  | ASN  |
| 2   | 3T    | 15  | GLN  |
| 2   | 3T    | 37  | HIS  |
| 2   | 3T    | 85  | GLN  |
| 2   | 3T    | 101 | ASN  |
| 2   | 3T    | 192 | HIS  |
| 2   | 3T    | 197 | ASN  |
| 2   | 3T    | 228 | ASN  |
| 2   | 3T    | 300 | ASN  |
| 2   | 3T    | 309 | HIS  |
| 2   | 3T    | 385 | GLN  |
| 2   | 3T    | 433 | GLN  |
| 2   | 3U    | 11  | GLN  |
| 2   | 3U    | 14  | ASN  |
| 2   | 3U    | 37  | HIS  |
| 2   | 3U    | 85  | GLN  |
| 2   | 3U    | 101 | ASN  |
| 2   | 3U    | 192 | HIS  |
| 2   | 3U    | 197 | ASN  |
| 2   | 3U    | 228 | ASN  |
| 2   | 3U    | 300 | ASN  |
| 2   | 3U    | 309 | HIS  |
| 2   | 3U    | 385 | GLN  |
| 2   | 3U    | 433 | GLN  |
| 2   | 3V    | 14  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3V    | 15  | GLN  |
| 2   | 3V    | 37  | HIS  |
| 2   | 3V    | 85  | GLN  |
| 2   | 3V    | 101 | ASN  |
| 2   | 3V    | 192 | HIS  |
| 2   | 3V    | 197 | ASN  |
| 2   | 3V    | 228 | ASN  |
| 2   | 3V    | 300 | ASN  |
| 2   | 3V    | 309 | HIS  |
| 2   | 3V    | 336 | GLN  |
| 2   | 3V    | 385 | GLN  |
| 2   | 3V    | 433 | GLN  |
| 2   | 3W    | 11  | GLN  |
| 2   | 3W    | 14  | ASN  |
| 2   | 3W    | 37  | HIS  |
| 2   | 3W    | 85  | GLN  |
| 2   | 3W    | 101 | ASN  |
| 2   | 3W    | 192 | HIS  |
| 2   | 3W    | 197 | ASN  |
| 2   | 3W    | 228 | ASN  |
| 2   | 3W    | 300 | ASN  |
| 2   | 3W    | 309 | HIS  |
| 2   | 3W    | 385 | GLN  |
| 2   | 3W    | 433 | GLN  |
| 2   | 3X    | 8   | GLN  |
| 2   | 3X    | 15  | GLN  |
| 2   | 3X    | 37  | HIS  |
| 2   | 3X    | 85  | GLN  |
| 2   | 3X    | 101 | ASN  |
| 2   | 3X    | 192 | HIS  |
| 2   | 3X    | 197 | ASN  |
| 2   | 3X    | 228 | ASN  |
| 2   | 3X    | 300 | ASN  |
| 2   | 3X    | 309 | HIS  |
| 2   | 3X    | 336 | GLN  |
| 2   | 3X    | 385 | GLN  |
| 2   | 3X    | 433 | GLN  |
| 2   | 3Y    | 14  | ASN  |
| 2   | 3Y    | 15  | GLN  |
| 2   | 3Y    | 37  | HIS  |
| 2   | 3Y    | 85  | GLN  |
| 2   | 3Y    | 101 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3Y    | 192 | HIS  |
| 2   | 3Y    | 197 | ASN  |
| 2   | 3Y    | 228 | ASN  |
| 2   | 3Y    | 300 | ASN  |
| 2   | 3Y    | 309 | HIS  |
| 2   | 3Y    | 336 | GLN  |
| 2   | 3Y    | 385 | GLN  |
| 2   | 3Y    | 433 | GLN  |
| 2   | 3Z    | 14  | ASN  |
| 2   | 3Z    | 15  | GLN  |
| 2   | 3Z    | 37  | HIS  |
| 2   | 3Z    | 85  | GLN  |
| 2   | 3Z    | 101 | ASN  |
| 2   | 3Z    | 133 | GLN  |
| 2   | 3Z    | 192 | HIS  |
| 2   | 3Z    | 197 | ASN  |
| 2   | 3Z    | 228 | ASN  |
| 2   | 3Z    | 300 | ASN  |
| 2   | 3Z    | 309 | HIS  |
| 2   | 3Z    | 385 | GLN  |
| 2   | 3Z    | 433 | GLN  |
| 1   | 4A    | 8   | HIS  |
| 1   | 4A    | 107 | HIS  |
| 1   | 4A    | 139 | HIS  |
| 1   | 4A    | 186 | ASN  |
| 1   | 4A    | 192 | HIS  |
| 1   | 4A    | 216 | ASN  |
| 1   | 4A    | 356 | ASN  |
| 1   | 4A    | 380 | ASN  |
| 1   | 4A    | 393 | HIS  |
| 1   | 4B    | 8   | HIS  |
| 1   | 4B    | 107 | HIS  |
| 1   | 4B    | 139 | HIS  |
| 1   | 4B    | 186 | ASN  |
| 1   | 4B    | 192 | HIS  |
| 1   | 4B    | 216 | ASN  |
| 1   | 4B    | 258 | ASN  |
| 1   | 4B    | 356 | ASN  |
| 1   | 4B    | 380 | ASN  |
| 1   | 4B    | 393 | HIS  |
| 1   | 4C    | 8   | HIS  |
| 1   | 4C    | 28  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4C    | 107 | HIS  |
| 1   | 4C    | 139 | HIS  |
| 1   | 4C    | 186 | ASN  |
| 1   | 4C    | 192 | HIS  |
| 1   | 4C    | 216 | ASN  |
| 1   | 4C    | 258 | ASN  |
| 1   | 4C    | 356 | ASN  |
| 1   | 4C    | 380 | ASN  |
| 1   | 4C    | 393 | HIS  |
| 1   | 4D    | 8   | HIS  |
| 1   | 4D    | 107 | HIS  |
| 1   | 4D    | 139 | HIS  |
| 1   | 4D    | 186 | ASN  |
| 1   | 4D    | 192 | HIS  |
| 1   | 4D    | 216 | ASN  |
| 1   | 4D    | 258 | ASN  |
| 1   | 4D    | 356 | ASN  |
| 1   | 4D    | 380 | ASN  |
| 1   | 4D    | 393 | HIS  |
| 1   | 4E    | 8   | HIS  |
| 1   | 4E    | 28  | HIS  |
| 1   | 4E    | 107 | HIS  |
| 1   | 4E    | 139 | HIS  |
| 1   | 4E    | 186 | ASN  |
| 1   | 4E    | 216 | ASN  |
| 1   | 4E    | 258 | ASN  |
| 1   | 4E    | 356 | ASN  |
| 1   | 4E    | 380 | ASN  |
| 1   | 4E    | 393 | HIS  |
| 1   | 4F    | 8   | HIS  |
| 1   | 4F    | 28  | HIS  |
| 1   | 4F    | 107 | HIS  |
| 1   | 4F    | 139 | HIS  |
| 1   | 4F    | 186 | ASN  |
| 1   | 4F    | 216 | ASN  |
| 1   | 4F    | 356 | ASN  |
| 1   | 4F    | 380 | ASN  |
| 1   | 4F    | 393 | HIS  |
| 1   | 4G    | 8   | HIS  |
| 1   | 4G    | 107 | HIS  |
| 1   | 4G    | 139 | HIS  |
| 1   | 4G    | 186 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4G    | 216 | ASN  |
| 1   | 4G    | 258 | ASN  |
| 1   | 4G    | 356 | ASN  |
| 1   | 4G    | 380 | ASN  |
| 1   | 4G    | 393 | HIS  |
| 1   | 4I    | 8   | HIS  |
| 1   | 4I    | 107 | HIS  |
| 1   | 4I    | 139 | HIS  |
| 1   | 4I    | 186 | ASN  |
| 1   | 4I    | 216 | ASN  |
| 1   | 4I    | 258 | ASN  |
| 1   | 4I    | 356 | ASN  |
| 1   | 4I    | 380 | ASN  |
| 1   | 4I    | 393 | HIS  |
| 1   | 4J    | 8   | HIS  |
| 1   | 4J    | 107 | HIS  |
| 1   | 4J    | 139 | HIS  |
| 1   | 4J    | 186 | ASN  |
| 1   | 4J    | 216 | ASN  |
| 1   | 4J    | 258 | ASN  |
| 1   | 4J    | 356 | ASN  |
| 1   | 4J    | 380 | ASN  |
| 1   | 4J    | 393 | HIS  |
| 1   | 4K    | 8   | HIS  |
| 1   | 4K    | 107 | HIS  |
| 1   | 4K    | 139 | HIS  |
| 1   | 4K    | 186 | ASN  |
| 1   | 4K    | 192 | HIS  |
| 1   | 4K    | 216 | ASN  |
| 1   | 4K    | 258 | ASN  |
| 1   | 4K    | 356 | ASN  |
| 1   | 4K    | 380 | ASN  |
| 1   | 4K    | 393 | HIS  |
| 1   | 4L    | 8   | HIS  |
| 1   | 4L    | 28  | HIS  |
| 1   | 4L    | 107 | HIS  |
| 1   | 4L    | 186 | ASN  |
| 1   | 4L    | 216 | ASN  |
| 1   | 4L    | 258 | ASN  |
| 1   | 4L    | 301 | GLN  |
| 1   | 4L    | 356 | ASN  |
| 1   | 4L    | 380 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4L    | 393 | HIS  |
| 1   | 4M    | 8   | HIS  |
| 1   | 4M    | 107 | HIS  |
| 1   | 4M    | 139 | HIS  |
| 1   | 4M    | 186 | ASN  |
| 1   | 4M    | 192 | HIS  |
| 1   | 4M    | 216 | ASN  |
| 1   | 4M    | 258 | ASN  |
| 1   | 4M    | 356 | ASN  |
| 1   | 4M    | 380 | ASN  |
| 1   | 4M    | 393 | HIS  |
| 1   | 4N    | 8   | HIS  |
| 1   | 4N    | 107 | HIS  |
| 1   | 4N    | 139 | HIS  |
| 1   | 4N    | 186 | ASN  |
| 1   | 4N    | 192 | HIS  |
| 1   | 4N    | 216 | ASN  |
| 1   | 4N    | 258 | ASN  |
| 1   | 4N    | 356 | ASN  |
| 1   | 4N    | 380 | ASN  |
| 1   | 4N    | 393 | HIS  |
| 2   | 4H    | 11  | GLN  |
| 2   | 4H    | 14  | ASN  |
| 2   | 4H    | 37  | HIS  |
| 2   | 4H    | 85  | GLN  |
| 2   | 4H    | 101 | ASN  |
| 2   | 4H    | 133 | GLN  |
| 2   | 4H    | 192 | HIS  |
| 2   | 4H    | 197 | ASN  |
| 2   | 4H    | 228 | ASN  |
| 2   | 4H    | 300 | ASN  |
| 2   | 4H    | 309 | HIS  |
| 2   | 4H    | 385 | GLN  |
| 2   | 4H    | 433 | GLN  |
| 2   | 4O    | 11  | GLN  |
| 2   | 4O    | 14  | ASN  |
| 2   | 4O    | 15  | GLN  |
| 2   | 4O    | 37  | HIS  |
| 2   | 4O    | 85  | GLN  |
| 2   | 4O    | 101 | ASN  |
| 2   | 4O    | 192 | HIS  |
| 2   | 4O    | 197 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 4O    | 228 | ASN  |
| 2   | 4O    | 300 | ASN  |
| 2   | 4O    | 309 | HIS  |
| 2   | 4O    | 336 | GLN  |
| 2   | 4O    | 385 | GLN  |
| 2   | 4O    | 433 | GLN  |
| 2   | 4P    | 11  | GLN  |
| 2   | 4P    | 14  | ASN  |
| 2   | 4P    | 15  | GLN  |
| 2   | 4P    | 37  | HIS  |
| 2   | 4P    | 85  | GLN  |
| 2   | 4P    | 101 | ASN  |
| 2   | 4P    | 192 | HIS  |
| 2   | 4P    | 197 | ASN  |
| 2   | 4P    | 228 | ASN  |
| 2   | 4P    | 300 | ASN  |
| 2   | 4P    | 309 | HIS  |
| 2   | 4P    | 385 | GLN  |
| 2   | 4P    | 433 | GLN  |
| 2   | 4Q    | 14  | ASN  |
| 2   | 4Q    | 15  | GLN  |
| 2   | 4Q    | 37  | HIS  |
| 2   | 4Q    | 85  | GLN  |
| 2   | 4Q    | 101 | ASN  |
| 2   | 4Q    | 192 | HIS  |
| 2   | 4Q    | 197 | ASN  |
| 2   | 4Q    | 228 | ASN  |
| 2   | 4Q    | 300 | ASN  |
| 2   | 4Q    | 309 | HIS  |
| 2   | 4Q    | 385 | GLN  |
| 2   | 4Q    | 433 | GLN  |
| 2   | 4R    | 14  | ASN  |
| 2   | 4R    | 15  | GLN  |
| 2   | 4R    | 37  | HIS  |
| 2   | 4R    | 85  | GLN  |
| 2   | 4R    | 101 | ASN  |
| 2   | 4R    | 192 | HIS  |
| 2   | 4R    | 197 | ASN  |
| 2   | 4R    | 228 | ASN  |
| 2   | 4R    | 300 | ASN  |
| 2   | 4R    | 309 | HIS  |
| 2   | 4R    | 336 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 4R    | 385 | GLN  |
| 2   | 4R    | 433 | GLN  |
| 2   | 4S    | 8   | GLN  |
| 2   | 4S    | 11  | GLN  |
| 2   | 4S    | 15  | GLN  |
| 2   | 4S    | 37  | HIS  |
| 2   | 4S    | 85  | GLN  |
| 2   | 4S    | 101 | ASN  |
| 2   | 4S    | 192 | HIS  |
| 2   | 4S    | 197 | ASN  |
| 2   | 4S    | 228 | ASN  |
| 2   | 4S    | 300 | ASN  |
| 2   | 4S    | 309 | HIS  |
| 2   | 4S    | 385 | GLN  |
| 2   | 4S    | 433 | GLN  |
| 2   | 4T    | 11  | GLN  |
| 2   | 4T    | 14  | ASN  |
| 2   | 4T    | 15  | GLN  |
| 2   | 4T    | 37  | HIS  |
| 2   | 4T    | 85  | GLN  |
| 2   | 4T    | 101 | ASN  |
| 2   | 4T    | 192 | HIS  |
| 2   | 4T    | 197 | ASN  |
| 2   | 4T    | 228 | ASN  |
| 2   | 4T    | 300 | ASN  |
| 2   | 4T    | 309 | HIS  |
| 2   | 4T    | 385 | GLN  |
| 2   | 4T    | 433 | GLN  |
| 2   | 4U    | 11  | GLN  |
| 2   | 4U    | 14  | ASN  |
| 2   | 4U    | 37  | HIS  |
| 2   | 4U    | 85  | GLN  |
| 2   | 4U    | 101 | ASN  |
| 2   | 4U    | 192 | HIS  |
| 2   | 4U    | 197 | ASN  |
| 2   | 4U    | 228 | ASN  |
| 2   | 4U    | 300 | ASN  |
| 2   | 4U    | 309 | HIS  |
| 2   | 4U    | 385 | GLN  |
| 2   | 4U    | 433 | GLN  |
| 2   | 4V    | 11  | GLN  |
| 2   | 4V    | 14  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 4V    | 37  | HIS  |
| 2   | 4V    | 85  | GLN  |
| 2   | 4V    | 101 | ASN  |
| 2   | 4V    | 192 | HIS  |
| 2   | 4V    | 197 | ASN  |
| 2   | 4V    | 228 | ASN  |
| 2   | 4V    | 300 | ASN  |
| 2   | 4V    | 309 | HIS  |
| 2   | 4V    | 336 | GLN  |
| 2   | 4V    | 385 | GLN  |
| 2   | 4V    | 433 | GLN  |
| 2   | 4W    | 11  | GLN  |
| 2   | 4W    | 14  | ASN  |
| 2   | 4W    | 37  | HIS  |
| 2   | 4W    | 85  | GLN  |
| 2   | 4W    | 101 | ASN  |
| 2   | 4W    | 192 | HIS  |
| 2   | 4W    | 197 | ASN  |
| 2   | 4W    | 228 | ASN  |
| 2   | 4W    | 300 | ASN  |
| 2   | 4W    | 309 | HIS  |
| 2   | 4W    | 385 | GLN  |
| 2   | 4W    | 433 | GLN  |
| 2   | 4X    | 8   | GLN  |
| 2   | 4X    | 11  | GLN  |
| 2   | 4X    | 37  | HIS  |
| 2   | 4X    | 85  | GLN  |
| 2   | 4X    | 101 | ASN  |
| 2   | 4X    | 192 | HIS  |
| 2   | 4X    | 197 | ASN  |
| 2   | 4X    | 228 | ASN  |
| 2   | 4X    | 300 | ASN  |
| 2   | 4X    | 309 | HIS  |
| 2   | 4X    | 336 | GLN  |
| 2   | 4X    | 385 | GLN  |
| 2   | 4X    | 433 | GLN  |
| 2   | 4Y    | 11  | GLN  |
| 2   | 4Y    | 14  | ASN  |
| 2   | 4Y    | 37  | HIS  |
| 2   | 4Y    | 85  | GLN  |
| 2   | 4Y    | 101 | ASN  |
| 2   | 4Y    | 192 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 4Y    | 197 | ASN  |
| 2   | 4Y    | 228 | ASN  |
| 2   | 4Y    | 300 | ASN  |
| 2   | 4Y    | 309 | HIS  |
| 2   | 4Y    | 385 | GLN  |
| 2   | 4Y    | 433 | GLN  |
| 2   | 4Z    | 11  | GLN  |
| 2   | 4Z    | 14  | ASN  |
| 2   | 4Z    | 37  | HIS  |
| 2   | 4Z    | 85  | GLN  |
| 2   | 4Z    | 101 | ASN  |
| 2   | 4Z    | 133 | GLN  |
| 2   | 4Z    | 192 | HIS  |
| 2   | 4Z    | 197 | ASN  |
| 2   | 4Z    | 228 | ASN  |
| 2   | 4Z    | 300 | ASN  |
| 2   | 4Z    | 309 | HIS  |
| 2   | 4Z    | 385 | GLN  |
| 2   | 4Z    | 433 | GLN  |

### 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 156 ligands modelled in this entry, 52 are monoatomic - leaving 104 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | GTP  | 3N    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 1Y    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 3   | GTP  | 1M    | 501 | 4    | 33,34,34     | 0.91 | 0           | 50,54,54    | 1.60 | 8 (16%)     |
| 3   | GTP  | 3J    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 1X    | 501 | -    | 29,30,30     | 1.19 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 3   | GTP  | 3L    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.58 | 8 (16%)     |
| 3   | GTP  | 2I    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 2G    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 3G    | 501 | 4    | 33,34,34     | 0.91 | 1 (3%)      | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 3K    | 501 | 4    | 33,34,34     | 0.91 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 3A    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 1K    | 501 | 4    | 33,34,34     | 0.91 | 1 (3%)      | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 3V    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 4S    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 5   | GDP  | 1P    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 5   | GDP  | 3X    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 4X    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 5   | GDP  | 4Y    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 1W    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 3   | GTP  | 4B    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 3F    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 4U    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 2T    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 3   | GTP  | 1L    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 4G    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 3P    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 3   | GTP  | 1C    | 501 | 4    | 33,34,34     | 0.91 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 3   | GTP  | 3M    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 3Z    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 2X    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 3   | GTP  | 4C    | 501 | 4    | 33,34,34     | 0.90 | 0           | 50,54,54    | 1.59 | 8 (16%)     |
| 5   | GDP  | 3T    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 5   | GDP  | 2H    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)     | 45,47,47    | 1.74 | 6 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | GTP  | 3I    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 4K    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 5   | GDP  | 2O    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 4N    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 1U    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 4L    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 1S    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 2N    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 4F    | 501 | 4    | 33,34,34     | 0.91 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 4P    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 4D    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 2P    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 2B    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 2U    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 1D    | 501 | 4    | 33,34,34     | 0.91 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 3D    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 3   | GTP  | 2J    | 501 | 4    | 33,34,34     | 0.91 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 3Q    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 1V    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 3S    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 4V    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 1F    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 3   | GTP  | 4M    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 1Q    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 3C    | 501 | 4    | 33,34,34     | 0.91 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 1T    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 3H    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 1Z    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 1E    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 3   | GTP  | 2C    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 2E    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 5   | GDP  | 3W    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 4E    | 501 | 4    | 33,34,34     | 0.89 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 1I    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 2Q    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | GDP  | 2Z    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 4T    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 2F    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 1N    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 2L    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 4W    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 2Y    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 2R    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 4Z    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 4R    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 1H    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 3O    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 1R    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 1J    | 501 | 4    | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 1O    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 4A    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 2D    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 2W    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 2A    | 501 | 4    | 33,34,34     | 0.91 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 3U    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 4H    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 3B    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 4J    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 5   | GDP  | 2S    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 3R    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 5   | GDP  | 4Q    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 3   | GTP  | 2K    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 1A    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 5   | GDP  | 2V    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 5   | GDP  | 3Y    | 501 | -    | 29,30,30     | 1.18 | 4 (13%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 3   | GTP  | 1B    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 3   | GTP  | 3E    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 2M    | 501 | 4    | 33,34,34     | 0.91 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 1G    | 501 | 4    | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 3   | GTP  | 4I    | 501 | 4    | 33,34,34     | 0.91 | 0        | 50,54,54    | 1.59 | 8 (16%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | GDP  | 4O    | 501 | -    | 29,30,30     | 1.17 | 4 (13%)  | 45,47,47    | 1.73 | 6 (13%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | GTP  | 3N    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1Y    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1M    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3J    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1X    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3L    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2I    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2G    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3G    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3K    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3A    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1K    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3V    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4S    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1P    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3X    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4X    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4Y    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1W    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4B    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3F    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 4U    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2T    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1L    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4G    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3P    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1C    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3M    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | GDP  | 3Z    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2X    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4C    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3T    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2H    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3I    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4K    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2O    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4N    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1U    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4L    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1S    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 2N    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4F    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 4P    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4D    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2P    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 2B    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2U    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1D    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3D    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2J    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3Q    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1V    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3S    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4V    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1F    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4M    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1Q    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3C    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1T    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3H    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1Z    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1E    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | GTP  | 2C    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2E    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3W    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4E    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1I    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2Q    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2Z    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4T    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 2F    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1N    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2L    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 4W    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2Y    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 2R    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4Z    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4R    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1H    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3O    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 1R    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1J    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 1O    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 4A    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2D    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2W    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 2A    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 3U    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4H    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 3B    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4J    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 2S    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3R    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 4Q    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 2K    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1A    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | GDP  | 2V    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 5   | GDP  | 3Y    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 3   | GTP  | 1B    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 3E    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 2M    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 1G    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 3   | GTP  | 4I    | 501 | 4    | -       | 6/22/38/38 | 0/3/3/3 |
| 5   | GDP  | 4O    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |

All (213) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 3H    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 3X    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 1X    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 3P    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 1U    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 1O    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 2Y    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 3T    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 4Y    | 501 | GDP  | C6-N1 | -2.78 | 1.33        | 1.38     |
| 5   | 2X    | 501 | GDP  | C5-C4 | 2.78  | 1.46        | 1.38     |
| 5   | 2O    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 1R    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 2Z    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 1S    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 3Q    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 3V    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 4H    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 2P    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 3U    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 1Z    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 2T    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 2V    | 501 | GDP  | C5-C4 | 2.77  | 1.46        | 1.38     |
| 5   | 3Z    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 3Y    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 1Y    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 1Q    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 4V    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 2R    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 4Q    | 501 | GDP  | C5-C4 | 2.76  | 1.46        | 1.38     |
| 5   | 4X    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 3Q    | 501 | GDP  | C6-N1 | -2.75 | 1.33        | 1.38     |
| 5   | 2H    | 501 | GDP  | C6-N1 | -2.75 | 1.33        | 1.38     |
| 5   | 2S    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 4P    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 4O    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 4Y    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 3W    | 501 | GDP  | C6-N1 | -2.75 | 1.33        | 1.38     |
| 5   | 1V    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 4W    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 1T    | 501 | GDP  | C6-N1 | -2.75 | 1.33        | 1.38     |
| 5   | 2U    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 1T    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 2W    | 501 | GDP  | C5-C4 | 2.75  | 1.46        | 1.38     |
| 5   | 1H    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 3S    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 4R    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 4U    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 4Z    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 4X    | 501 | GDP  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 5   | 1P    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 2P    | 501 | GDP  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 5   | 1W    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 2R    | 501 | GDP  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 5   | 3T    | 501 | GDP  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 5   | 4U    | 501 | GDP  | C6-N1 | -2.74 | 1.33        | 1.38     |
| 5   | 3R    | 501 | GDP  | C5-C4 | 2.74  | 1.46        | 1.38     |
| 5   | 1U    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 4Z    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 2V    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 3O    | 501 | GDP  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 5   | 3X    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 3W    | 501 | GDP  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 5   | 1S    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 2Q    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 4S    | 501 | GDP  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 5   | 2H    | 501 | GDP  | C5-C4 | 2.73  | 1.46        | 1.38     |
| 5   | 2W    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 2U    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 1X    | 501 | GDP  | C6-N1 | -2.73 | 1.33        | 1.38     |
| 5   | 2Q    | 501 | GDP  | C5-C4 | 2.73  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 2S    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 4T    | 501 | GDP  | C5-C4 | 2.72  | 1.46        | 1.38     |
| 5   | 4P    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 1R    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 4R    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 3U    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 4H    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 3P    | 501 | GDP  | C6-N1 | -2.72 | 1.33        | 1.38     |
| 5   | 4V    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 2T    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 3Y    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 1O    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 3V    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 1Z    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 3S    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 2Z    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 2O    | 501 | GDP  | C6-N1 | -2.71 | 1.33        | 1.38     |
| 5   | 1V    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 1W    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 1Y    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 4W    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 1Q    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 4S    | 501 | GDP  | C6-N1 | -2.70 | 1.33        | 1.38     |
| 5   | 3Z    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 4Q    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 2Y    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 1H    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 3R    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 4O    | 501 | GDP  | C6-N1 | -2.69 | 1.33        | 1.38     |
| 5   | 2X    | 501 | GDP  | C6-N1 | -2.68 | 1.33        | 1.38     |
| 5   | 3O    | 501 | GDP  | C6-N1 | -2.68 | 1.33        | 1.38     |
| 5   | 3H    | 501 | GDP  | C6-N1 | -2.68 | 1.33        | 1.38     |
| 5   | 1P    | 501 | GDP  | C6-N1 | -2.67 | 1.33        | 1.38     |
| 5   | 4T    | 501 | GDP  | C6-N1 | -2.66 | 1.33        | 1.38     |
| 5   | 1P    | 501 | GDP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 5   | 1Q    | 501 | GDP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 5   | 4H    | 501 | GDP  | C5-N7 | -2.33 | 1.34        | 1.39     |
| 5   | 3H    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 3S    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 2Z    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 2X    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 1H    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 1Y    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 3X    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 4W    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 2O    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 2Y    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 1R    | 501 | GDP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 5   | 3O    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 1X    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 3T    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 4Z    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 4T    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 4R    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 4P    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 2P    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 3P    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 3R    | 501 | GDP  | C5-N7 | -2.31 | 1.34        | 1.39     |
| 5   | 2S    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 2T    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 3Z    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 1W    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 3Q    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 1V    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 2V    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 1Z    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 3Y    | 501 | GDP  | C5-N7 | -2.30 | 1.34        | 1.39     |
| 5   | 1O    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 3W    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 4S    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 1S    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 2Q    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 2H    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 4V    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 2W    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 1U    | 501 | GDP  | C5-N7 | -2.29 | 1.34        | 1.39     |
| 5   | 3U    | 501 | GDP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 5   | 2U    | 501 | GDP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 5   | 4X    | 501 | GDP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 5   | 4Q    | 501 | GDP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 5   | 4U    | 501 | GDP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 5   | 4O    | 501 | GDP  | C5-N7 | -2.27 | 1.34        | 1.39     |
| 5   | 3V    | 501 | GDP  | C5-N7 | -2.26 | 1.34        | 1.39     |
| 5   | 1T    | 501 | GDP  | C5-N7 | -2.26 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 2R    | 501 | GDP  | C5-N7 | -2.26 | 1.34        | 1.39     |
| 5   | 4Y    | 501 | GDP  | C5-N7 | -2.24 | 1.34        | 1.39     |
| 5   | 1R    | 501 | GDP  | C4-N9 | -2.19 | 1.32        | 1.38     |
| 5   | 2Q    | 501 | GDP  | C4-N9 | -2.18 | 1.32        | 1.38     |
| 5   | 3P    | 501 | GDP  | C4-N9 | -2.18 | 1.32        | 1.38     |
| 5   | 4W    | 501 | GDP  | C4-N9 | -2.18 | 1.32        | 1.38     |
| 5   | 2T    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 1Q    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 2Z    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 1O    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 3Z    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 3W    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 4U    | 501 | GDP  | C4-N9 | -2.17 | 1.32        | 1.38     |
| 5   | 2P    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 3S    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 4Q    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 2W    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 1X    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 4H    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 2H    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 4V    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 3H    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 4O    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 4S    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 2X    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 3Y    | 501 | GDP  | C4-N9 | -2.16 | 1.32        | 1.38     |
| 5   | 1Z    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 3R    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 4T    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 3O    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 4Y    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 2Y    | 501 | GDP  | C4-N9 | -2.15 | 1.32        | 1.38     |
| 5   | 1S    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 3Q    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 1W    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 4X    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 3U    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 2O    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 4Z    | 501 | GDP  | C4-N9 | -2.14 | 1.32        | 1.38     |
| 5   | 2V    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 1P    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 2S    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 3T    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 1Y    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 3X    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 2R    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 1H    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 2U    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 3V    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 1V    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 4R    | 501 | GDP  | C4-N9 | -2.13 | 1.32        | 1.38     |
| 5   | 1U    | 501 | GDP  | C4-N9 | -2.12 | 1.32        | 1.38     |
| 5   | 1T    | 501 | GDP  | C4-N9 | -2.12 | 1.32        | 1.38     |
| 5   | 4P    | 501 | GDP  | C4-N9 | -2.12 | 1.32        | 1.38     |
| 3   | 2A    | 501 | GTP  | C2-N3 | 2.03  | 1.38        | 1.33     |
| 3   | 1J    | 501 | GTP  | C2-N3 | 2.00  | 1.38        | 1.33     |
| 3   | 2M    | 501 | GTP  | C2-N3 | 2.00  | 1.38        | 1.33     |
| 3   | 1K    | 501 | GTP  | C2-N3 | 2.00  | 1.38        | 1.33     |
| 3   | 3G    | 501 | GTP  | C2-N3 | 2.00  | 1.38        | 1.33     |

All (728) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 1O    | 501 | GDP  | C5-C4-N3 | -5.76 | 119.22      | 128.39   |
| 5   | 1R    | 501 | GDP  | C5-C4-N3 | -5.76 | 119.23      | 128.39   |
| 5   | 3P    | 501 | GDP  | C5-C4-N3 | -5.76 | 119.23      | 128.39   |
| 5   | 4V    | 501 | GDP  | C5-C4-N3 | -5.76 | 119.23      | 128.39   |
| 5   | 4U    | 501 | GDP  | C5-C4-N3 | -5.76 | 119.23      | 128.39   |
| 5   | 2W    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.23      | 128.39   |
| 5   | 4Q    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.23      | 128.39   |
| 5   | 2H    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.23      | 128.39   |
| 5   | 4Y    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.23      | 128.39   |
| 5   | 2O    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.24      | 128.39   |
| 5   | 1Q    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.24      | 128.39   |
| 5   | 3Z    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.24      | 128.39   |
| 5   | 3R    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.24      | 128.39   |
| 5   | 1X    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.25      | 128.39   |
| 5   | 2P    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.25      | 128.39   |
| 5   | 3Q    | 501 | GDP  | C5-C4-N3 | -5.75 | 119.25      | 128.39   |
| 5   | 2Y    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |
| 5   | 2R    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |
| 5   | 2Z    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |
| 5   | 4X    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |
| 5   | 3V    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 3Y    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.25      | 128.39   |
| 5   | 2X    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.26      | 128.39   |
| 5   | 1S    | 501 | GDP  | C5-C4-N3 | -5.74 | 119.26      | 128.39   |
| 5   | 2S    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.26      | 128.39   |
| 5   | 3W    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 2Q    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 1T    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 4H    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 1V    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 1Y    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 4T    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 2T    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 3U    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 4O    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 4S    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 1W    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.27      | 128.39   |
| 5   | 3S    | 501 | GDP  | C5-C4-N3 | -5.73 | 119.28      | 128.39   |
| 5   | 1Z    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 3H    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 3T    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 2V    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 3X    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 4W    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.28      | 128.39   |
| 5   | 1U    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.29      | 128.39   |
| 5   | 1P    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.29      | 128.39   |
| 5   | 3O    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.29      | 128.39   |
| 5   | 4P    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.29      | 128.39   |
| 5   | 4R    | 501 | GDP  | C5-C4-N3 | -5.72 | 119.29      | 128.39   |
| 5   | 1H    | 501 | GDP  | C5-C4-N3 | -5.71 | 119.30      | 128.39   |
| 5   | 2U    | 501 | GDP  | C5-C4-N3 | -5.71 | 119.31      | 128.39   |
| 5   | 4Z    | 501 | GDP  | C5-C4-N3 | -5.71 | 119.31      | 128.39   |
| 3   | 1F    | 501 | GTP  | C5-C4-N3 | -5.04 | 120.38      | 128.39   |
| 3   | 2E    | 501 | GTP  | C5-C4-N3 | -5.04 | 120.38      | 128.39   |
| 3   | 3D    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.38      | 128.39   |
| 3   | 2C    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.38      | 128.39   |
| 3   | 2B    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.38      | 128.39   |
| 3   | 4J    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.39      | 128.39   |
| 3   | 1E    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.39      | 128.39   |
| 3   | 1M    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.39      | 128.39   |
| 3   | 4F    | 501 | GTP  | C5-C4-N3 | -5.03 | 120.39      | 128.39   |
| 3   | 3B    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.39      | 128.39   |
| 3   | 1N    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.40      | 128.39   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 4K    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.40      | 128.39   |
| 3   | 1B    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.40      | 128.39   |
| 3   | 2K    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.40      | 128.39   |
| 3   | 2N    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.41      | 128.39   |
| 3   | 3G    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.41      | 128.39   |
| 3   | 1L    | 501 | GTP  | C5-C4-N3 | -5.02 | 120.41      | 128.39   |
| 3   | 2L    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.41      | 128.39   |
| 3   | 3C    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.41      | 128.39   |
| 3   | 4M    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.41      | 128.39   |
| 3   | 1K    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.41      | 128.39   |
| 3   | 3A    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.41      | 128.39   |
| 3   | 2A    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 2D    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 4N    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 4A    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 3F    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 1G    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 4C    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 4I    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 2F    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 1I    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 2G    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 3E    | 501 | GTP  | C5-C4-N3 | -5.01 | 120.42      | 128.39   |
| 3   | 2J    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 3I    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 3K    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 4G    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 4L    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 3M    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 1C    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.43      | 128.39   |
| 3   | 1A    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.44      | 128.39   |
| 3   | 2I    | 501 | GTP  | C5-C4-N3 | -5.00 | 120.44      | 128.39   |
| 3   | 4E    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.44      | 128.39   |
| 3   | 2M    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 3J    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 4B    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 3N    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 4D    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 1D    | 501 | GTP  | C5-C4-N3 | -4.99 | 120.45      | 128.39   |
| 3   | 1J    | 501 | GTP  | C5-C4-N3 | -4.98 | 120.47      | 128.39   |
| 3   | 3L    | 501 | GTP  | C5-C4-N3 | -4.98 | 120.47      | 128.39   |
| 5   | 3Q    | 501 | GDP  | C2-N3-C4 | 4.93  | 120.80      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5   | 2O    | 501 | GDP  | C2-N3-C4 | 4.93 | 120.78      | 112.30   |
| 5   | 1Q    | 501 | GDP  | C2-N3-C4 | 4.92 | 120.78      | 112.30   |
| 5   | 2S    | 501 | GDP  | C2-N3-C4 | 4.92 | 120.77      | 112.30   |
| 5   | 4V    | 501 | GDP  | C2-N3-C4 | 4.92 | 120.77      | 112.30   |
| 5   | 3Y    | 501 | GDP  | C2-N3-C4 | 4.92 | 120.77      | 112.30   |
| 5   | 2V    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.77      | 112.30   |
| 5   | 3P    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.76      | 112.30   |
| 5   | 4Q    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.76      | 112.30   |
| 5   | 1R    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.76      | 112.30   |
| 5   | 2X    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.76      | 112.30   |
| 5   | 3Z    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 2W    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 1Y    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 2R    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 3R    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 4Y    | 501 | GDP  | C2-N3-C4 | 4.91 | 120.75      | 112.30   |
| 5   | 3V    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.75      | 112.30   |
| 5   | 4P    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.75      | 112.30   |
| 5   | 1H    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 1T    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 1X    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 2Z    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 4H    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 1O    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 1P    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 4T    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.74      | 112.30   |
| 5   | 1S    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 3X    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 4U    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 3W    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 4O    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 4X    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 1W    | 501 | GDP  | C2-N3-C4 | 4.90 | 120.73      | 112.30   |
| 5   | 4W    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.73      | 112.30   |
| 5   | 3T    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.73      | 112.30   |
| 5   | 4S    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.73      | 112.30   |
| 5   | 2T    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 3H    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 2Y    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 2H    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 3U    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 2P    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5   | 2Q    | 501 | GDP  | C2-N3-C4 | 4.89 | 120.72      | 112.30   |
| 5   | 1V    | 501 | GDP  | C2-N3-C4 | 4.88 | 120.71      | 112.30   |
| 5   | 4R    | 501 | GDP  | C2-N3-C4 | 4.88 | 120.71      | 112.30   |
| 5   | 1U    | 501 | GDP  | C2-N3-C4 | 4.88 | 120.71      | 112.30   |
| 5   | 3O    | 501 | GDP  | C2-N3-C4 | 4.88 | 120.71      | 112.30   |
| 5   | 2U    | 501 | GDP  | C2-N3-C4 | 4.87 | 120.70      | 112.30   |
| 5   | 1Z    | 501 | GDP  | C2-N3-C4 | 4.87 | 120.69      | 112.30   |
| 5   | 4Z    | 501 | GDP  | C2-N3-C4 | 4.87 | 120.69      | 112.30   |
| 5   | 3S    | 501 | GDP  | C2-N3-C4 | 4.87 | 120.69      | 112.30   |
| 3   | 2C    | 501 | GTP  | C2-N3-C4 | 4.67 | 120.34      | 112.30   |
| 3   | 3I    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.33      | 112.30   |
| 3   | 1E    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.33      | 112.30   |
| 3   | 2K    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.33      | 112.30   |
| 3   | 1F    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.33      | 112.30   |
| 3   | 2E    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.32      | 112.30   |
| 3   | 4A    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.32      | 112.30   |
| 3   | 1B    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.32      | 112.30   |
| 3   | 4F    | 501 | GTP  | C2-N3-C4 | 4.66 | 120.32      | 112.30   |
| 3   | 4G    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.31      | 112.30   |
| 3   | 3D    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.31      | 112.30   |
| 3   | 3C    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.31      | 112.30   |
| 3   | 3M    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.30      | 112.30   |
| 3   | 4J    | 501 | GTP  | C2-N3-C4 | 4.65 | 120.30      | 112.30   |
| 3   | 1G    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.30      | 112.30   |
| 3   | 1L    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.30      | 112.30   |
| 3   | 4N    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.30      | 112.30   |
| 3   | 2F    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.30      | 112.30   |
| 3   | 3F    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.29      | 112.30   |
| 3   | 2B    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.29      | 112.30   |
| 3   | 2J    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.29      | 112.30   |
| 3   | 2L    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.29      | 112.30   |
| 3   | 4B    | 501 | GTP  | C2-N3-C4 | 4.64 | 120.29      | 112.30   |
| 3   | 3A    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 3B    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 4K    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 4C    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 1M    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 2A    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.28      | 112.30   |
| 3   | 1A    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 3K    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 1C    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 2G    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | 3G    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 4L    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 1D    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 4E    | 501 | GTP  | C2-N3-C4 | 4.63 | 120.27      | 112.30   |
| 3   | 2N    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.27      | 112.30   |
| 3   | 3J    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.27      | 112.30   |
| 3   | 2D    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 2M    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 1J    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 1K    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 4D    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 1N    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.26      | 112.30   |
| 3   | 3L    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.25      | 112.30   |
| 3   | 3N    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.25      | 112.30   |
| 3   | 1I    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.25      | 112.30   |
| 3   | 4M    | 501 | GTP  | C2-N3-C4 | 4.62 | 120.25      | 112.30   |
| 3   | 3E    | 501 | GTP  | C2-N3-C4 | 4.61 | 120.25      | 112.30   |
| 3   | 2I    | 501 | GTP  | C2-N3-C4 | 4.61 | 120.24      | 112.30   |
| 3   | 4I    | 501 | GTP  | C2-N3-C4 | 4.61 | 120.24      | 112.30   |
| 5   | 4V    | 501 | GDP  | N9-C4-N3 | 4.16 | 134.27      | 125.95   |
| 5   | 1X    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.25      | 125.95   |
| 5   | 1Q    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.25      | 125.95   |
| 5   | 2Z    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.25      | 125.95   |
| 5   | 3T    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.25      | 125.95   |
| 5   | 3V    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.25      | 125.95   |
| 5   | 1T    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.24      | 125.95   |
| 5   | 3Q    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.24      | 125.95   |
| 5   | 2O    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.24      | 125.95   |
| 5   | 4X    | 501 | GDP  | N9-C4-N3 | 4.15 | 134.24      | 125.95   |
| 5   | 4H    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.24      | 125.95   |
| 5   | 3P    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.24      | 125.95   |
| 5   | 3Y    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.24      | 125.95   |
| 5   | 3Z    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.24      | 125.95   |
| 5   | 1S    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 1O    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 2S    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 1R    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 4Y    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 2Y    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.23      | 125.95   |
| 5   | 2T    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.22      | 125.95   |
| 5   | 1Y    | 501 | GDP  | N9-C4-N3 | 4.14 | 134.22      | 125.95   |
| 5   | 4P    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.22      | 125.95   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5   | 2H    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.22      | 125.95   |
| 5   | 2X    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.22      | 125.95   |
| 5   | 3U    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.22      | 125.95   |
| 5   | 4U    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.22      | 125.95   |
| 5   | 2R    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 2W    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 4Q    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 1U    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 2V    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 4W    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 1Z    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.21      | 125.95   |
| 5   | 3X    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.20      | 125.95   |
| 5   | 3H    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.20      | 125.95   |
| 5   | 3R    | 501 | GDP  | N9-C4-N3 | 4.13 | 134.20      | 125.95   |
| 5   | 3W    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.20      | 125.95   |
| 5   | 1H    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.20      | 125.95   |
| 5   | 4R    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.19      | 125.95   |
| 5   | 4O    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.19      | 125.95   |
| 5   | 2Q    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.19      | 125.95   |
| 5   | 2P    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.19      | 125.95   |
| 5   | 3S    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.19      | 125.95   |
| 5   | 4T    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.18      | 125.95   |
| 5   | 1P    | 501 | GDP  | N9-C4-N3 | 4.12 | 134.18      | 125.95   |
| 5   | 1V    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.18      | 125.95   |
| 5   | 1W    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.18      | 125.95   |
| 5   | 2U    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.17      | 125.95   |
| 5   | 4S    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.17      | 125.95   |
| 5   | 3O    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.17      | 125.95   |
| 5   | 4Z    | 501 | GDP  | N9-C4-N3 | 4.11 | 134.17      | 125.95   |
| 5   | 3X    | 501 | GDP  | C6-C5-N7 | 3.54 | 136.73      | 130.29   |
| 5   | 2P    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.72      | 130.29   |
| 5   | 2V    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.72      | 130.29   |
| 5   | 3H    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 1O    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 2X    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 1U    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 2O    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 1V    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 1X    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 4Z    | 501 | GDP  | C6-C5-N7 | 3.53 | 136.71      | 130.29   |
| 5   | 2Z    | 501 | GDP  | C6-C5-N7 | 3.52 | 136.70      | 130.29   |
| 5   | 4H    | 501 | GDP  | C6-C5-N7 | 3.52 | 136.70      | 130.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 2U    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 2Y    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 3P    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 1S    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 2S    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 4R    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 2R    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 1Z    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 3T    | 501 | GDP  | C6-C5-N7 | 3.52  | 136.69      | 130.29   |
| 5   | 3Y    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 1H    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 1R    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 3Q    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 3V    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 4W    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 1Q    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 2T    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 4U    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 2H    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.68      | 130.29   |
| 5   | 3Z    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.67      | 130.29   |
| 5   | 1Y    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.67      | 130.29   |
| 5   | 4P    | 501 | GDP  | C6-C5-N7 | 3.51  | 136.67      | 130.29   |
| 5   | 3S    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.67      | 130.29   |
| 5   | 4Y    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.67      | 130.29   |
| 5   | 1T    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 3W    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 3U    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 3R    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 4O    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 4V    | 501 | GDP  | C6-C5-N7 | 3.50  | 136.66      | 130.29   |
| 5   | 1W    | 501 | GDP  | C6-C5-N7 | 3.49  | 136.65      | 130.29   |
| 5   | 3O    | 501 | GDP  | C6-C5-N7 | 3.49  | 136.65      | 130.29   |
| 5   | 4Q    | 501 | GDP  | C6-C5-N7 | 3.49  | 136.64      | 130.29   |
| 5   | 1P    | 501 | GDP  | C6-C5-N7 | 3.49  | 136.64      | 130.29   |
| 5   | 2W    | 501 | GDP  | C6-C5-N7 | 3.49  | 136.64      | 130.29   |
| 5   | 4S    | 501 | GDP  | C6-C5-N7 | 3.48  | 136.63      | 130.29   |
| 5   | 4T    | 501 | GDP  | C6-C5-N7 | 3.48  | 136.63      | 130.29   |
| 5   | 4X    | 501 | GDP  | C6-C5-N7 | 3.48  | 136.62      | 130.29   |
| 5   | 2Q    | 501 | GDP  | C6-C5-N7 | 3.48  | 136.62      | 130.29   |
| 3   | 4J    | 501 | GTP  | C2-N1-C6 | -3.17 | 119.36      | 125.11   |
| 3   | 4I    | 501 | GTP  | C2-N1-C6 | -3.16 | 119.37      | 125.11   |
| 3   | 1I    | 501 | GTP  | C2-N1-C6 | -3.16 | 119.39      | 125.11   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 3F    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.39      | 125.11   |
| 3   | 3D    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.39      | 125.11   |
| 3   | 4B    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.39      | 125.11   |
| 3   | 1F    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.39      | 125.11   |
| 3   | 4A    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.40      | 125.11   |
| 3   | 3B    | 501 | GTP  | C2-N1-C6 | -3.15 | 119.40      | 125.11   |
| 3   | 1B    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.41      | 125.11   |
| 3   | 4N    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.41      | 125.11   |
| 3   | 1E    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.41      | 125.11   |
| 3   | 4G    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.41      | 125.11   |
| 3   | 3E    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.41      | 125.11   |
| 3   | 4K    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2D    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 1N    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 3A    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 1J    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2N    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2K    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 1D    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 1M    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 4E    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 3G    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2E    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2L    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 3L    | 501 | GTP  | C2-N1-C6 | -3.14 | 119.42      | 125.11   |
| 3   | 2G    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.43      | 125.11   |
| 3   | 4M    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.43      | 125.11   |
| 3   | 4C    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.43      | 125.11   |
| 3   | 2M    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.43      | 125.11   |
| 3   | 3M    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.43      | 125.11   |
| 3   | 3J    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 1C    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 2I    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 3C    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 1K    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 2J    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 3N    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 3I    | 501 | GTP  | C2-N1-C6 | -3.13 | 119.44      | 125.11   |
| 3   | 4D    | 501 | GTP  | C2-N1-C6 | -3.12 | 119.44      | 125.11   |
| 3   | 1A    | 501 | GTP  | C2-N1-C6 | -3.12 | 119.44      | 125.11   |
| 3   | 3K    | 501 | GTP  | C2-N1-C6 | -3.12 | 119.45      | 125.11   |
| 3   | 1G    | 501 | GTP  | C2-N1-C6 | -3.12 | 119.46      | 125.11   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 4L    | 501 | GTP  | C2-N1-C6 | -3.12 | 119.46      | 125.11   |
| 3   | 4F    | 501 | GTP  | C2-N1-C6 | -3.11 | 119.47      | 125.11   |
| 3   | 2C    | 501 | GTP  | C2-N1-C6 | -3.11 | 119.47      | 125.11   |
| 3   | 2F    | 501 | GTP  | C2-N1-C6 | -3.11 | 119.48      | 125.11   |
| 3   | 1L    | 501 | GTP  | C2-N1-C6 | -3.11 | 119.48      | 125.11   |
| 3   | 2B    | 501 | GTP  | C2-N1-C6 | -3.10 | 119.48      | 125.11   |
| 3   | 2A    | 501 | GTP  | C2-N1-C6 | -3.10 | 119.49      | 125.11   |
| 3   | 4A    | 501 | GTP  | N9-C4-N3 | 3.05  | 132.06      | 125.95   |
| 3   | 4N    | 501 | GTP  | N9-C4-N3 | 3.05  | 132.06      | 125.95   |
| 3   | 1F    | 501 | GTP  | N9-C4-N3 | 3.05  | 132.04      | 125.95   |
| 3   | 2C    | 501 | GTP  | N9-C4-N3 | 3.05  | 132.04      | 125.95   |
| 3   | 3I    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.04      | 125.95   |
| 3   | 4F    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 2G    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 2K    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 3K    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 4K    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 3C    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 1I    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 3J    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.03      | 125.95   |
| 3   | 1K    | 501 | GTP  | N9-C4-N3 | 3.04  | 132.02      | 125.95   |
| 3   | 4G    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.02      | 125.95   |
| 3   | 1B    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.02      | 125.95   |
| 3   | 3M    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.02      | 125.95   |
| 3   | 4J    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 3A    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 1G    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 1C    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 3D    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 4B    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 2L    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.01      | 125.95   |
| 3   | 3G    | 501 | GTP  | N9-C4-N3 | 3.03  | 132.00      | 125.95   |
| 3   | 4C    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 1N    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 2F    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 2B    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 2J    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 3F    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 4L    | 501 | GTP  | N9-C4-N3 | 3.02  | 132.00      | 125.95   |
| 3   | 2D    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 1L    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 1M    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 3B    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 3E    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 1D    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 1E    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.99      | 125.95   |
| 3   | 4M    | 501 | GTP  | N9-C4-N3 | 3.02  | 131.98      | 125.95   |
| 3   | 2E    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.98      | 125.95   |
| 3   | 2A    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.98      | 125.95   |
| 3   | 3N    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.97      | 125.95   |
| 3   | 4I    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.97      | 125.95   |
| 3   | 2N    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.97      | 125.95   |
| 3   | 4E    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.97      | 125.95   |
| 3   | 3L    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.97      | 125.95   |
| 3   | 1A    | 501 | GTP  | N9-C4-N3 | 3.01  | 131.96      | 125.95   |
| 3   | 4D    | 501 | GTP  | N9-C4-N3 | 3.00  | 131.96      | 125.95   |
| 3   | 2I    | 501 | GTP  | N9-C4-N3 | 3.00  | 131.95      | 125.95   |
| 3   | 1J    | 501 | GTP  | N9-C4-N3 | 2.99  | 131.94      | 125.95   |
| 3   | 2M    | 501 | GTP  | N9-C4-N3 | 2.99  | 131.93      | 125.95   |
| 3   | 2J    | 501 | GTP  | N9-C8-N7 | -2.86 | 108.09      | 113.40   |
| 3   | 4K    | 501 | GTP  | N9-C8-N7 | -2.86 | 108.10      | 113.40   |
| 3   | 1D    | 501 | GTP  | N9-C8-N7 | -2.86 | 108.11      | 113.40   |
| 3   | 4J    | 501 | GTP  | N9-C8-N7 | -2.86 | 108.11      | 113.40   |
| 3   | 1B    | 501 | GTP  | N9-C8-N7 | -2.85 | 108.12      | 113.40   |
| 3   | 1N    | 501 | GTP  | N9-C8-N7 | -2.85 | 108.12      | 113.40   |
| 3   | 3D    | 501 | GTP  | N9-C8-N7 | -2.85 | 108.12      | 113.40   |
| 3   | 4F    | 501 | GTP  | N9-C8-N7 | -2.85 | 108.12      | 113.40   |
| 3   | 2G    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 1K    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 1M    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 4D    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 1A    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 1I    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 2E    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 4N    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.13      | 113.40   |
| 3   | 3C    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.14      | 113.40   |
| 3   | 3I    | 501 | GTP  | N9-C8-N7 | -2.84 | 108.14      | 113.40   |
| 3   | 3J    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.14      | 113.40   |
| 3   | 4G    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.14      | 113.40   |
| 3   | 1J    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.14      | 113.40   |
| 3   | 3N    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.14      | 113.40   |
| 3   | 1E    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.15      | 113.40   |
| 3   | 2C    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.15      | 113.40   |
| 3   | 2B    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.15      | 113.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 2I    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 1L    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 3F    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 4I    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 2D    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 1C    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 3B    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 3E    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 1G    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 2N    | 501 | GTP  | N9-C8-N7 | -2.83 | 108.16      | 113.40   |
| 3   | 4E    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.16      | 113.40   |
| 3   | 3A    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 3K    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 2A    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 2F    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 4L    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 3L    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 1F    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.17      | 113.40   |
| 3   | 2L    | 501 | GTP  | N9-C8-N7 | -2.82 | 108.18      | 113.40   |
| 3   | 4B    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.18      | 113.40   |
| 3   | 3M    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.18      | 113.40   |
| 3   | 4C    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.18      | 113.40   |
| 3   | 4M    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.18      | 113.40   |
| 3   | 3G    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.19      | 113.40   |
| 3   | 2M    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.19      | 113.40   |
| 3   | 2K    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.19      | 113.40   |
| 3   | 4A    | 501 | GTP  | N9-C8-N7 | -2.81 | 108.20      | 113.40   |
| 3   | 1F    | 501 | GTP  | C5-C6-N1 | 2.68  | 120.06      | 113.25   |
| 3   | 4G    | 501 | GTP  | C5-C6-N1 | 2.68  | 120.06      | 113.25   |
| 3   | 1J    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.05      | 113.25   |
| 3   | 1M    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 1D    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 3D    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 4J    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 4I    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 1B    | 501 | GTP  | C5-C6-N1 | 2.67  | 120.04      | 113.25   |
| 3   | 2K    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.03      | 113.25   |
| 3   | 2E    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.03      | 113.25   |
| 3   | 3L    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.03      | 113.25   |
| 3   | 3M    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.02      | 113.25   |
| 3   | 2D    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.02      | 113.25   |
| 3   | 4K    | 501 | GTP  | C5-C6-N1 | 2.66  | 120.02      | 113.25   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | 1E    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.02      | 113.25   |
| 3   | 1I    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.02      | 113.25   |
| 3   | 1G    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.02      | 113.25   |
| 3   | 3I    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.02      | 113.25   |
| 3   | 2M    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.01      | 113.25   |
| 3   | 4N    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.01      | 113.25   |
| 3   | 1C    | 501 | GTP  | C5-C6-N1 | 2.66 | 120.01      | 113.25   |
| 3   | 2F    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.01      | 113.25   |
| 3   | 2G    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.01      | 113.25   |
| 3   | 3A    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.01      | 113.25   |
| 3   | 4B    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.01      | 113.25   |
| 3   | 1N    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 3B    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 4A    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 4C    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 1A    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 3F    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 3G    | 501 | GTP  | C5-C6-N1 | 2.65 | 120.00      | 113.25   |
| 3   | 4J    | 501 | GTP  | C8-N7-C5 | 2.65 | 108.98      | 104.26   |
| 3   | 2L    | 501 | GTP  | C5-C6-N1 | 2.65 | 119.99      | 113.25   |
| 3   | 3K    | 501 | GTP  | C5-C6-N1 | 2.65 | 119.99      | 113.25   |
| 3   | 2J    | 501 | GTP  | C5-C6-N1 | 2.65 | 119.99      | 113.25   |
| 3   | 2C    | 501 | GTP  | C5-C6-N1 | 2.65 | 119.99      | 113.25   |
| 3   | 1K    | 501 | GTP  | C5-C6-N1 | 2.65 | 119.99      | 113.25   |
| 3   | 4L    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.98      | 113.25   |
| 3   | 4M    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.98      | 113.25   |
| 3   | 4E    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.98      | 113.25   |
| 3   | 2N    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.98      | 113.25   |
| 3   | 2I    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 3J    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 3N    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 1L    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 4D    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 4F    | 501 | GTP  | C5-C6-N1 | 2.64 | 119.97      | 113.25   |
| 3   | 1A    | 501 | GTP  | C8-N7-C5 | 2.63 | 108.95      | 104.26   |
| 3   | 1K    | 501 | GTP  | C8-N7-C5 | 2.63 | 108.95      | 104.26   |
| 3   | 2A    | 501 | GTP  | C5-C6-N1 | 2.63 | 119.96      | 113.25   |
| 3   | 3E    | 501 | GTP  | C5-C6-N1 | 2.63 | 119.96      | 113.25   |
| 3   | 3C    | 501 | GTP  | C5-C6-N1 | 2.63 | 119.95      | 113.25   |
| 3   | 1B    | 501 | GTP  | C8-N7-C5 | 2.63 | 108.95      | 104.26   |
| 3   | 1M    | 501 | GTP  | C8-N7-C5 | 2.63 | 108.94      | 104.26   |
| 3   | 2E    | 501 | GTP  | C8-N7-C5 | 2.63 | 108.94      | 104.26   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 2B    | 501 | GTP  | C5-C6-N1 | 2.63  | 119.94      | 113.25   |
| 3   | 4K    | 501 | GTP  | C8-N7-C5 | 2.63  | 108.94      | 104.26   |
| 3   | 1J    | 501 | GTP  | C8-N7-C5 | 2.63  | 108.94      | 104.26   |
| 3   | 1D    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 1N    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 3D    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 2D    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 2G    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 4N    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 1E    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.93      | 104.26   |
| 3   | 4F    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.92      | 104.26   |
| 3   | 3B    | 501 | GTP  | C8-N7-C5 | 2.62  | 108.92      | 104.26   |
| 3   | 2J    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 4D    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 1G    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 3C    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 4G    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 4L    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 3E    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 3J    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.91      | 104.26   |
| 3   | 1I    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.90      | 104.26   |
| 3   | 1F    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.90      | 104.26   |
| 3   | 3N    | 501 | GTP  | C8-N7-C5 | 2.61  | 108.90      | 104.26   |
| 3   | 3M    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.90      | 104.26   |
| 3   | 2L    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.90      | 104.26   |
| 3   | 4B    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.89      | 104.26   |
| 3   | 2K    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.89      | 104.26   |
| 3   | 4I    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.89      | 104.26   |
| 3   | 4E    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.89      | 104.26   |
| 3   | 1C    | 501 | GTP  | C8-N7-C5 | 2.60  | 108.89      | 104.26   |
| 3   | 1L    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.88      | 104.26   |
| 3   | 2M    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.88      | 104.26   |
| 5   | 1O    | 501 | GDP  | C4-C5-N7 | -2.59 | 106.56      | 110.67   |
| 3   | 2A    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.88      | 104.26   |
| 3   | 2N    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.88      | 104.26   |
| 3   | 2B    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 2F    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 3K    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 3G    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 4A    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 3A    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |
| 3   | 2I    | 501 | GTP  | C8-N7-C5 | 2.59  | 108.87      | 104.26   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 3I    | 501 | GTP  | C8-N7-C5 | 2.58  | 108.86      | 104.26   |
| 5   | 2P    | 501 | GDP  | C4-C5-N7 | -2.58 | 106.58      | 110.67   |
| 5   | 3X    | 501 | GDP  | C4-C5-N7 | -2.58 | 106.58      | 110.67   |
| 3   | 3F    | 501 | GTP  | C8-N7-C5 | 2.58  | 108.86      | 104.26   |
| 3   | 4M    | 501 | GTP  | C8-N7-C5 | 2.58  | 108.86      | 104.26   |
| 5   | 1V    | 501 | GDP  | C4-C5-N7 | -2.58 | 106.58      | 110.67   |
| 5   | 4U    | 501 | GDP  | C4-C5-N7 | -2.58 | 106.58      | 110.67   |
| 5   | 1R    | 501 | GDP  | C4-C5-N7 | -2.58 | 106.59      | 110.67   |
| 3   | 4C    | 501 | GTP  | C8-N7-C5 | 2.57  | 108.85      | 104.26   |
| 5   | 3R    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.59      | 110.67   |
| 5   | 2X    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.59      | 110.67   |
| 5   | 2O    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.59      | 110.67   |
| 5   | 2R    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.59      | 110.67   |
| 5   | 3V    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 3   | 2C    | 501 | GTP  | C8-N7-C5 | 2.57  | 108.84      | 104.26   |
| 5   | 2H    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 3P    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 3Z    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 4H    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 4Y    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 2V    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 2Z    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 2Y    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 1Z    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 5   | 3W    | 501 | GDP  | C4-C5-N7 | -2.57 | 106.60      | 110.67   |
| 3   | 3L    | 501 | GTP  | C8-N7-C5 | 2.57  | 108.83      | 104.26   |
| 5   | 4V    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.61      | 110.67   |
| 5   | 1U    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.61      | 110.67   |
| 5   | 1S    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.61      | 110.67   |
| 5   | 4Z    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.61      | 110.67   |
| 5   | 4Q    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.61      | 110.67   |
| 5   | 2S    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.62      | 110.67   |
| 5   | 3U    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.62      | 110.67   |
| 5   | 1Q    | 501 | GDP  | C4-C5-N7 | -2.56 | 106.62      | 110.67   |
| 5   | 4O    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 2T    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 2W    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 3T    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 1Y    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 2U    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 1W    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.62      | 110.67   |
| 5   | 3H    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 3Y    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |
| 5   | 4R    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |
| 5   | 3O    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |
| 5   | 1X    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |
| 5   | 3Q    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.63      | 110.67   |
| 5   | 1H    | 501 | GDP  | C4-C5-N7 | -2.55 | 106.64      | 110.67   |
| 5   | 1T    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.64      | 110.67   |
| 5   | 2Q    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.64      | 110.67   |
| 5   | 4S    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.64      | 110.67   |
| 5   | 4W    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.64      | 110.67   |
| 5   | 4T    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.64      | 110.67   |
| 5   | 3S    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.65      | 110.67   |
| 5   | 4X    | 501 | GDP  | C4-C5-N7 | -2.54 | 106.65      | 110.67   |
| 5   | 4P    | 501 | GDP  | C4-C5-N7 | -2.53 | 106.66      | 110.67   |
| 5   | 1P    | 501 | GDP  | C4-C5-N7 | -2.53 | 106.67      | 110.67   |
| 3   | 1M    | 501 | GTP  | O6-C6-C5 | -2.31 | 120.43      | 126.53   |
| 3   | 1F    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.45      | 126.53   |
| 3   | 2K    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.45      | 126.53   |
| 3   | 3D    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.45      | 126.53   |
| 3   | 3N    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.46      | 126.53   |
| 3   | 4M    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.46      | 126.53   |
| 3   | 4G    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.46      | 126.53   |
| 3   | 1J    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 4E    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 4C    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 1E    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 2A    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 4L    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 1C    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 2B    | 501 | GTP  | O6-C6-C5 | -2.30 | 120.47      | 126.53   |
| 3   | 1G    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.47      | 126.53   |
| 3   | 2M    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 1D    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 1B    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 2C    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 2D    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 4N    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 2F    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.48      | 126.53   |
| 3   | 3B    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.49      | 126.53   |
| 3   | 3A    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.49      | 126.53   |
| 3   | 3F    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.49      | 126.53   |
| 3   | 4I    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.49      | 126.53   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 2E    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.49      | 126.53   |
| 3   | 3I    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.50      | 126.53   |
| 3   | 3M    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.50      | 126.53   |
| 3   | 1N    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.50      | 126.53   |
| 3   | 2I    | 501 | GTP  | O6-C6-C5 | -2.29 | 120.50      | 126.53   |
| 3   | 2G    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.50      | 126.53   |
| 3   | 4K    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.50      | 126.53   |
| 3   | 1I    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.51      | 126.53   |
| 3   | 2L    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.51      | 126.53   |
| 3   | 4J    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.51      | 126.53   |
| 3   | 1L    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.51      | 126.53   |
| 3   | 1K    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.51      | 126.53   |
| 3   | 4A    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 4B    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 1A    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 3J    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 3K    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 3L    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.52      | 126.53   |
| 3   | 2J    | 501 | GTP  | O6-C6-C5 | -2.28 | 120.53      | 126.53   |
| 3   | 4D    | 501 | GTP  | O6-C6-C5 | -2.27 | 120.53      | 126.53   |
| 3   | 2N    | 501 | GTP  | O6-C6-C5 | -2.27 | 120.54      | 126.53   |
| 3   | 3G    | 501 | GTP  | O6-C6-C5 | -2.27 | 120.54      | 126.53   |
| 3   | 4F    | 501 | GTP  | O6-C6-C5 | -2.27 | 120.54      | 126.53   |
| 3   | 3C    | 501 | GTP  | O6-C6-C5 | -2.27 | 120.55      | 126.53   |
| 3   | 3E    | 501 | GTP  | O6-C6-C5 | -2.26 | 120.56      | 126.53   |
| 5   | 3Q    | 501 | GDP  | O6-C6-C5 | -2.15 | 120.86      | 126.53   |
| 5   | 1X    | 501 | GDP  | O6-C6-C5 | -2.15 | 120.86      | 126.53   |
| 5   | 4Y    | 501 | GDP  | O6-C6-C5 | -2.15 | 120.86      | 126.53   |
| 5   | 1T    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.88      | 126.53   |
| 5   | 4Z    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 4R    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 2H    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 2W    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 3S    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 3X    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 2U    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.89      | 126.53   |
| 5   | 2V    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.90      | 126.53   |
| 5   | 3H    | 501 | GDP  | O6-C6-C5 | -2.14 | 120.90      | 126.53   |
| 5   | 1U    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.90      | 126.53   |
| 5   | 4X    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.90      | 126.53   |
| 5   | 3P    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.90      | 126.53   |
| 5   | 2Y    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | 2O    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |
| 5   | 3Y    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |
| 5   | 4U    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |
| 5   | 2P    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |
| 5   | 2S    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.91      | 126.53   |
| 5   | 1Y    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.92      | 126.53   |
| 5   | 4Q    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.92      | 126.53   |
| 5   | 2T    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.92      | 126.53   |
| 5   | 1S    | 501 | GDP  | O6-C6-C5 | -2.13 | 120.92      | 126.53   |
| 5   | 3V    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.92      | 126.53   |
| 5   | 3T    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.92      | 126.53   |
| 5   | 2Z    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 3U    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 4P    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 1Q    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 4W    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 4V    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 1H    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 1V    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.93      | 126.53   |
| 5   | 4O    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 2R    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 1Z    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 2X    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 3Z    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 1P    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 4H    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 1O    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.94      | 126.53   |
| 5   | 1R    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.95      | 126.53   |
| 5   | 3O    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.95      | 126.53   |
| 5   | 1W    | 501 | GDP  | O6-C6-C5 | -2.12 | 120.95      | 126.53   |
| 5   | 3W    | 501 | GDP  | O6-C6-C5 | -2.11 | 120.95      | 126.53   |
| 5   | 4S    | 501 | GDP  | O6-C6-C5 | -2.11 | 120.95      | 126.53   |
| 5   | 2Q    | 501 | GDP  | O6-C6-C5 | -2.11 | 120.96      | 126.53   |
| 5   | 3R    | 501 | GDP  | O6-C6-C5 | -2.11 | 120.96      | 126.53   |
| 5   | 4T    | 501 | GDP  | O6-C6-C5 | -2.10 | 120.99      | 126.53   |

There are no chirality outliers.

All (520) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 1A    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1A    | 501 | GTP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 1A    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1B    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1B    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1B    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1C    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1C    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1C    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1D    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1D    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1D    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1E    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1E    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1E    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1F    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1F    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1F    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1G    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1G    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1G    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1I    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1I    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1I    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1J    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1J    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1J    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1K    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1K    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1K    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1L    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1L    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1L    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1M    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1M    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1M    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 1N    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 1N    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 1N    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2A    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2A    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2A    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2B    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2B    | 501 | GTP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 2B    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2C    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2C    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2C    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2D    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2D    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2D    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2E    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2E    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2E    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2F    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2F    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2F    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2G    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2G    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2G    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2I    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2I    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2I    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2J    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2J    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2J    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2K    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2K    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2K    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2L    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2L    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2L    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2M    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2M    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2M    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 2N    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 2N    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 2N    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3A    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3A    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3A    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3B    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3B    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3B    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3C    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3C    | 501 | GTP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 3C    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3D    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3D    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3D    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3E    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3E    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3E    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3F    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3F    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3F    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3G    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3G    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3G    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3I    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3I    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3I    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3J    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3J    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3J    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3K    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3K    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3K    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3L    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3L    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3L    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3M    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3M    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3M    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 3N    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 3N    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 3N    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4A    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4A    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4A    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4B    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4B    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4B    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4C    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4C    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4C    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4D    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4D    | 501 | GTP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 4D    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4E    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4E    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4E    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4F    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4F    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4F    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4G    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4G    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4G    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4I    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4I    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4I    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4J    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4J    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4J    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4K    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4K    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4K    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4L    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4L    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4L    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4M    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4M    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4M    | 501 | GTP  | C5'-O5'-PA-O2A |
| 3   | 4N    | 501 | GTP  | C5'-O5'-PA-O3A |
| 3   | 4N    | 501 | GTP  | C5'-O5'-PA-O1A |
| 3   | 4N    | 501 | GTP  | C5'-O5'-PA-O2A |
| 5   | 1H    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1O    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1P    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1Q    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1R    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1S    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1T    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1U    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1V    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1W    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1X    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1Y    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 1Z    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2H    | 501 | GDP  | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 5   | 2O    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2P    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2Q    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2R    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2S    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2T    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2U    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2V    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2W    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2X    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2Y    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 2Z    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3H    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3O    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3P    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3Q    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3R    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3S    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3T    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3U    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3V    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3W    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3X    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3Y    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 3Z    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4H    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4O    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4P    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4Q    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4R    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4S    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4T    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4U    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4V    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4W    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4X    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4Y    | 501 | GDP  | C5'-O5'-PA-O1A |
| 5   | 4Z    | 501 | GDP  | C5'-O5'-PA-O1A |
| 3   | 1A    | 501 | GTP  | PB-O3A-PA-O1A  |
| 3   | 1B    | 501 | GTP  | PB-O3A-PA-O1A  |
| 3   | 1C    | 501 | GTP  | PB-O3A-PA-O1A  |
| 3   | 1D    | 501 | GTP  | PB-O3A-PA-O1A  |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | 1E    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1F    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1G    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1I    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1J    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1K    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1L    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1M    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 1N    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2A    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2B    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2C    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2D    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2E    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2F    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2G    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2I    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2J    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2K    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2L    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2M    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 2N    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3A    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3B    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3C    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3D    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3E    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3F    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3G    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3I    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3J    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3K    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3L    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3M    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 3N    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4A    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4B    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4C    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4D    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4E    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4F    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4G    | 501 | GTP  | PB-O3A-PA-O1A |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | 4I    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4J    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4K    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4L    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4M    | 501 | GTP  | PB-O3A-PA-O1A |
| 3   | 4N    | 501 | GTP  | PB-O3A-PA-O1A |
| 5   | 1H    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1O    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1P    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1Q    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1R    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1S    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1T    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1U    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1V    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1W    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1X    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1Y    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 1Z    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2H    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2O    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2P    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2Q    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2R    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2S    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2T    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2U    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2V    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2W    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2X    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2Y    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 2Z    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3H    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3O    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3P    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3Q    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3R    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3S    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3T    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3U    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3V    | 501 | GDP  | PB-O3A-PA-O2A |
| 5   | 3W    | 501 | GDP  | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 5   | 3X    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 3Y    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 3Z    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4H    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4O    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4P    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4Q    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4R    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4S    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4T    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4U    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4V    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4W    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4X    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4Y    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 4Z    | 501 | GDP  | PB-O3A-PA-O2A  |
| 5   | 1H    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1H    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1O    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1O    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1P    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1P    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1Q    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1Q    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1R    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1R    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1S    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1S    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1T    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1T    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1U    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1U    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1V    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1V    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1W    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1W    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1X    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1X    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1Y    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1Y    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 1Z    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 1Z    | 501 | GDP  | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 5   | 2H    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2H    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2O    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2O    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2P    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2P    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2Q    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2Q    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2R    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2R    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2S    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2S    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2T    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2T    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2U    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2U    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2V    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2V    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2W    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2W    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2X    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2X    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2Y    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2Y    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 2Z    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 2Z    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3H    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3H    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3O    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3O    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3P    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3P    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3Q    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3Q    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3R    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3R    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3S    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3S    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3T    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3T    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3U    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3U    | 501 | GDP  | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 5   | 3V    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3V    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3W    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3W    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3X    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3X    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3Y    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3Y    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 3Z    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 3Z    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4H    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4H    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4O    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4O    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4P    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4P    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4Q    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4Q    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4R    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4R    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4S    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4S    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4T    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4T    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4U    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4U    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4V    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4V    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4W    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4W    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4X    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4X    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4Y    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4Y    | 501 | GDP  | C5'-O5'-PA-O2A |
| 5   | 4Z    | 501 | GDP  | C5'-O5'-PA-O3A |
| 5   | 4Z    | 501 | GDP  | C5'-O5'-PA-O2A |
| 3   | 1A    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1B    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1C    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1D    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1E    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1F    | 501 | GTP  | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 1G    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1I    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1J    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1K    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1L    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1M    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1N    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2A    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2B    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2C    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2D    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2E    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2F    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2G    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2I    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2J    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2K    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2L    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2M    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 2N    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3A    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3B    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3C    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3D    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3E    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3F    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3G    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3I    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3J    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3K    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3L    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3M    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 3N    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4A    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4B    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4C    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4D    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4E    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4F    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4G    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4I    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4J    | 501 | GTP  | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 3   | 4K    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4L    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4M    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 4N    | 501 | GTP  | C4'-C5'-O5'-PA |
| 3   | 1A    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1B    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1C    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1D    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1E    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1F    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1G    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1I    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1J    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1K    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1L    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1M    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 1N    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2A    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2B    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2C    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2D    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2E    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2F    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2G    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2I    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2J    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2K    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2L    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2M    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 2N    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3A    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3B    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3C    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3D    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3E    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3F    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3G    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3I    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3J    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3K    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3L    | 501 | GTP  | PB-O3A-PA-O2A  |
| 3   | 3M    | 501 | GTP  | PB-O3A-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | 3N    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4A    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4B    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4C    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4D    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4E    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4F    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4G    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4I    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4J    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4K    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4L    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4M    | 501 | GTP  | PB-O3A-PA-O2A |
| 3   | 4N    | 501 | GTP  | PB-O3A-PA-O2A |

There are no ring outliers.

104 monomers are involved in 391 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | 3N    | 501 | GTP  | 2       | 0            |
| 5   | 1Y    | 501 | GDP  | 5       | 0            |
| 3   | 1M    | 501 | GTP  | 2       | 0            |
| 3   | 3J    | 501 | GTP  | 2       | 0            |
| 5   | 1X    | 501 | GDP  | 5       | 0            |
| 3   | 3L    | 501 | GTP  | 2       | 0            |
| 3   | 2I    | 501 | GTP  | 2       | 0            |
| 3   | 2G    | 501 | GTP  | 2       | 0            |
| 3   | 3G    | 501 | GTP  | 2       | 0            |
| 3   | 3K    | 501 | GTP  | 2       | 0            |
| 3   | 3A    | 501 | GTP  | 2       | 0            |
| 3   | 1K    | 501 | GTP  | 2       | 0            |
| 5   | 3V    | 501 | GDP  | 3       | 0            |
| 5   | 4S    | 501 | GDP  | 7       | 0            |
| 5   | 1P    | 501 | GDP  | 3       | 0            |
| 5   | 3X    | 501 | GDP  | 3       | 0            |
| 5   | 4X    | 501 | GDP  | 6       | 0            |
| 5   | 4Y    | 501 | GDP  | 6       | 0            |
| 5   | 1W    | 501 | GDP  | 4       | 0            |
| 3   | 4B    | 501 | GTP  | 2       | 0            |
| 3   | 3F    | 501 | GTP  | 2       | 0            |
| 5   | 4U    | 501 | GDP  | 7       | 0            |
| 5   | 2T    | 501 | GDP  | 8       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | 1L    | 501 | GTP  | 2       | 0            |
| 3   | 4G    | 501 | GTP  | 2       | 0            |
| 5   | 3P    | 501 | GDP  | 3       | 0            |
| 3   | 1C    | 501 | GTP  | 2       | 0            |
| 3   | 3M    | 501 | GTP  | 2       | 0            |
| 5   | 3Z    | 501 | GDP  | 3       | 0            |
| 5   | 2X    | 501 | GDP  | 8       | 0            |
| 3   | 4C    | 501 | GTP  | 2       | 0            |
| 5   | 3T    | 501 | GDP  | 3       | 0            |
| 5   | 2H    | 501 | GDP  | 7       | 0            |
| 3   | 3I    | 501 | GTP  | 2       | 0            |
| 3   | 4K    | 501 | GTP  | 2       | 0            |
| 5   | 2O    | 501 | GDP  | 7       | 0            |
| 3   | 4N    | 501 | GTP  | 2       | 0            |
| 5   | 1U    | 501 | GDP  | 3       | 0            |
| 3   | 4L    | 501 | GTP  | 2       | 0            |
| 5   | 1S    | 501 | GDP  | 3       | 0            |
| 3   | 2N    | 501 | GTP  | 2       | 0            |
| 3   | 4F    | 501 | GTP  | 2       | 0            |
| 5   | 4P    | 501 | GDP  | 9       | 0            |
| 3   | 4D    | 501 | GTP  | 2       | 0            |
| 5   | 2P    | 501 | GDP  | 7       | 0            |
| 3   | 2B    | 501 | GTP  | 2       | 0            |
| 5   | 2U    | 501 | GDP  | 8       | 0            |
| 3   | 1D    | 501 | GTP  | 2       | 0            |
| 3   | 3D    | 501 | GTP  | 2       | 0            |
| 3   | 2J    | 501 | GTP  | 2       | 0            |
| 5   | 3Q    | 501 | GDP  | 3       | 0            |
| 5   | 1V    | 501 | GDP  | 4       | 0            |
| 5   | 3S    | 501 | GDP  | 3       | 0            |
| 5   | 4V    | 501 | GDP  | 7       | 0            |
| 3   | 1F    | 501 | GTP  | 2       | 0            |
| 3   | 4M    | 501 | GTP  | 2       | 0            |
| 5   | 1Q    | 501 | GDP  | 3       | 0            |
| 3   | 3C    | 501 | GTP  | 2       | 0            |
| 5   | 1T    | 501 | GDP  | 3       | 0            |
| 5   | 3H    | 501 | GDP  | 3       | 0            |
| 5   | 1Z    | 501 | GDP  | 6       | 0            |
| 3   | 1E    | 501 | GTP  | 2       | 0            |
| 3   | 2C    | 501 | GTP  | 2       | 0            |
| 3   | 2E    | 501 | GTP  | 2       | 0            |
| 5   | 3W    | 501 | GDP  | 3       | 0            |

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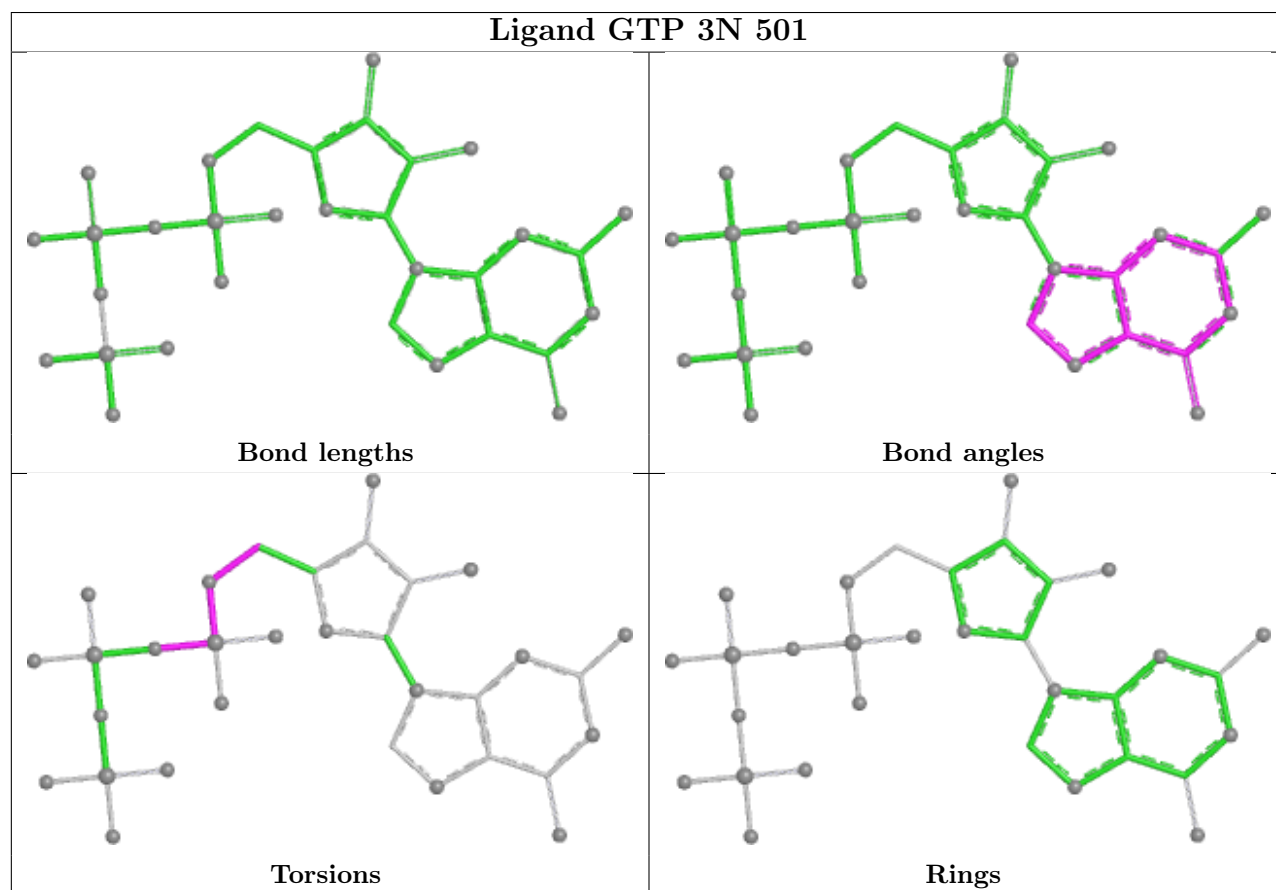
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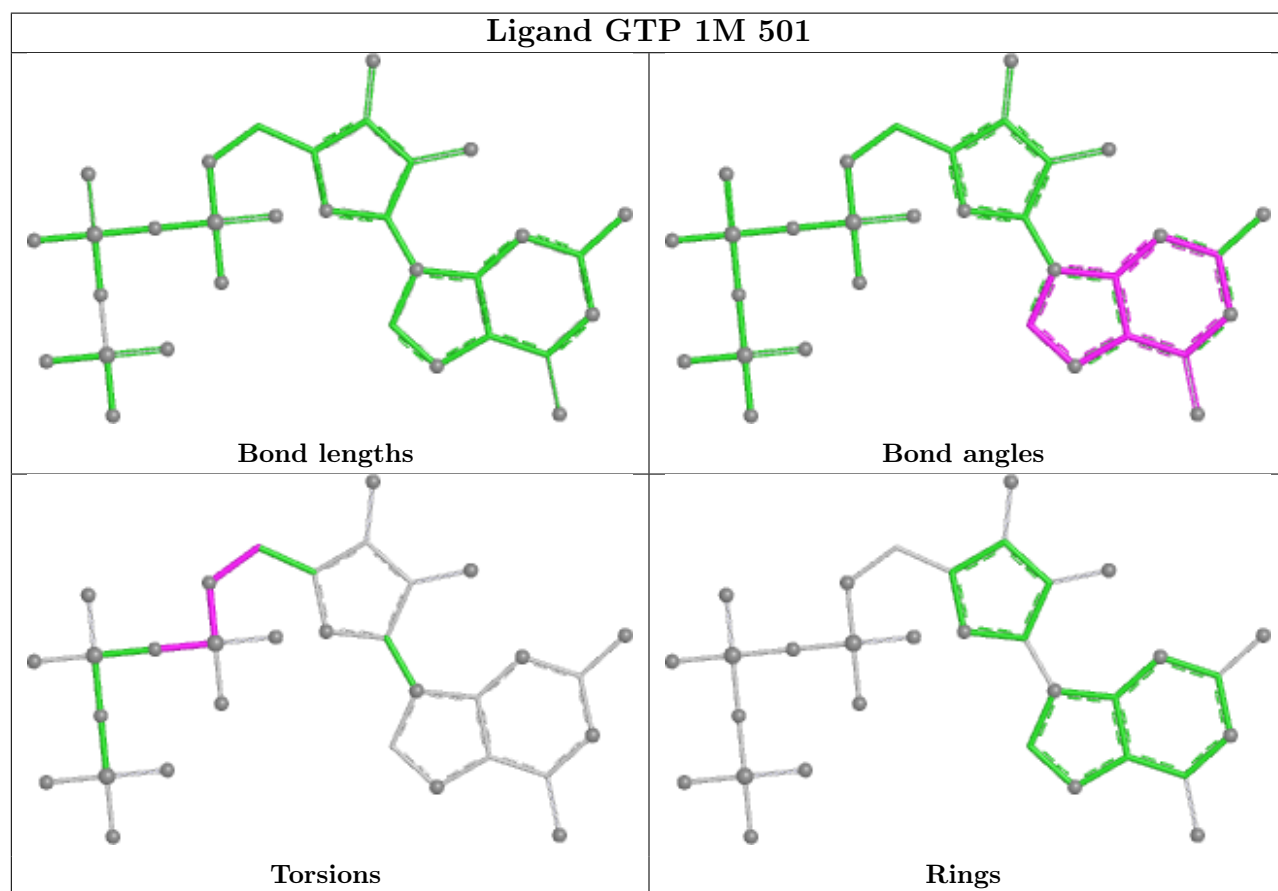
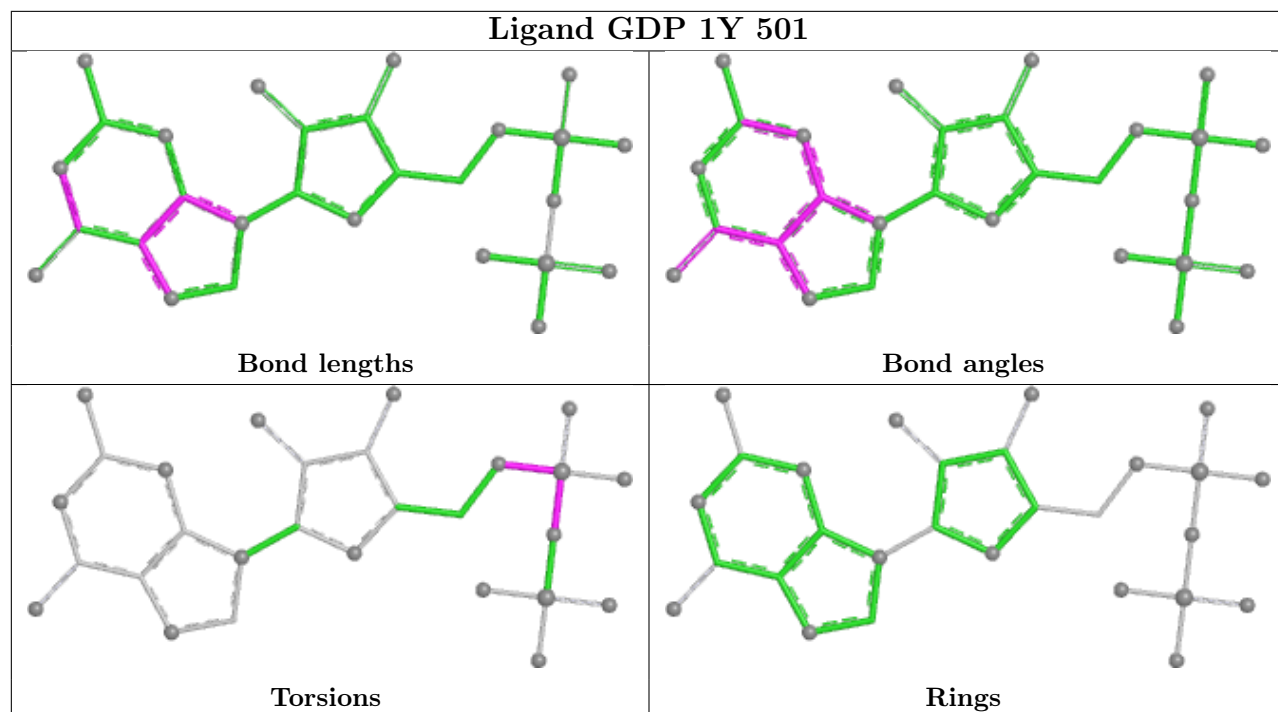
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | 4E    | 501 | GTP  | 2       | 0            |
| 3   | 1I    | 501 | GTP  | 2       | 0            |
| 5   | 2Q    | 501 | GDP  | 7       | 0            |
| 5   | 2Z    | 501 | GDP  | 7       | 0            |
| 5   | 4T    | 501 | GDP  | 7       | 0            |
| 3   | 2F    | 501 | GTP  | 2       | 0            |
| 3   | 1N    | 501 | GTP  | 2       | 0            |
| 3   | 2L    | 501 | GTP  | 2       | 0            |
| 5   | 4W    | 501 | GDP  | 6       | 0            |
| 5   | 2Y    | 501 | GDP  | 8       | 0            |
| 5   | 2R    | 501 | GDP  | 7       | 0            |
| 5   | 4Z    | 501 | GDP  | 8       | 0            |
| 5   | 4R    | 501 | GDP  | 9       | 0            |
| 5   | 1H    | 501 | GDP  | 5       | 0            |
| 5   | 3O    | 501 | GDP  | 3       | 0            |
| 5   | 1R    | 501 | GDP  | 3       | 0            |
| 3   | 1J    | 501 | GTP  | 2       | 0            |
| 5   | 1O    | 501 | GDP  | 4       | 0            |
| 3   | 4A    | 501 | GTP  | 2       | 0            |
| 3   | 2D    | 501 | GTP  | 2       | 0            |
| 5   | 2W    | 501 | GDP  | 8       | 0            |
| 3   | 2A    | 501 | GTP  | 2       | 0            |
| 5   | 3U    | 501 | GDP  | 3       | 0            |
| 5   | 4H    | 501 | GDP  | 8       | 0            |
| 3   | 3B    | 501 | GTP  | 2       | 0            |
| 3   | 4J    | 501 | GTP  | 2       | 0            |
| 5   | 2S    | 501 | GDP  | 8       | 0            |
| 5   | 3R    | 501 | GDP  | 3       | 0            |
| 5   | 4Q    | 501 | GDP  | 10      | 0            |
| 3   | 2K    | 501 | GTP  | 2       | 0            |
| 3   | 1A    | 501 | GTP  | 2       | 0            |
| 5   | 2V    | 501 | GDP  | 8       | 0            |
| 5   | 3Y    | 501 | GDP  | 3       | 0            |
| 3   | 1B    | 501 | GTP  | 2       | 0            |
| 3   | 3E    | 501 | GTP  | 2       | 0            |
| 3   | 2M    | 501 | GTP  | 2       | 0            |
| 3   | 1G    | 501 | GTP  | 2       | 0            |
| 3   | 4I    | 501 | GTP  | 2       | 0            |
| 5   | 4O    | 501 | GDP  | 9       | 0            |

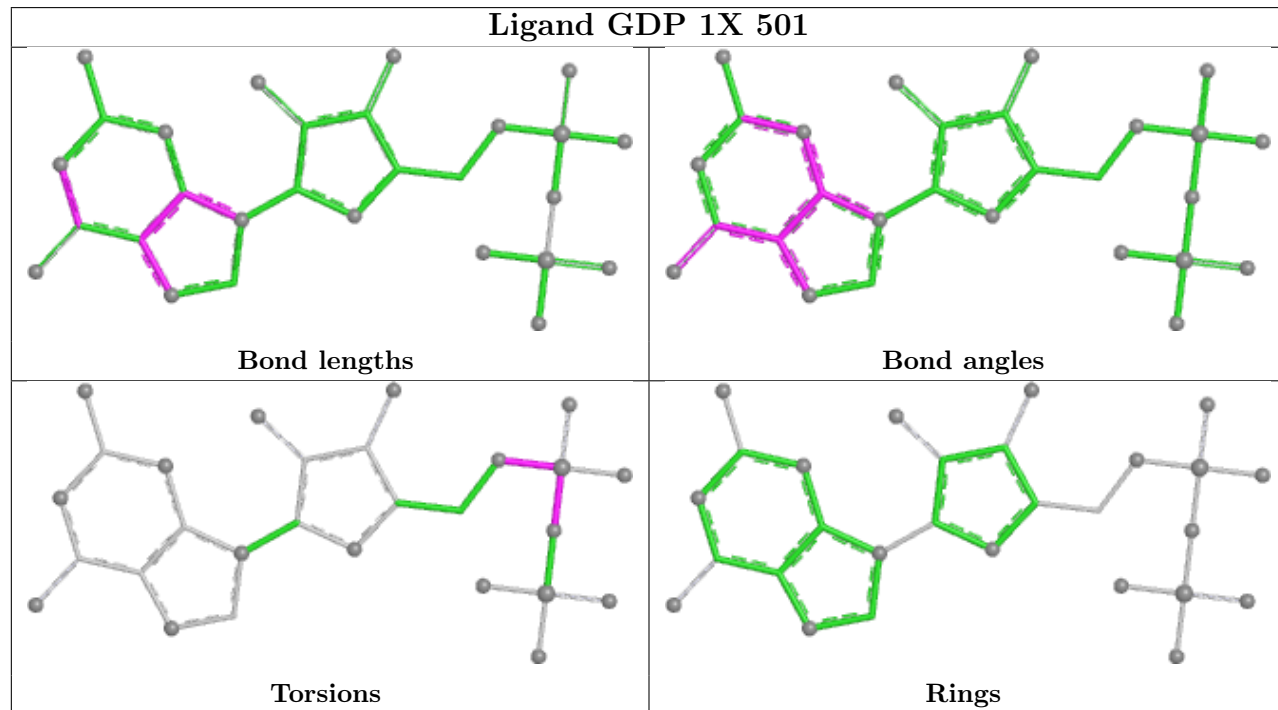
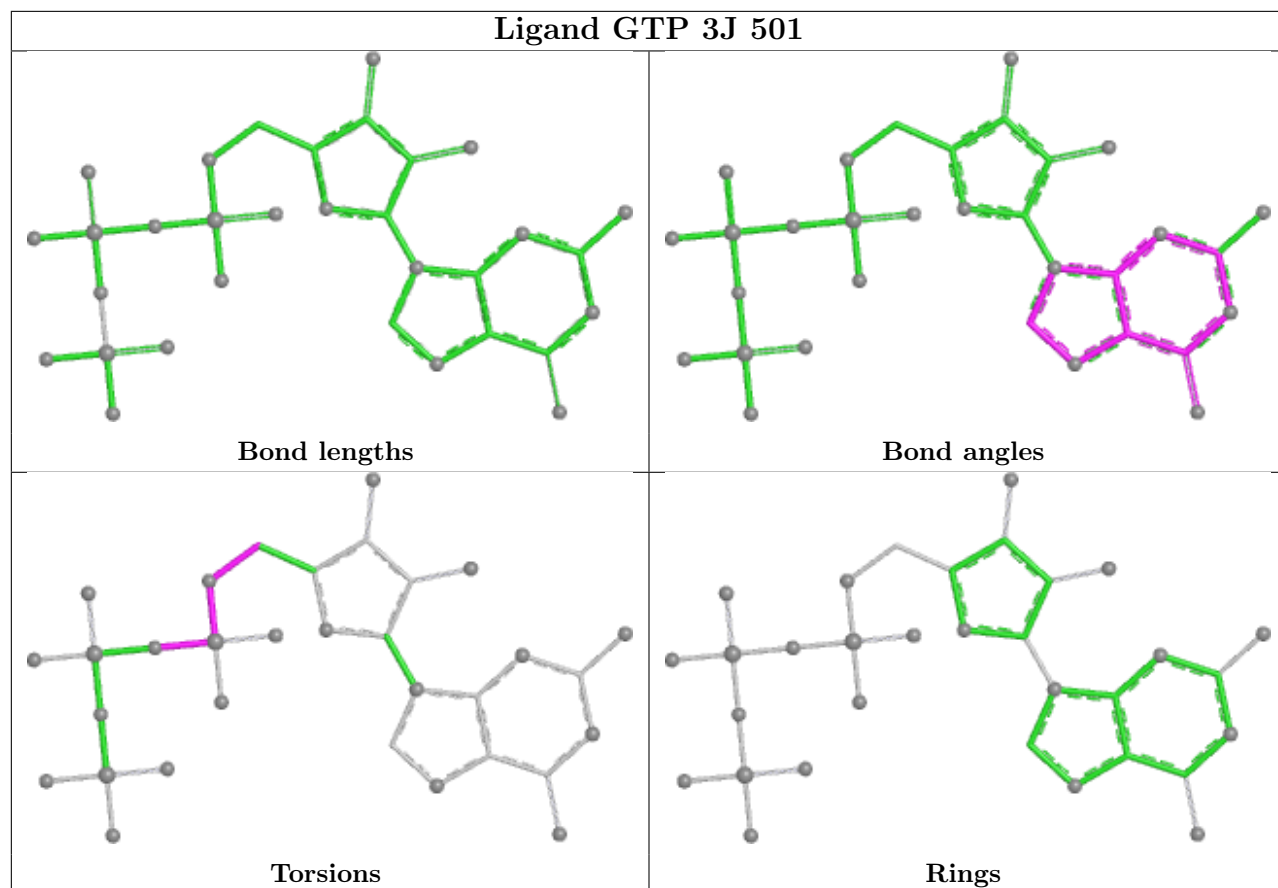
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will



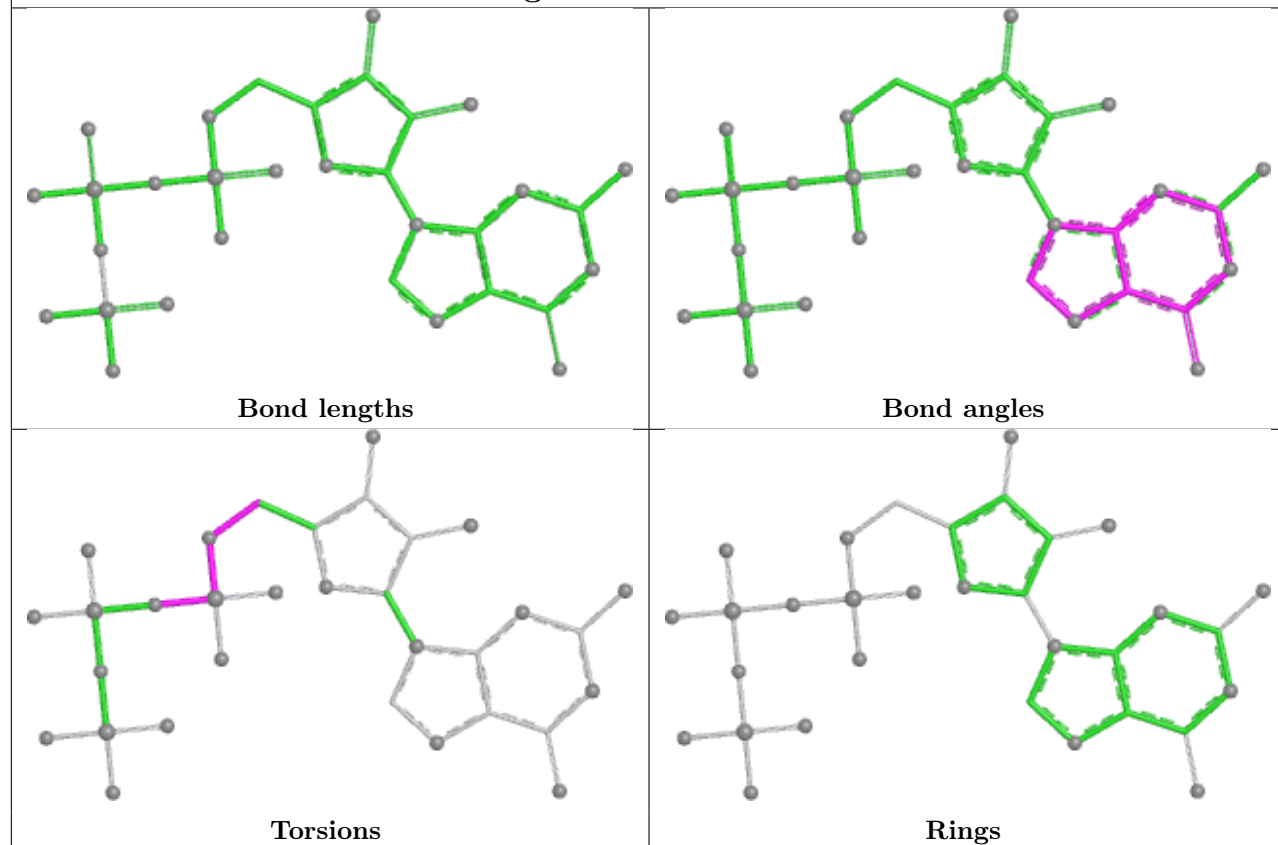
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



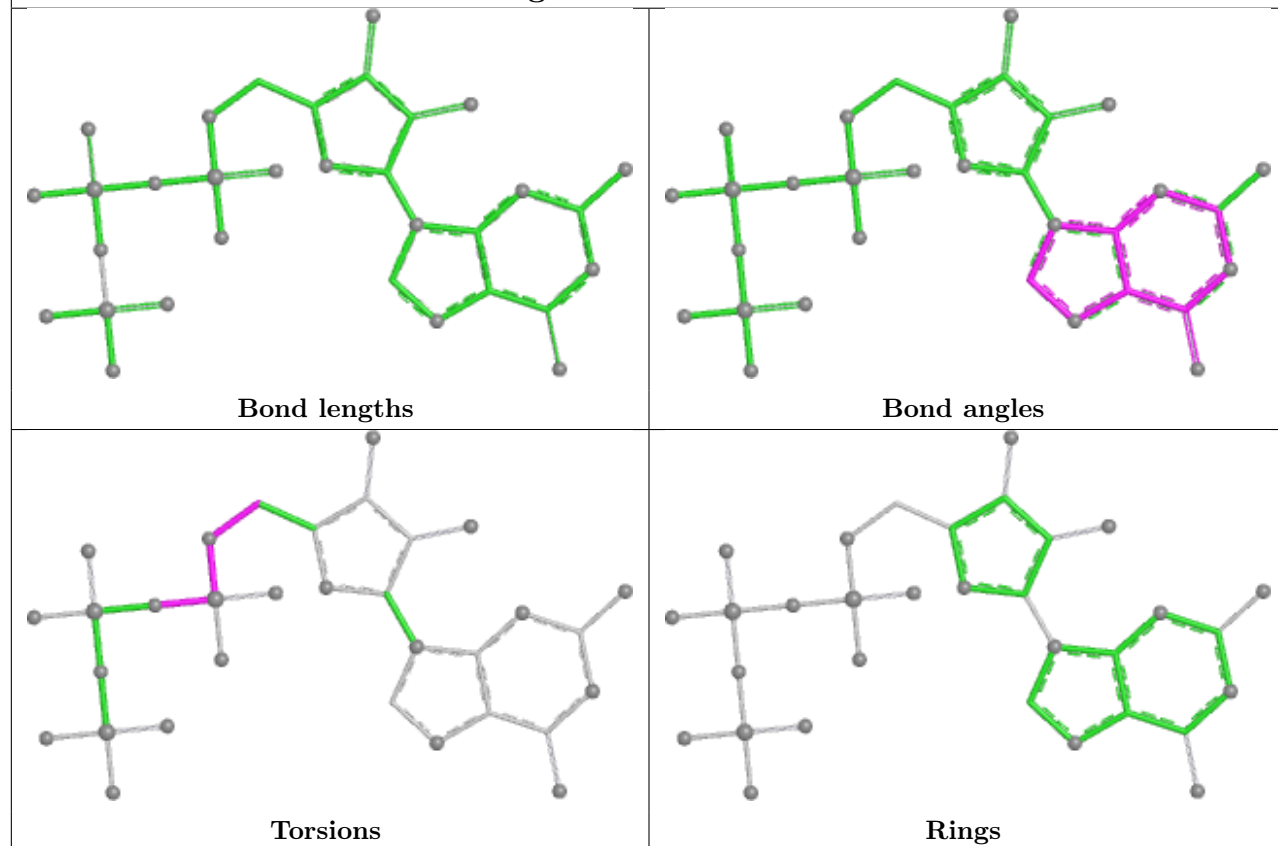




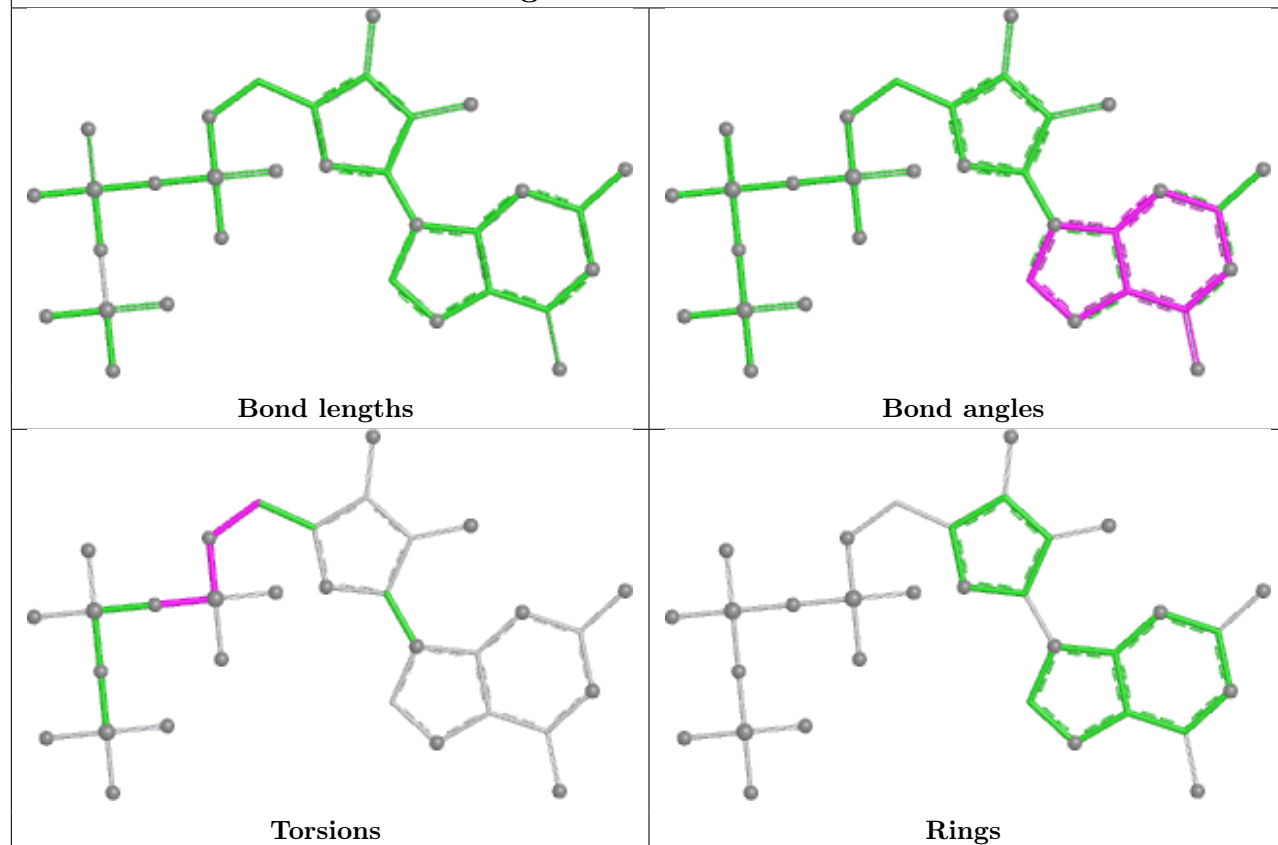
## Ligand GTP 3L 501



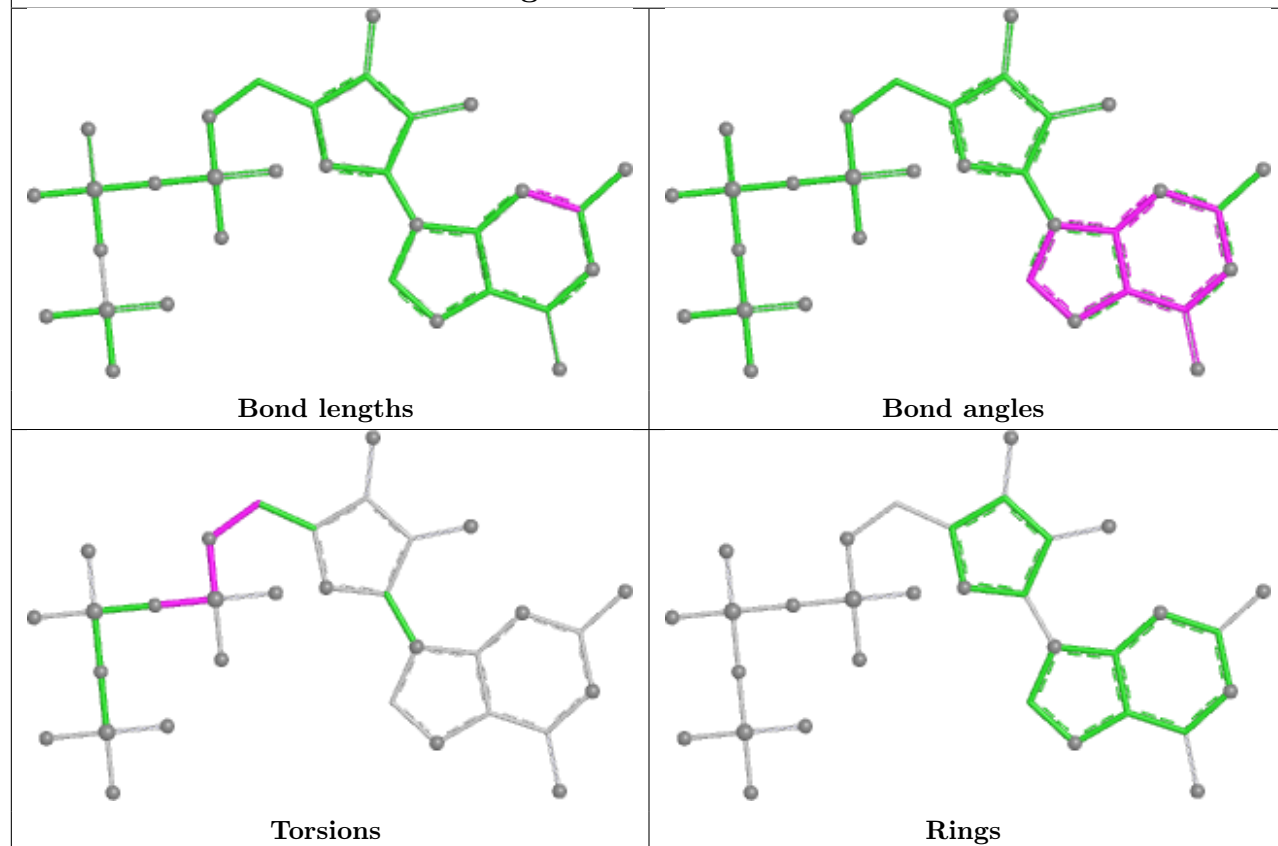
## Ligand GTP 2I 501



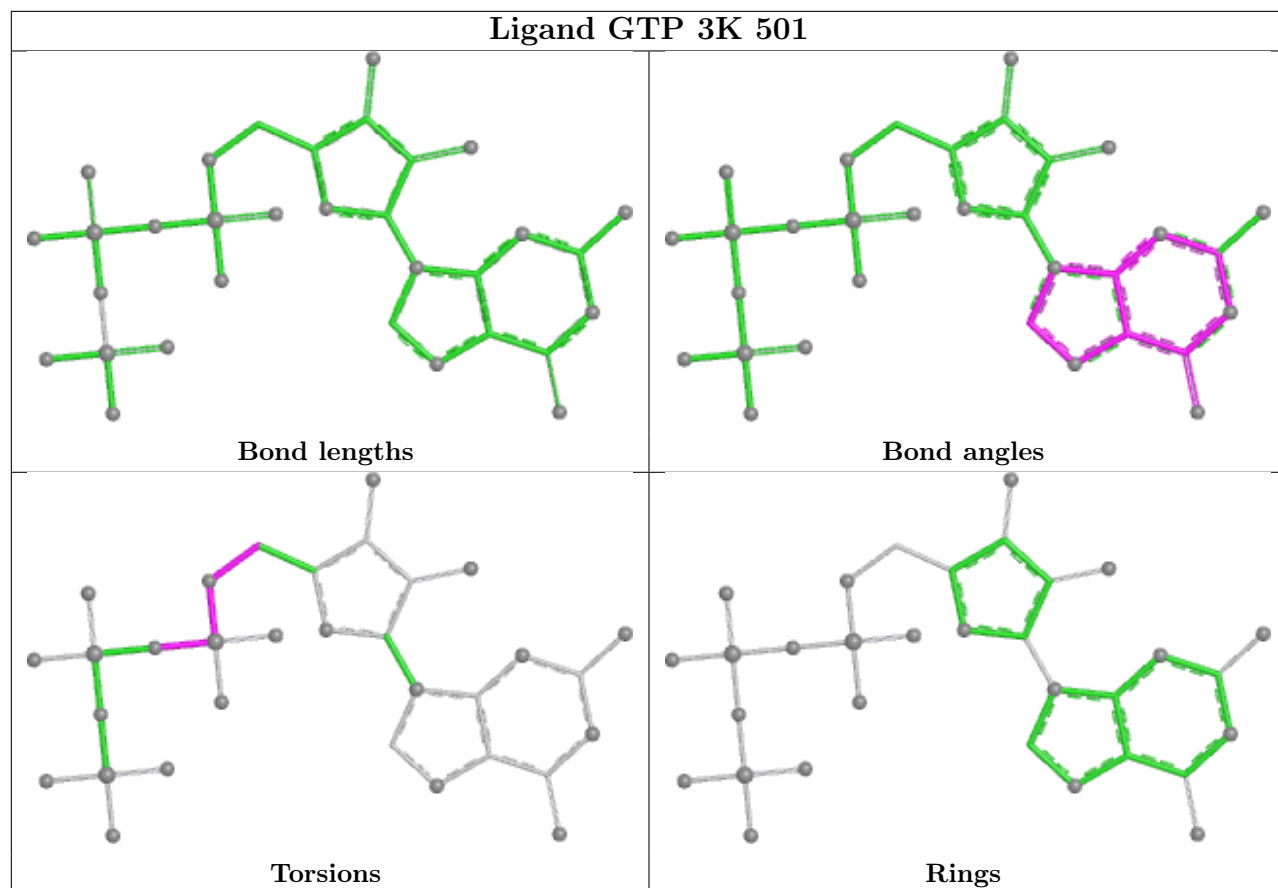
## Ligand GTP 2G 501



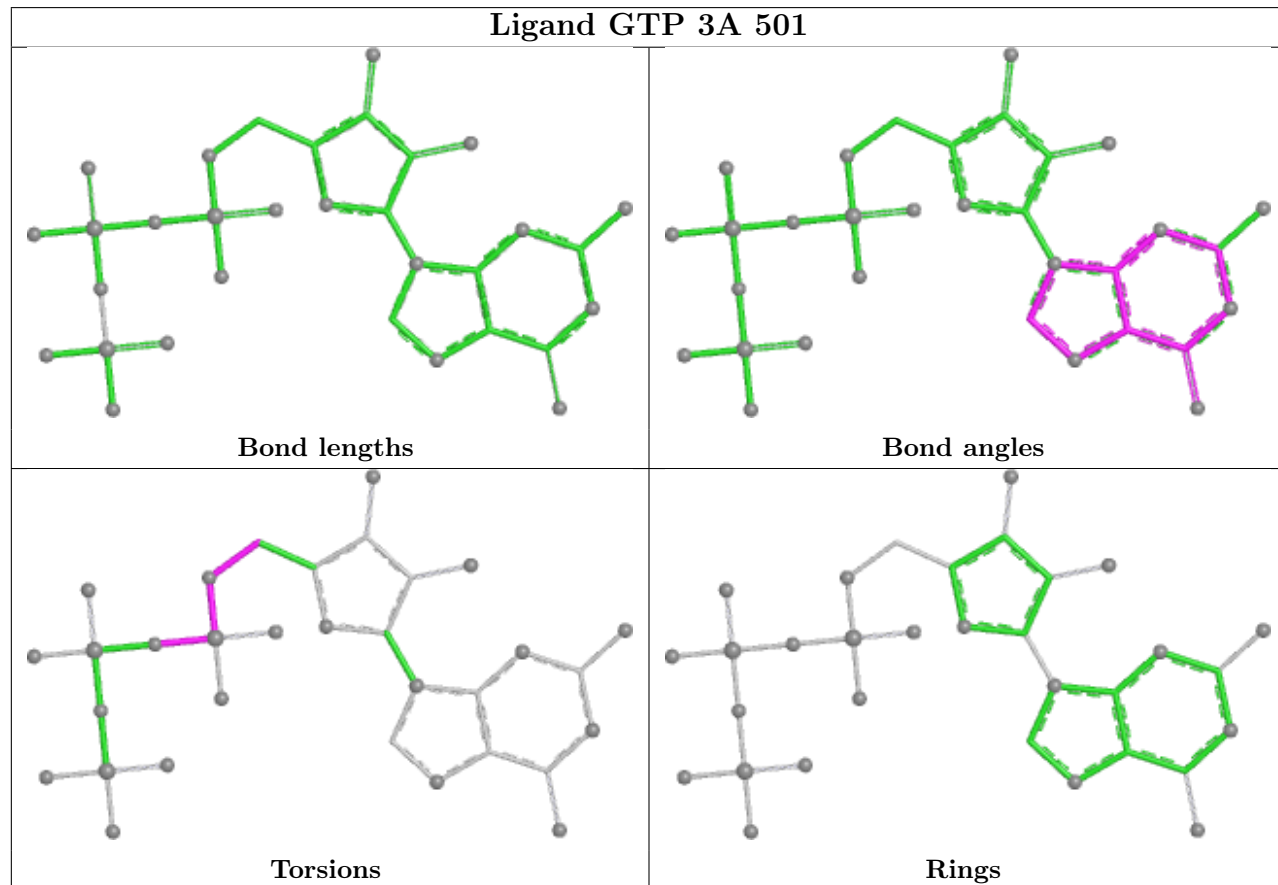
## Ligand GTP 3G 501

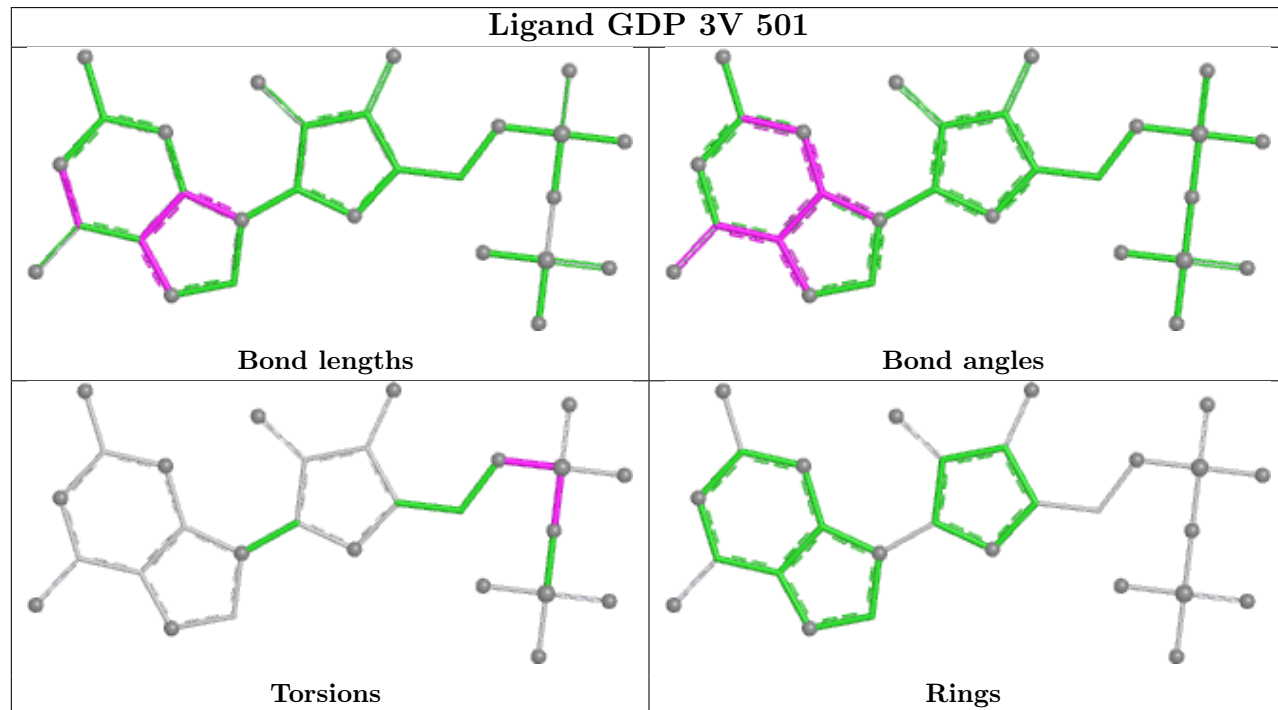
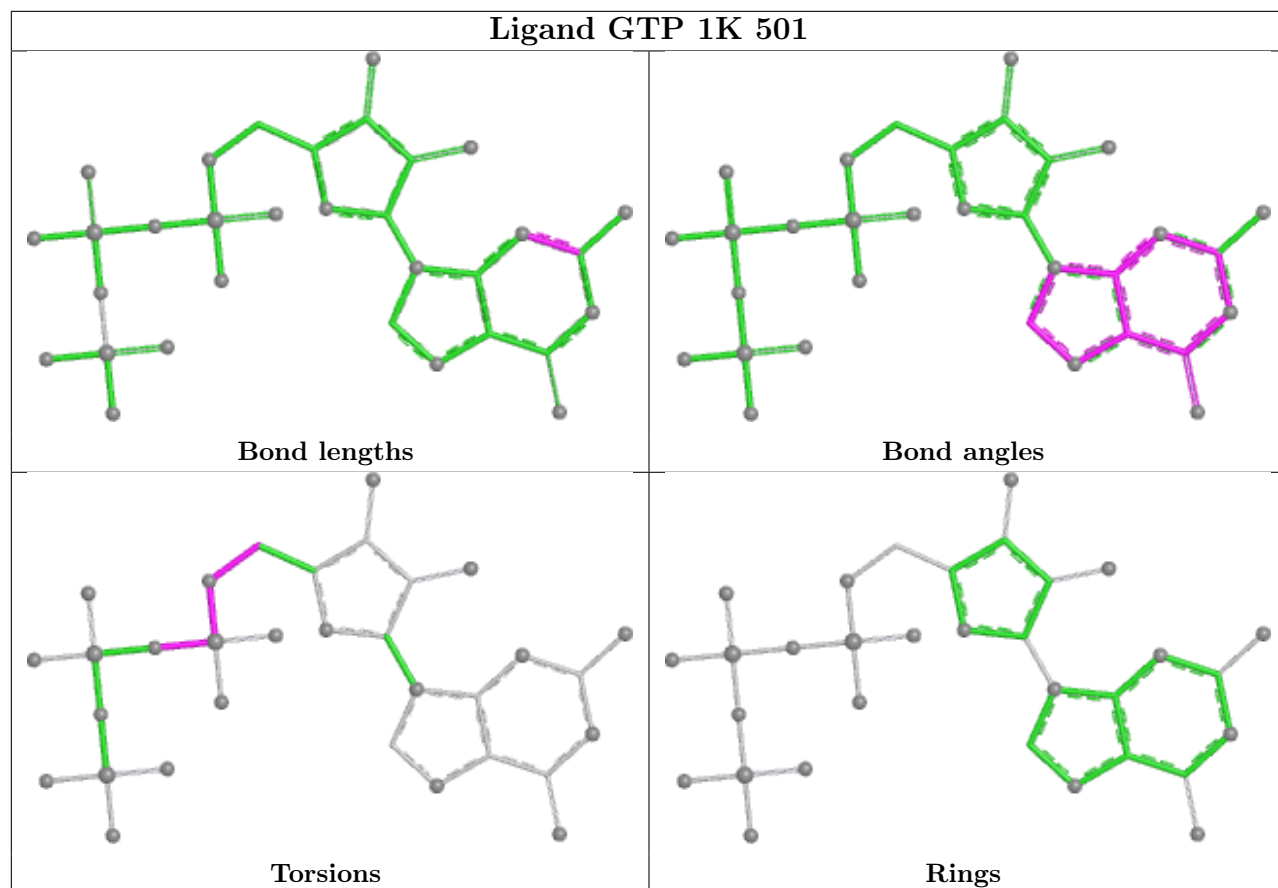


## Ligand GTP 3K 501

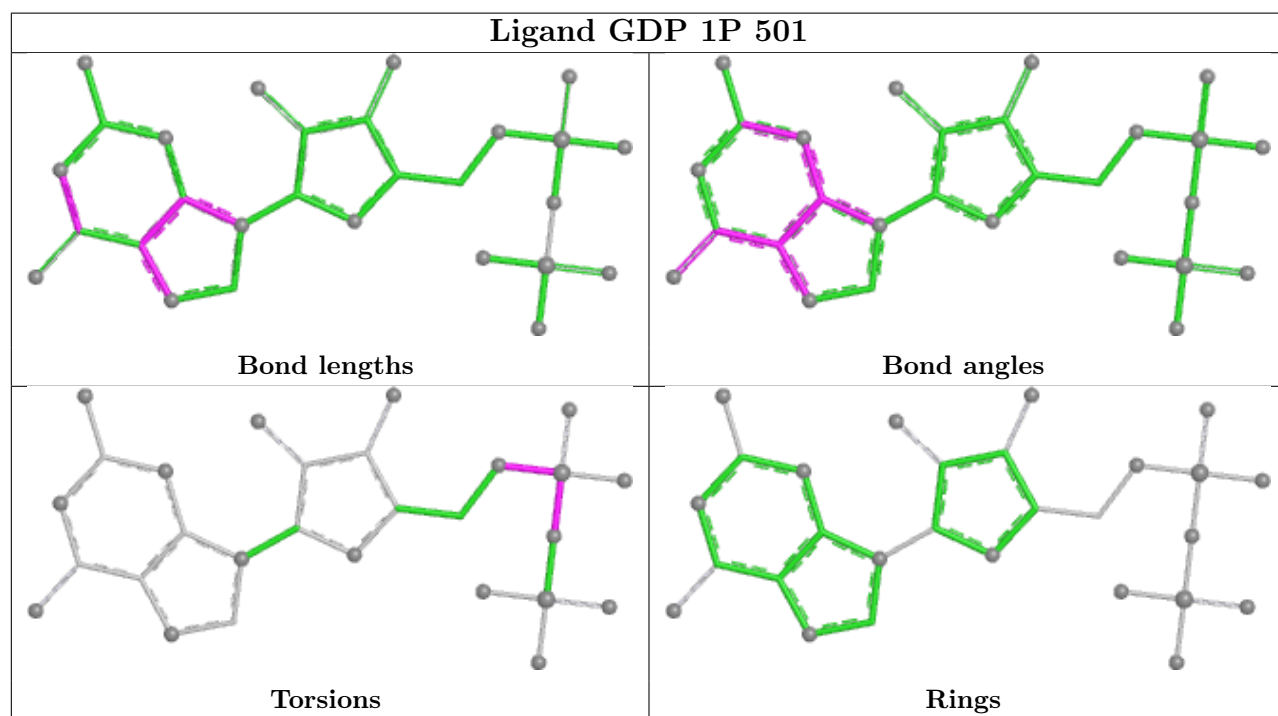
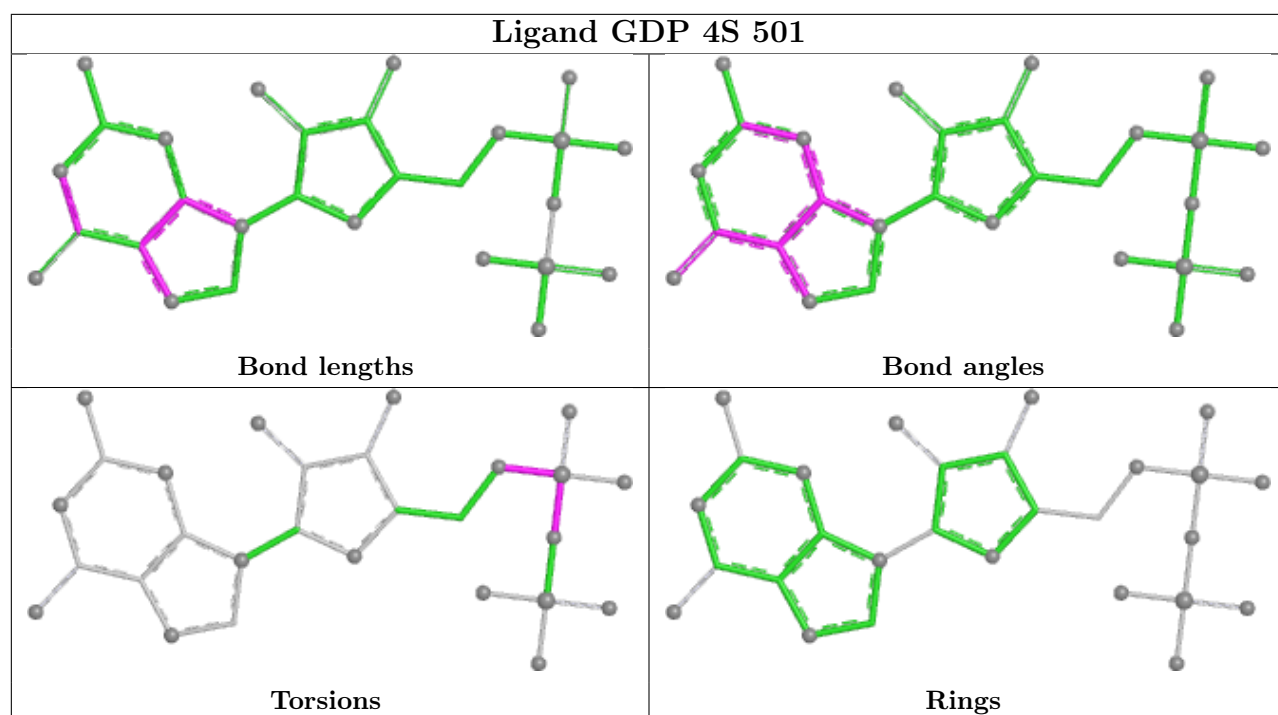


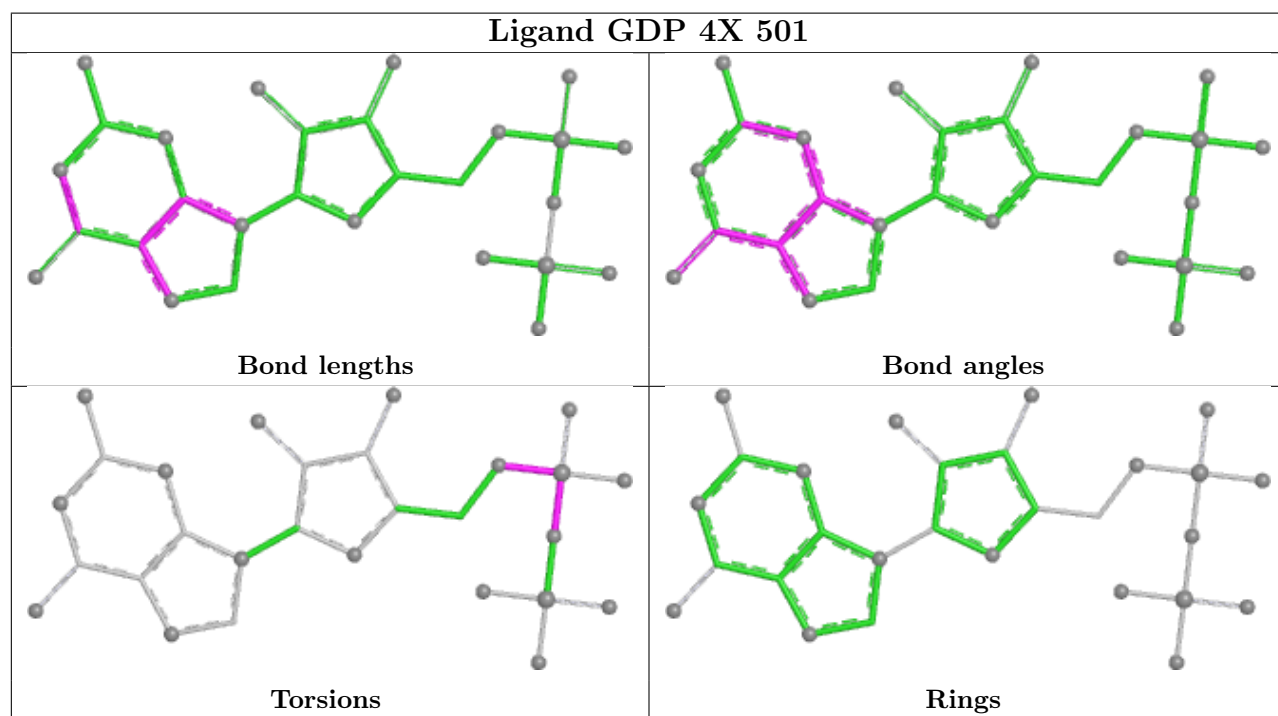
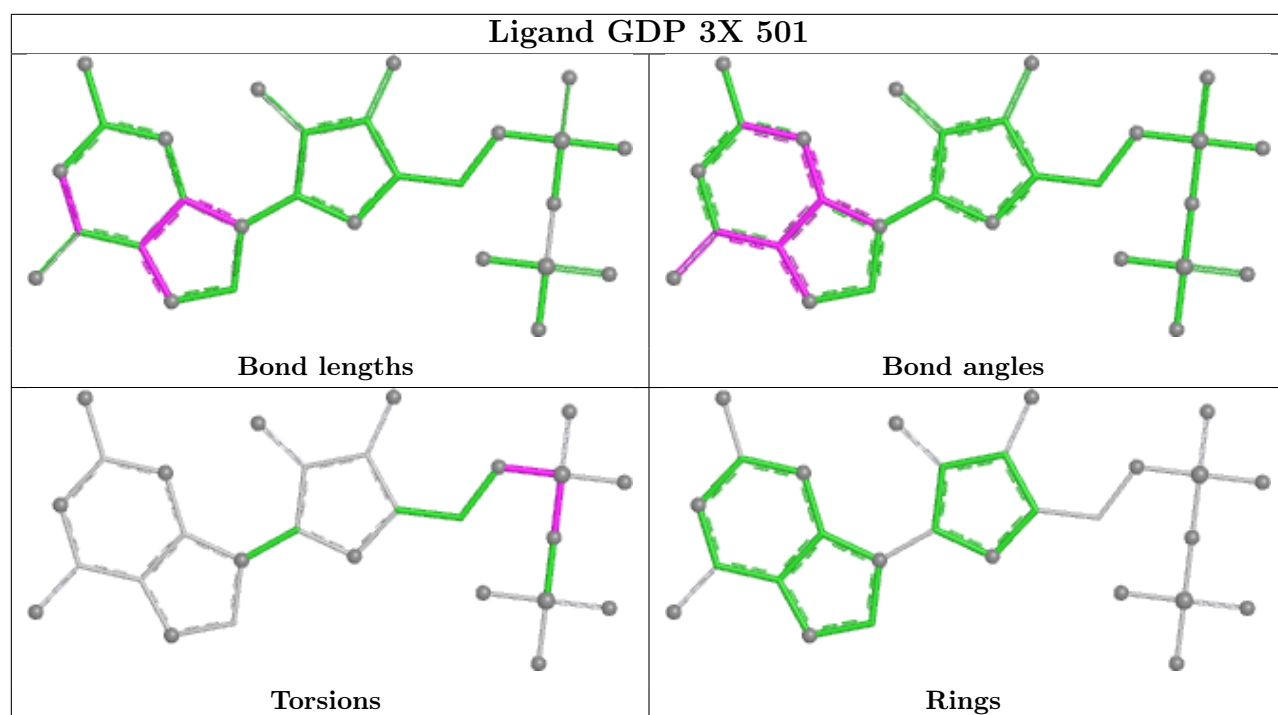
## Ligand GTP 3A 501

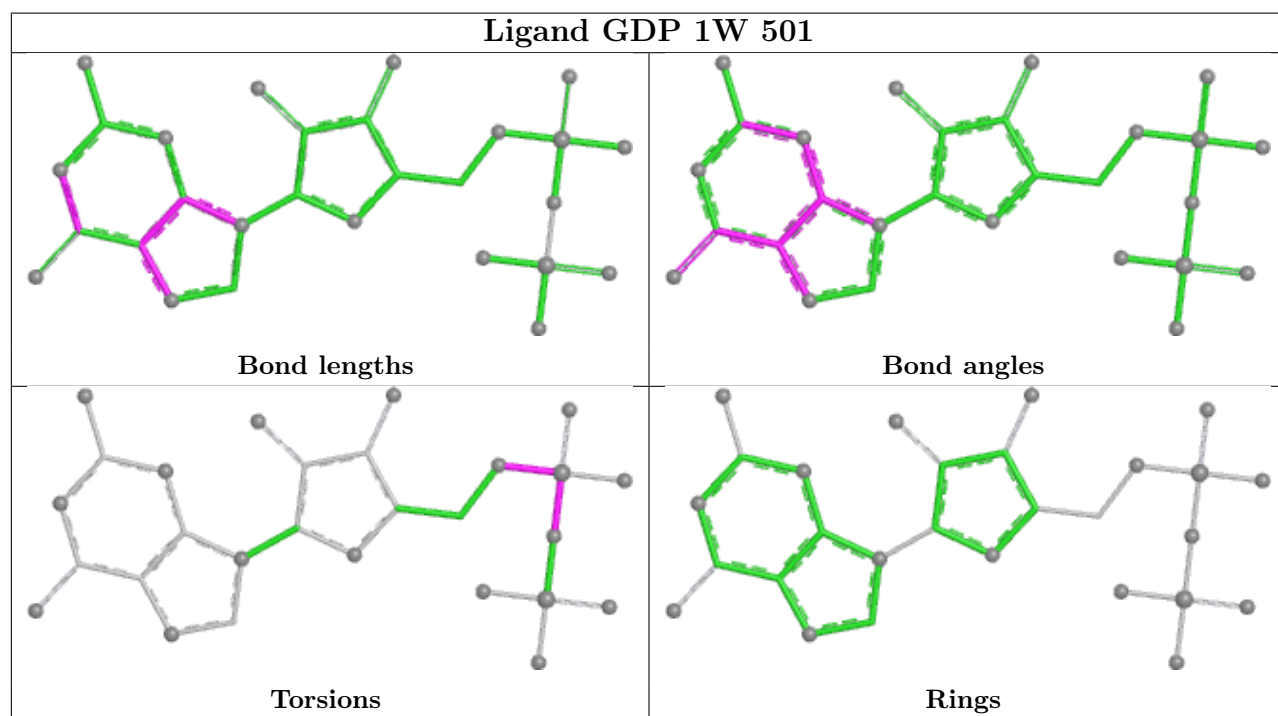
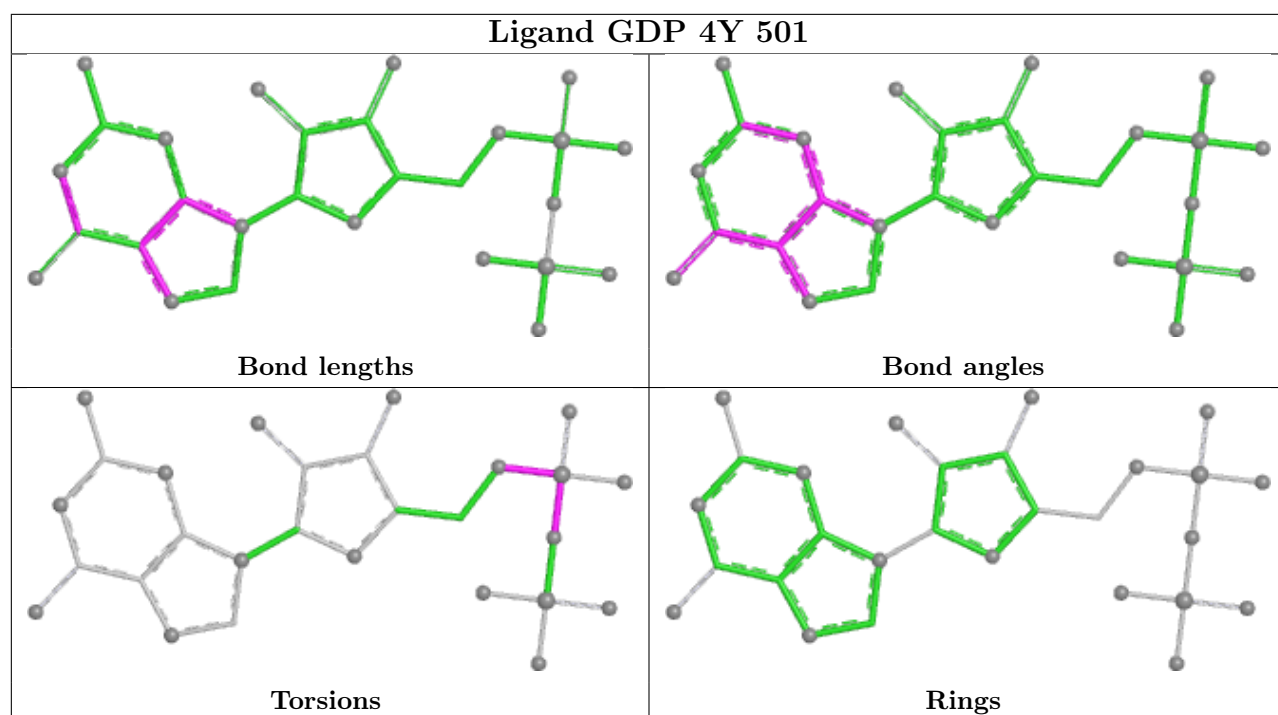




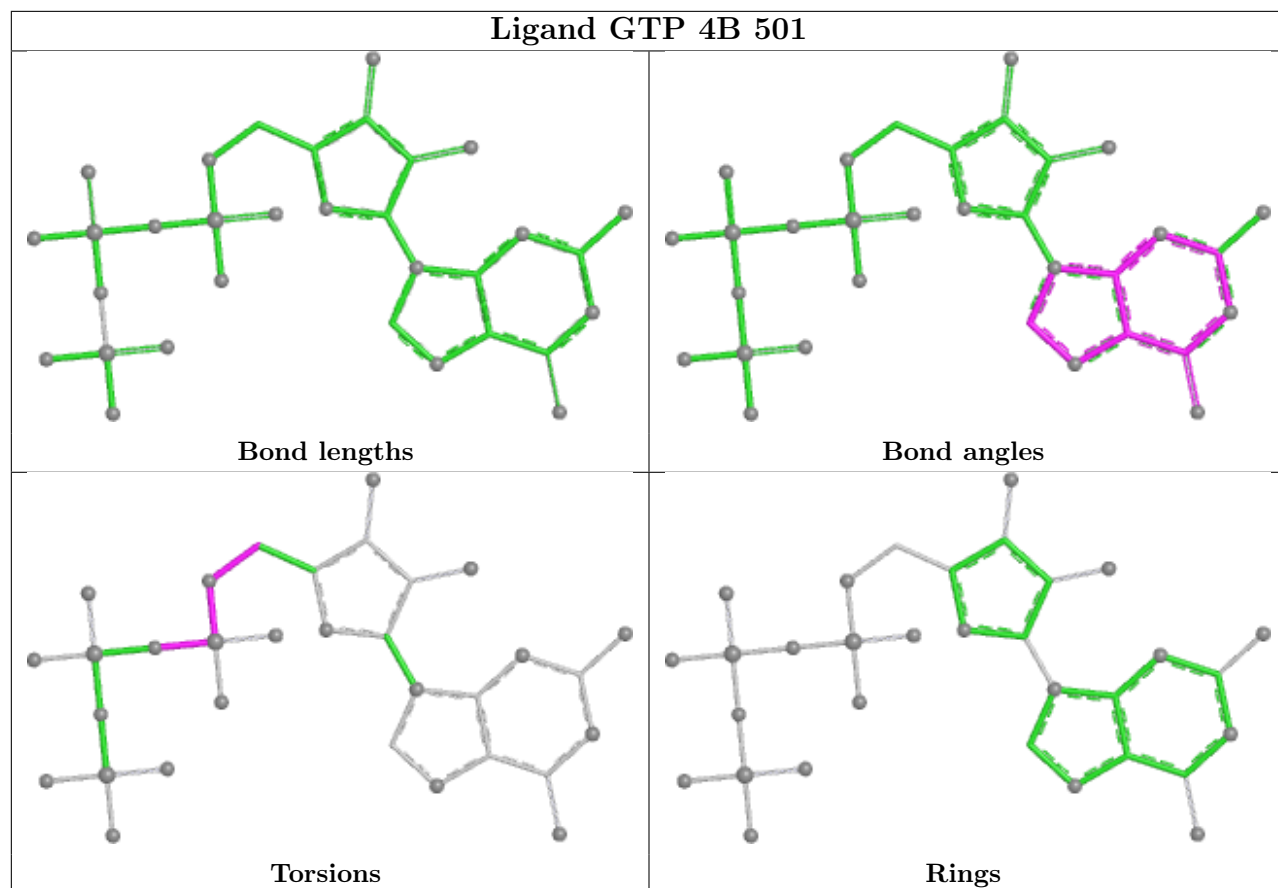




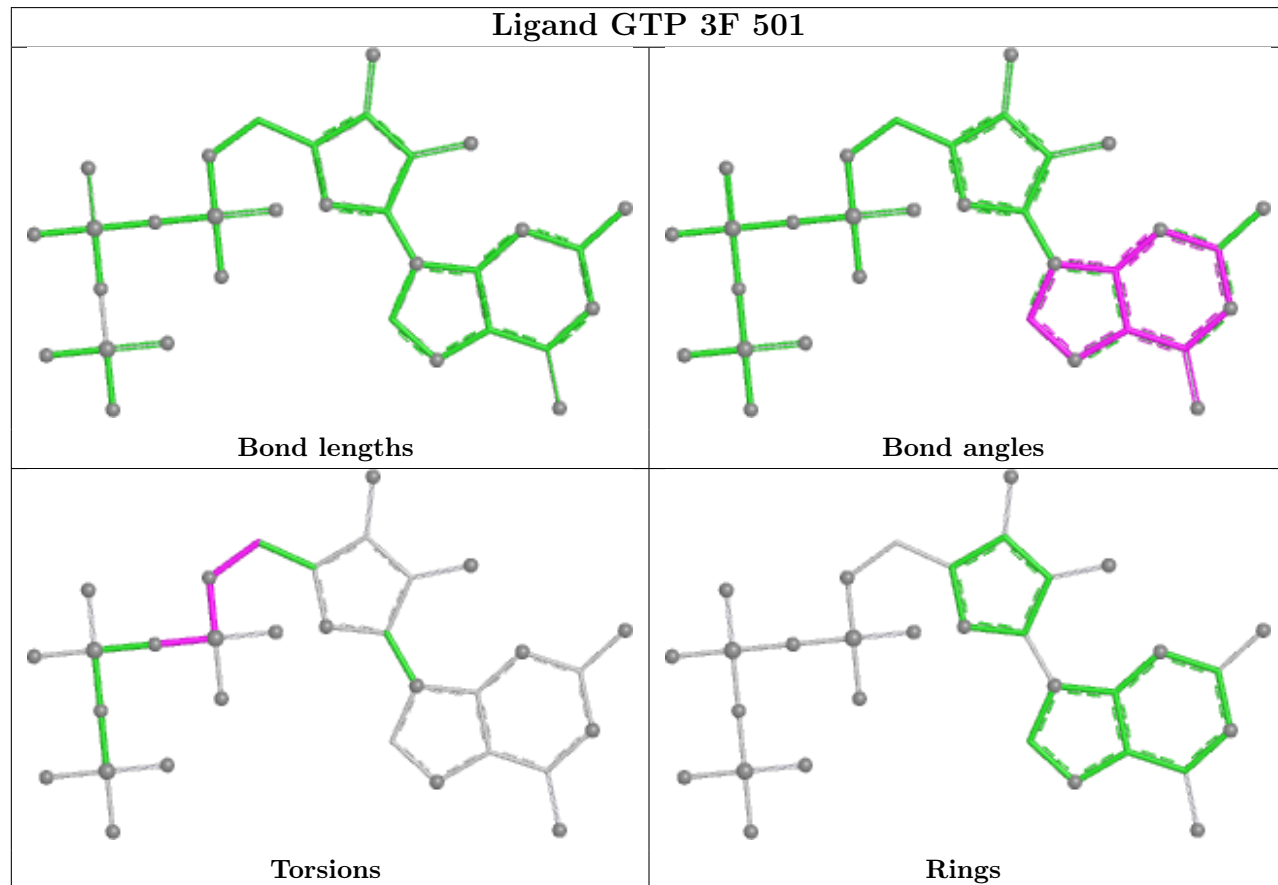


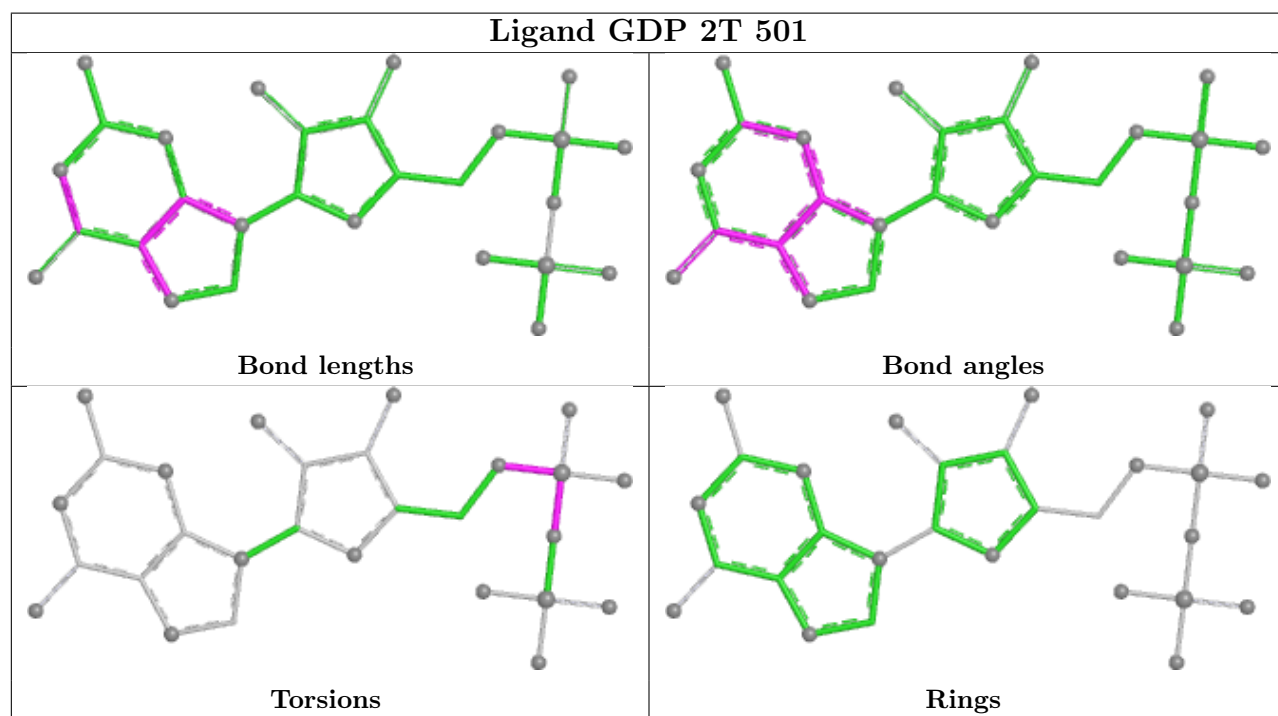
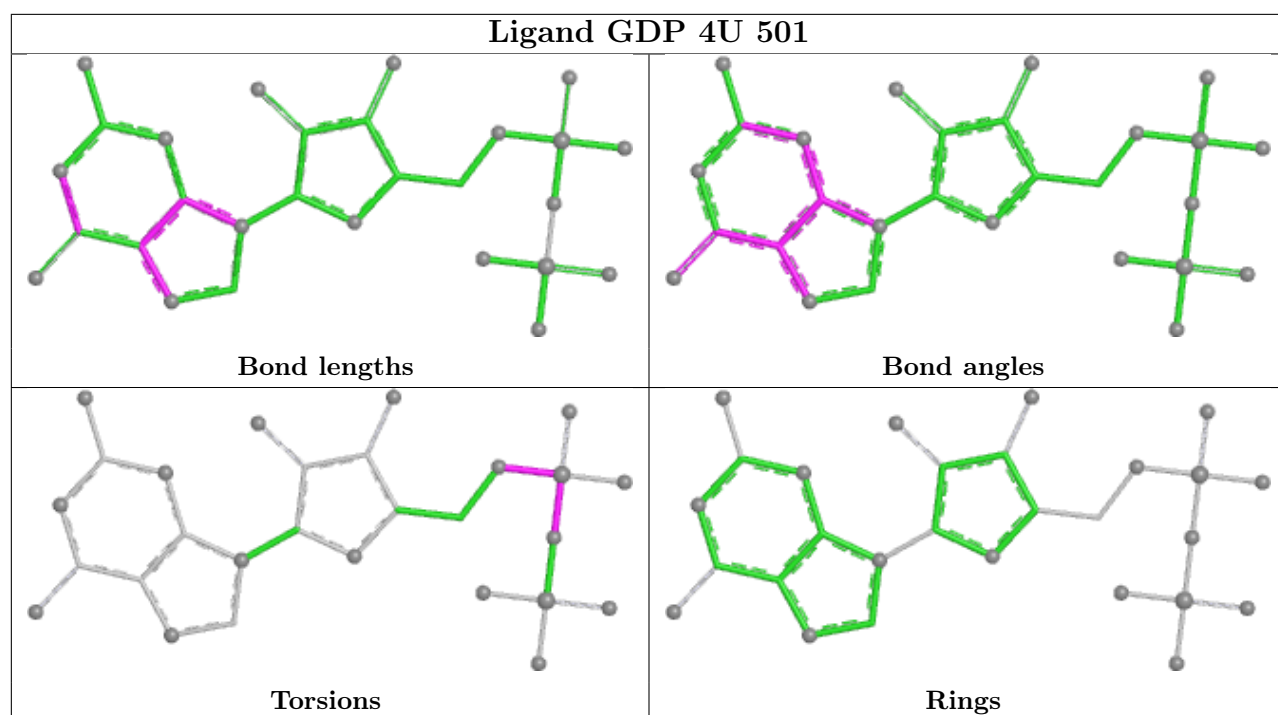


## Ligand GTP 4B 501

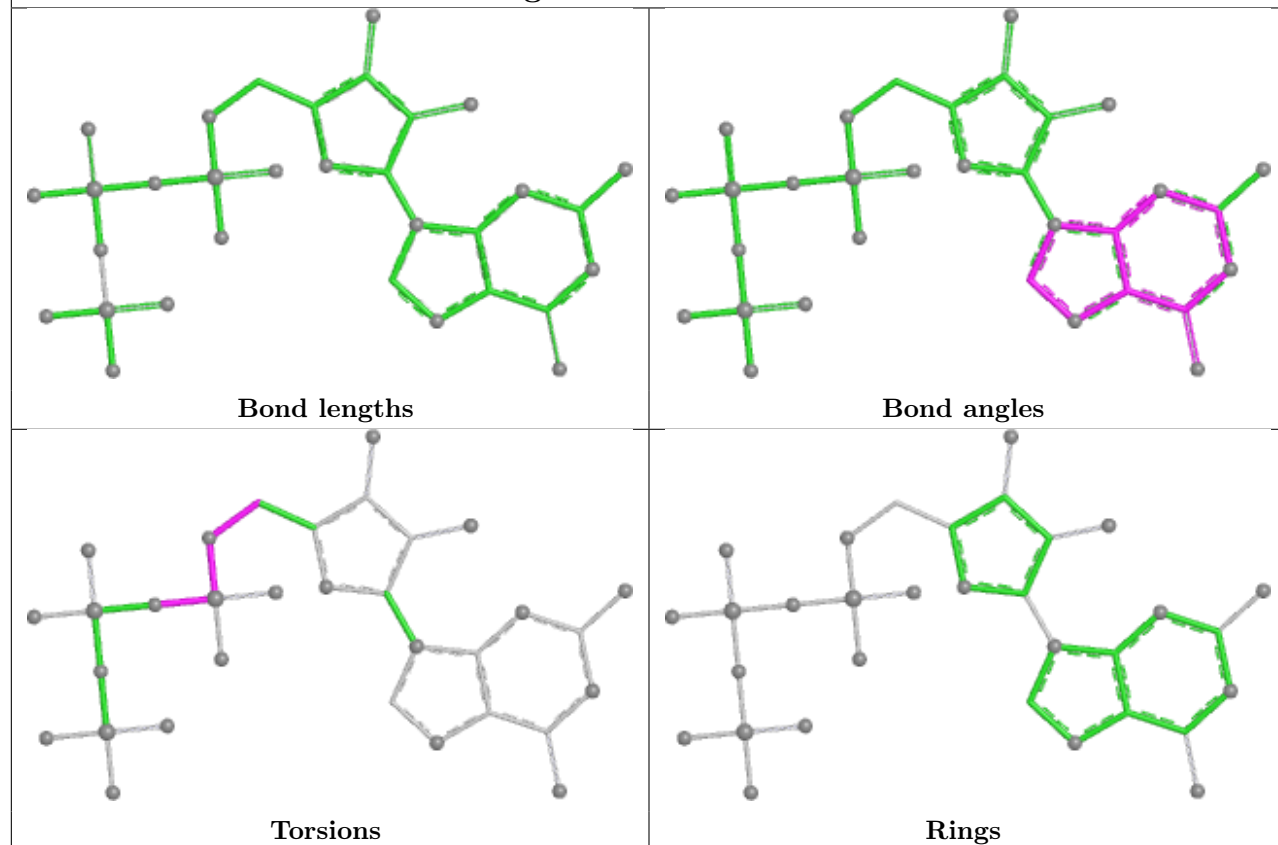


## Ligand GTP 3F 501

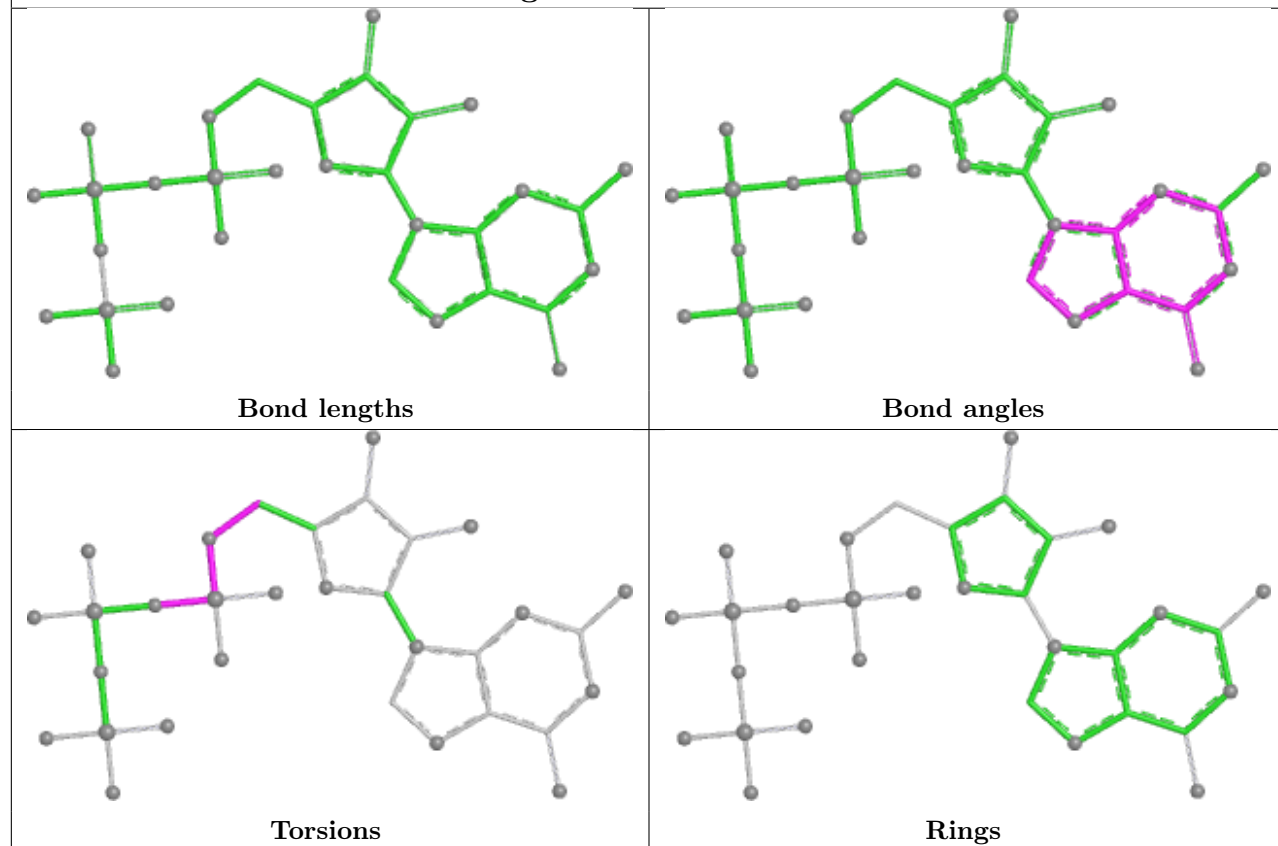


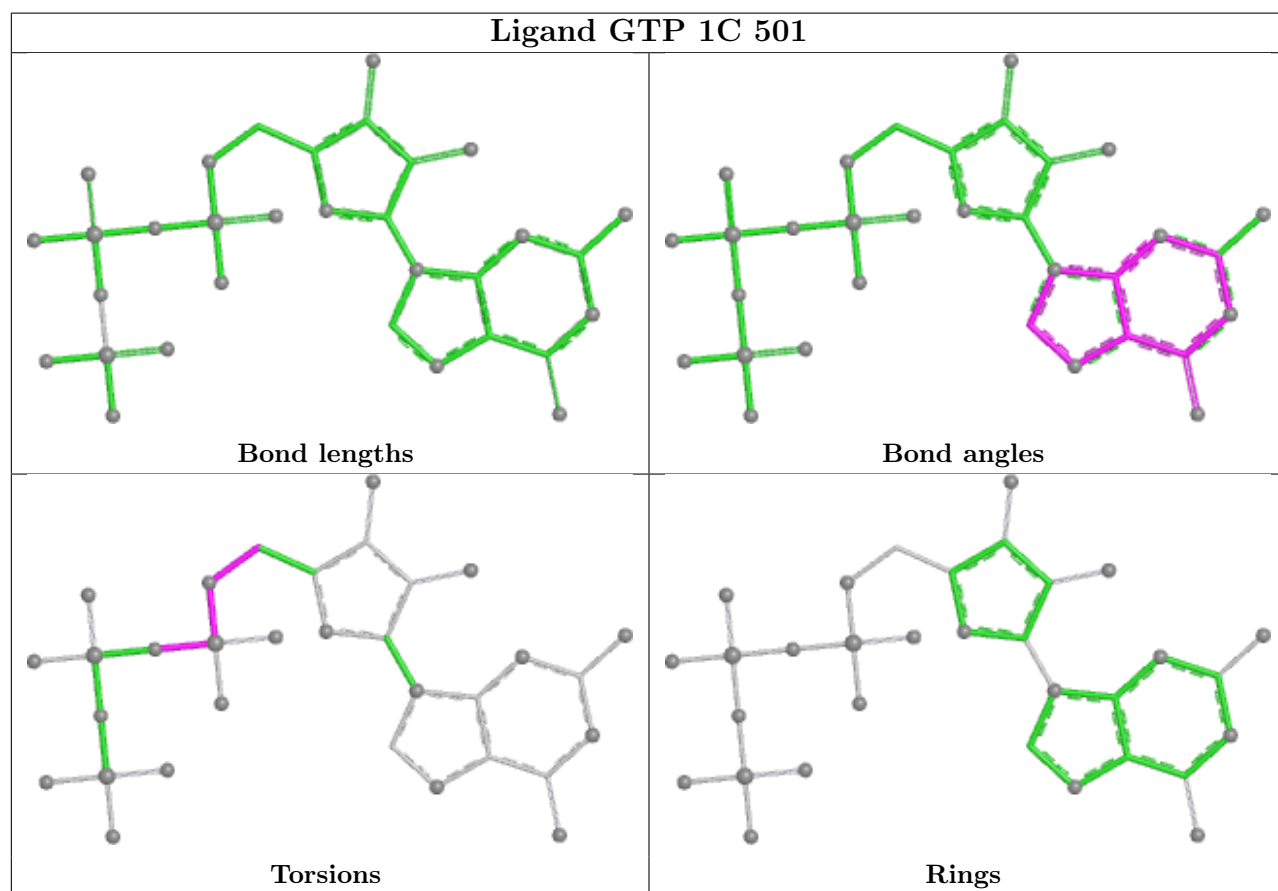
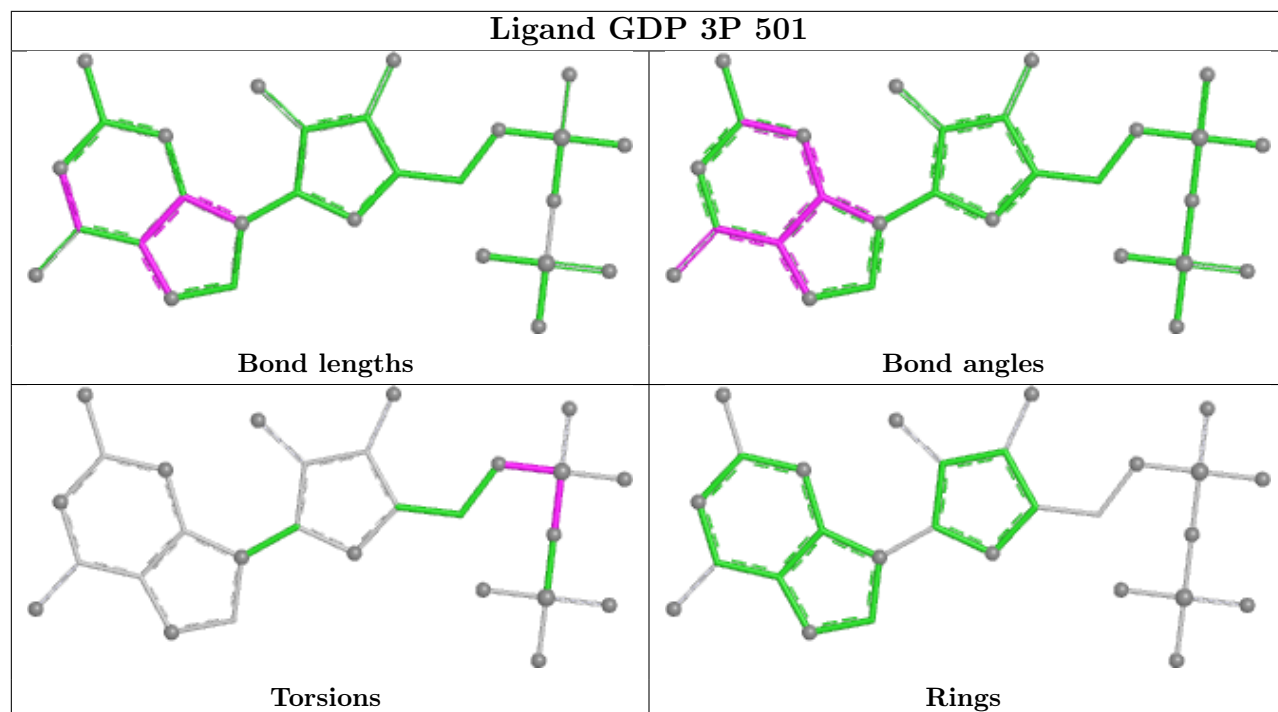


## Ligand GTP 1L 501



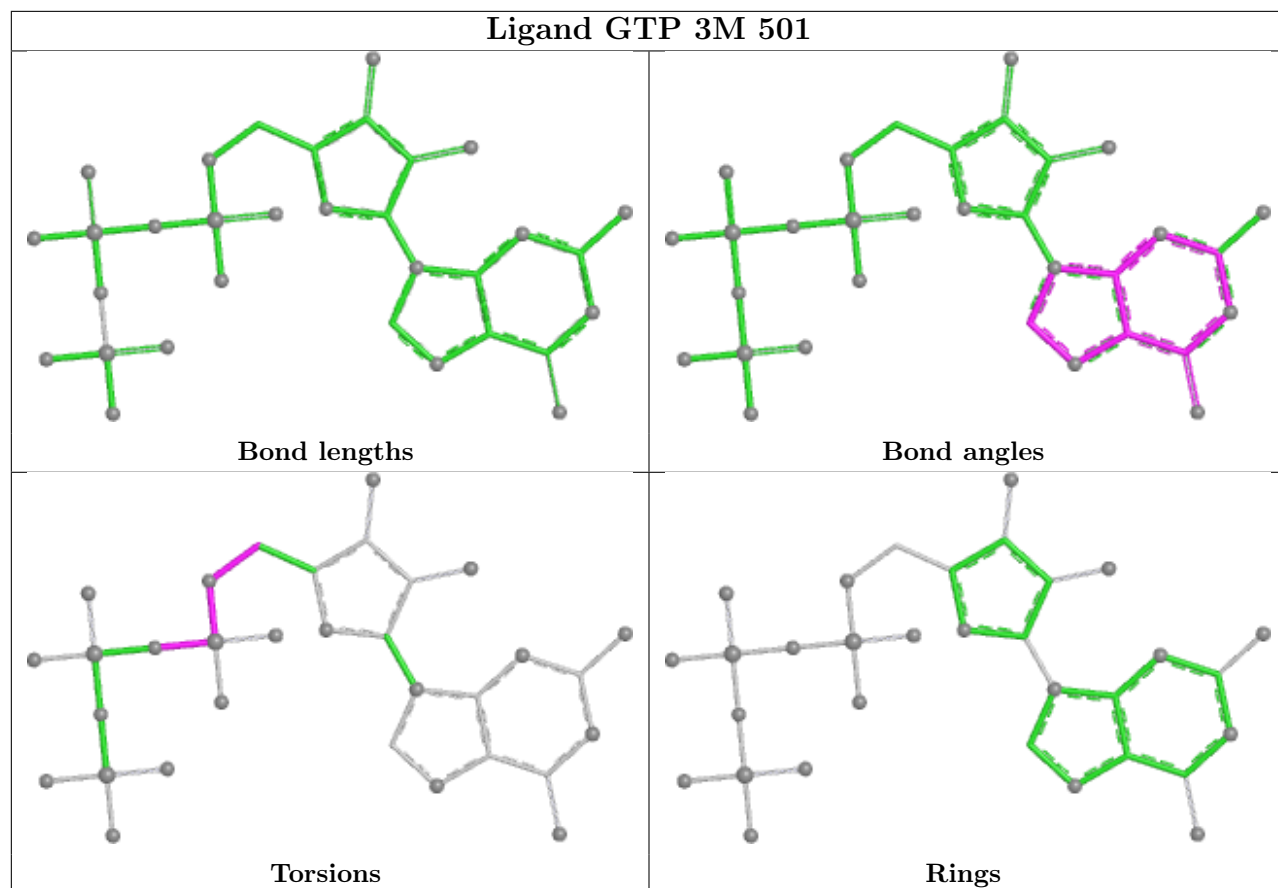
## Ligand GTP 4G 501



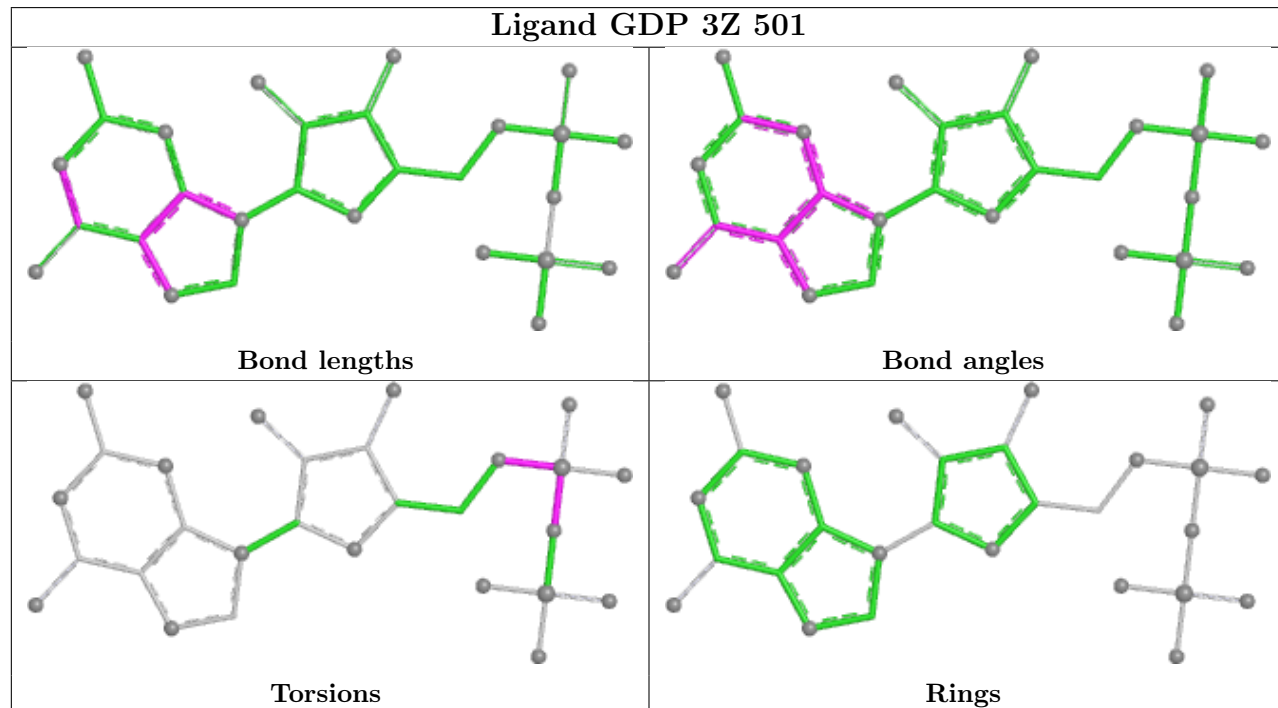


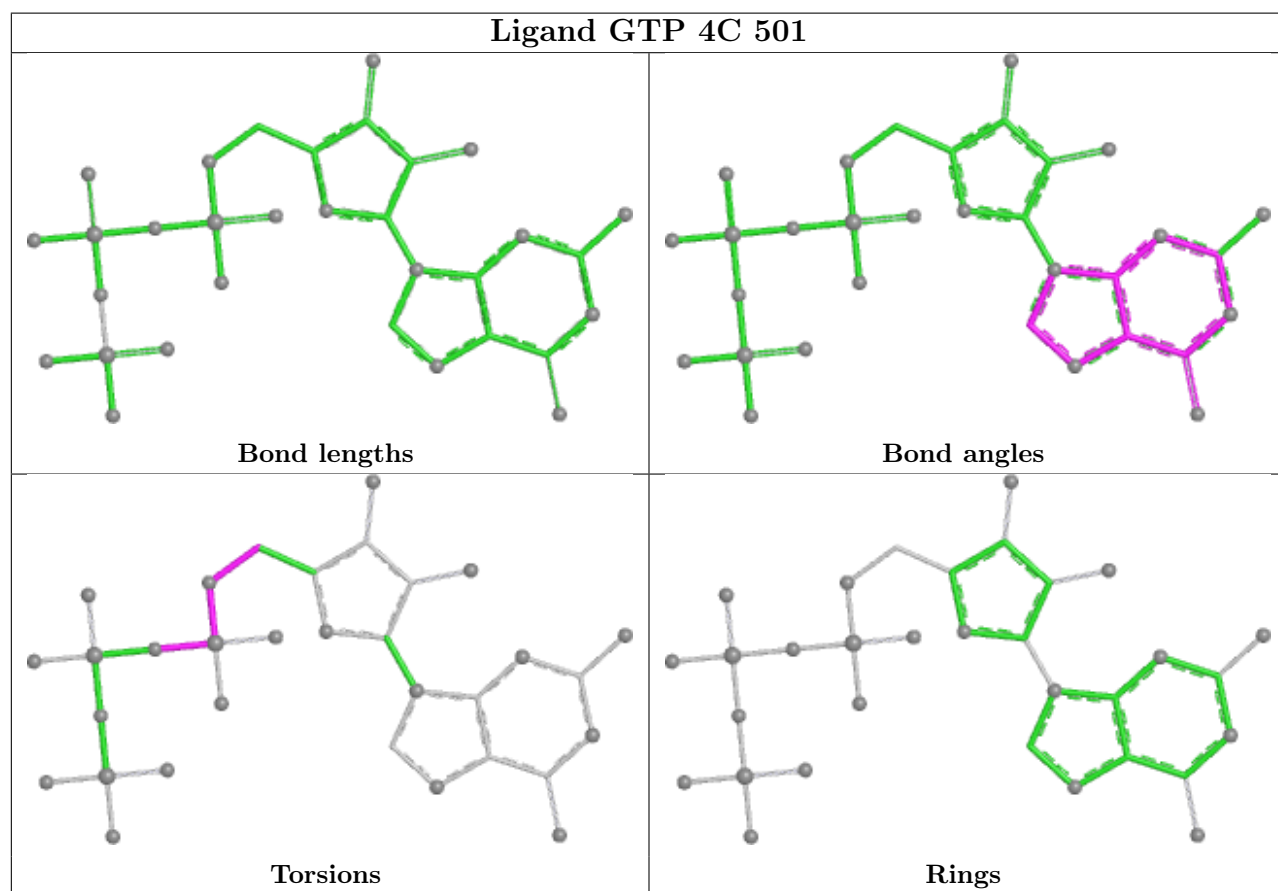
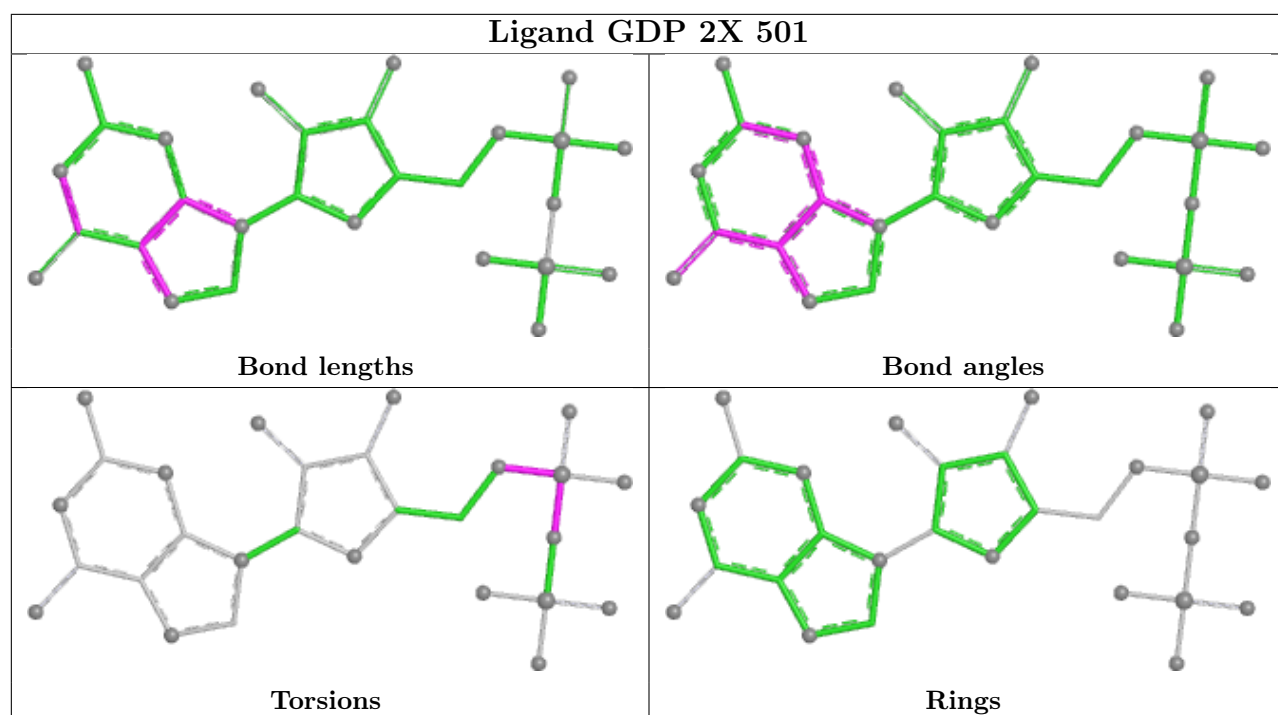


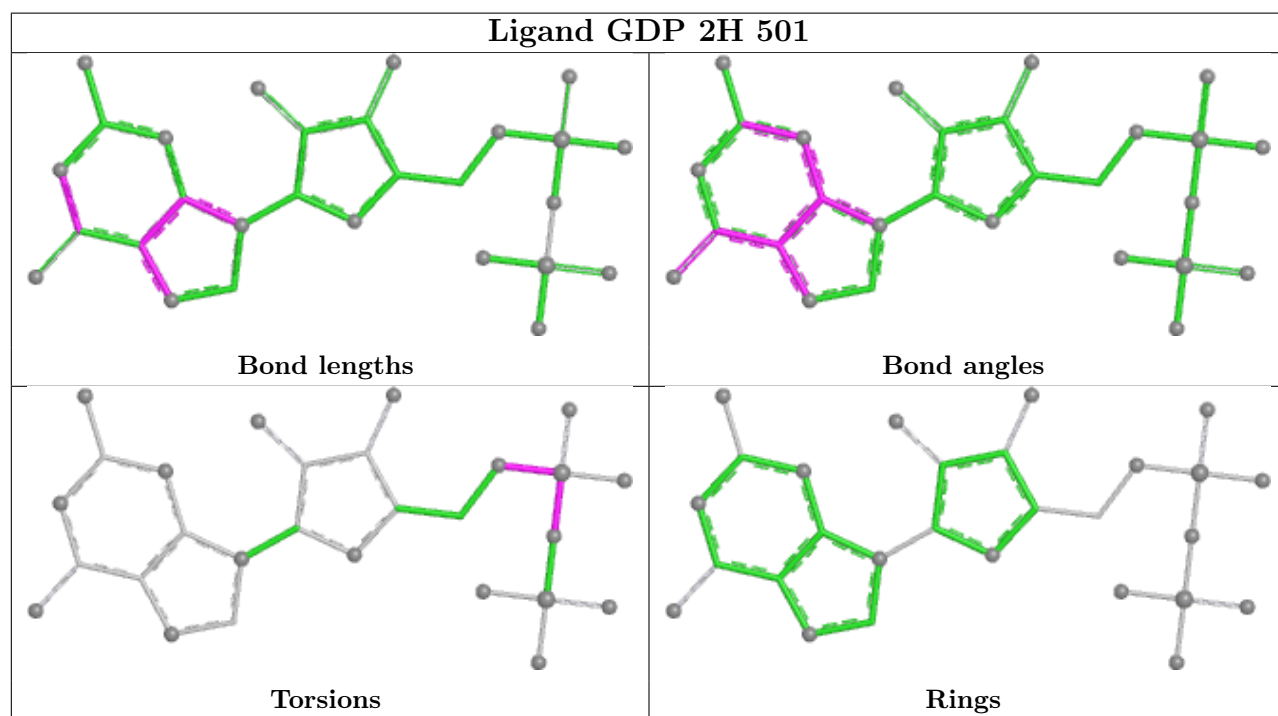
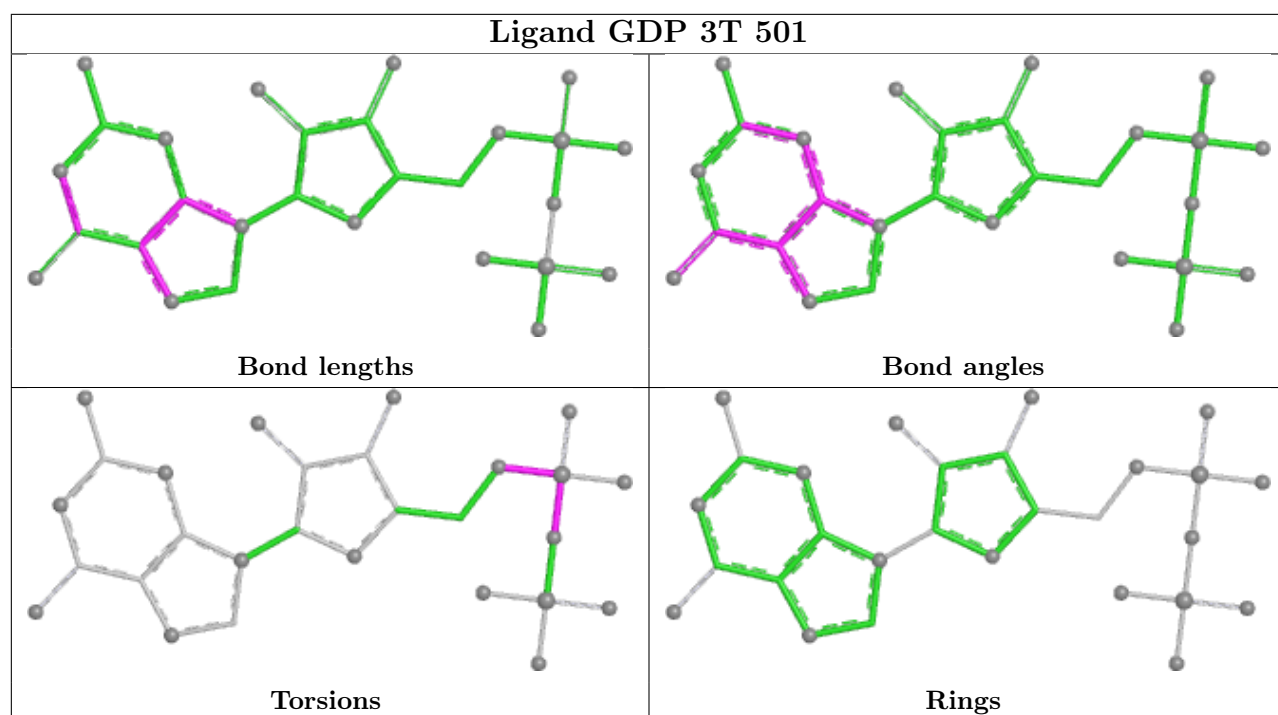
## Ligand GTP 3M 501

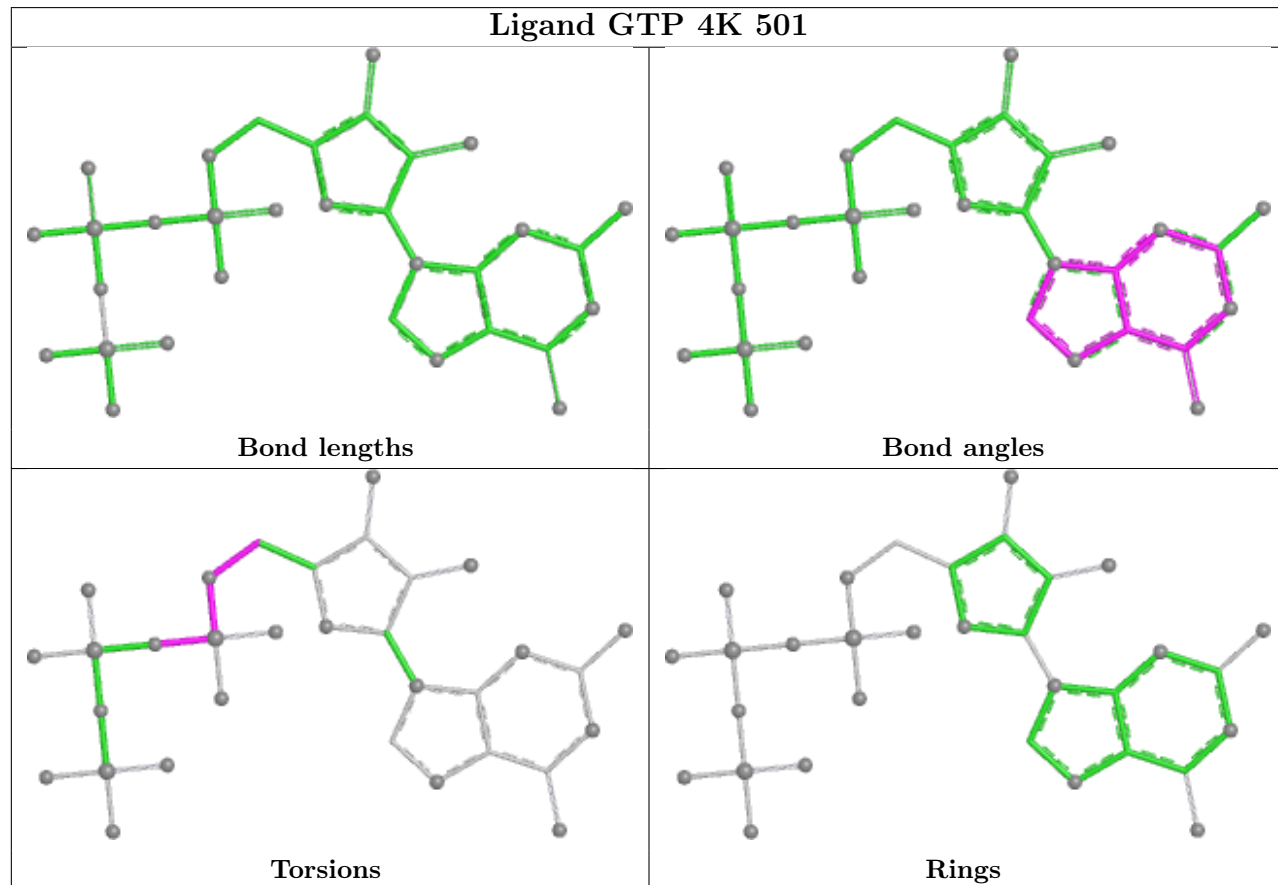
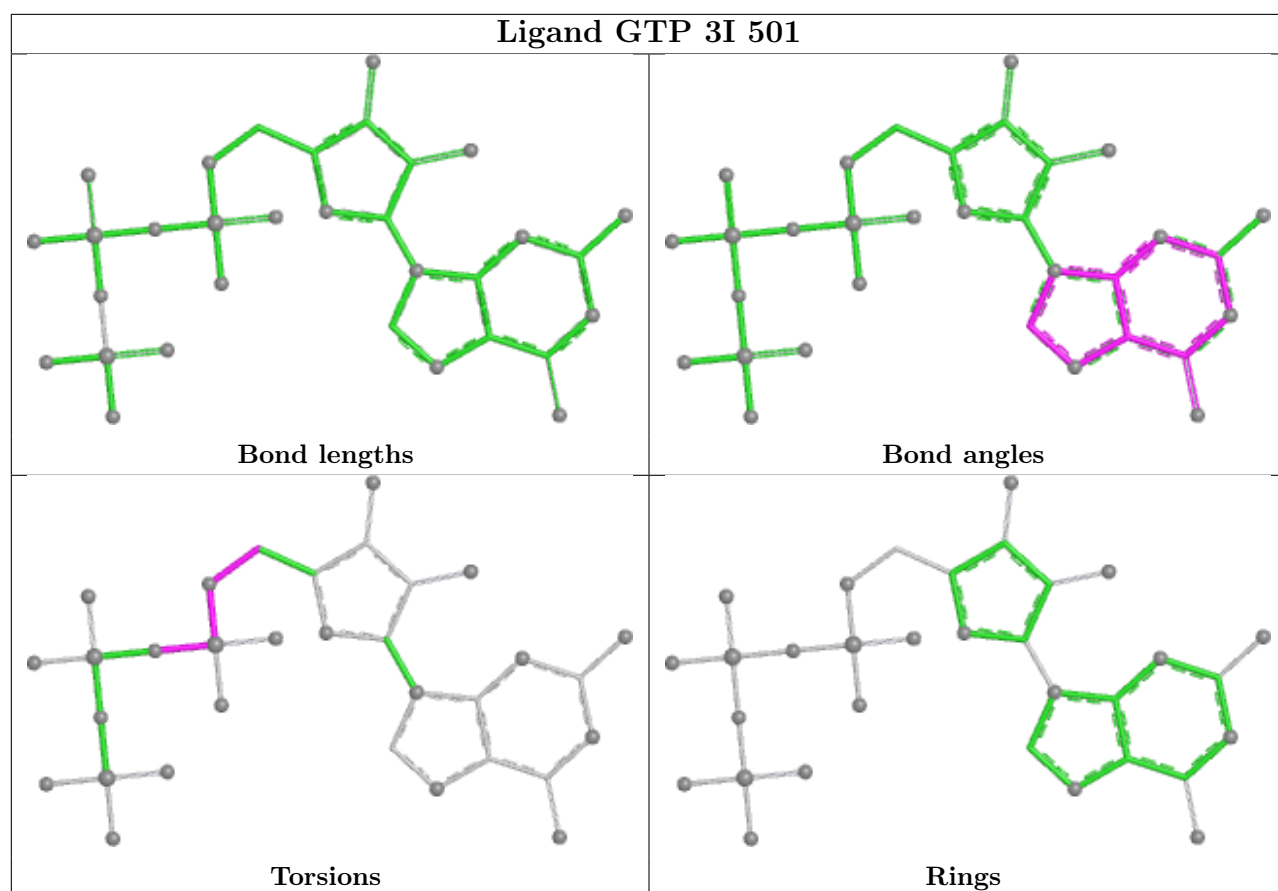


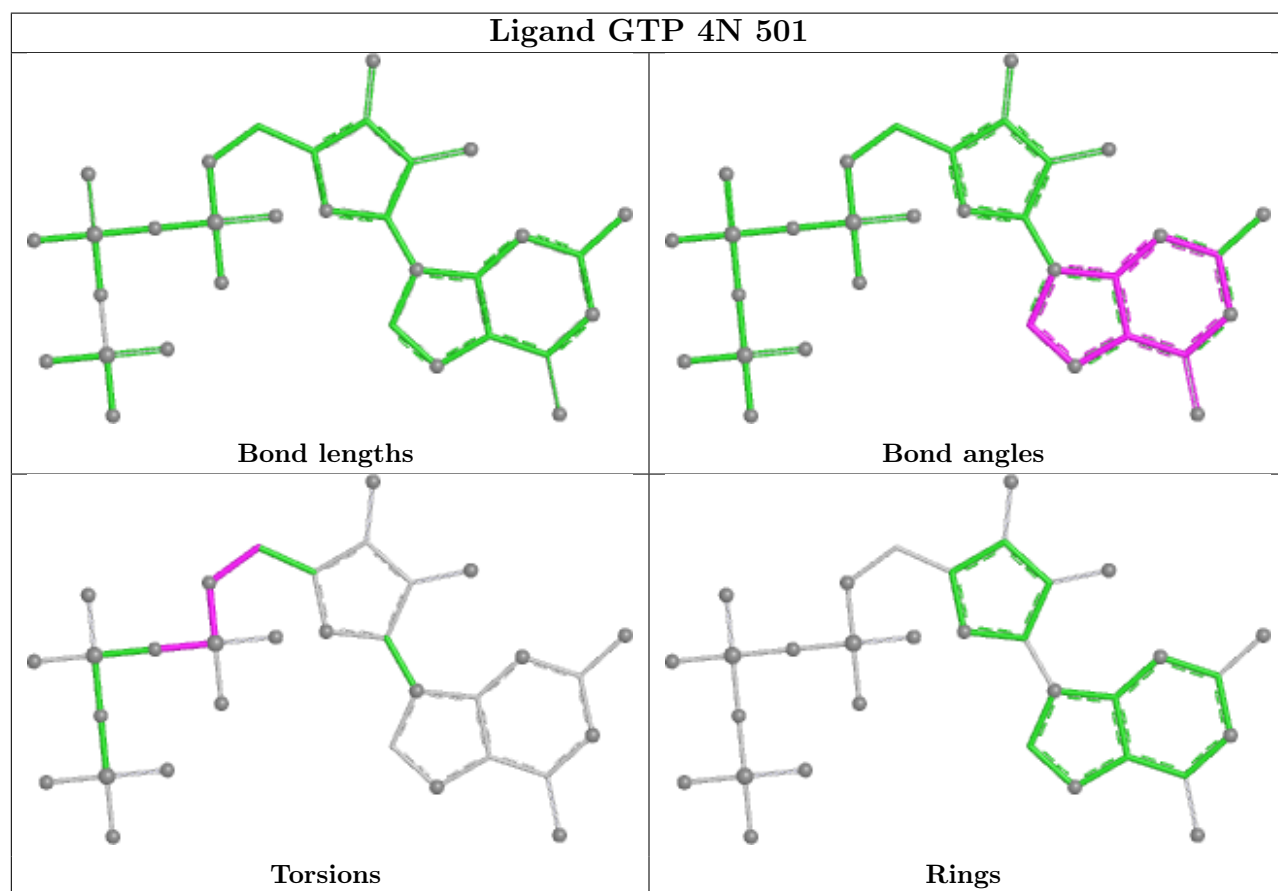
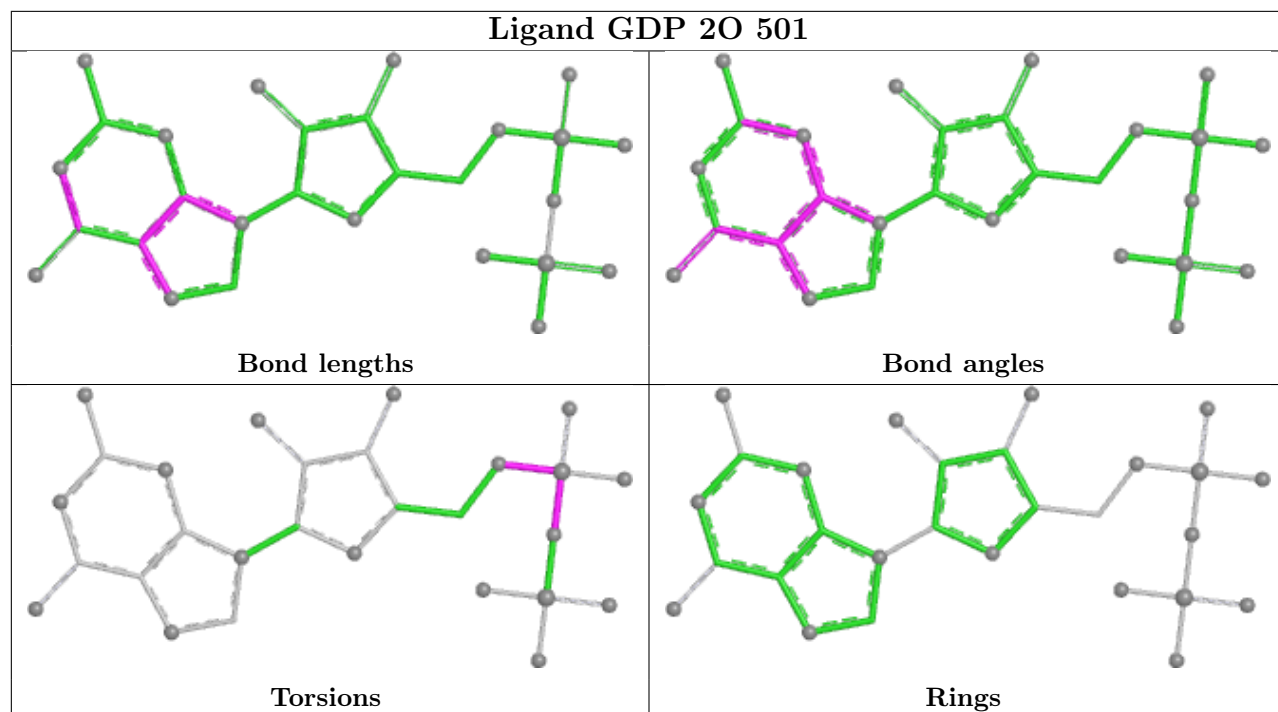
## Ligand GDP 3Z 501

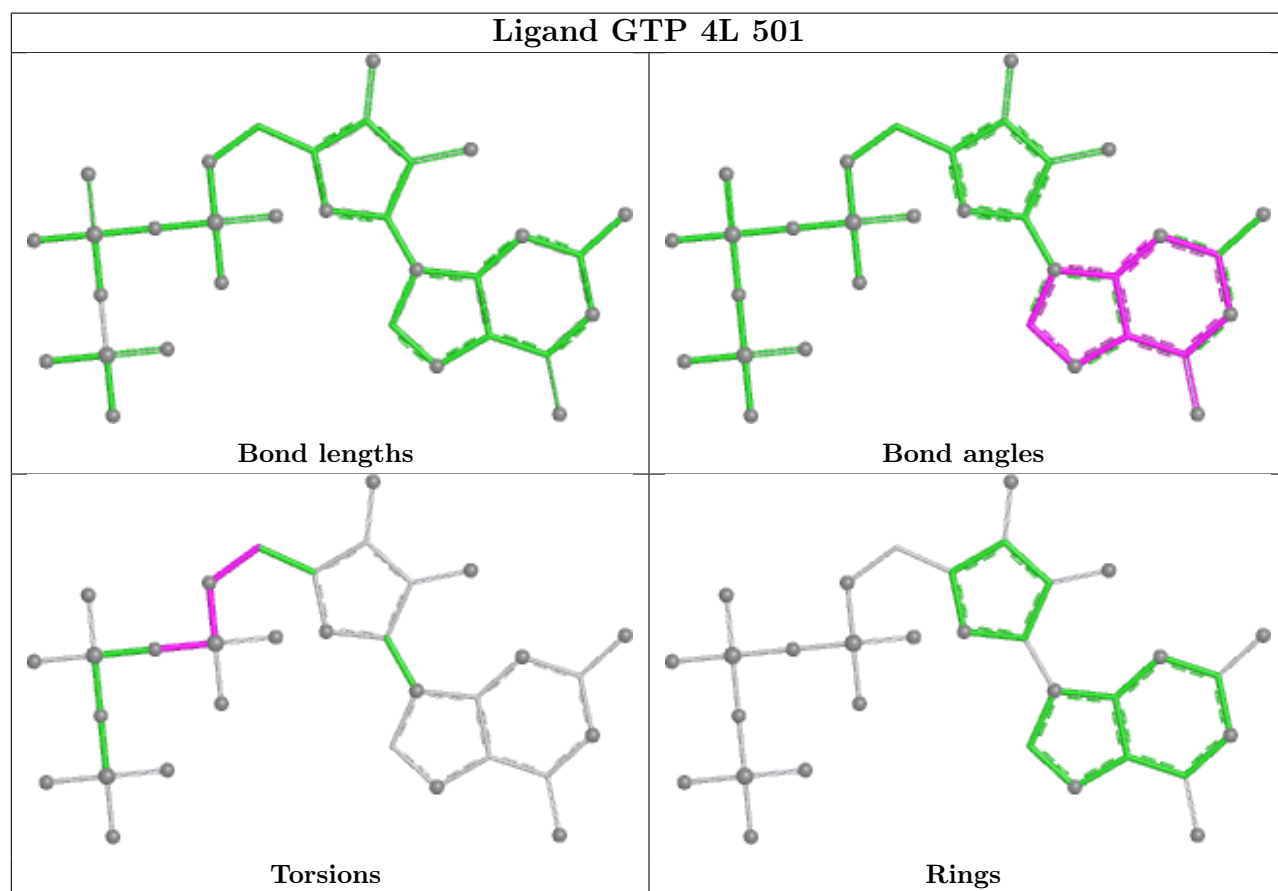
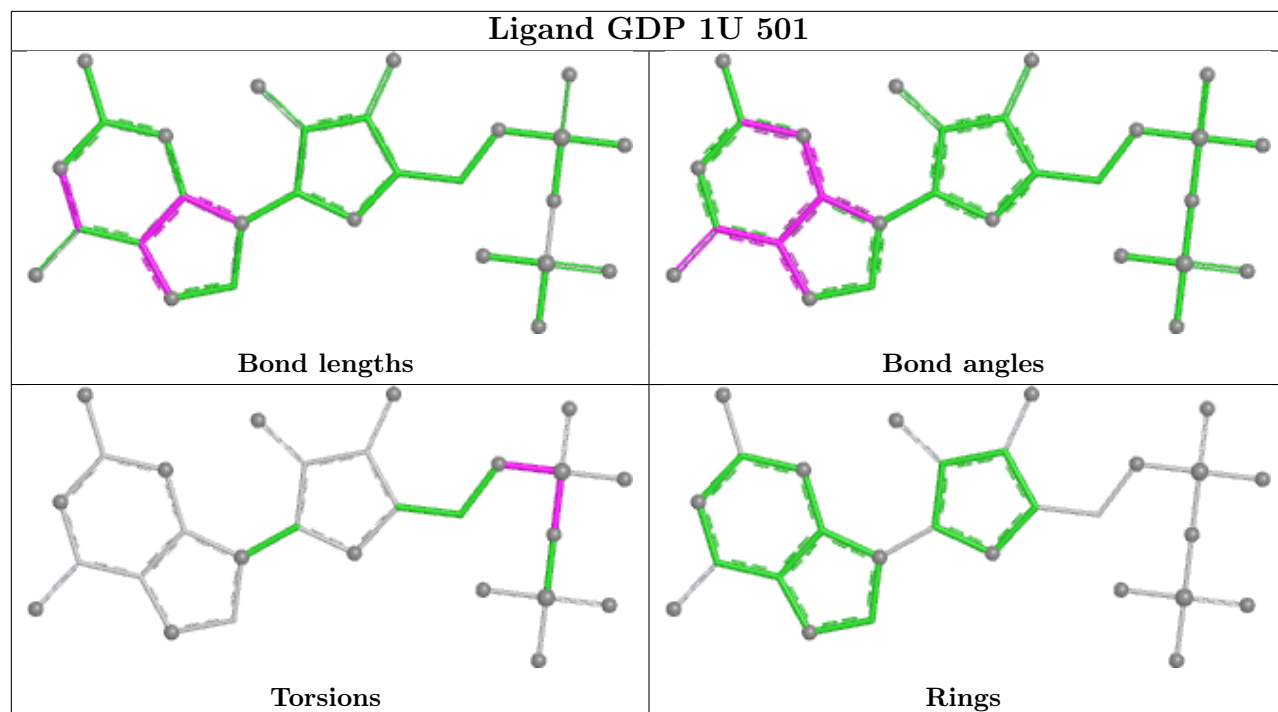


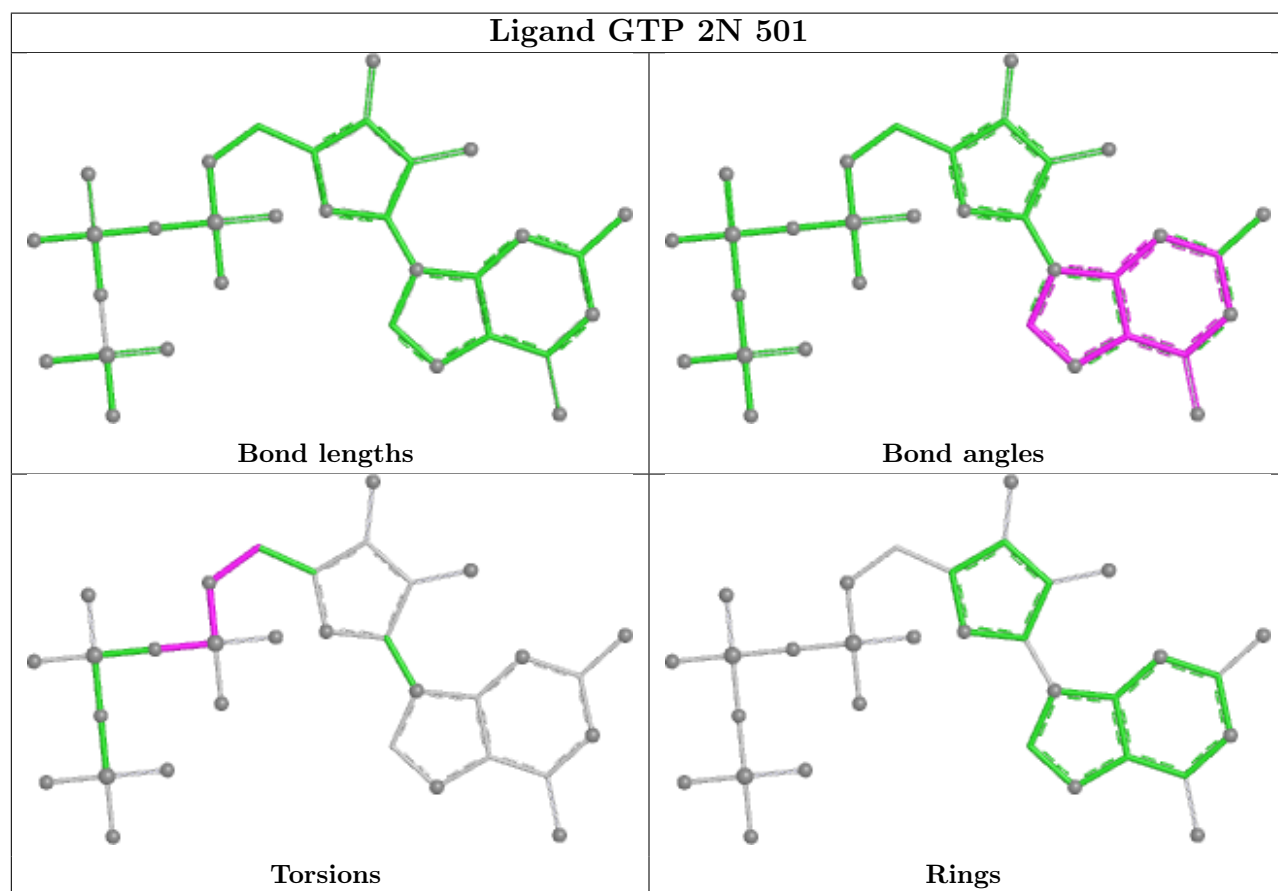
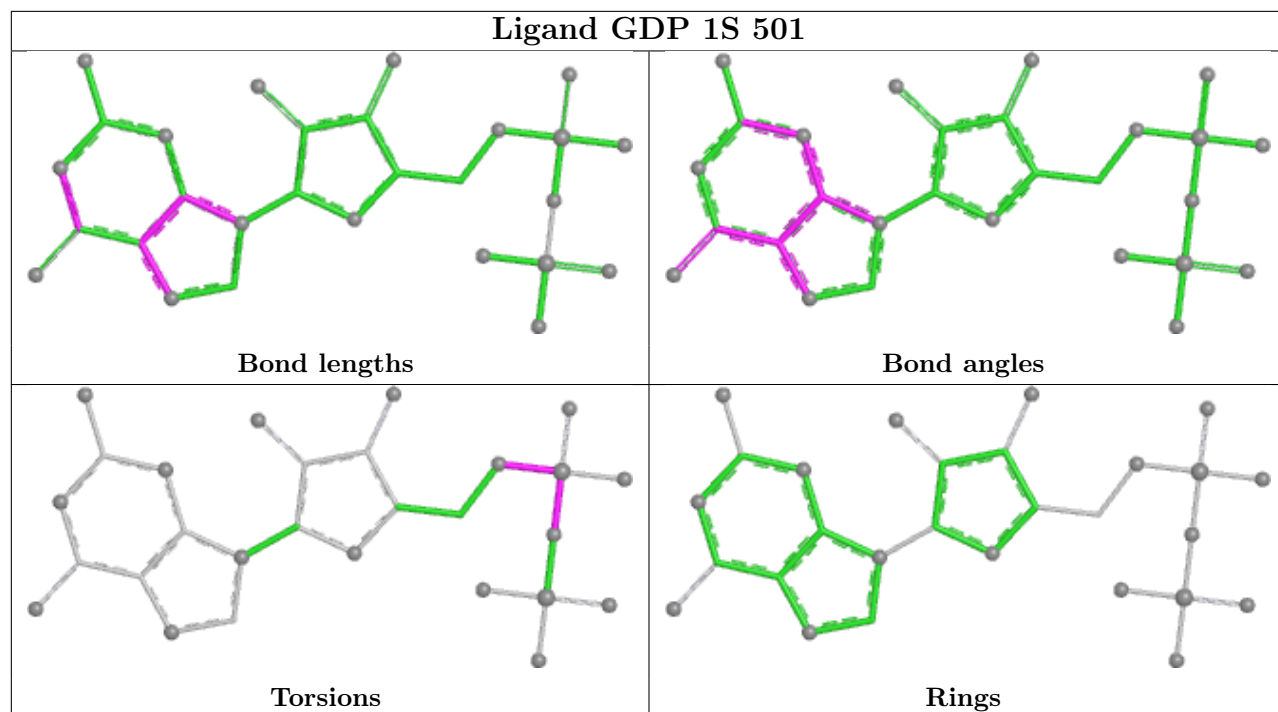




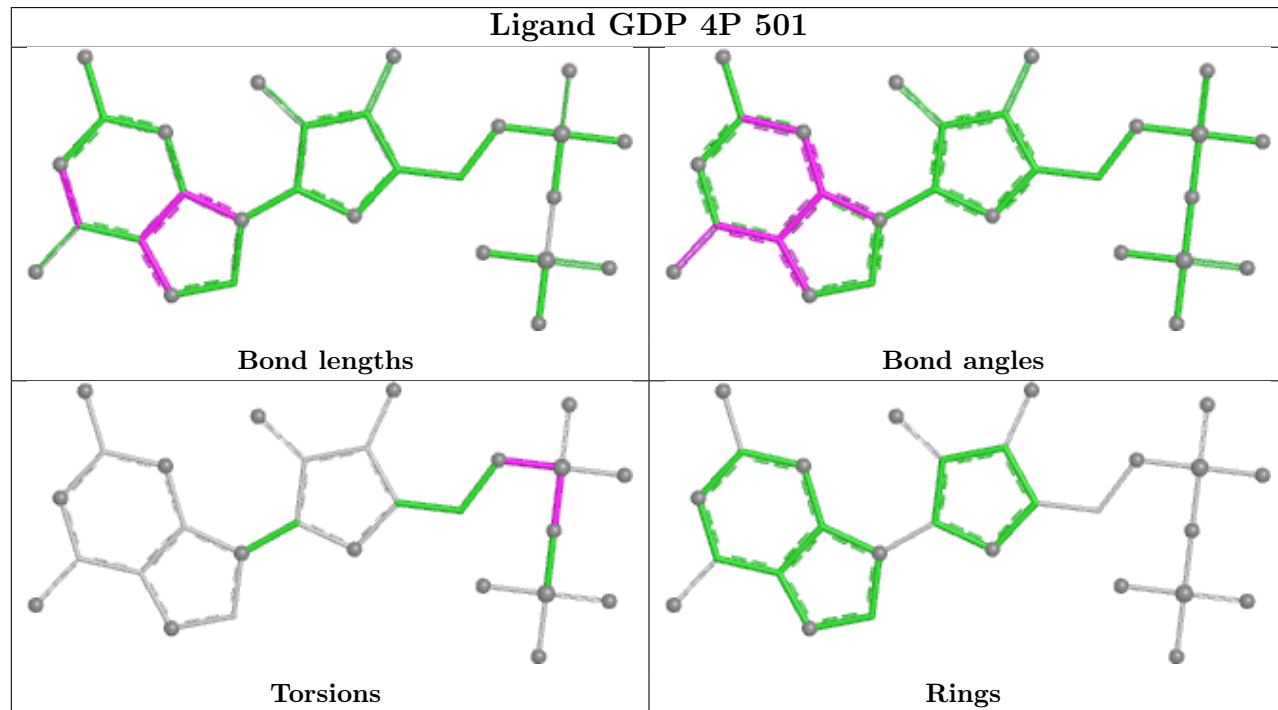
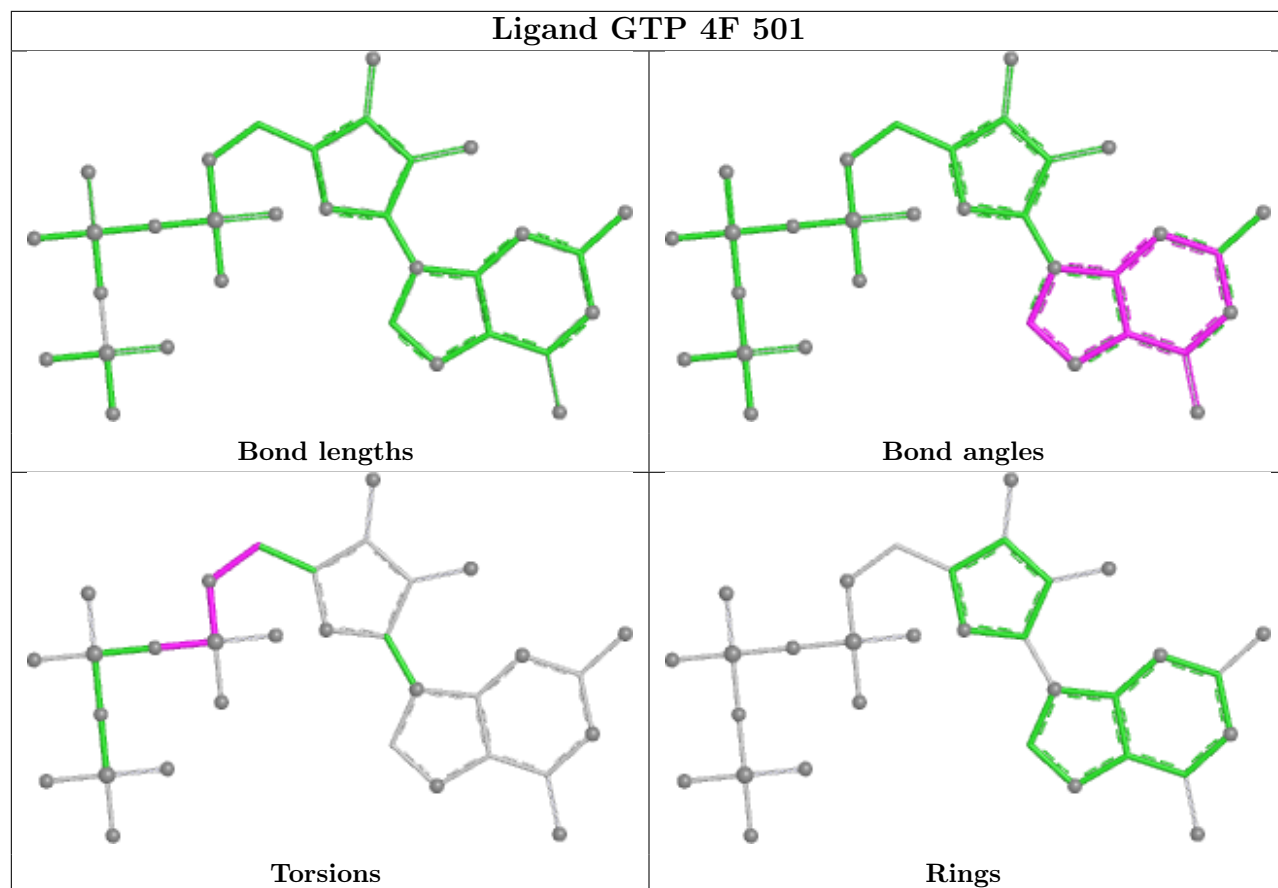


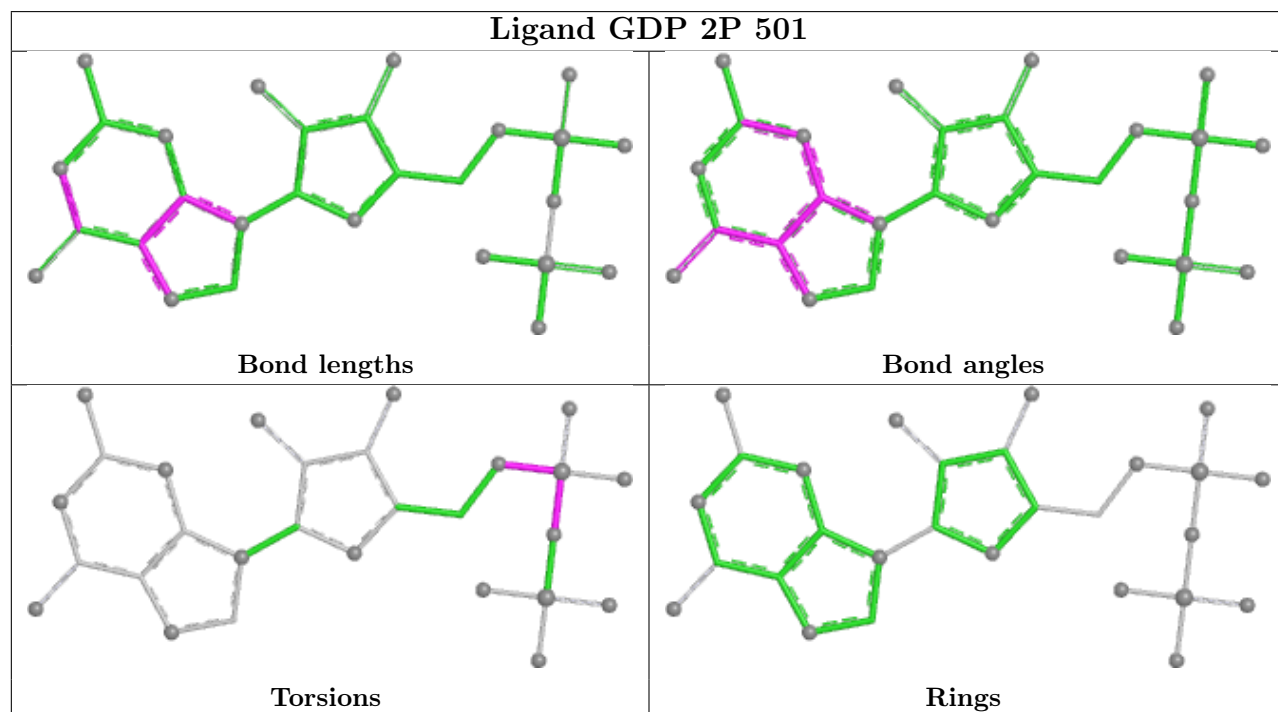
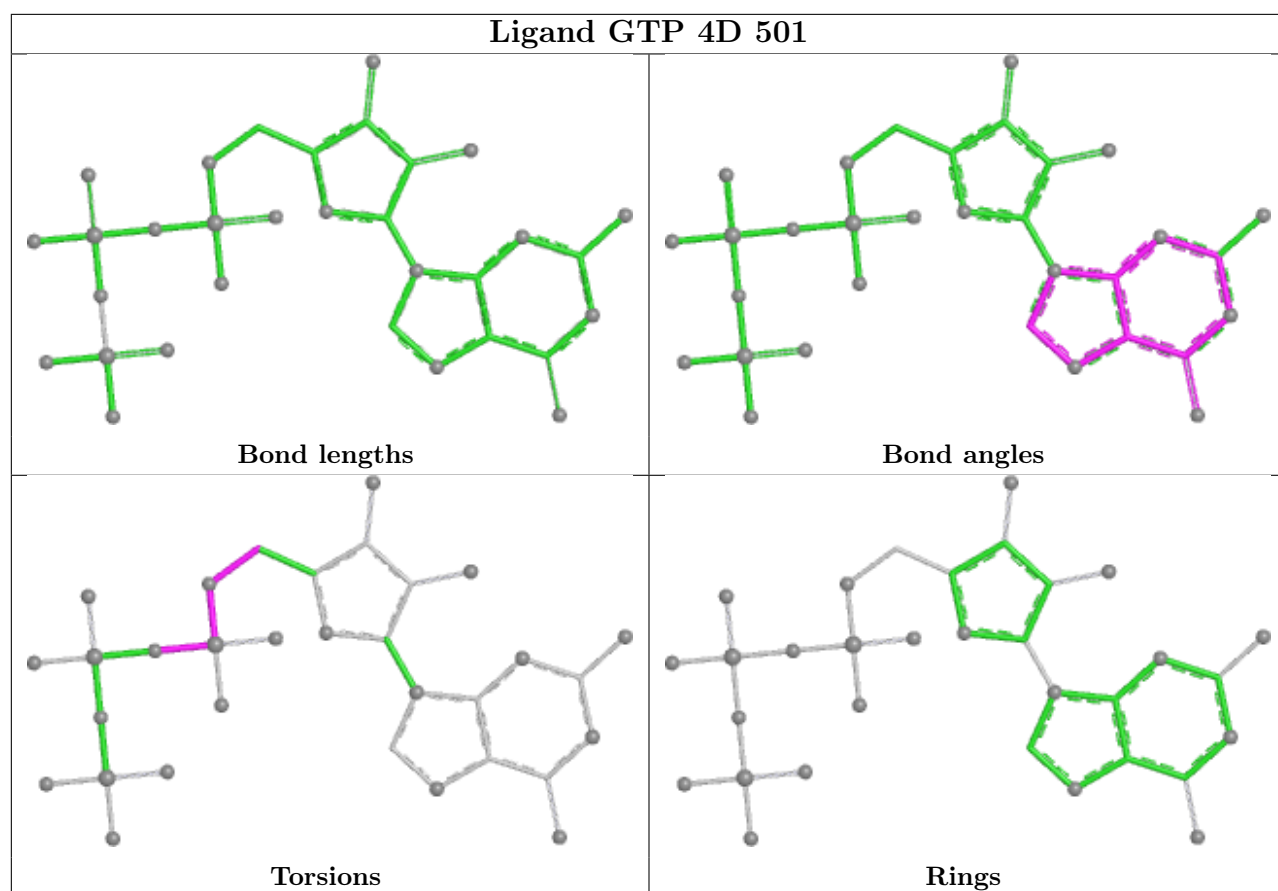


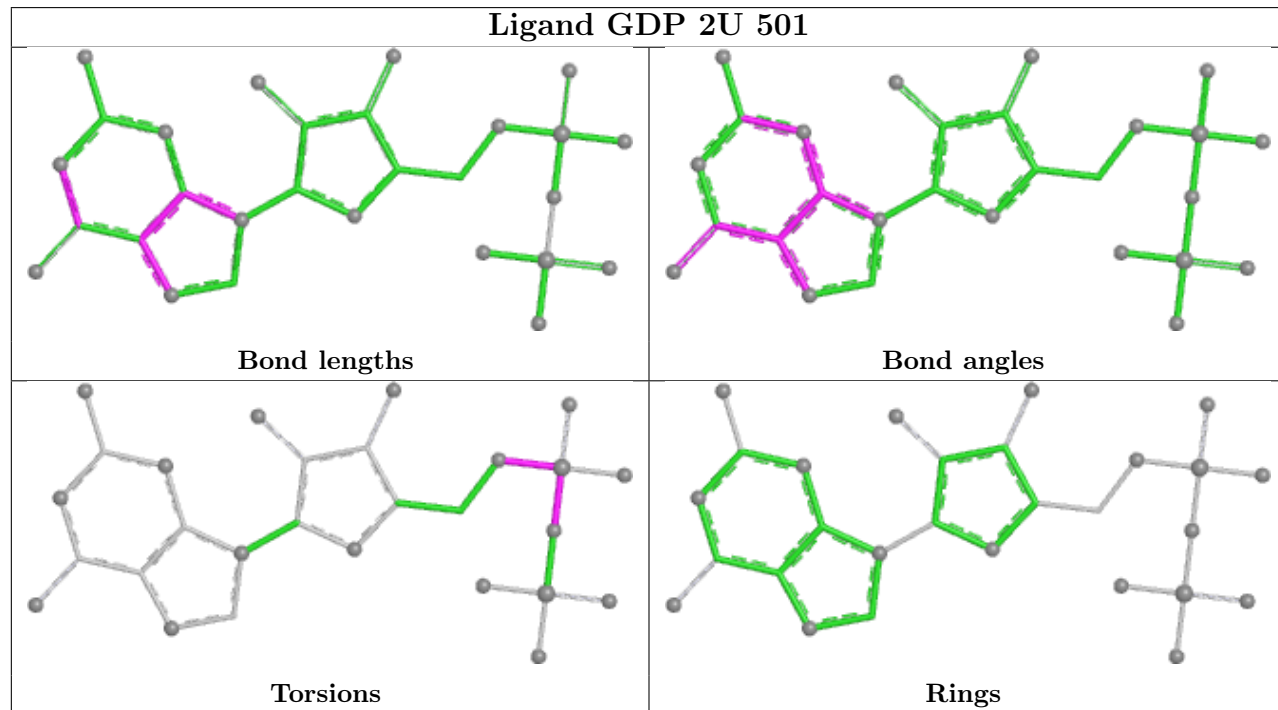
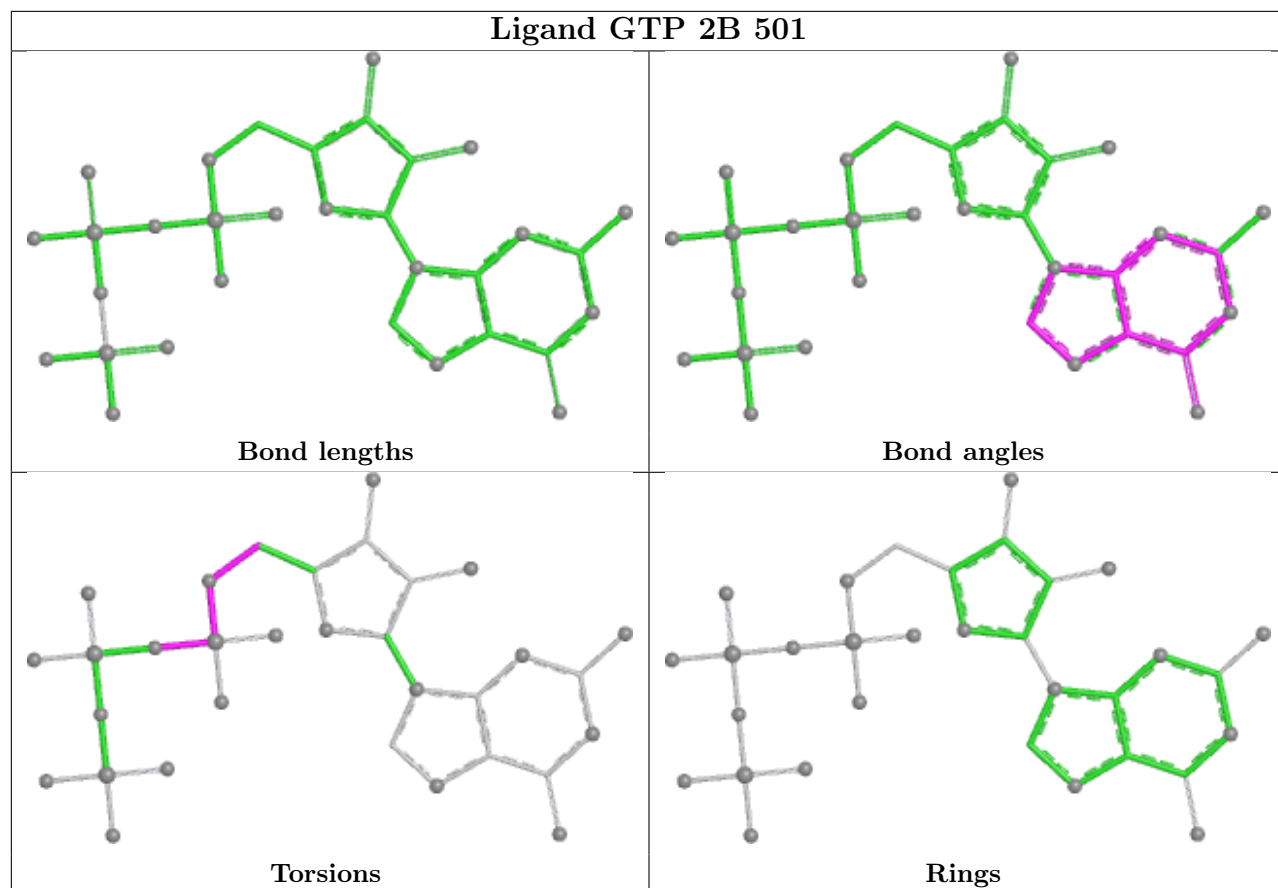




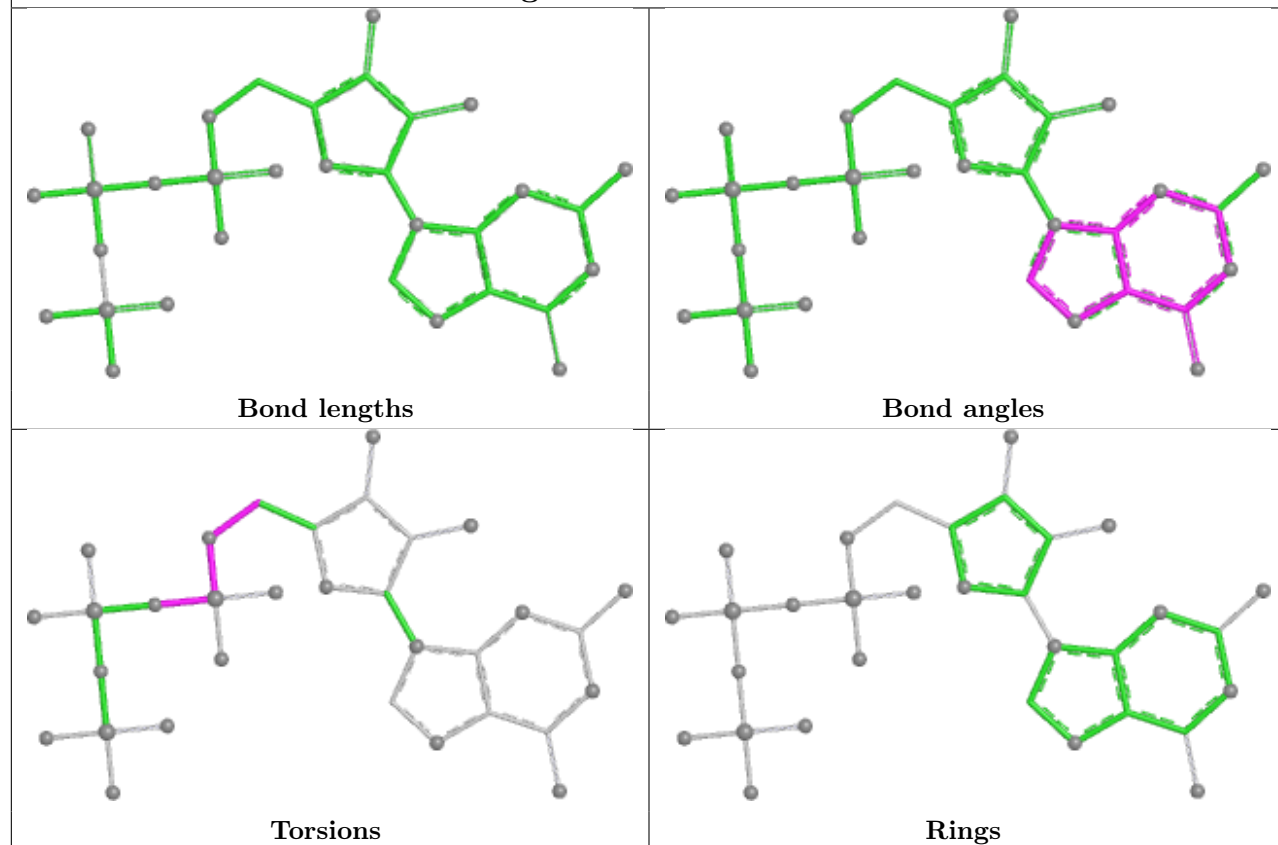




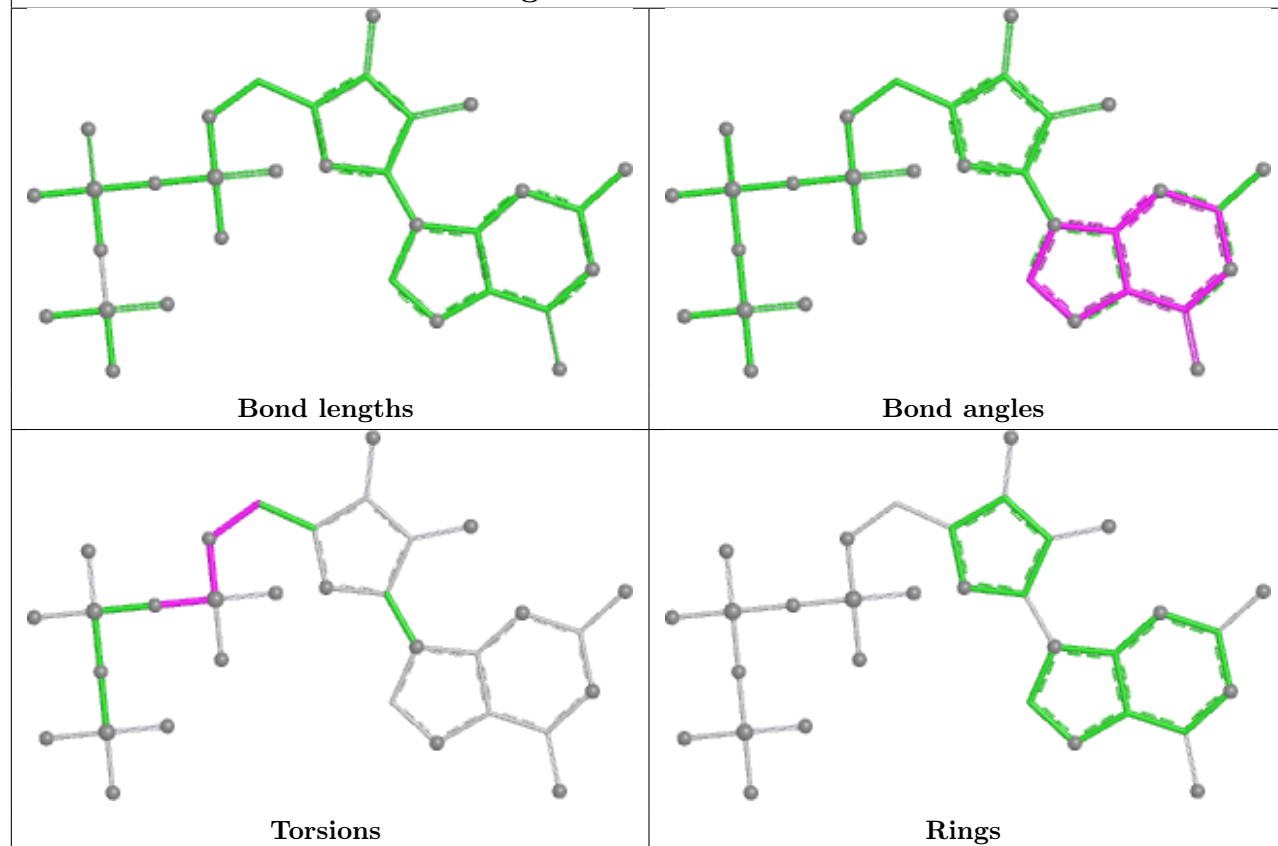


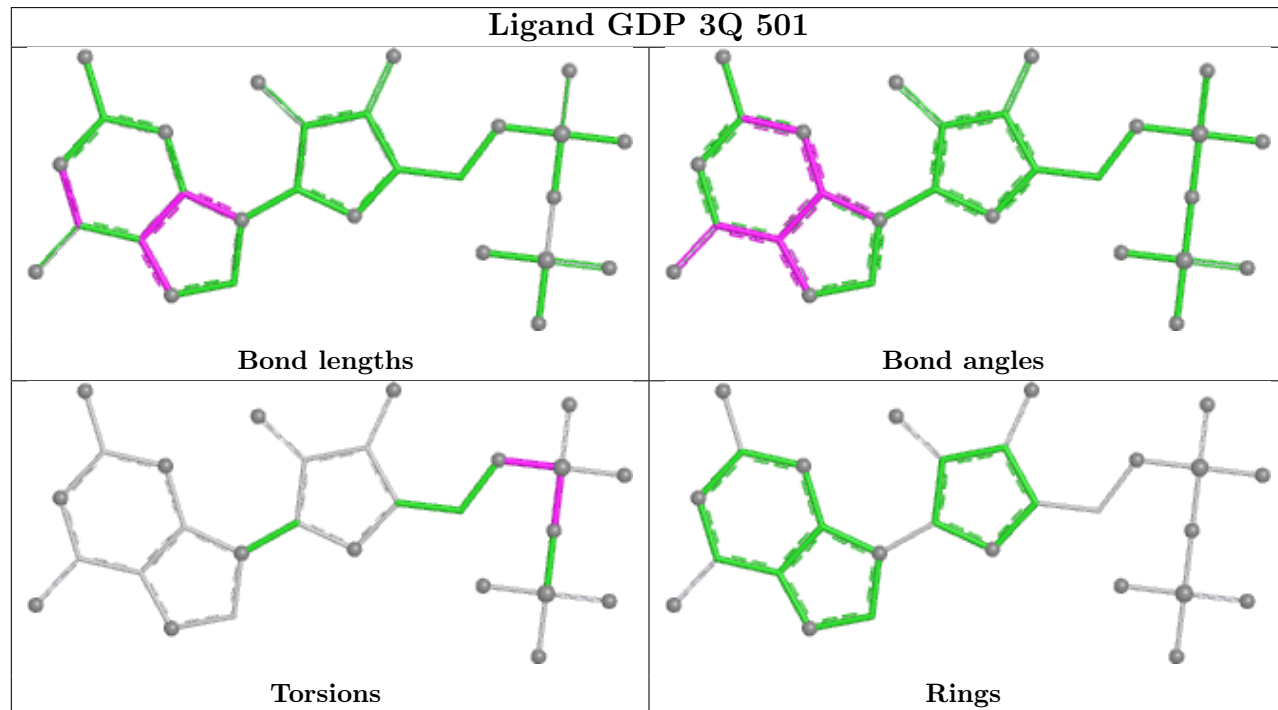
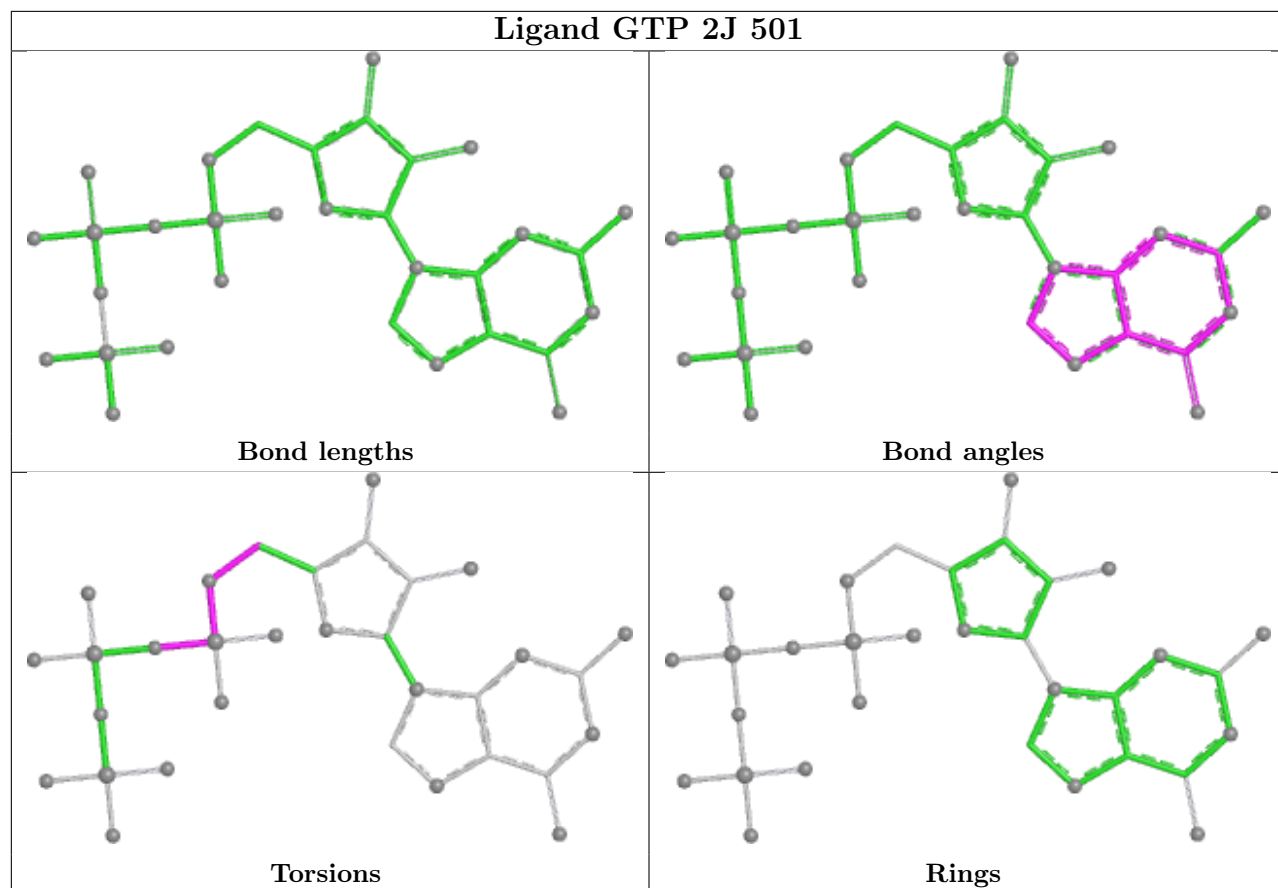


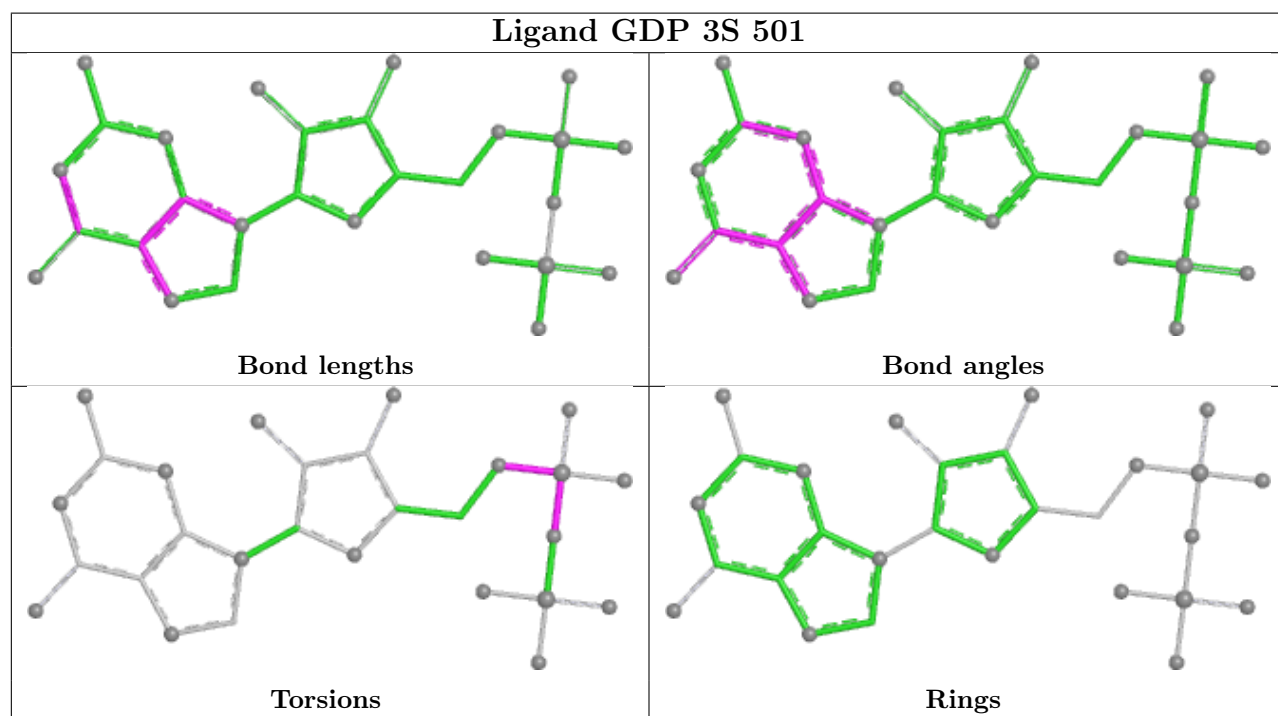
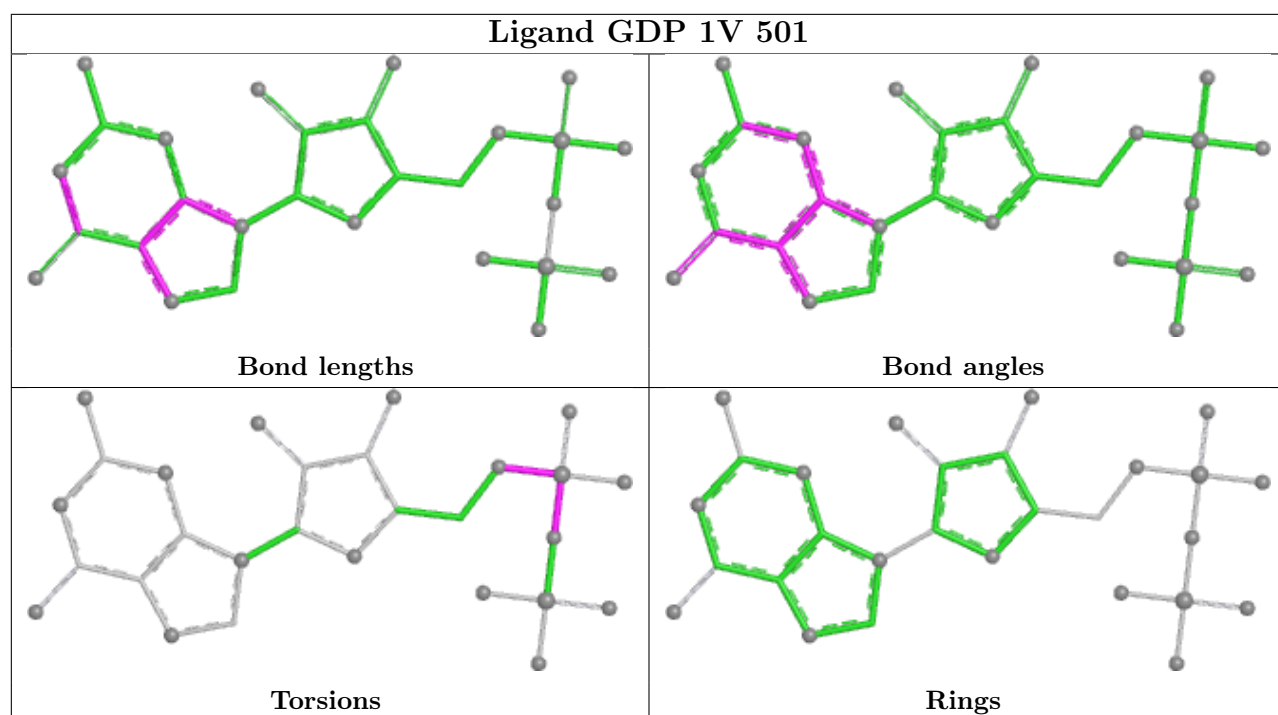
## Ligand GTP 1D 501

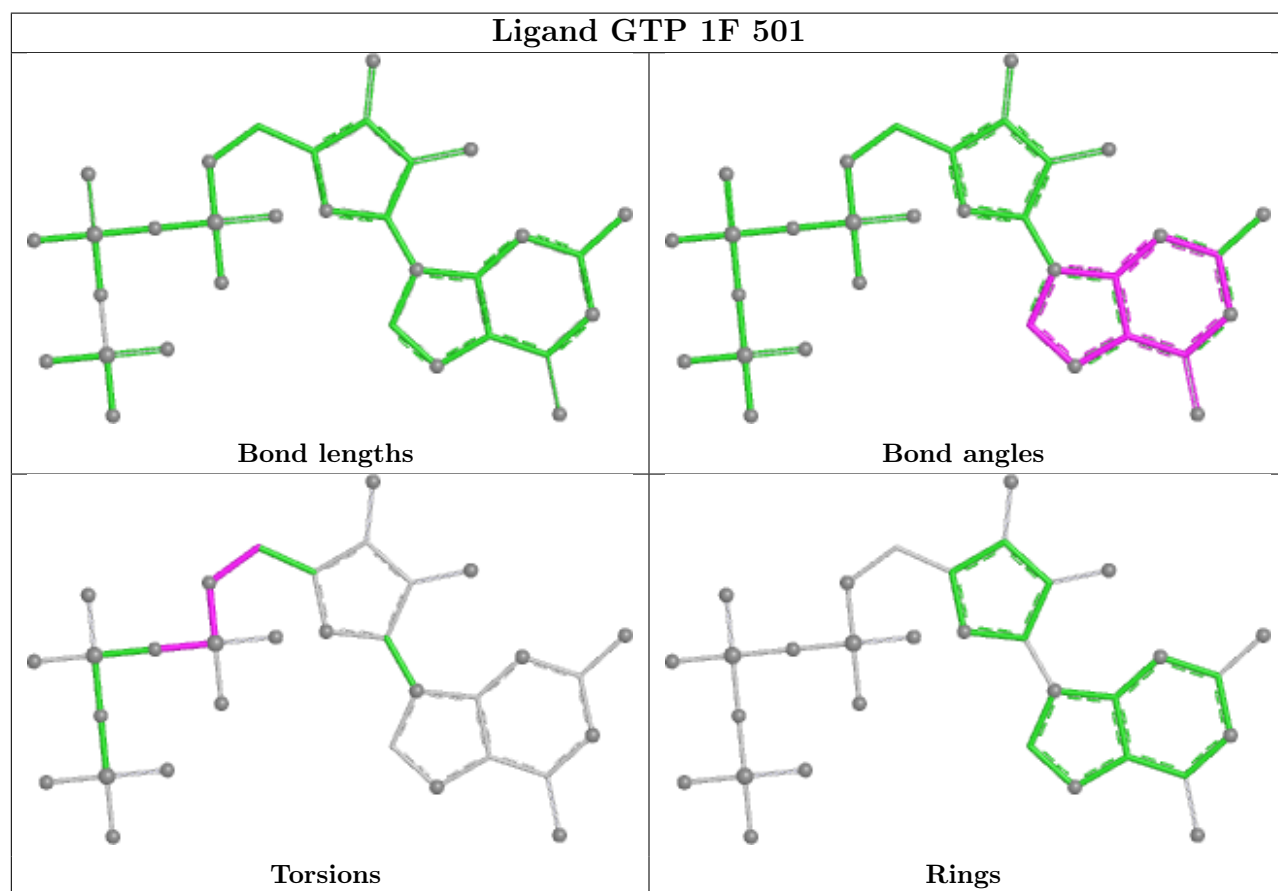
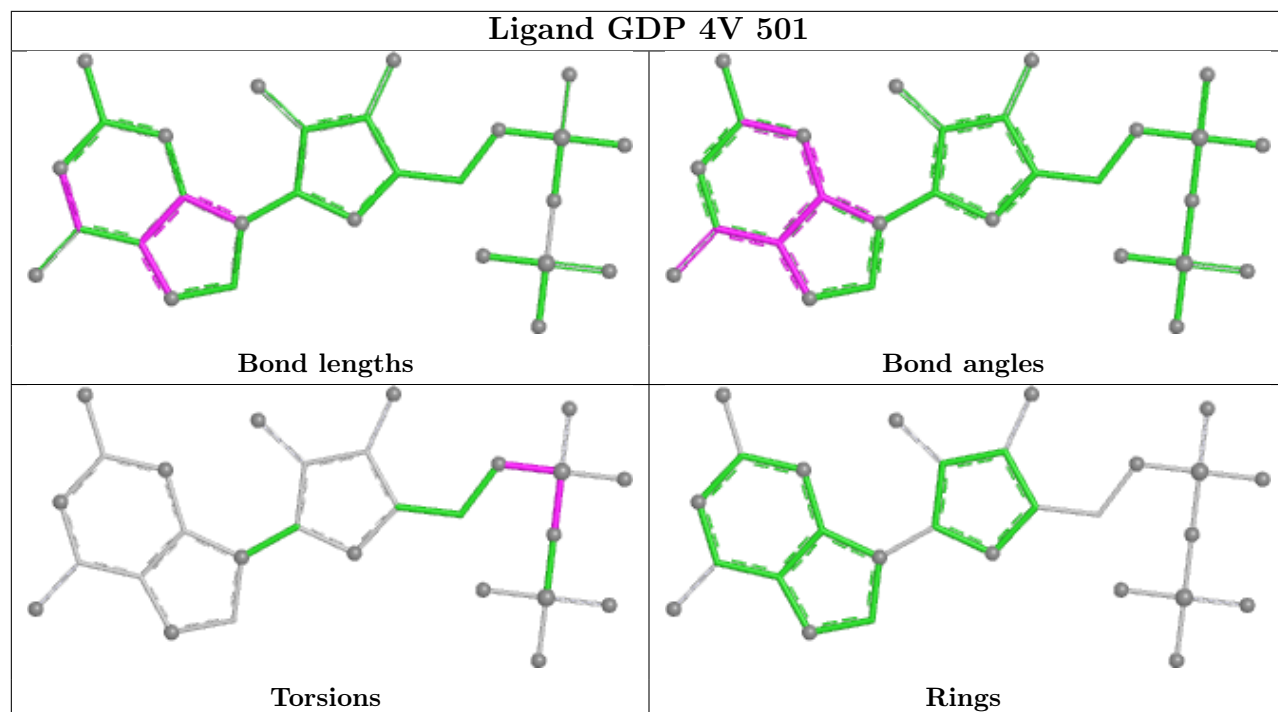


## Ligand GTP 3D 501

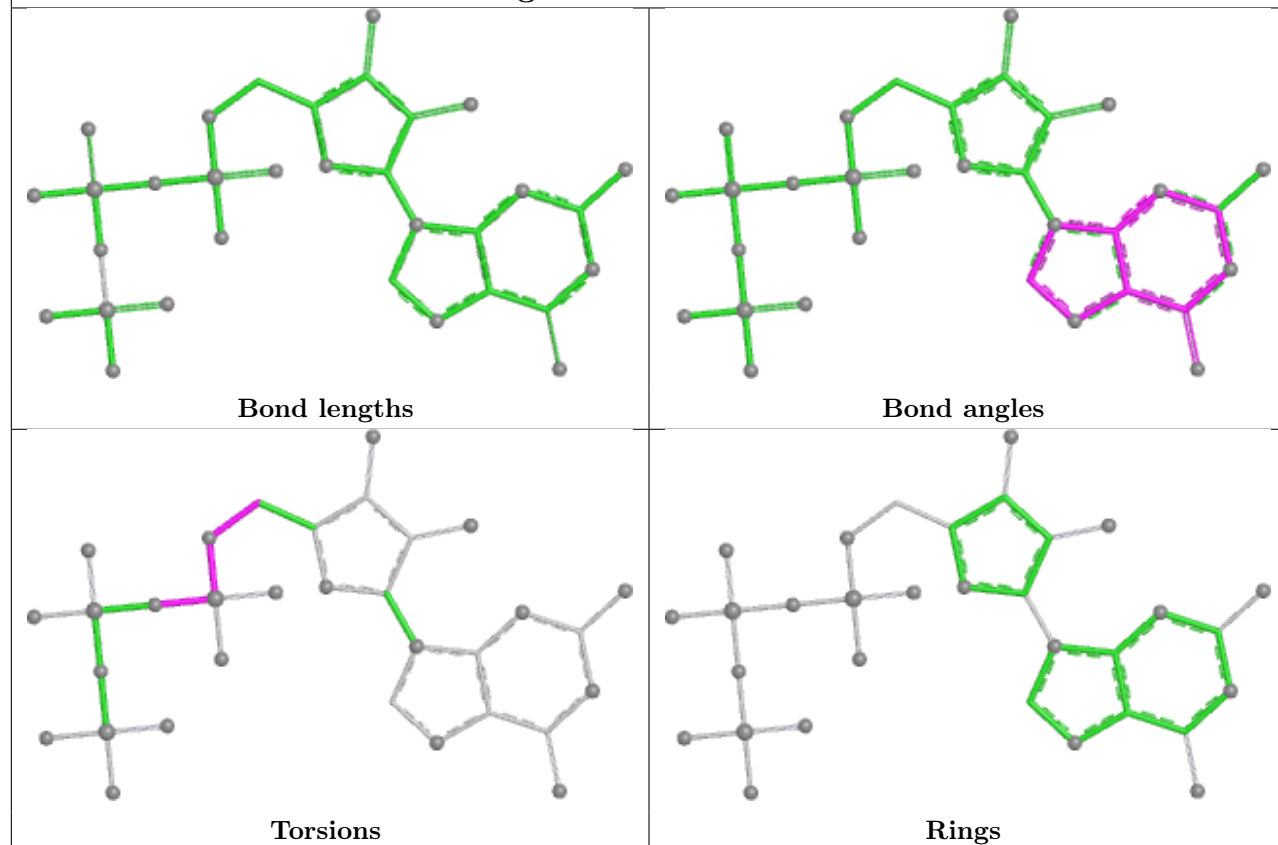




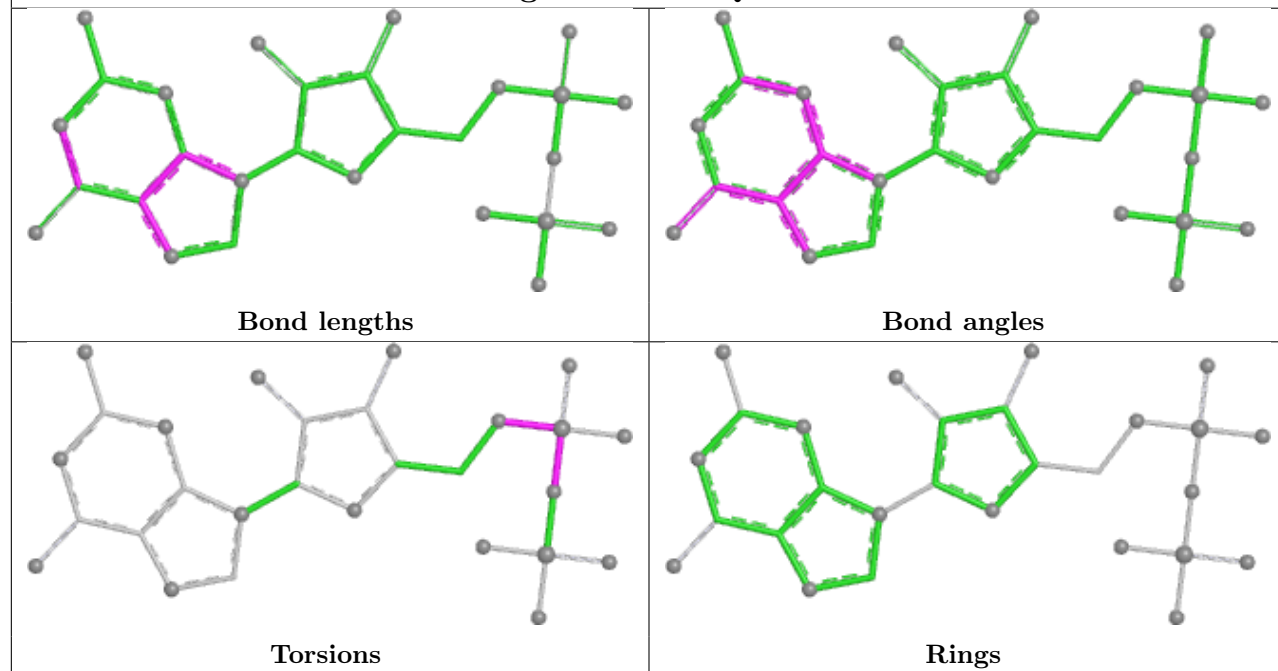




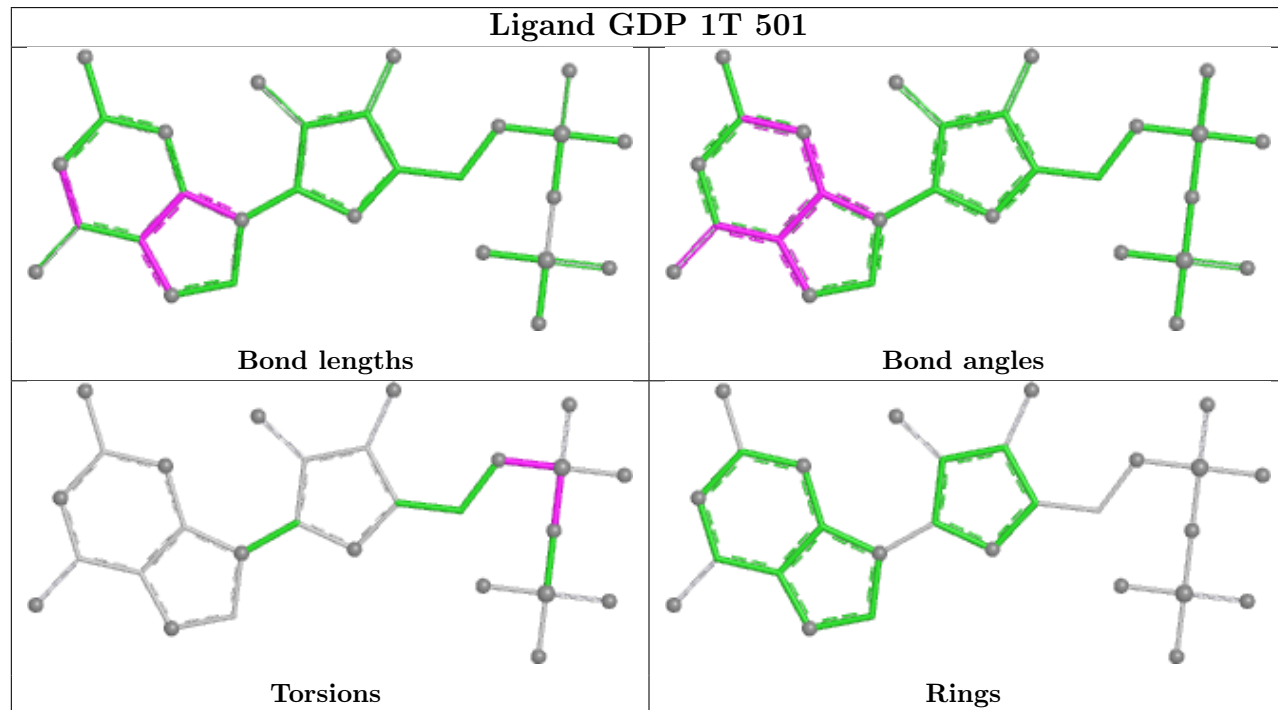
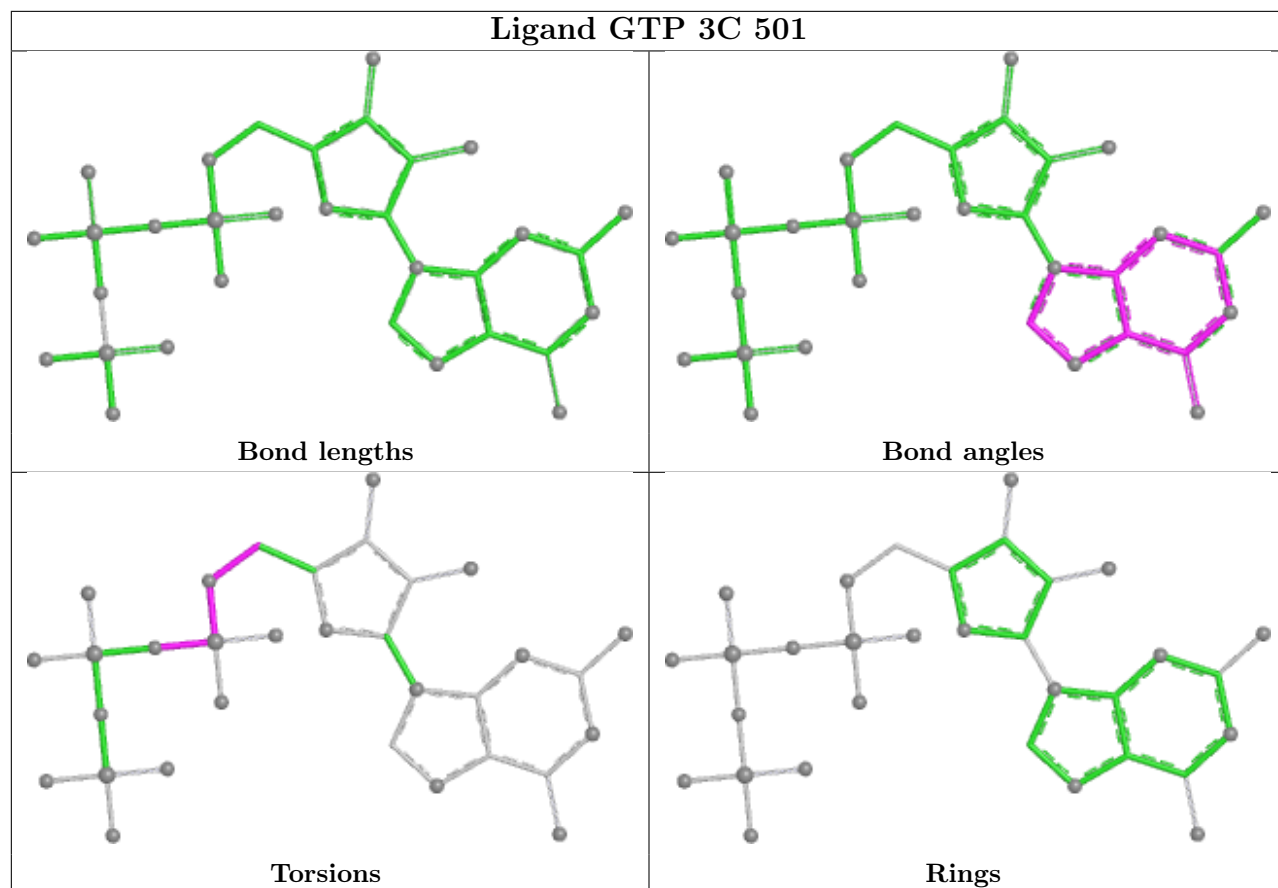
## Ligand GTP 4M 501

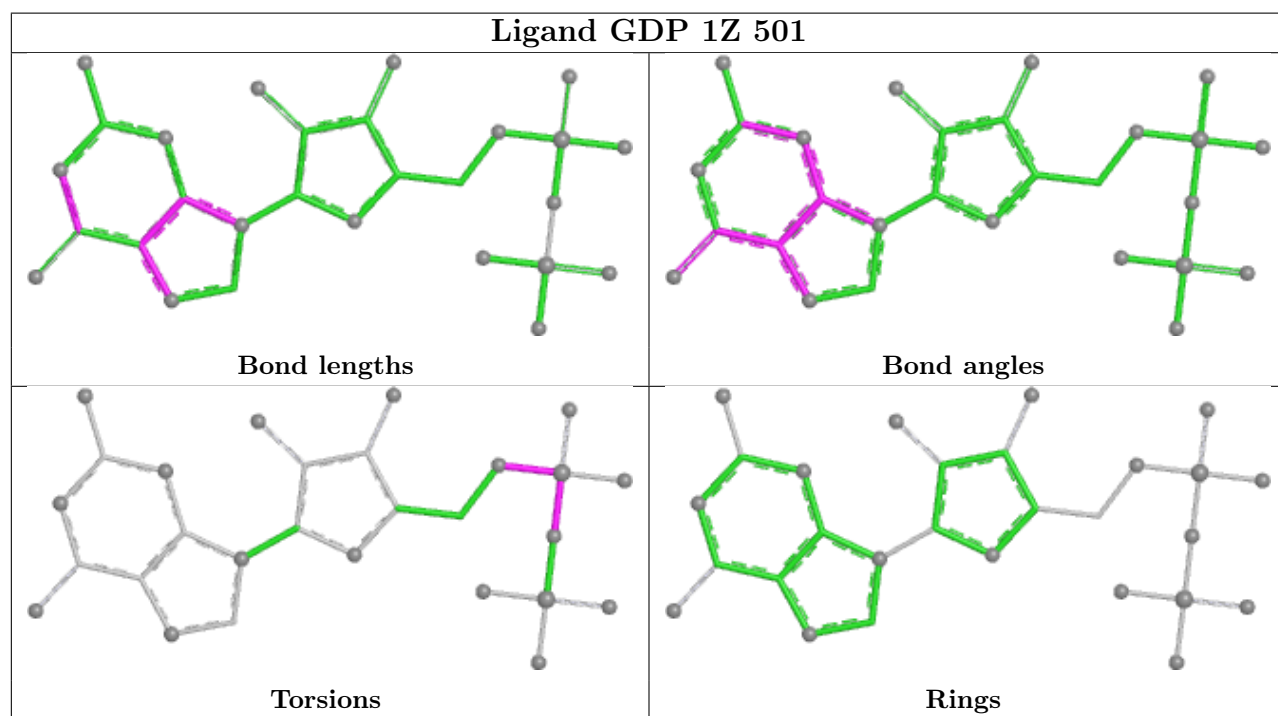
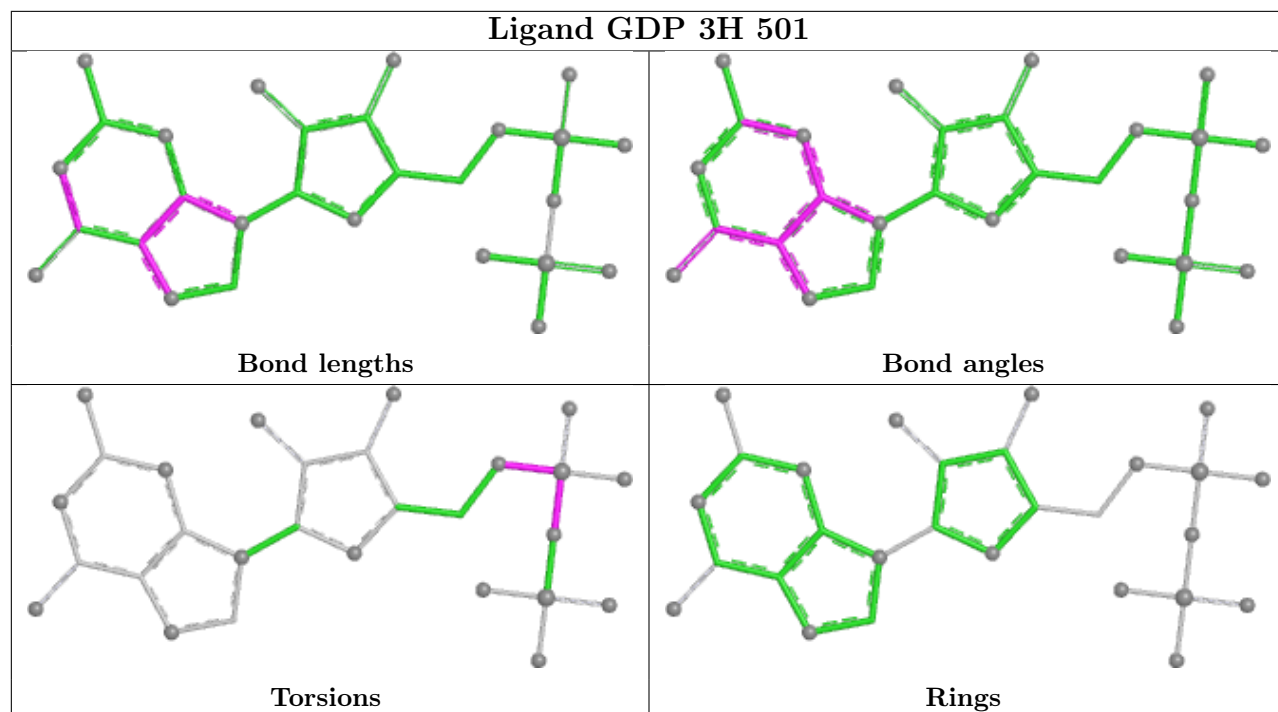


## Ligand GDP 1Q 501

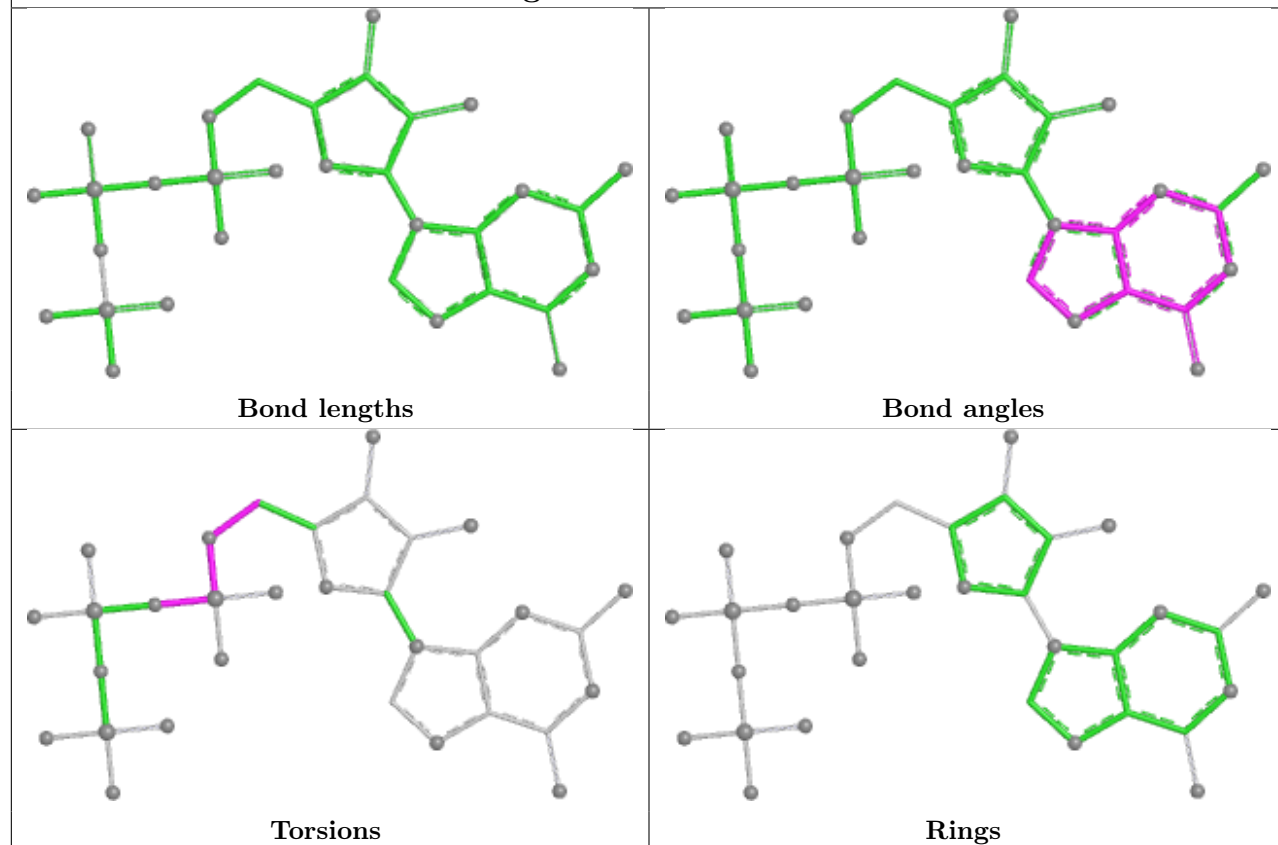




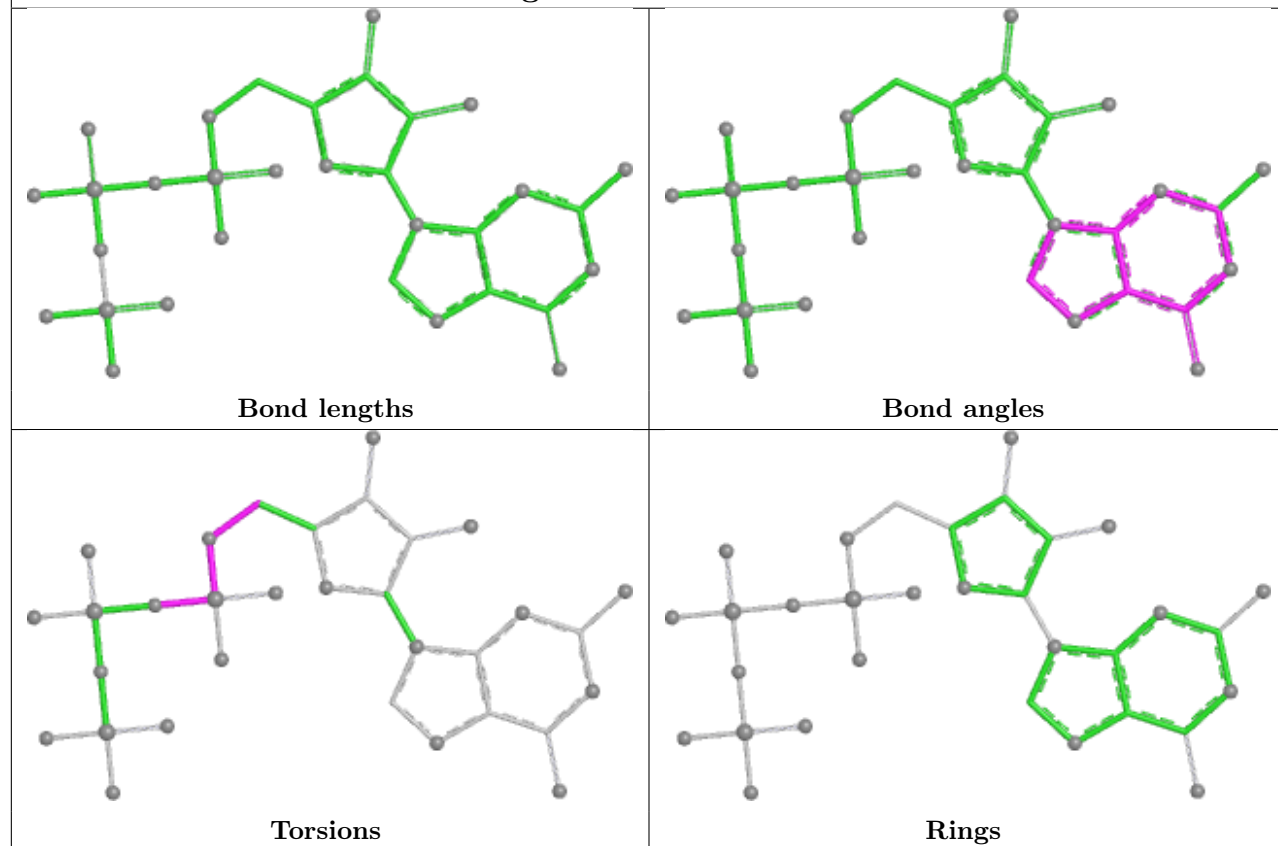


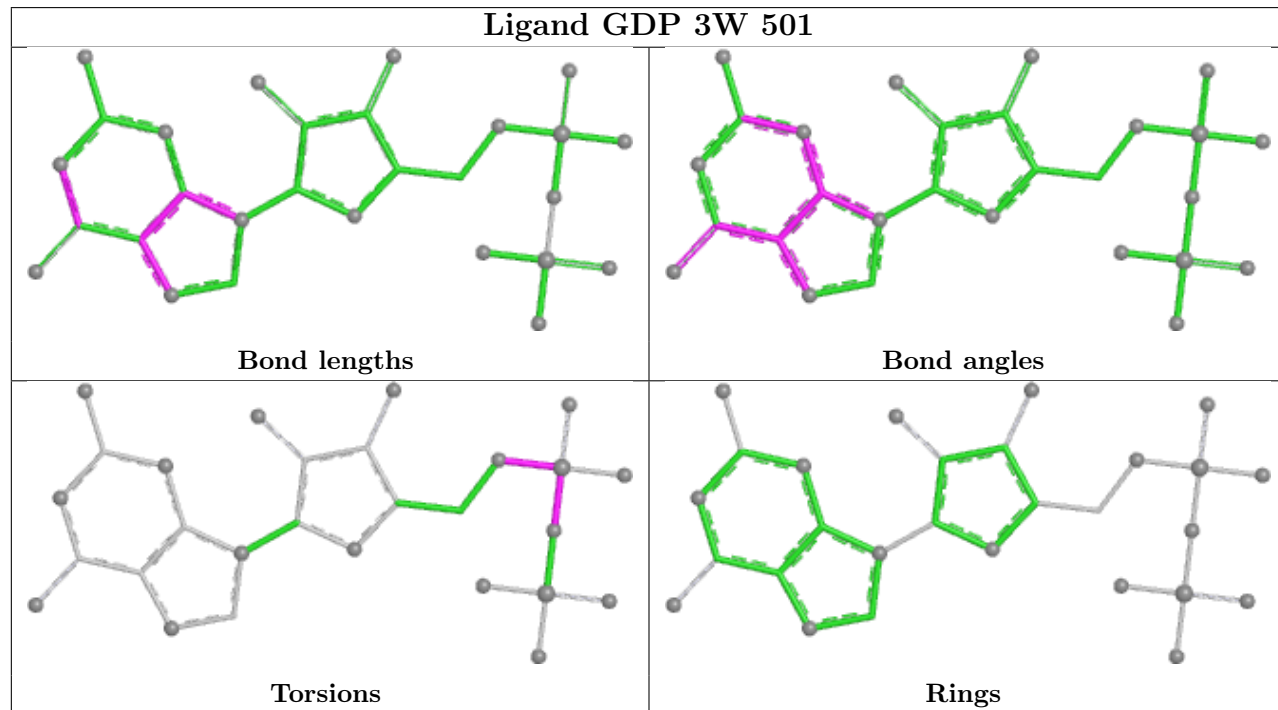
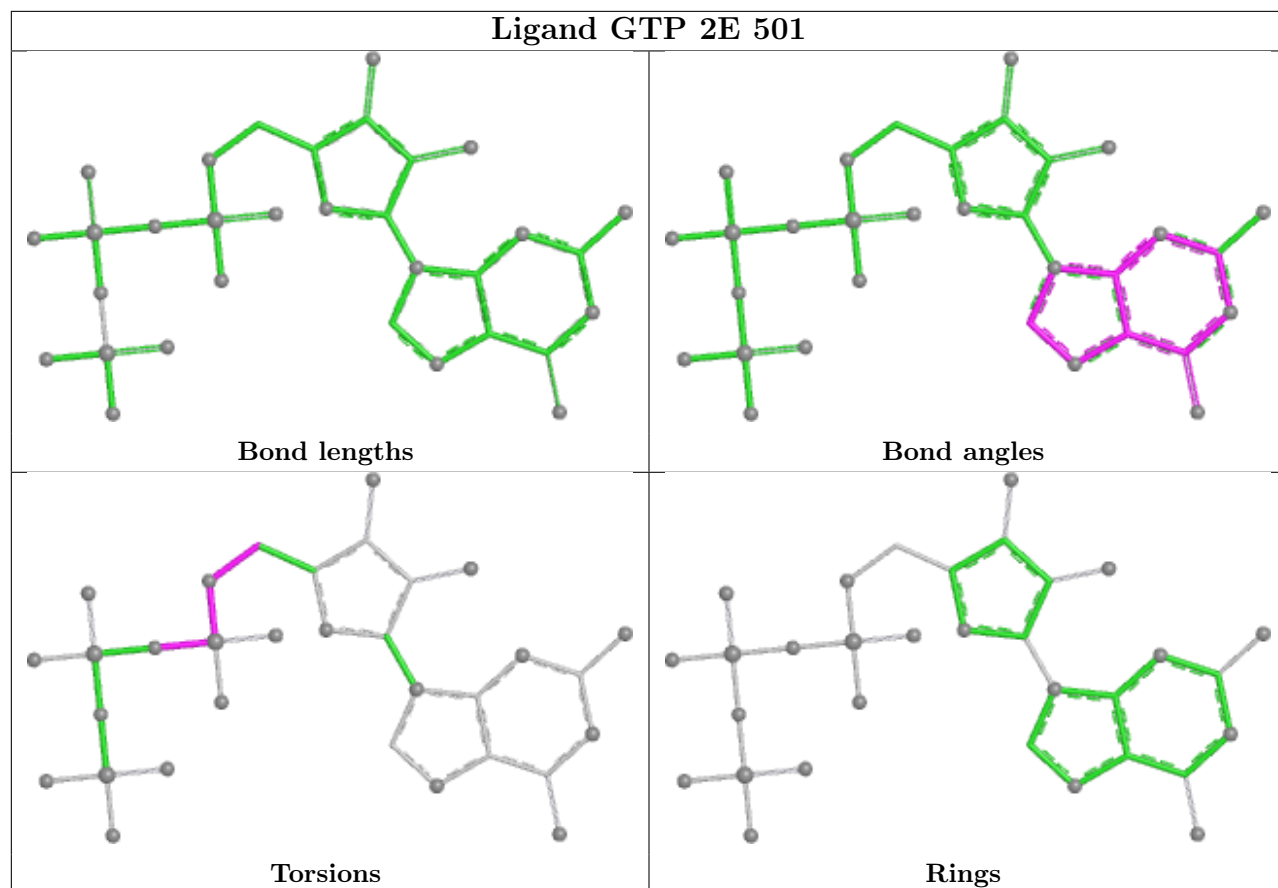


## Ligand GTP 1E 501

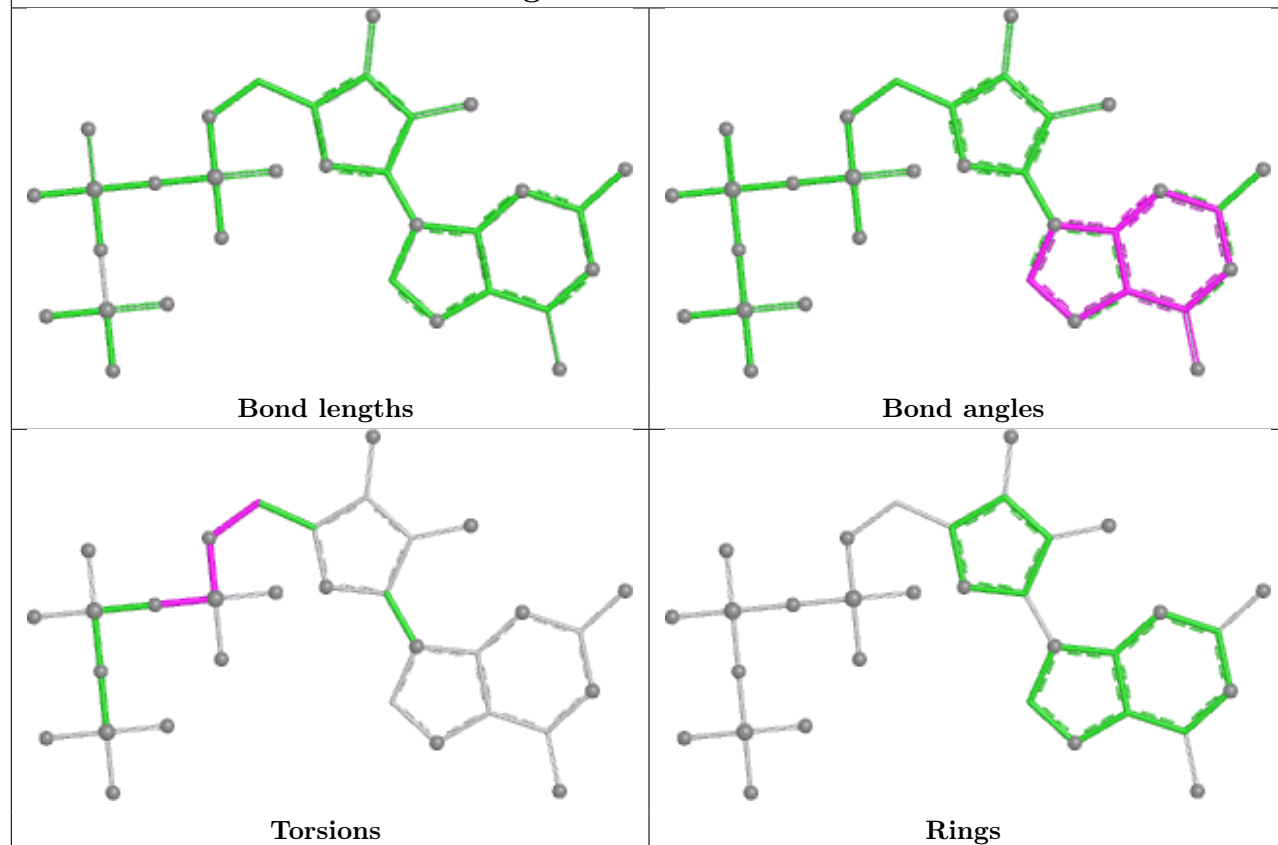


## Ligand GTP 2C 501

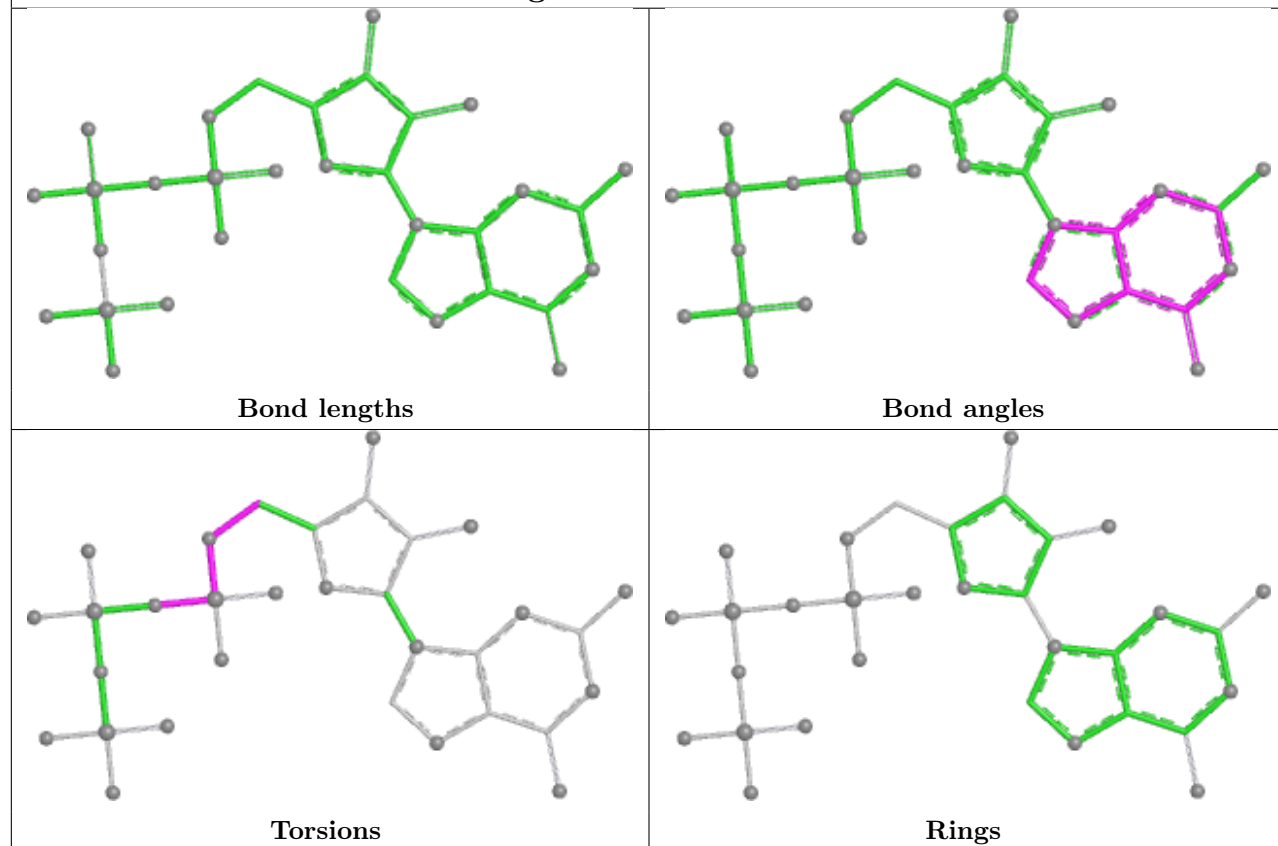


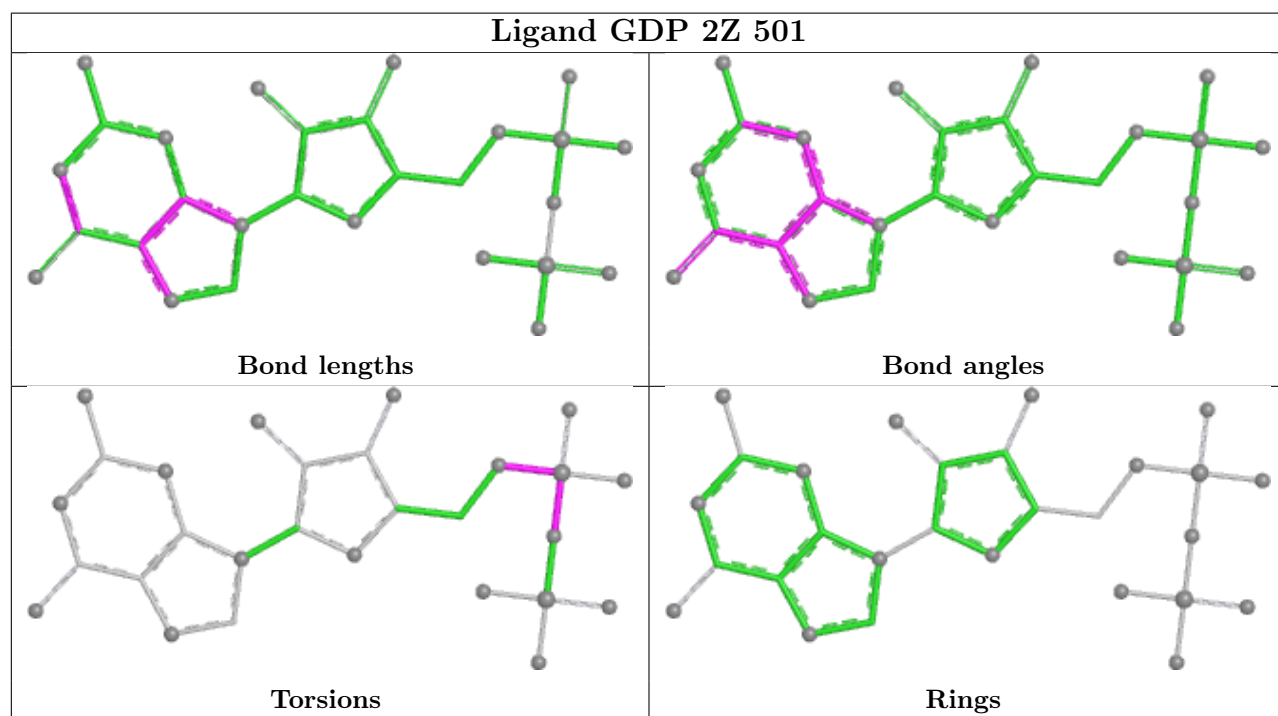
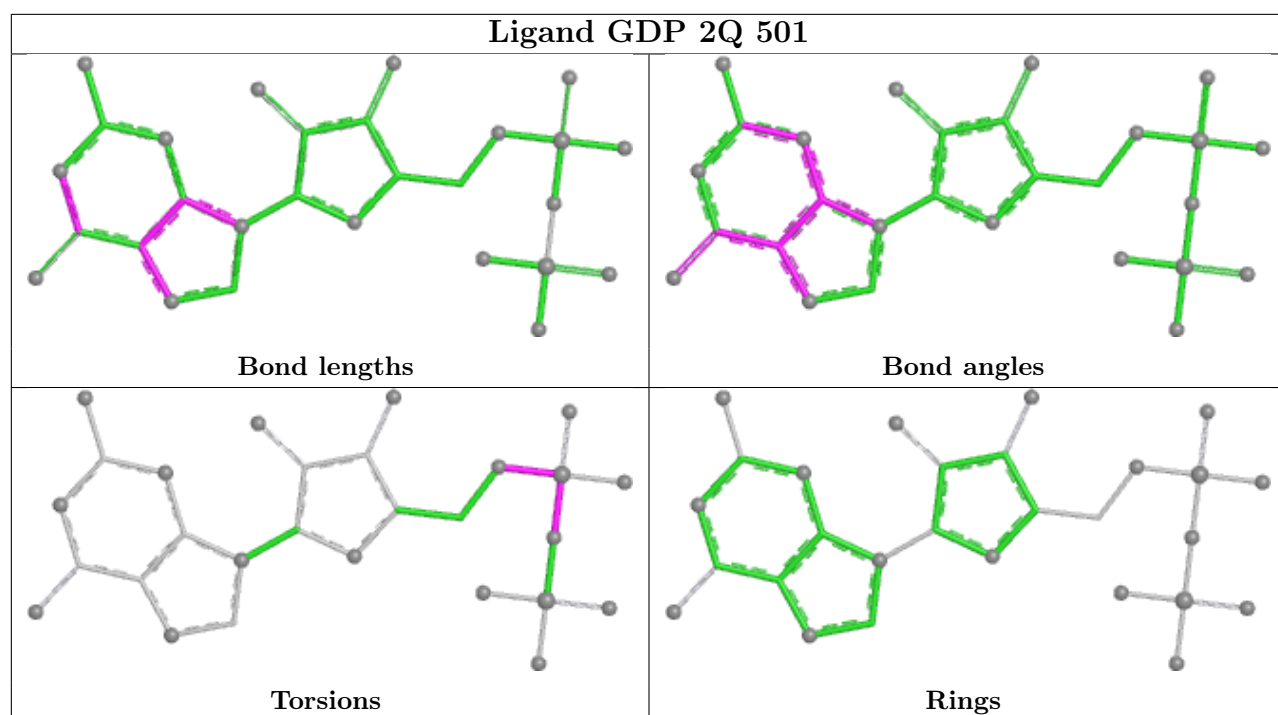


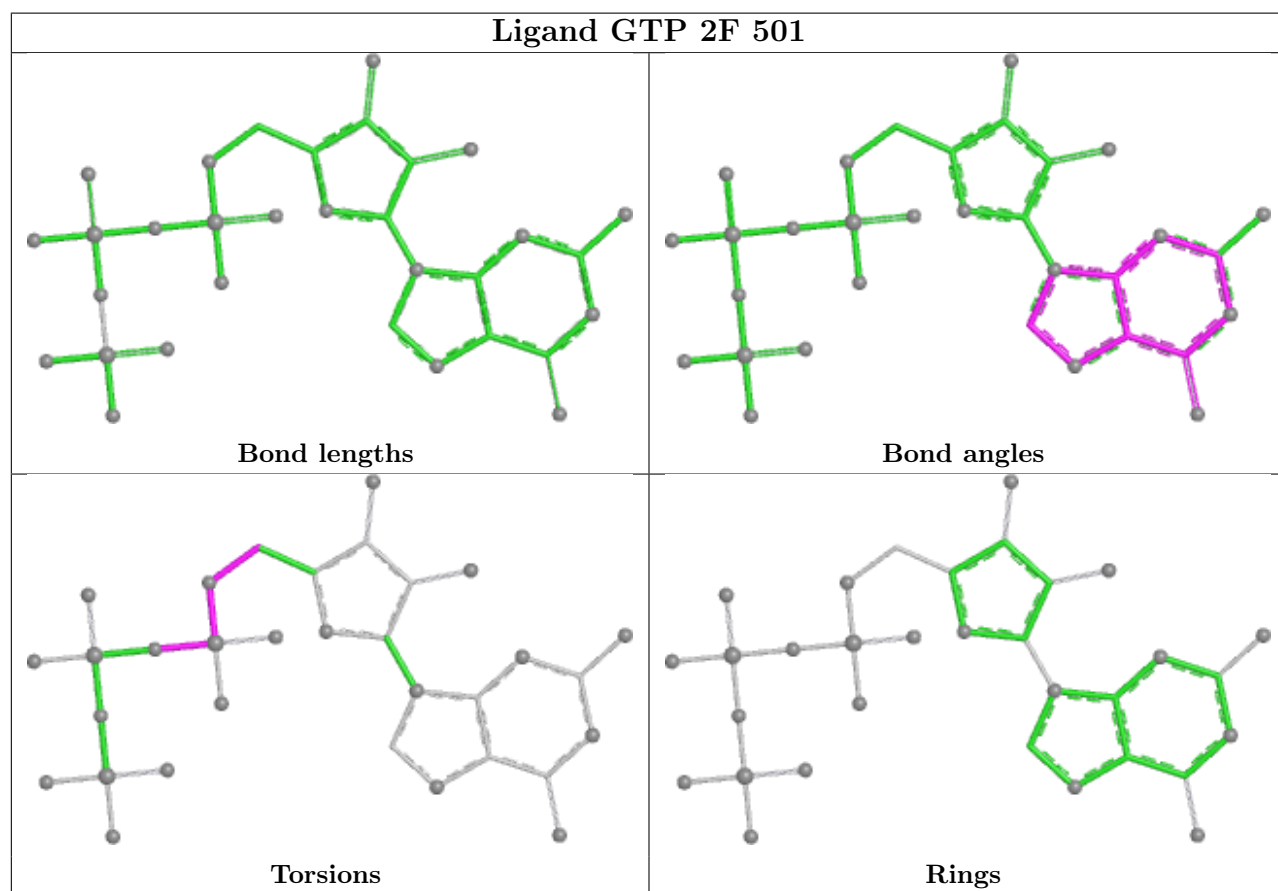
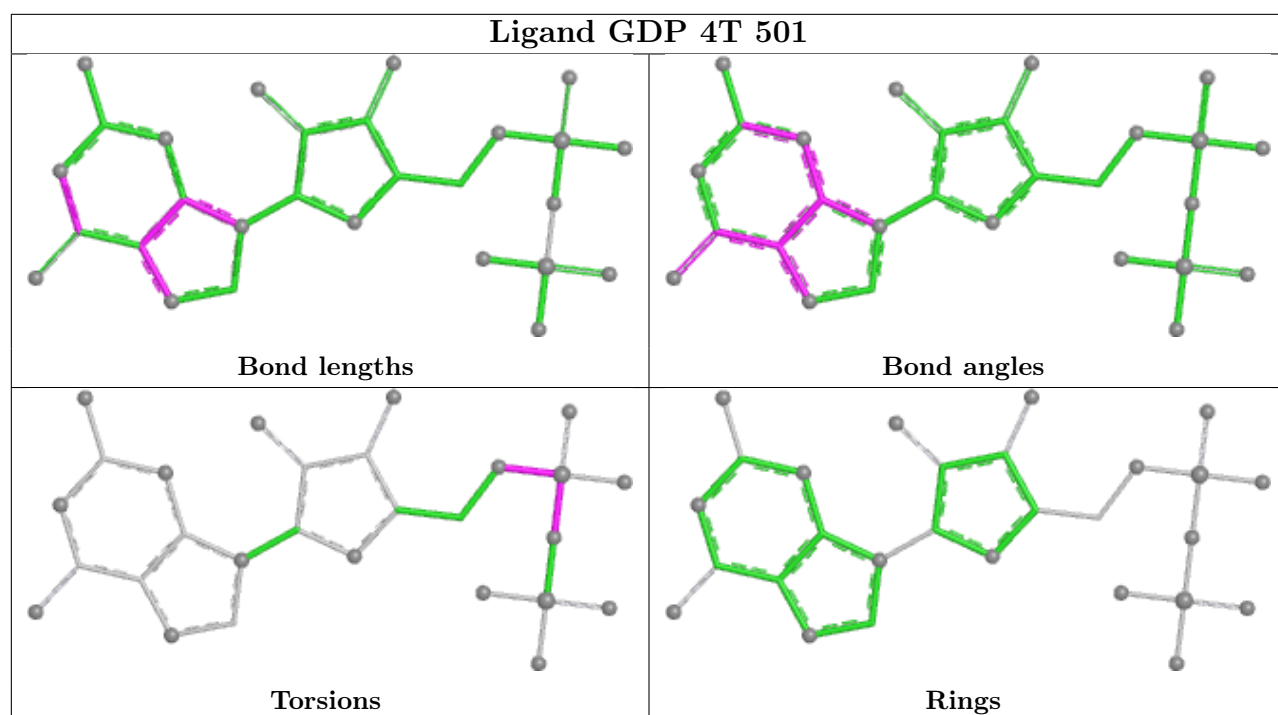
## Ligand GTP 4E 501



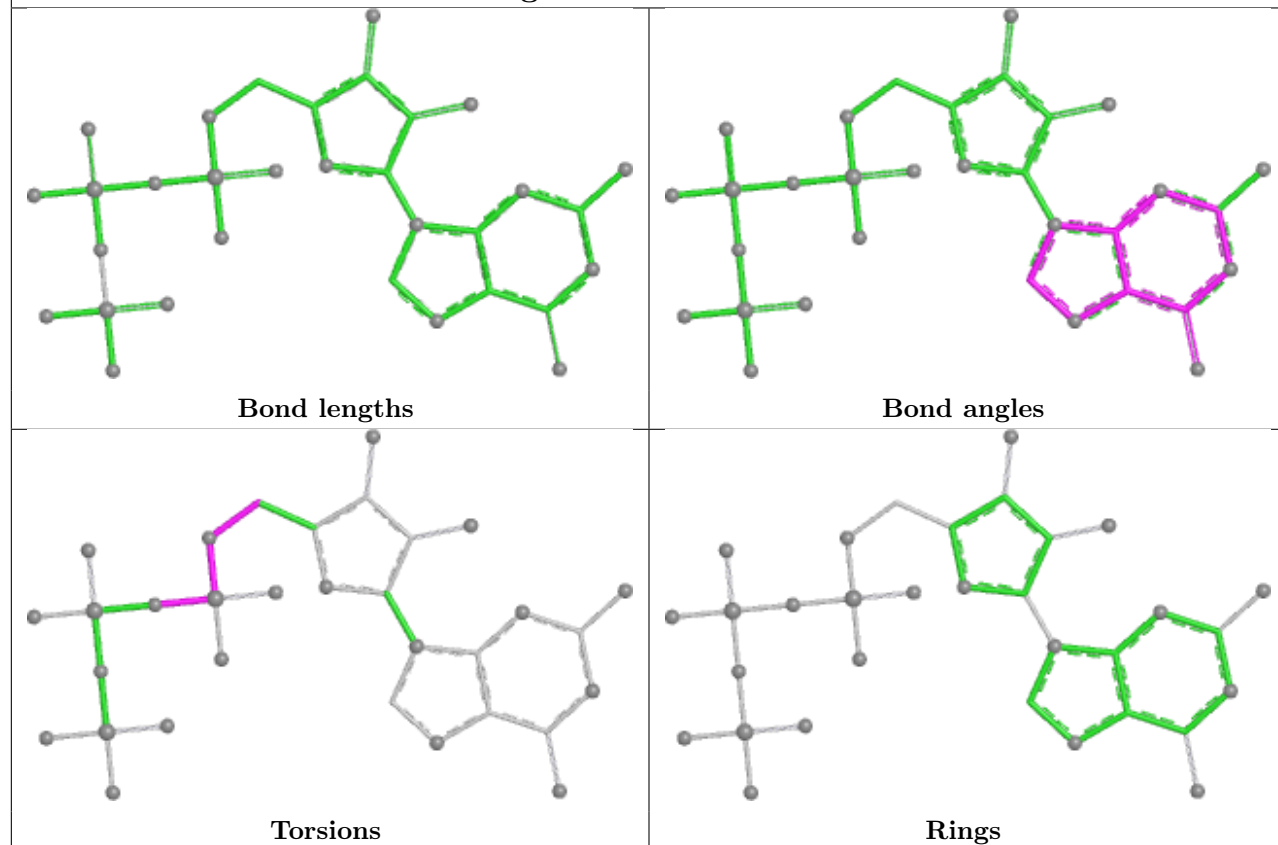
## Ligand GTP 1I 501



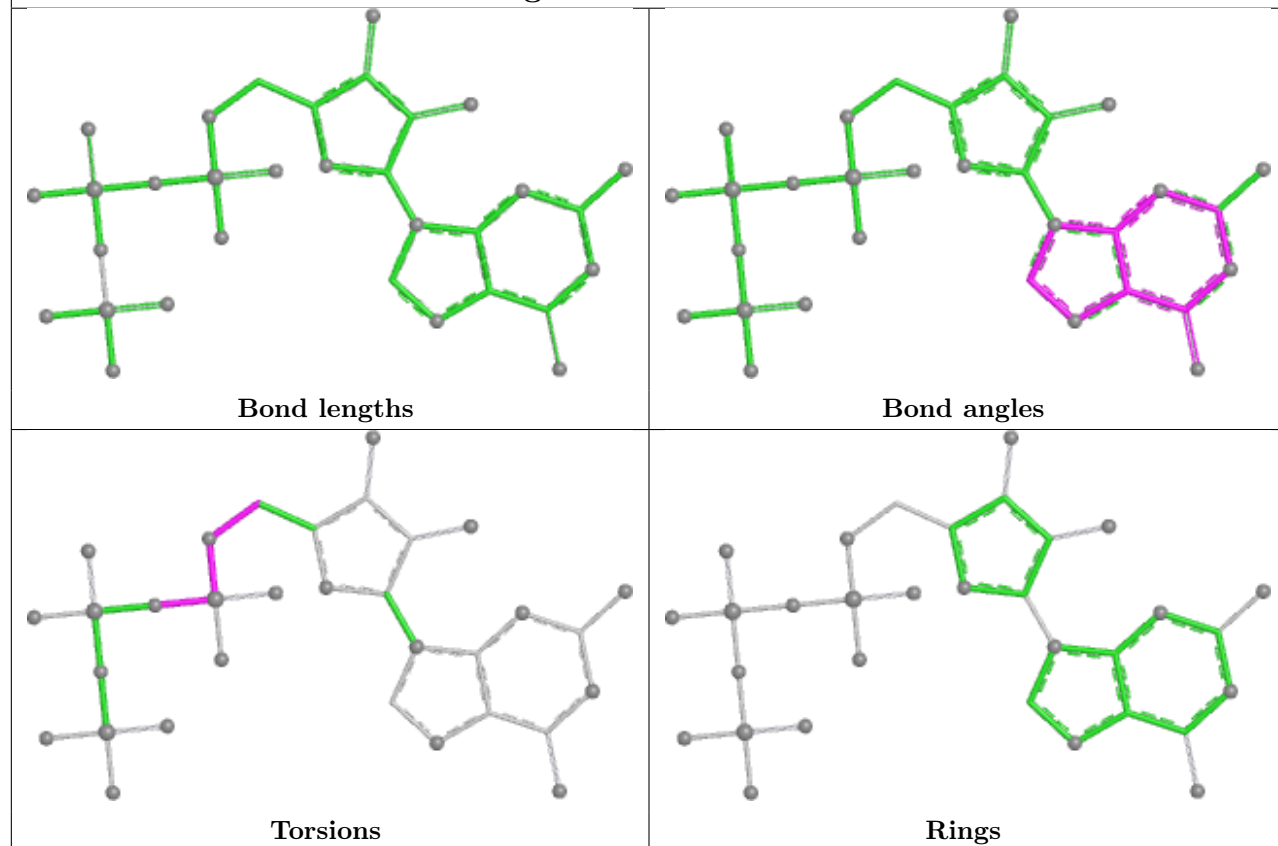




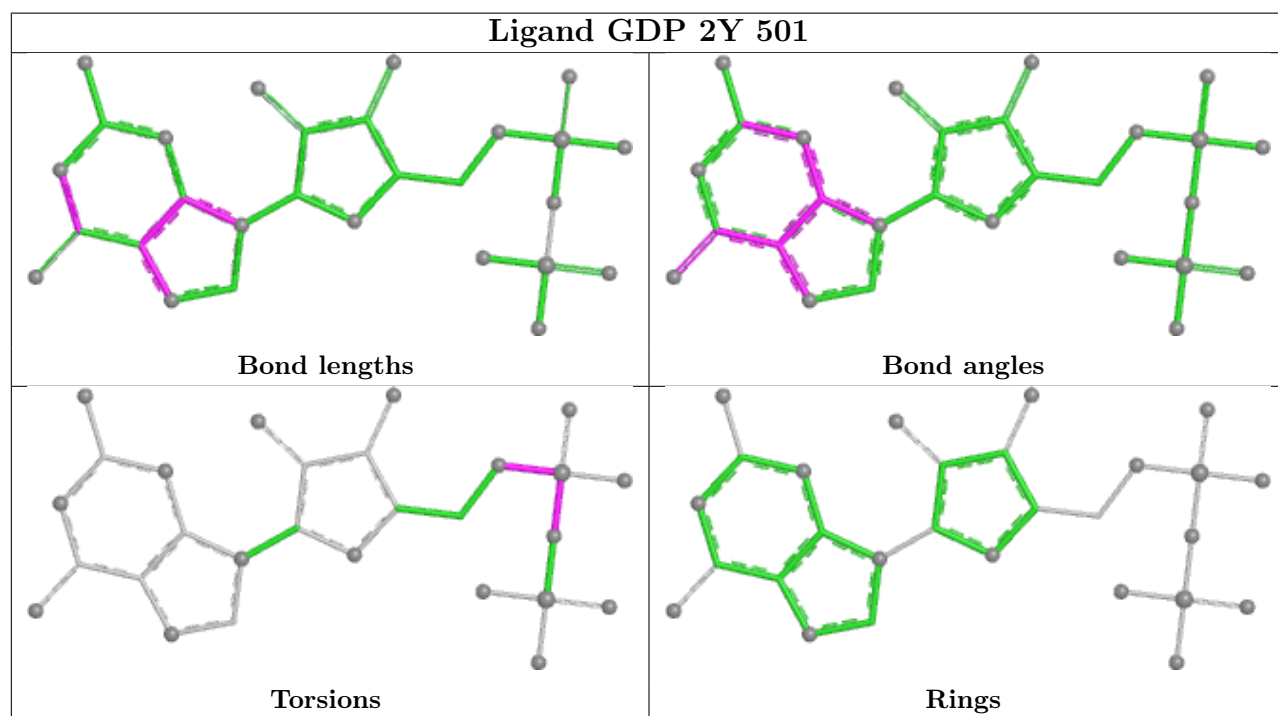
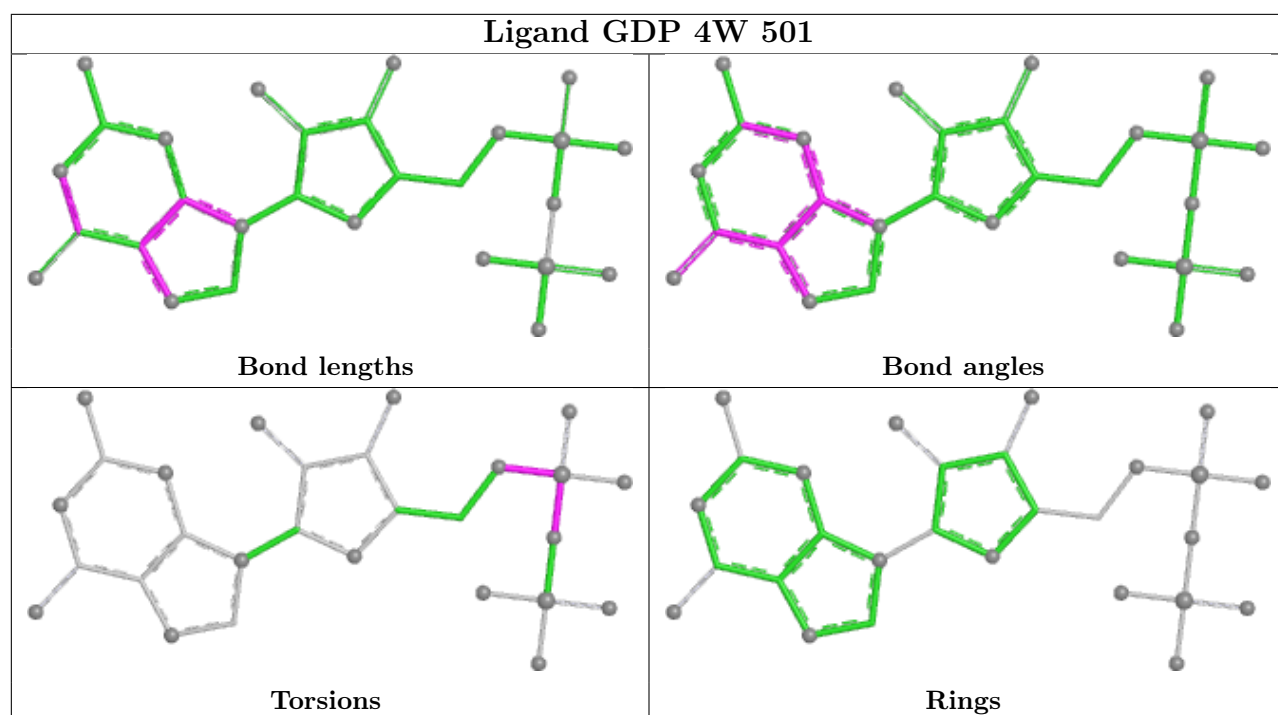
## Ligand GTP 1N 501

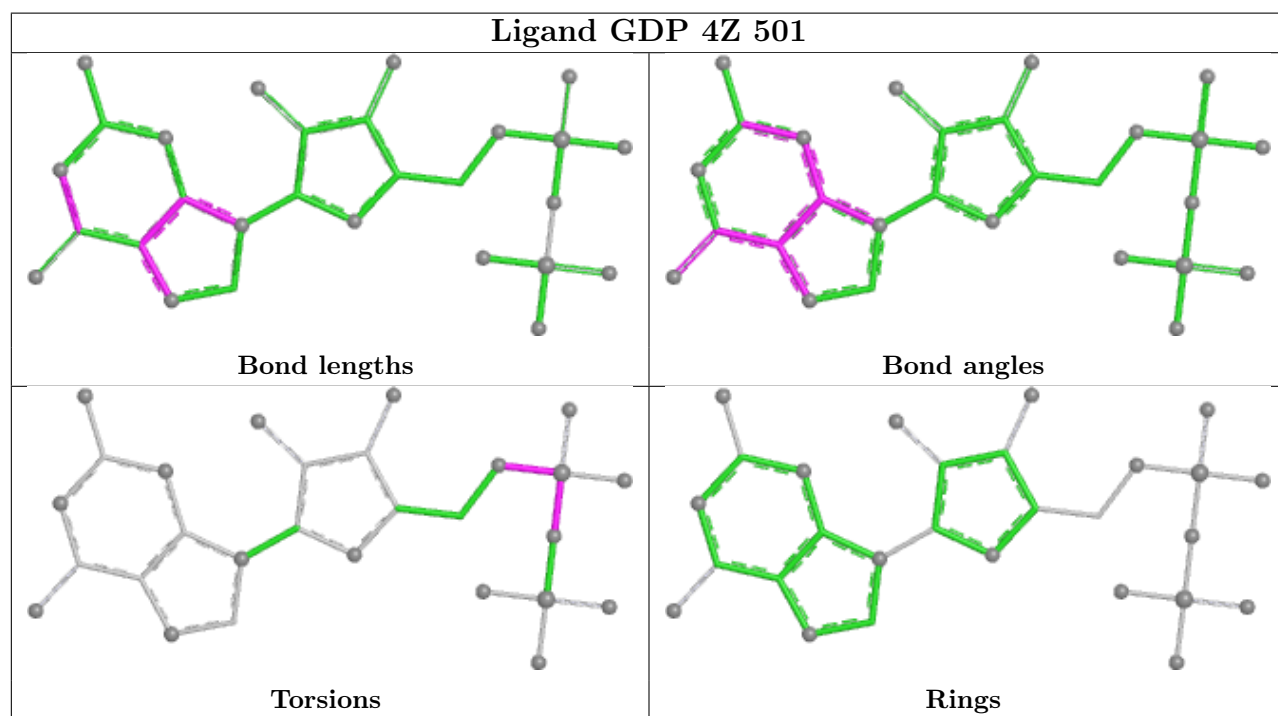
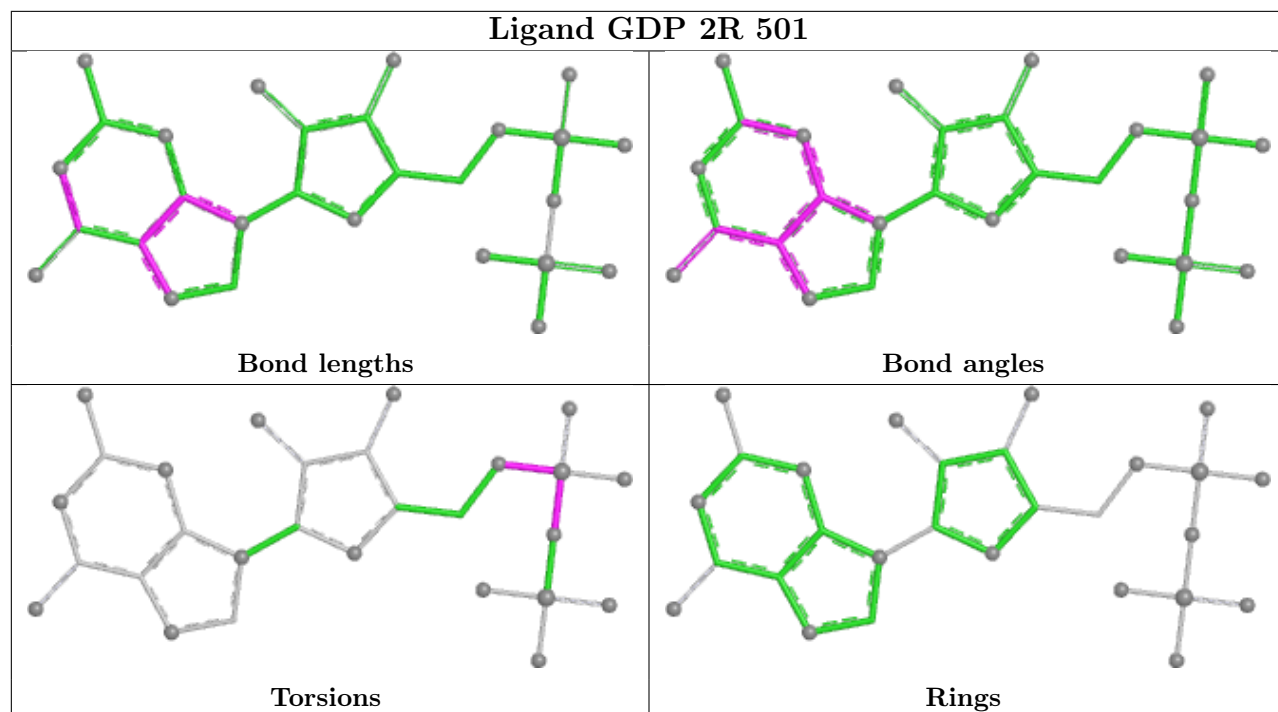


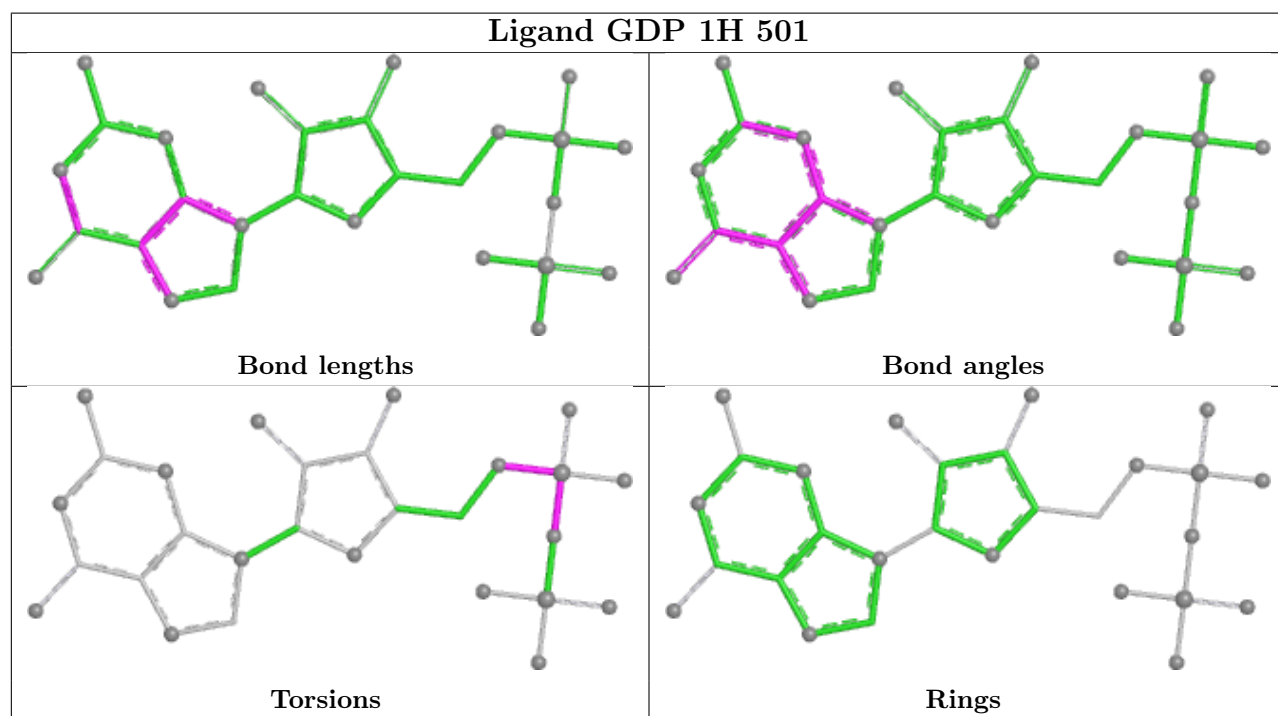
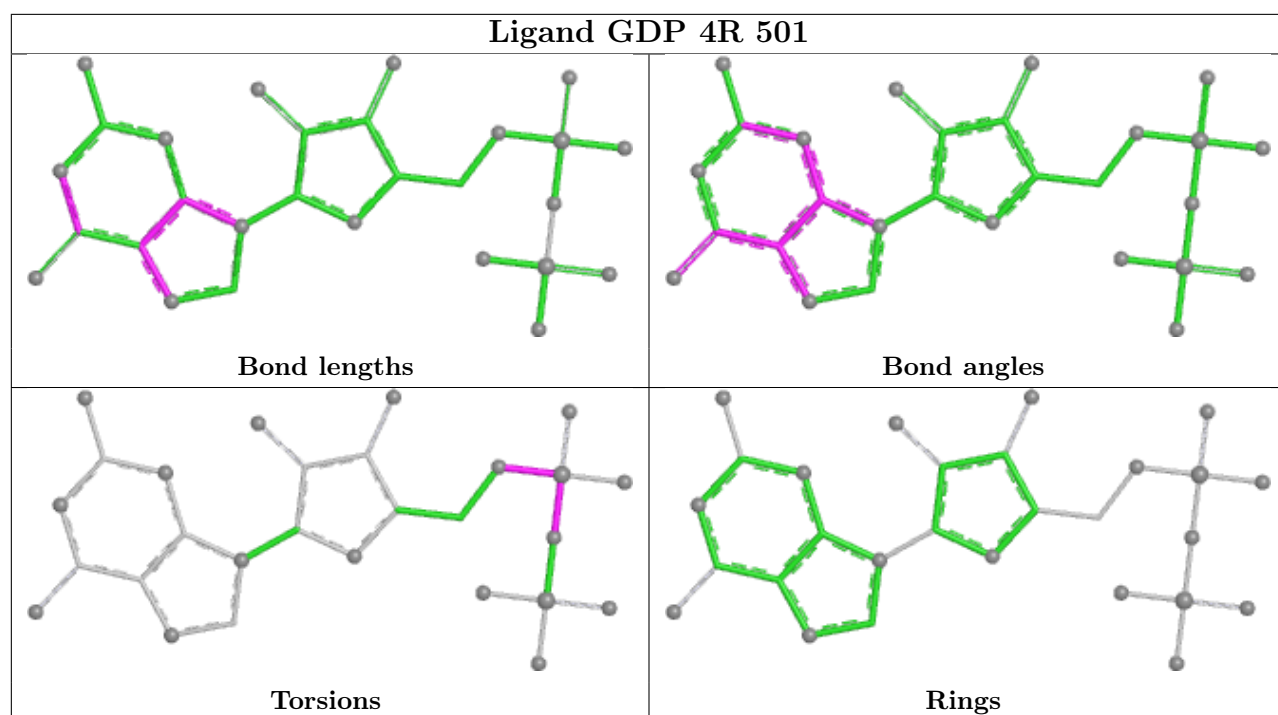
## Ligand GTP 2L 501

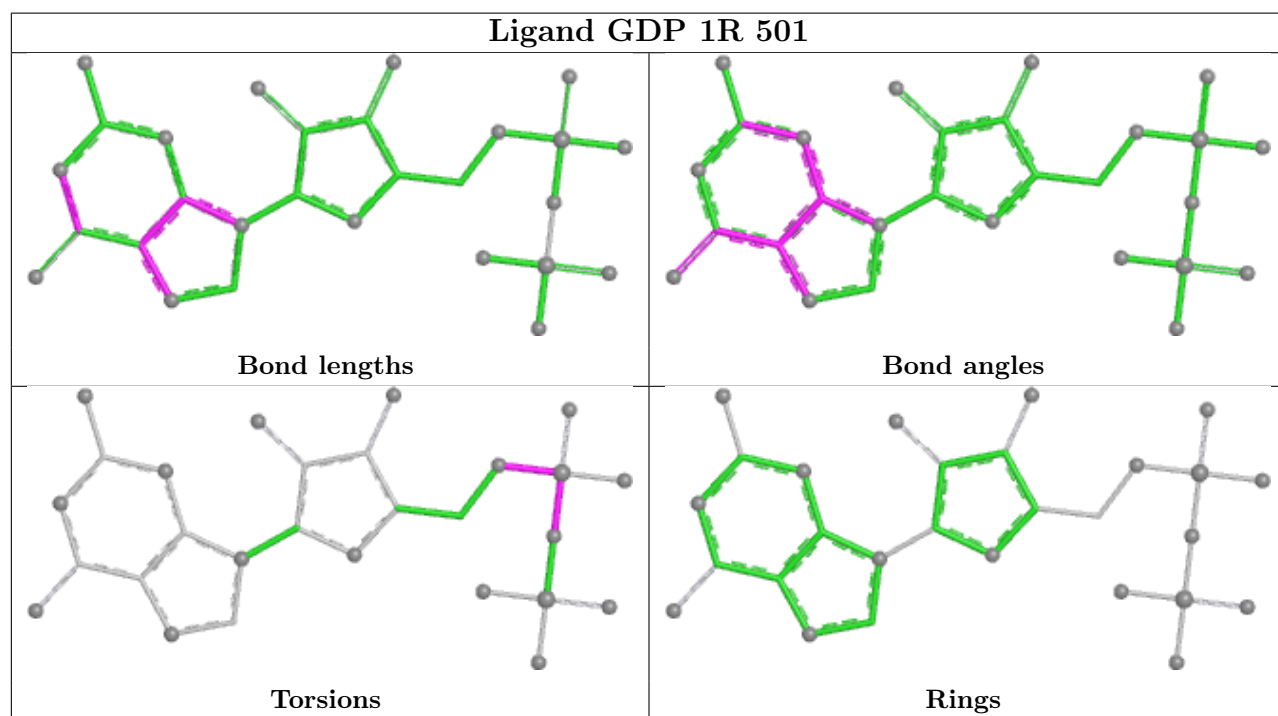
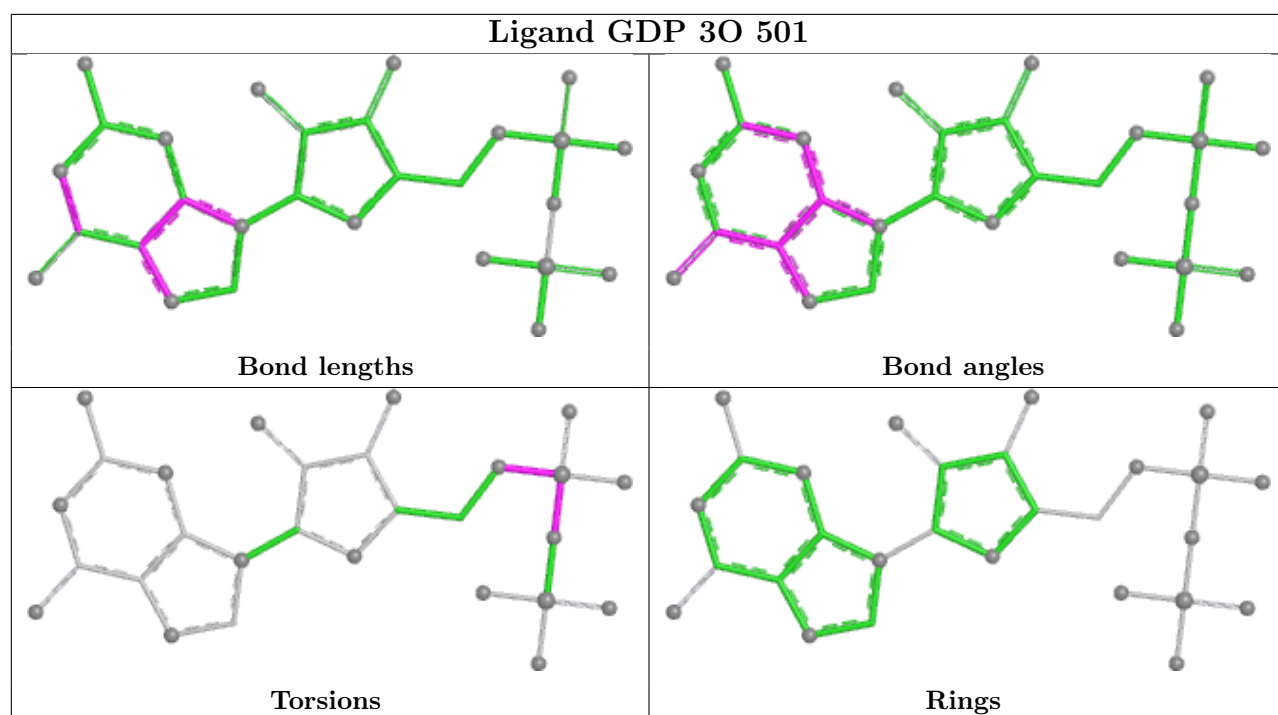


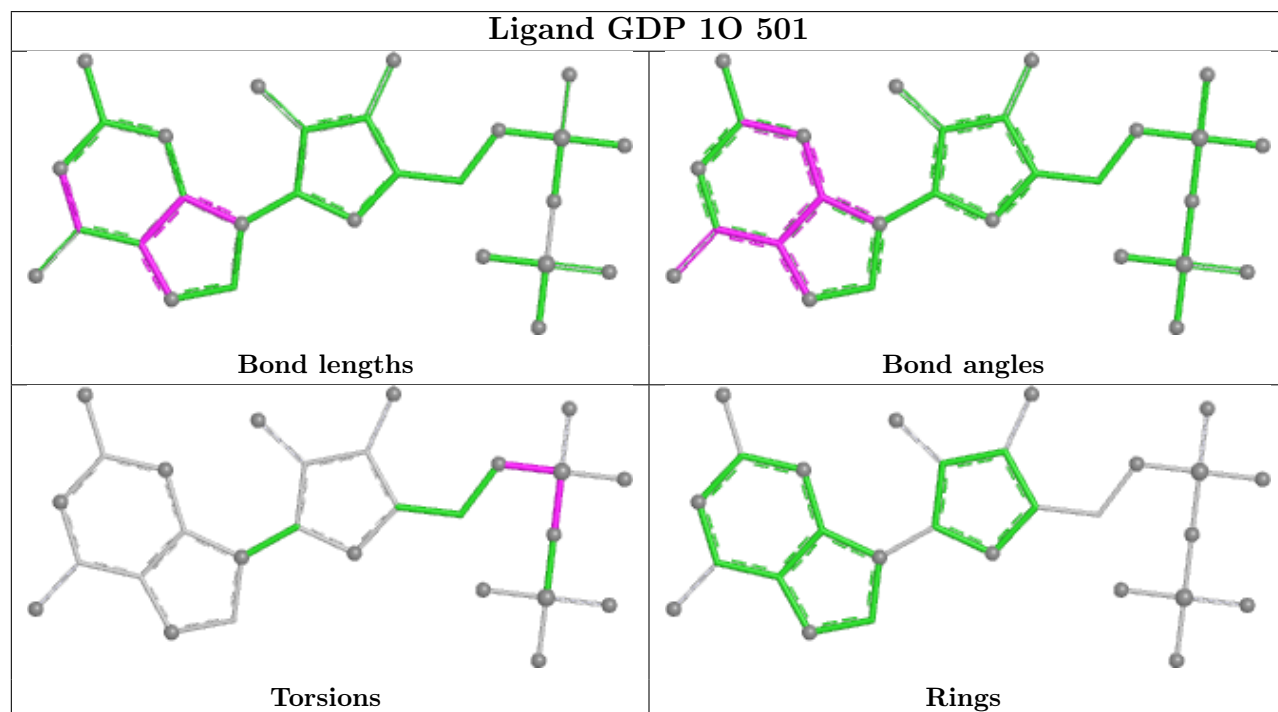
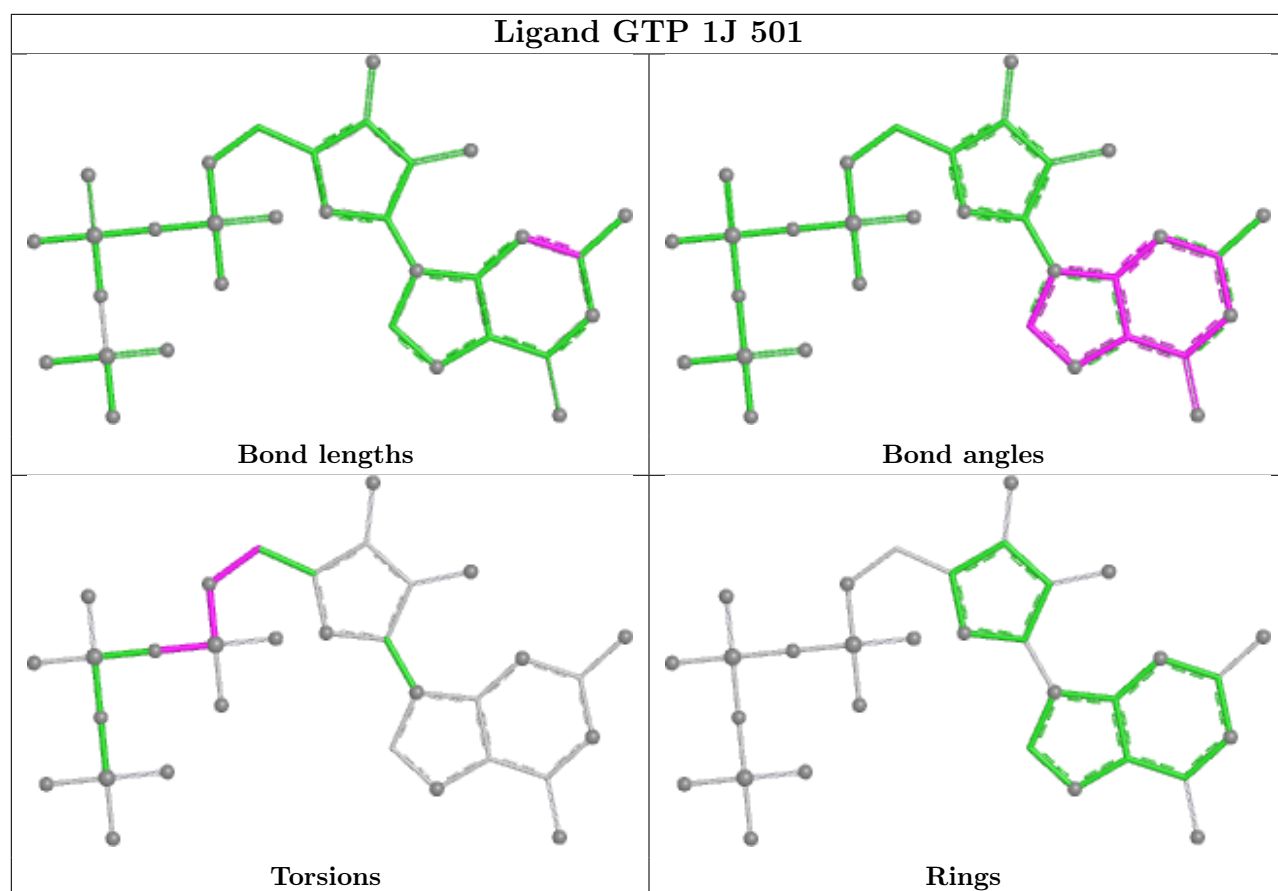




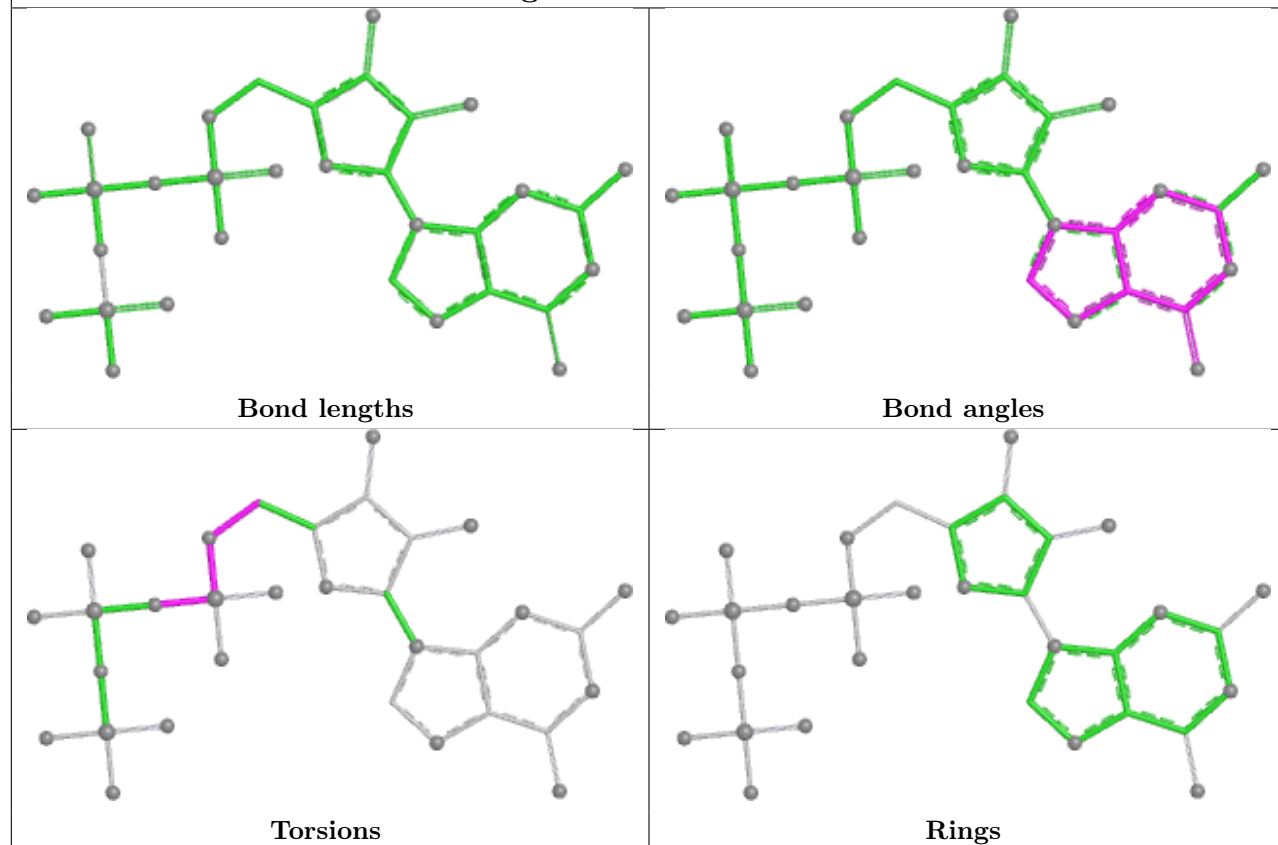




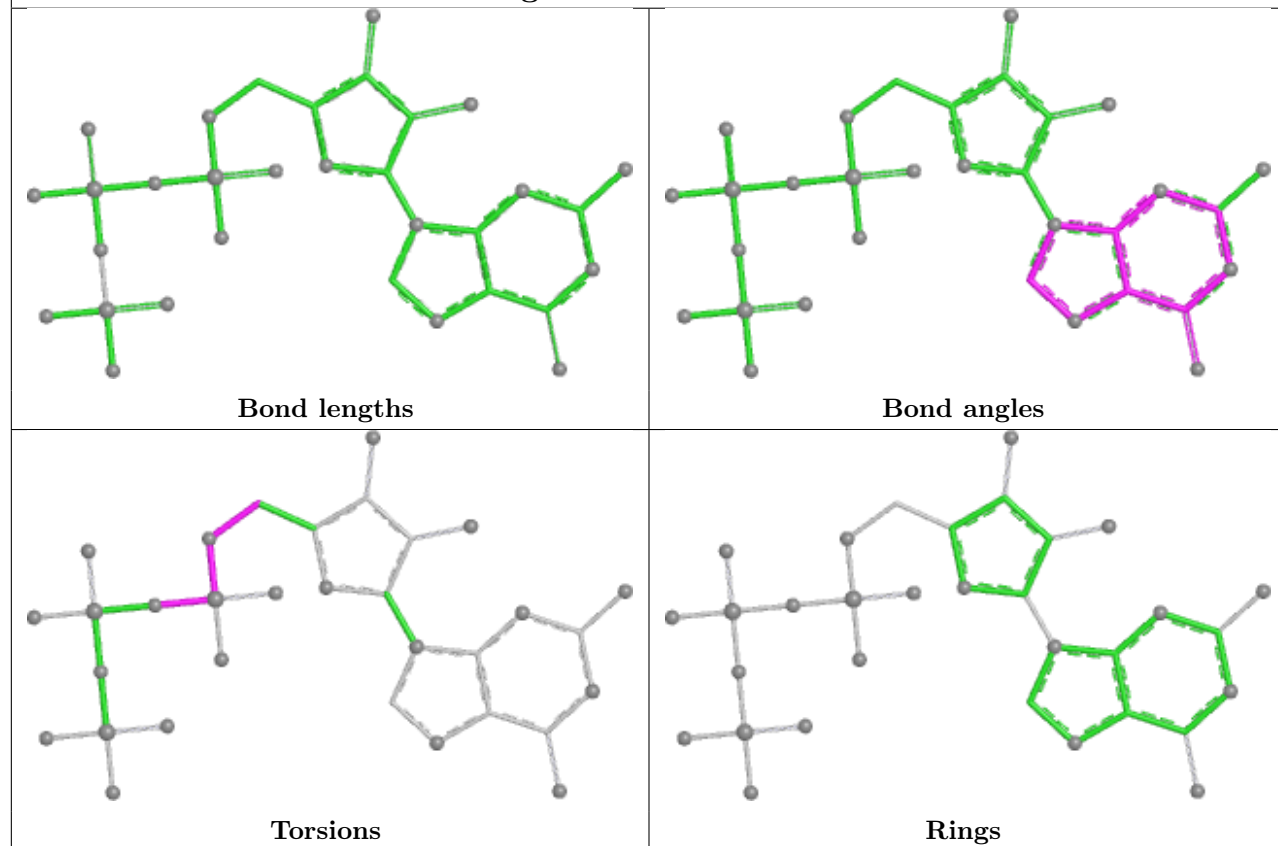


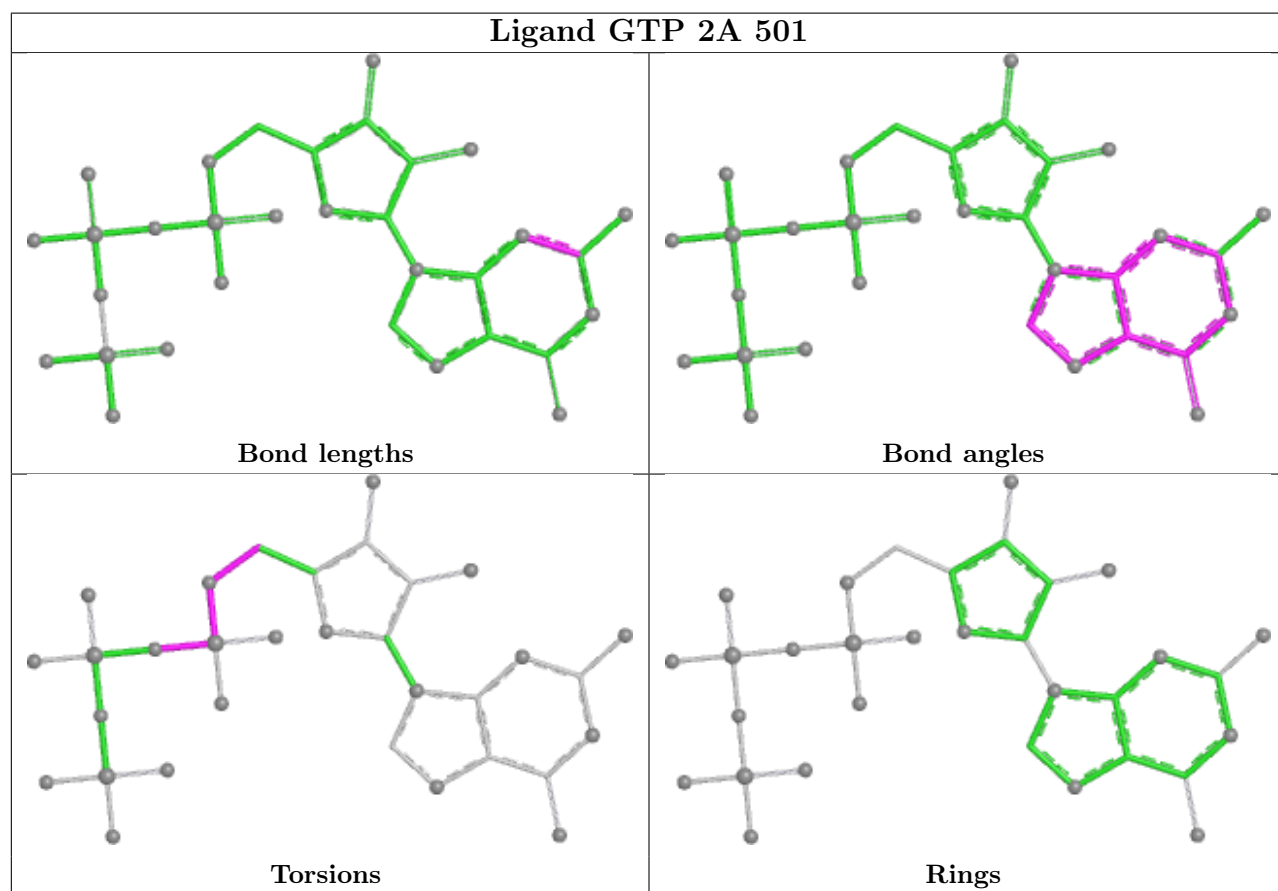
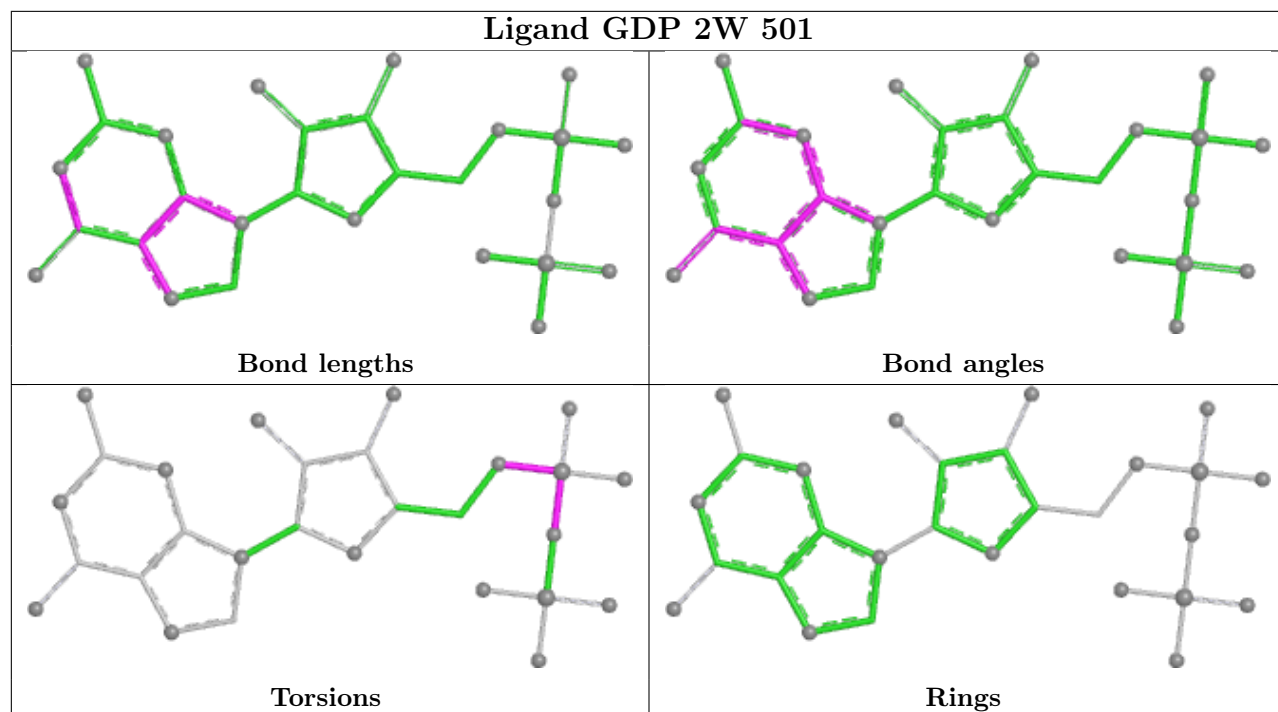


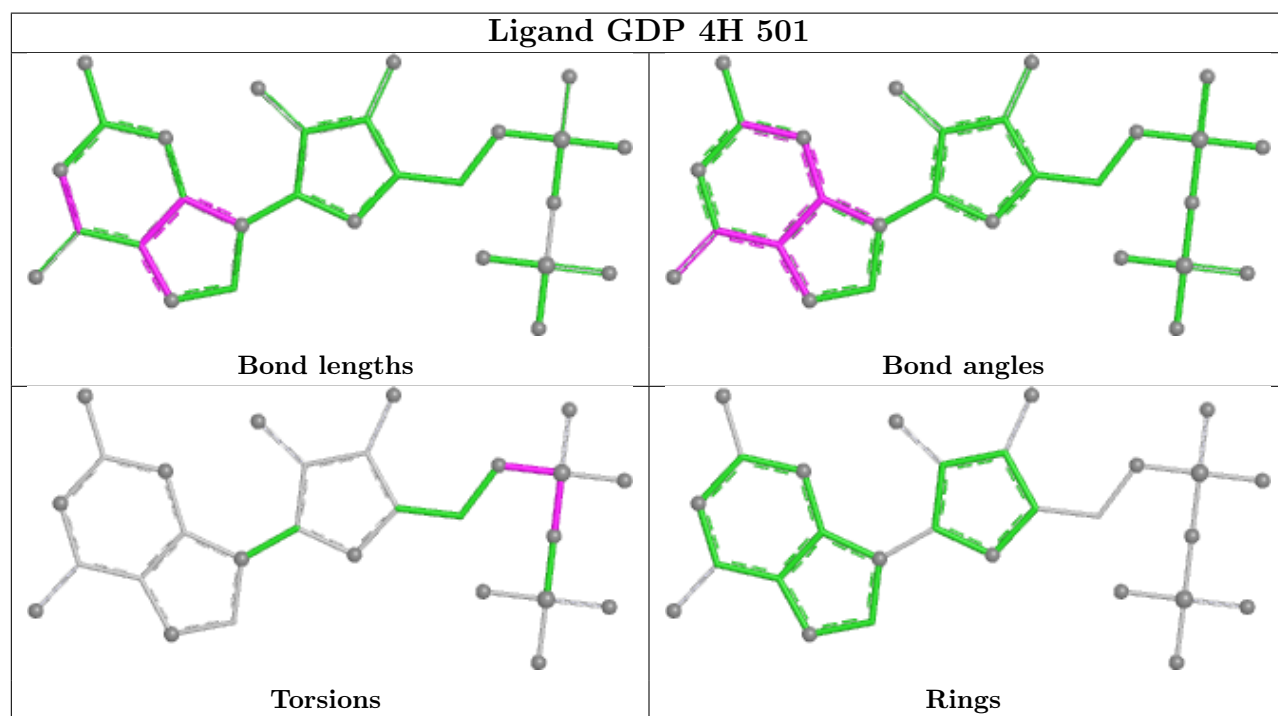
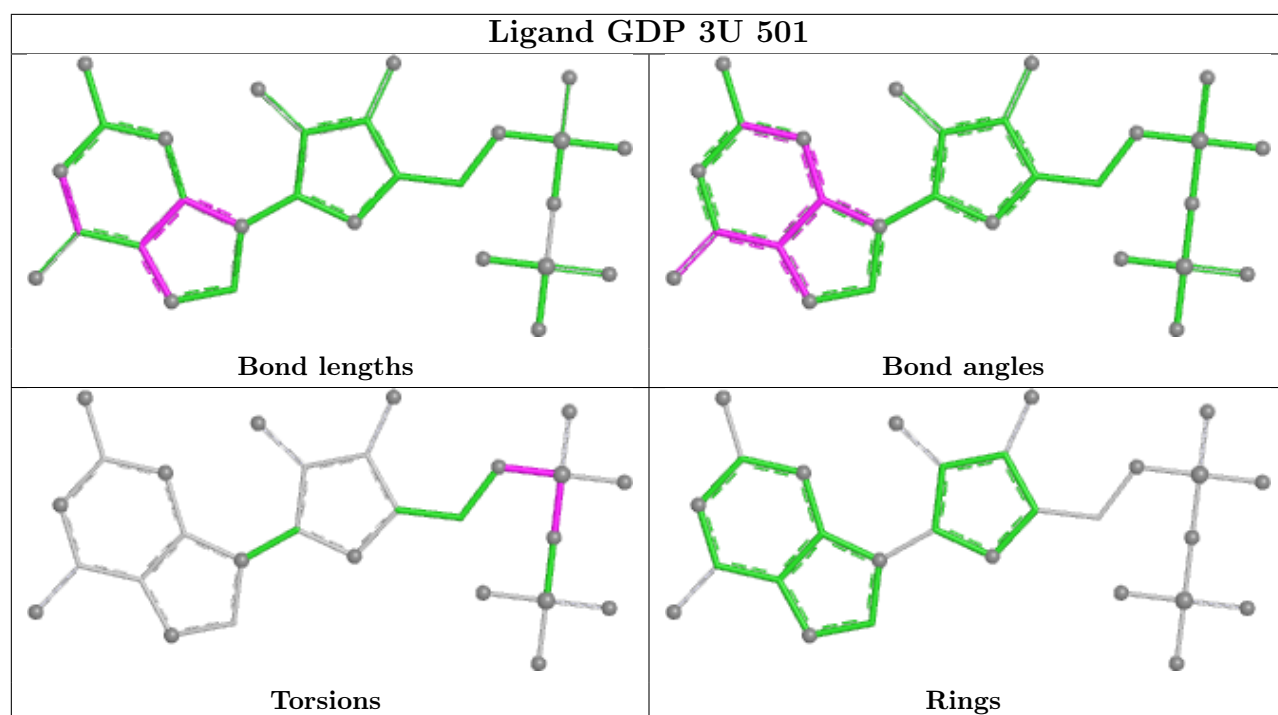
## Ligand GTP 4A 501



## Ligand GTP 2D 501

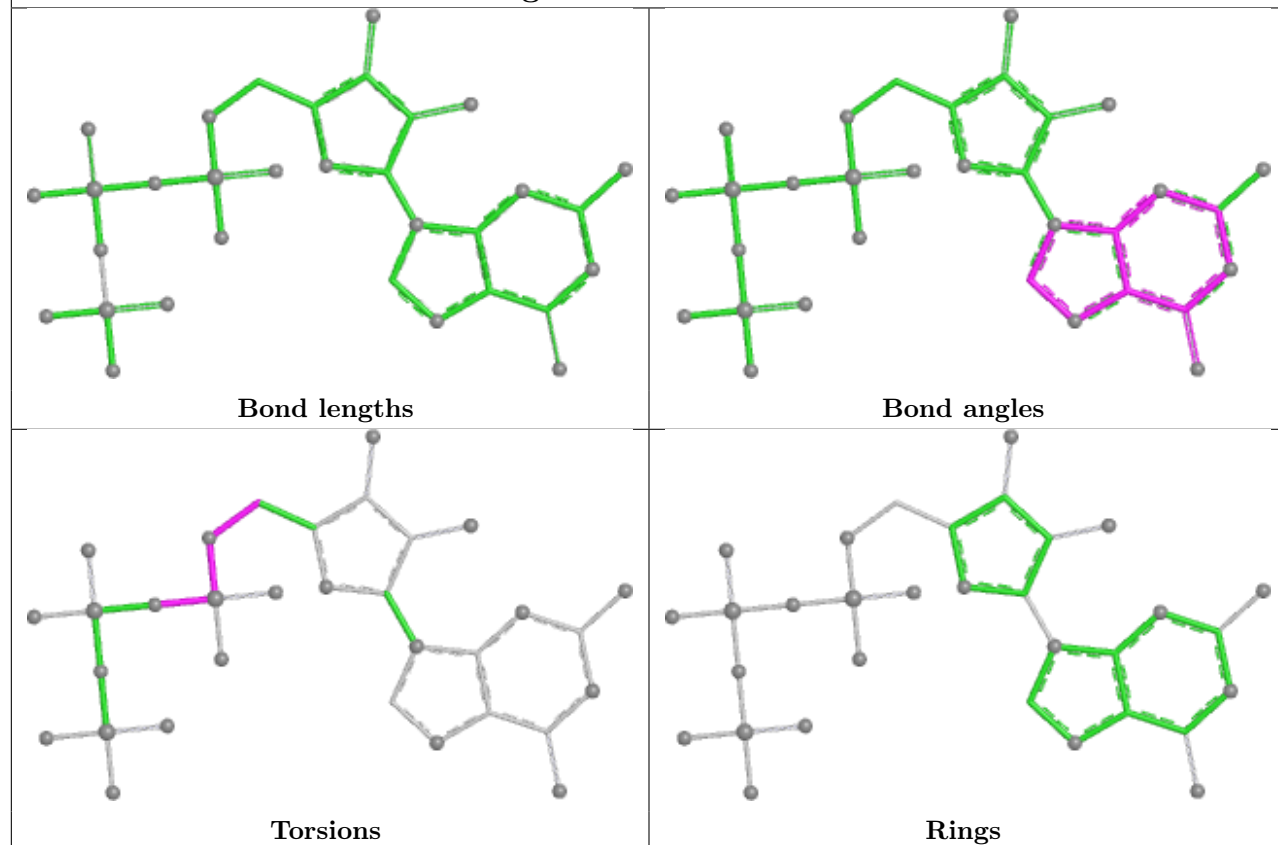




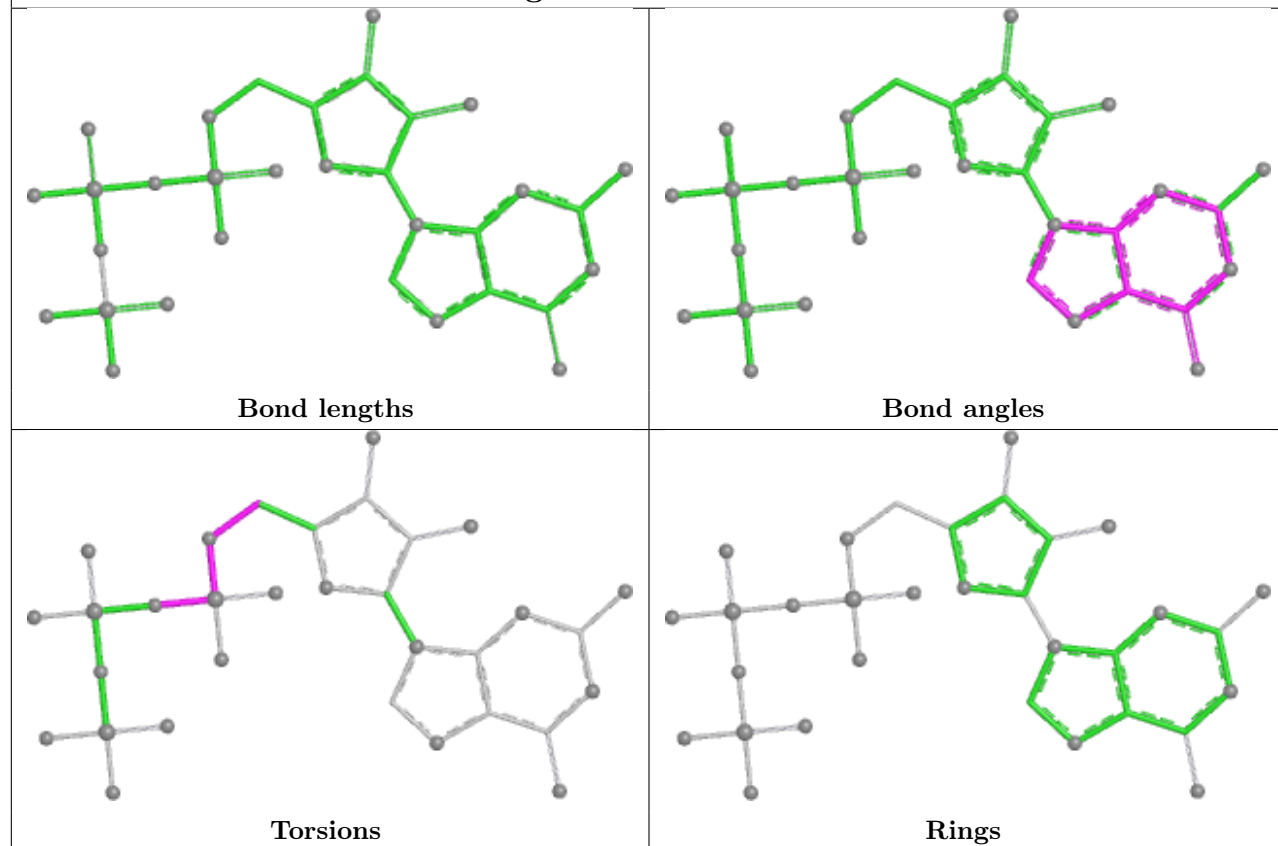


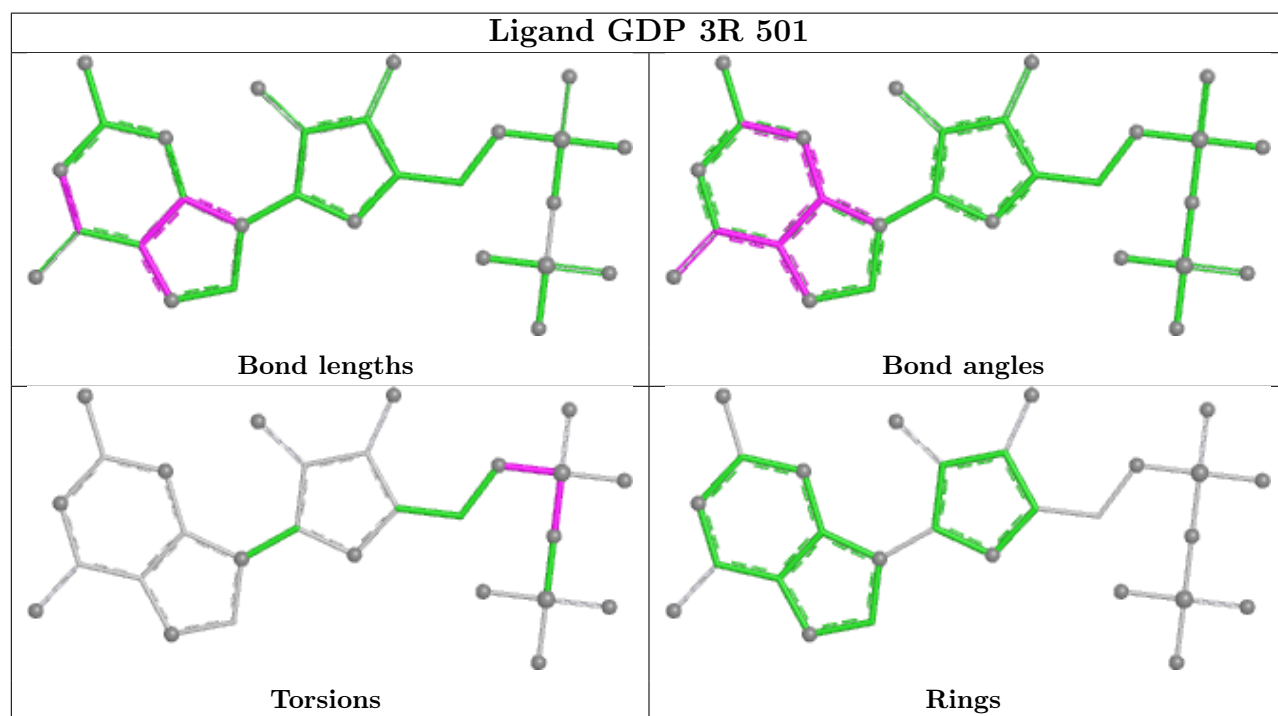
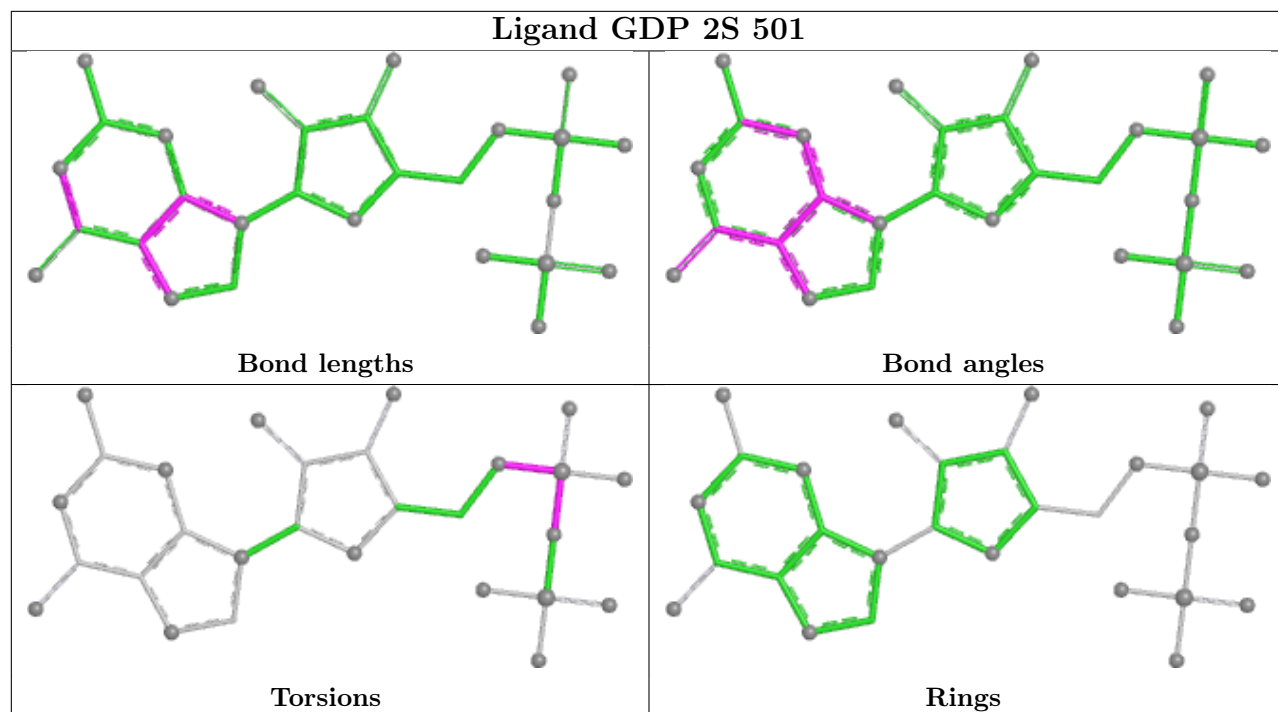


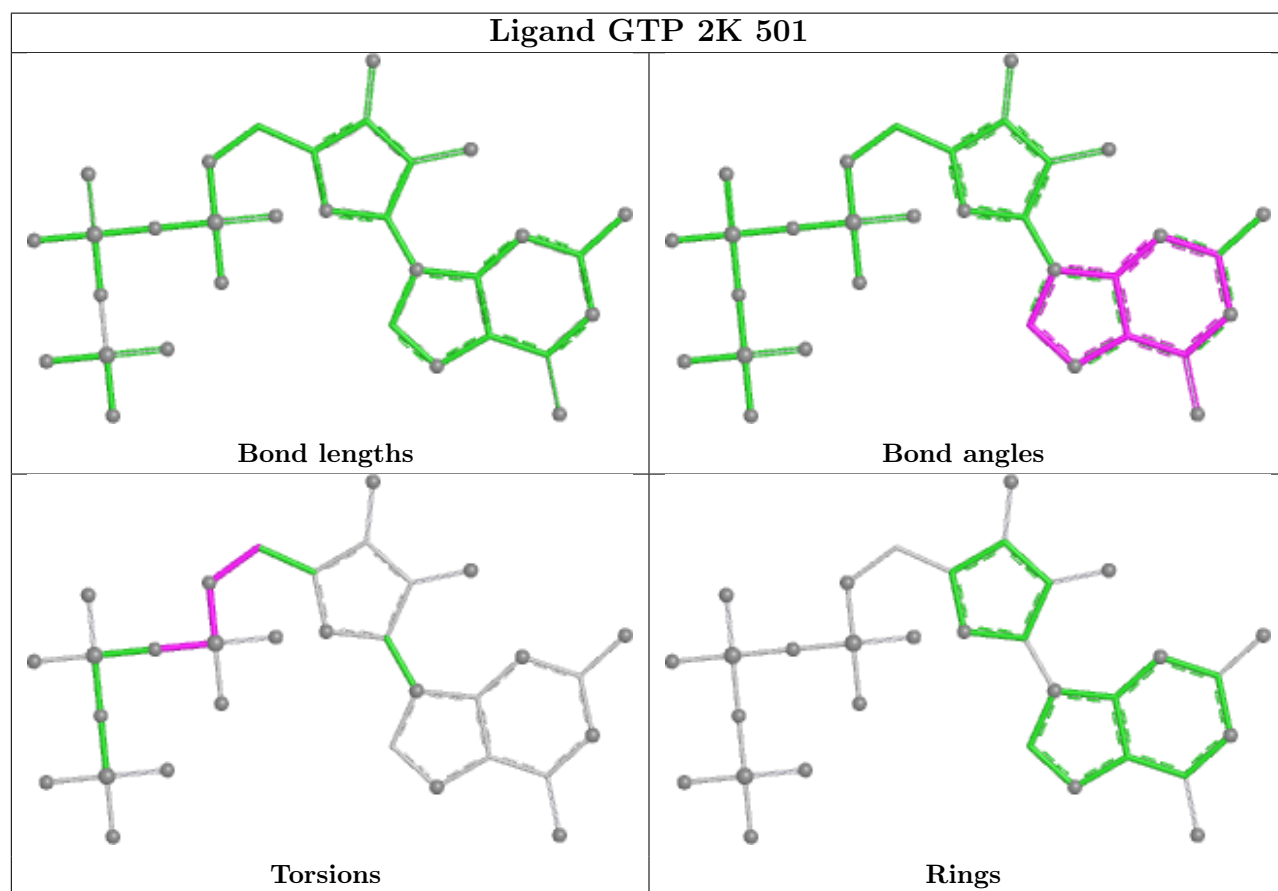
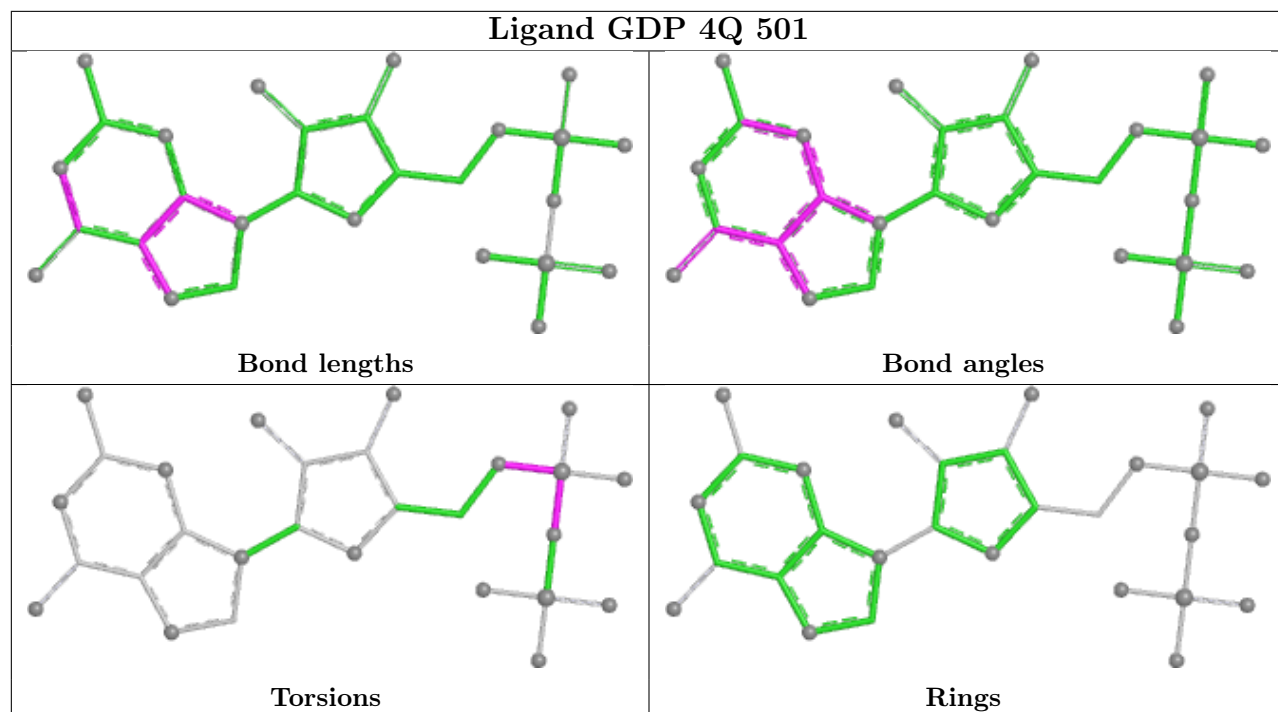
## Ligand GTP 3B 501

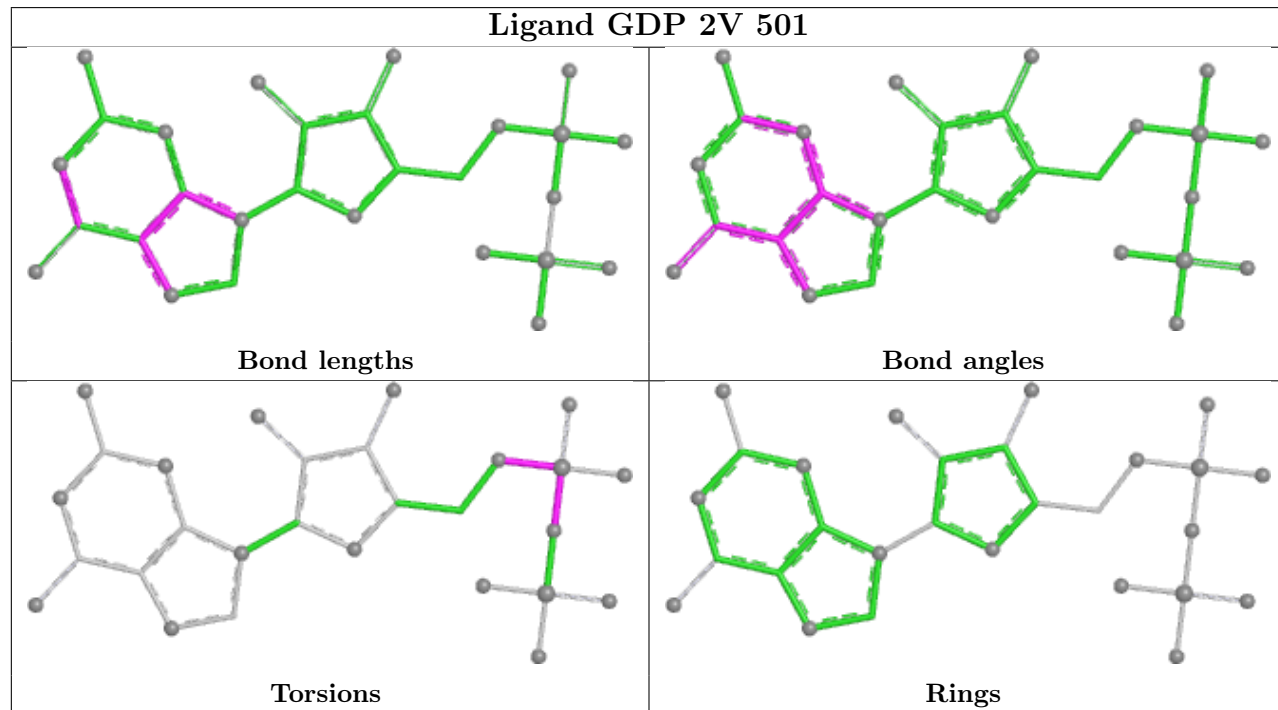
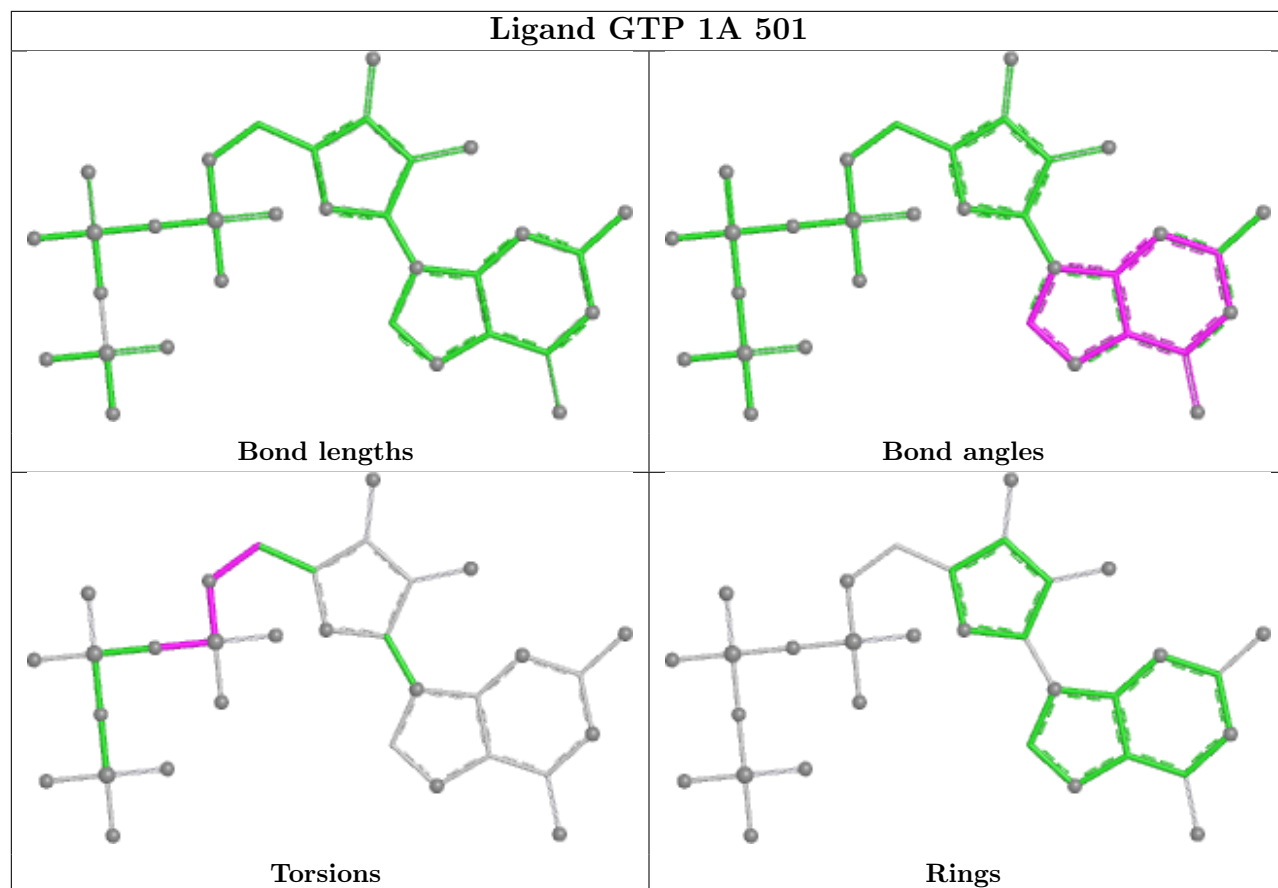


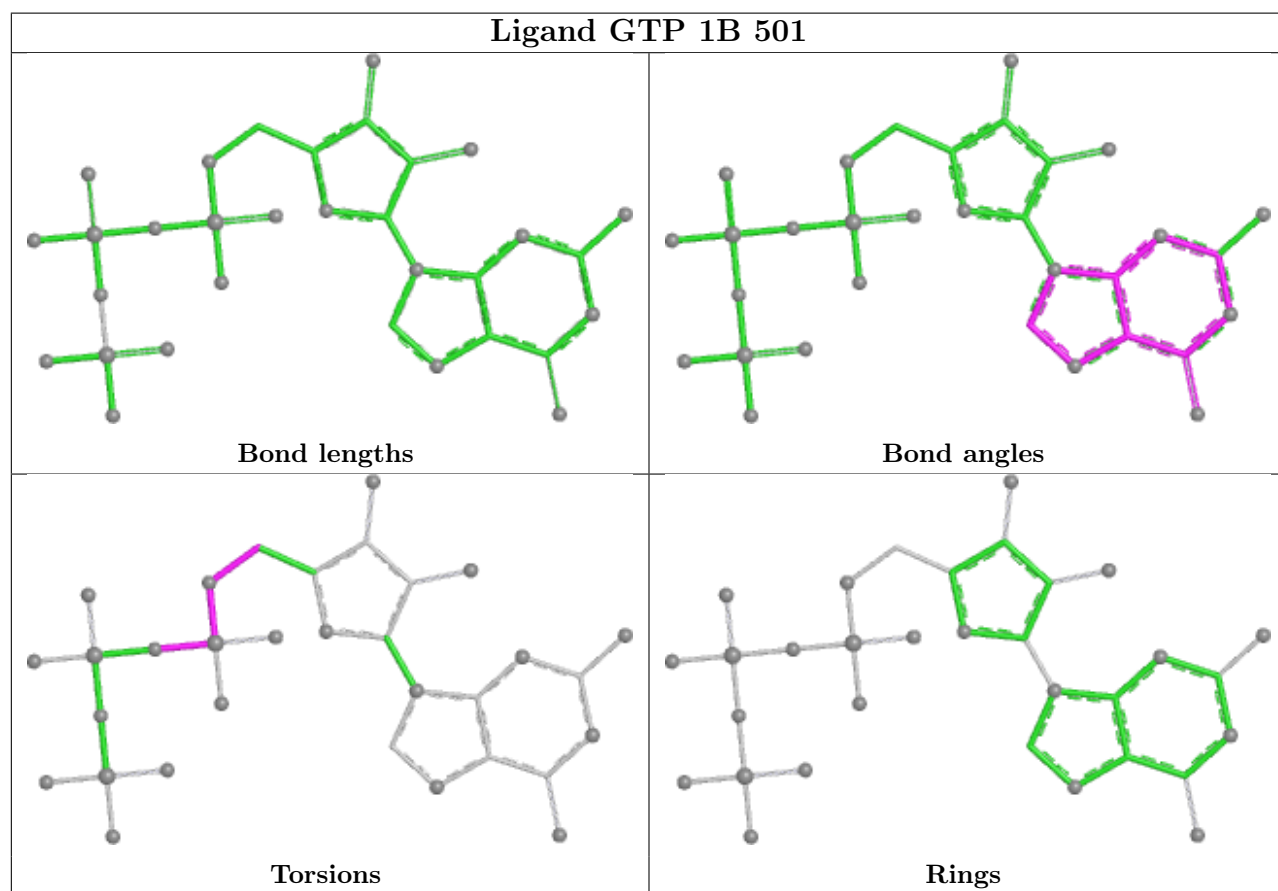
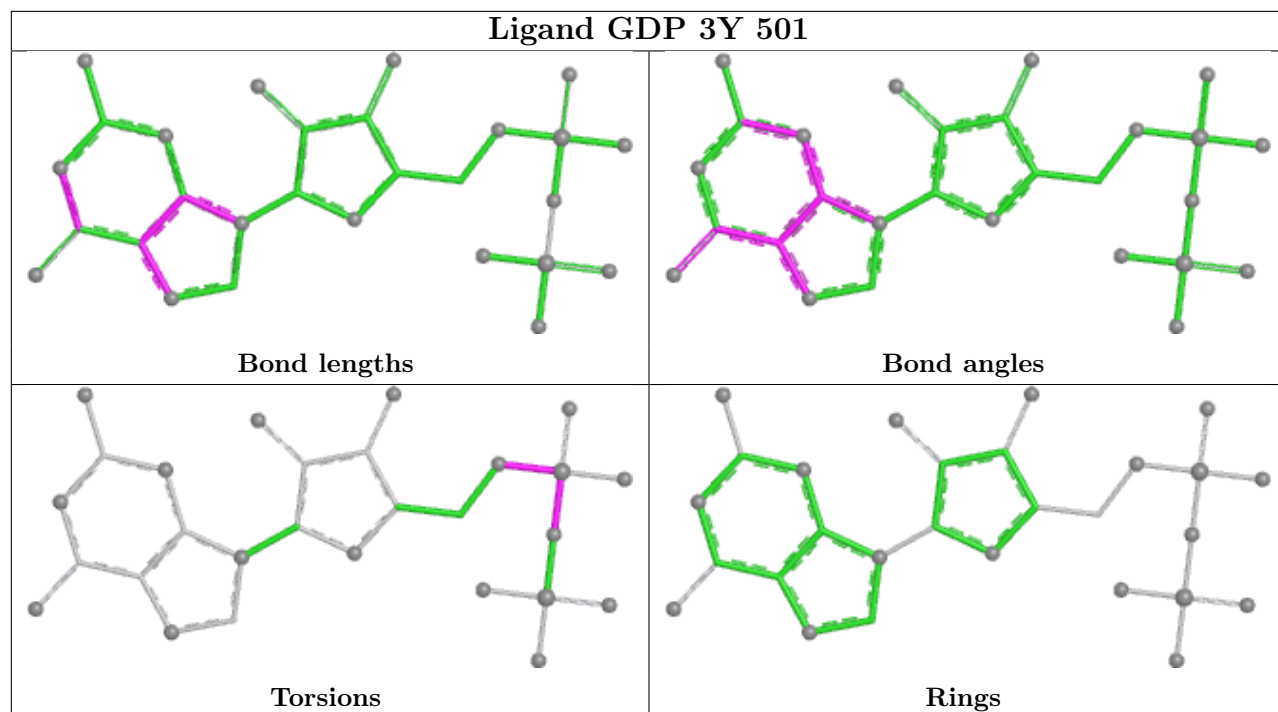
## Ligand GTP 4J 501



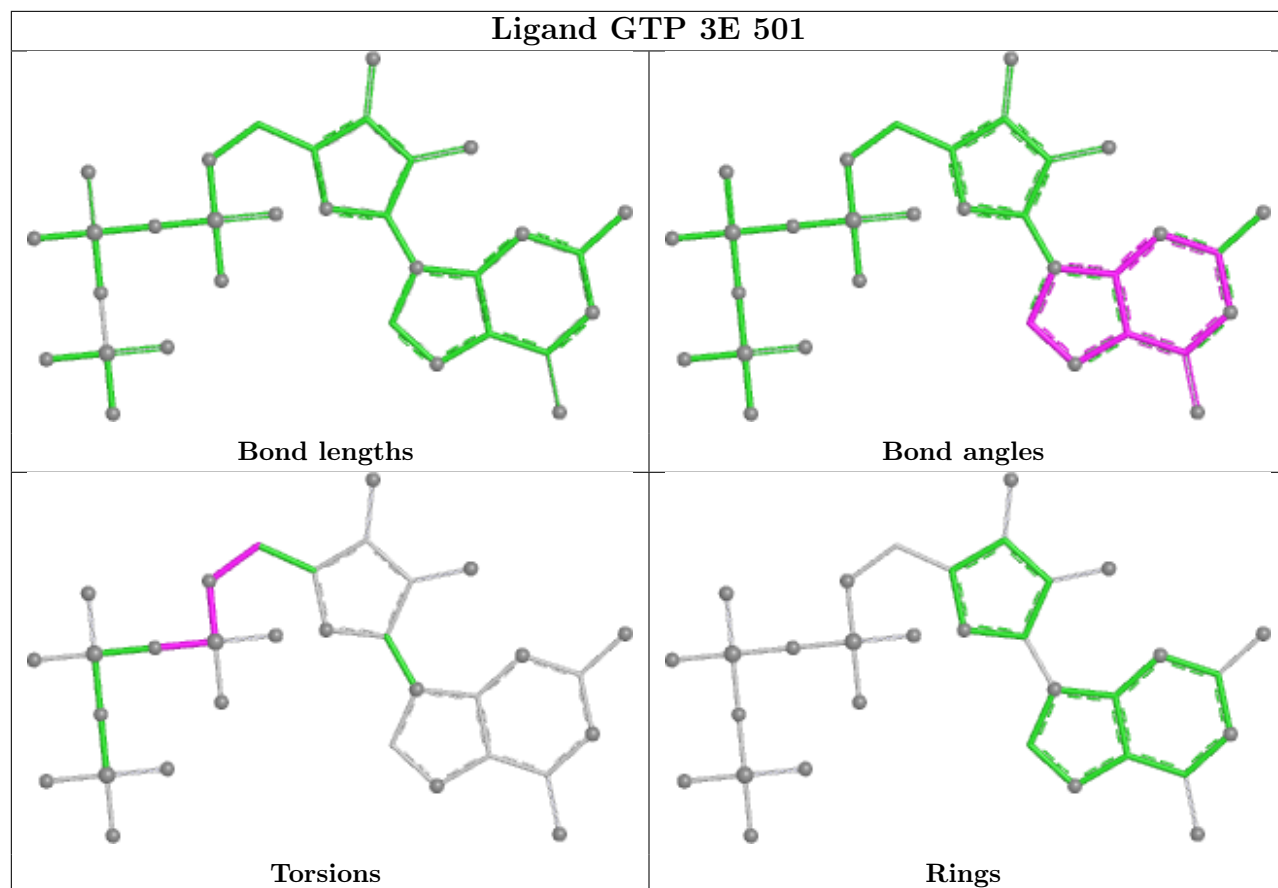




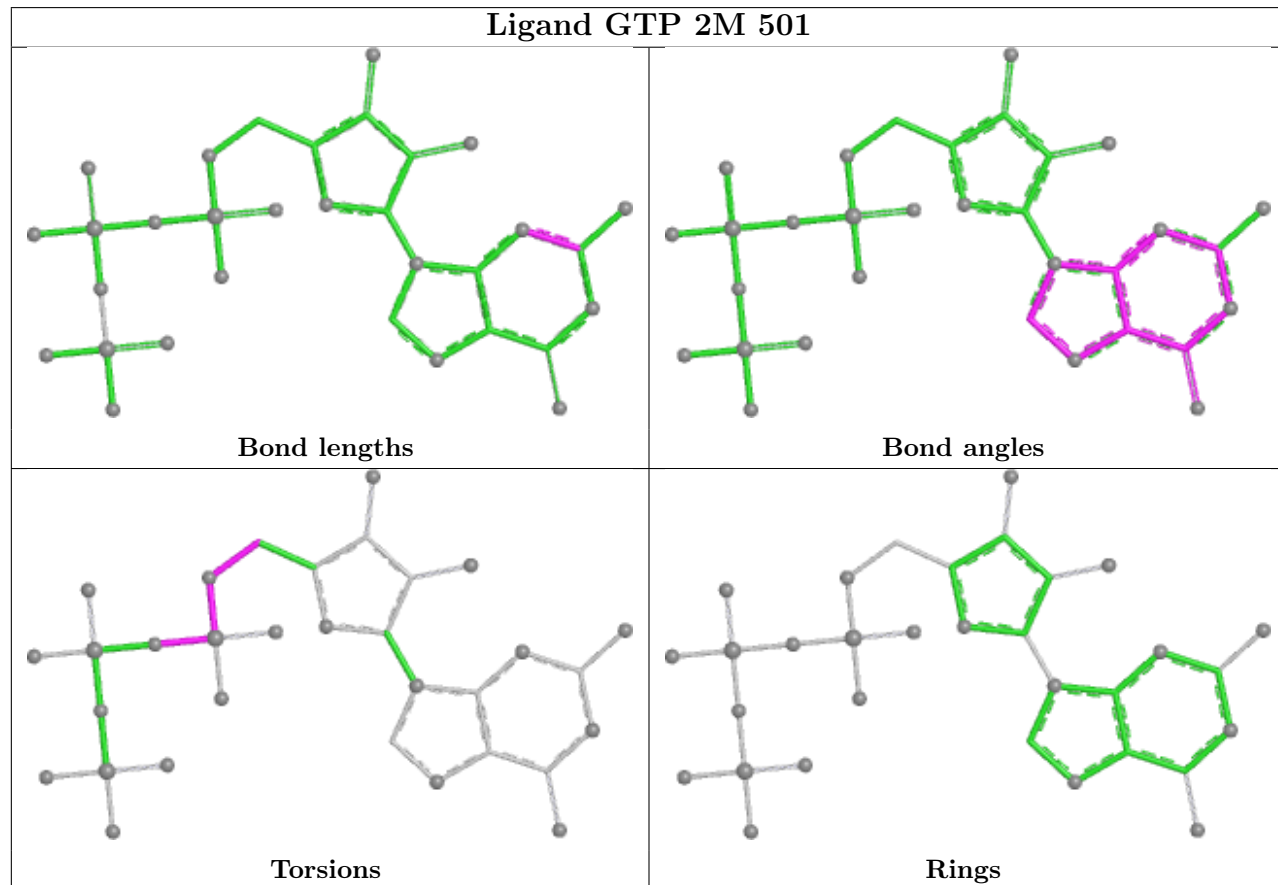




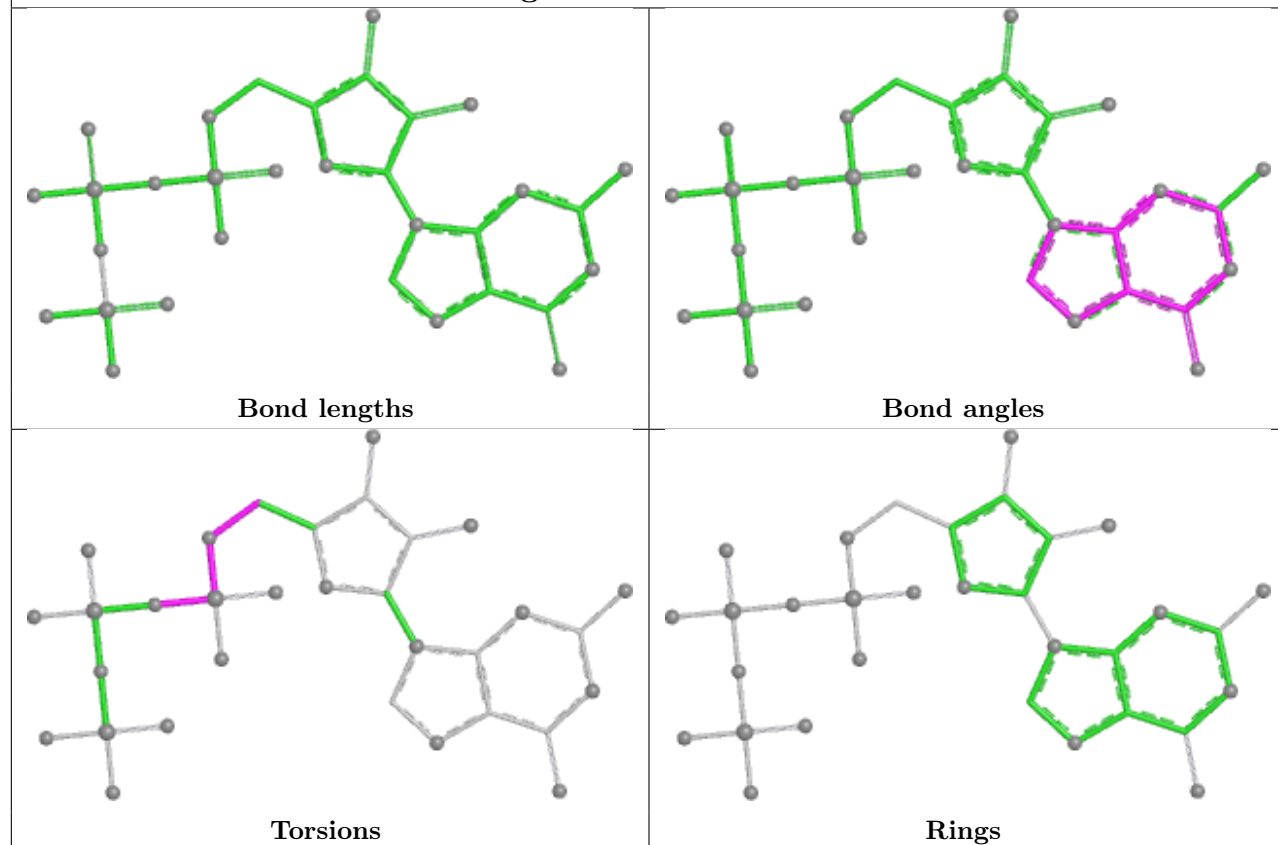
## Ligand GTP 3E 501



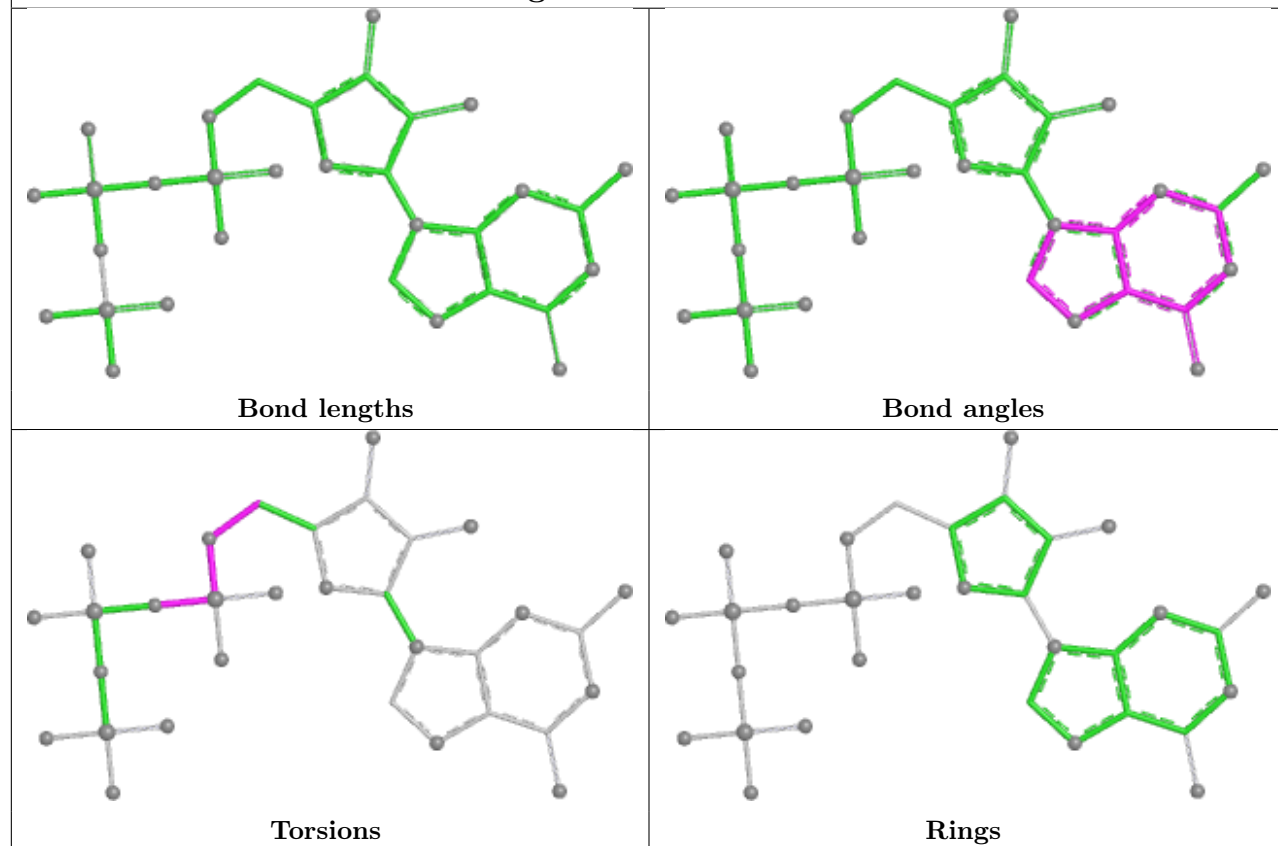
## Ligand GTP 2M 501

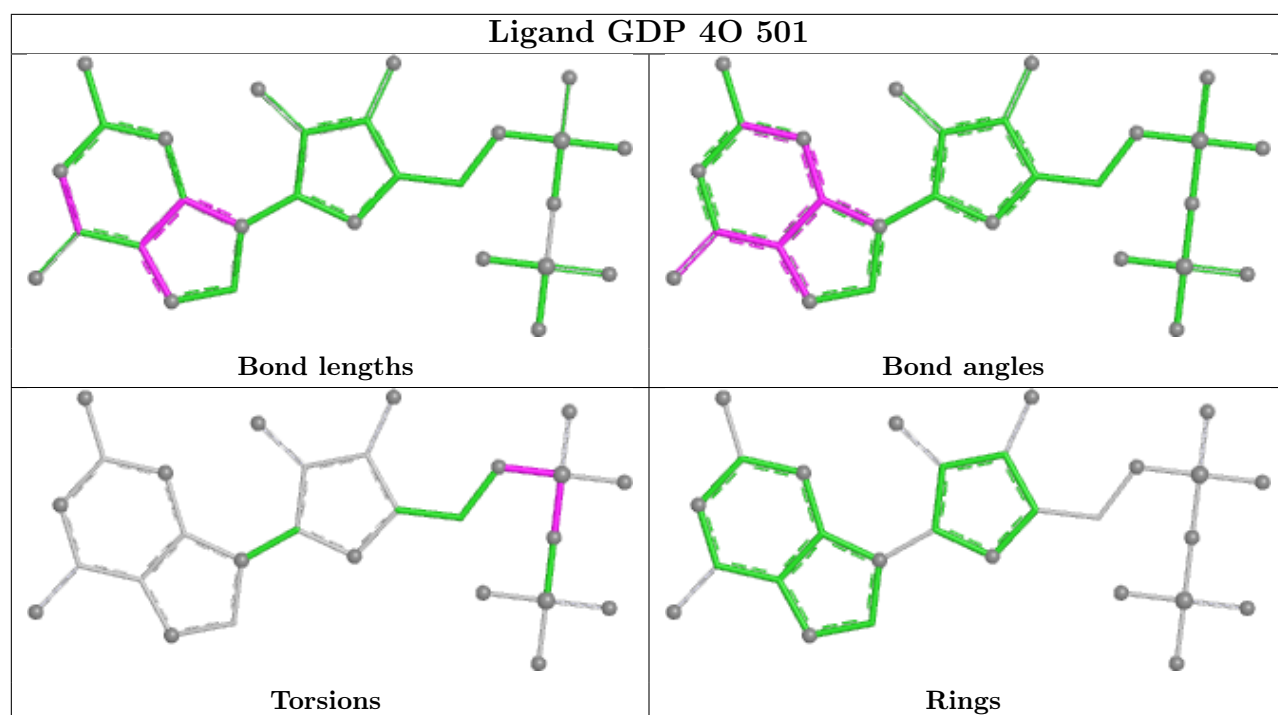


## Ligand GTP 1G 501



## Ligand GTP 4I 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.



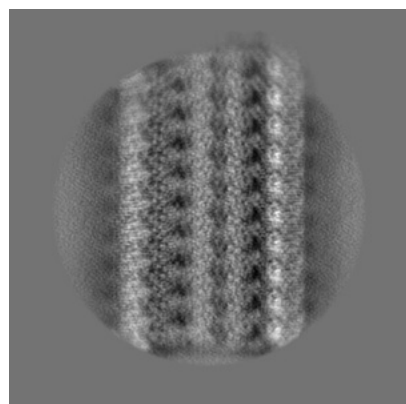
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0615. These allow visual inspection of the internal detail of the map and identification of artifacts.

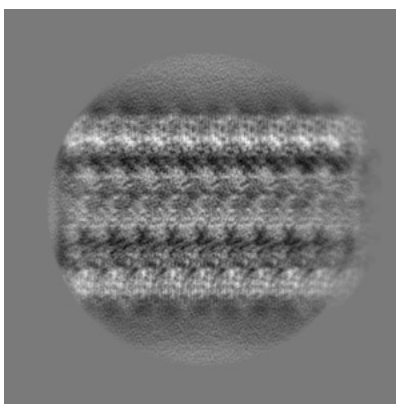
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

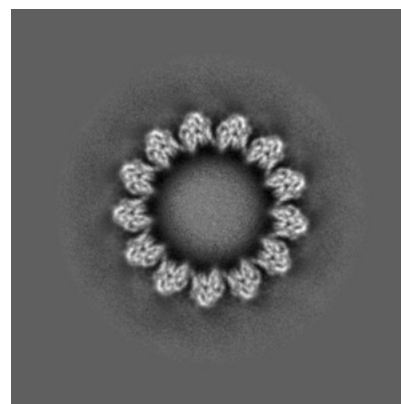
#### 6.1.1 Primary map



X

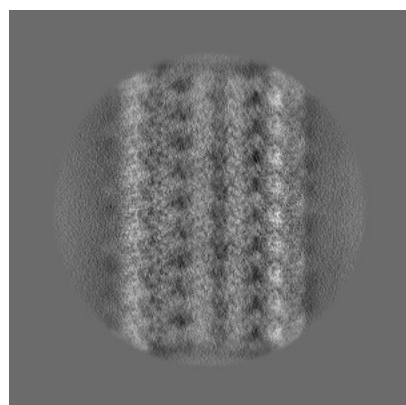


Y

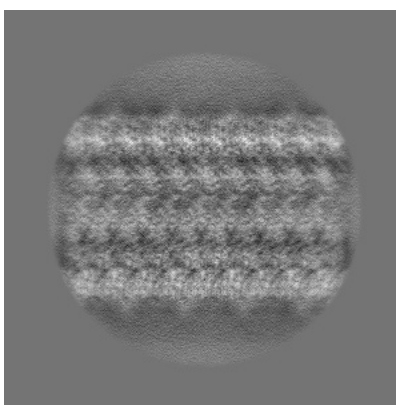


Z

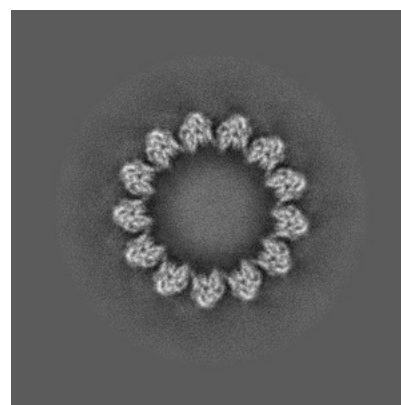
#### 6.1.2 Raw map



X



Y

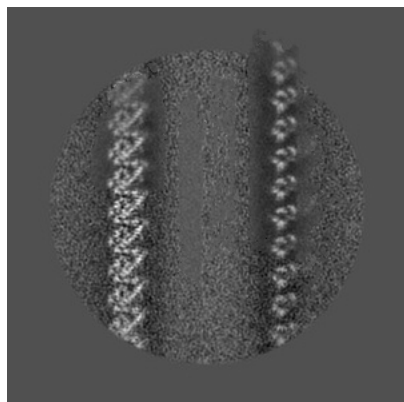


Z

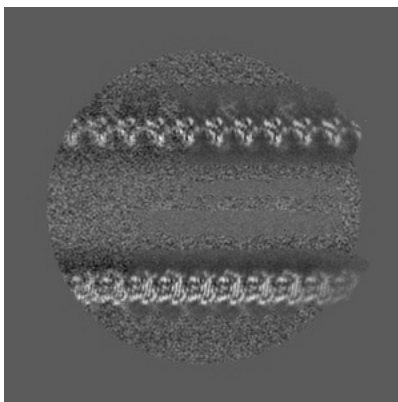
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

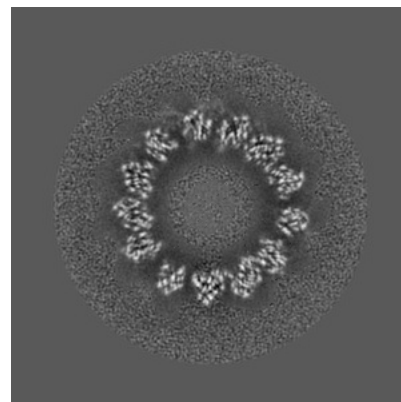
### 6.2.1 Primary map



X Index: 256

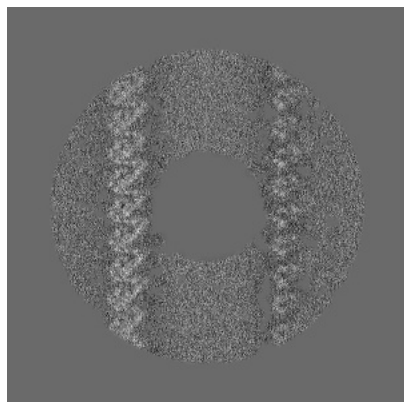


Y Index: 256

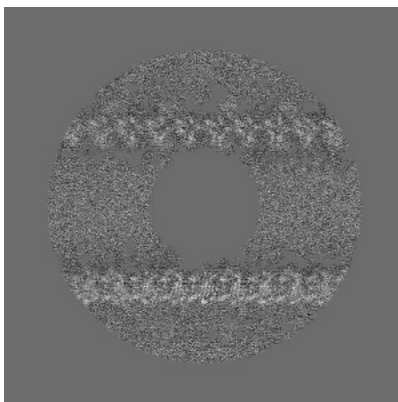


Z Index: 256

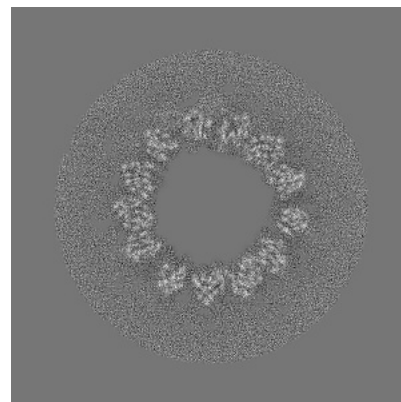
### 6.2.2 Raw map



X Index: 256



Y Index: 256

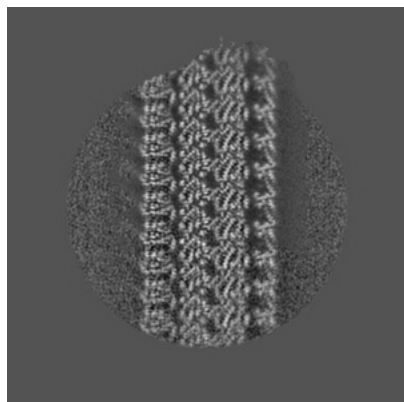


Z Index: 256

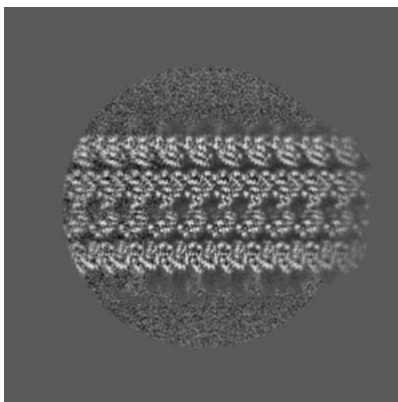
The images above show central slices of the map in three orthogonal directions.

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

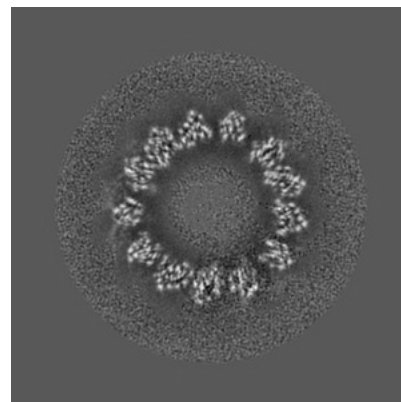
### 6.3.1 Primary map



X Index: 346

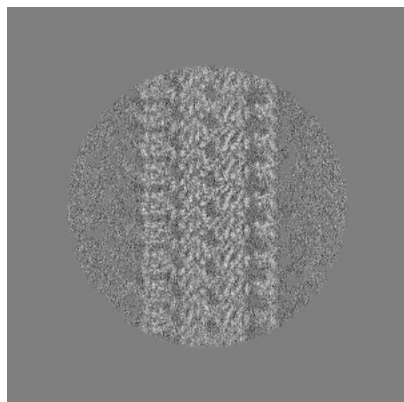


Y Index: 343

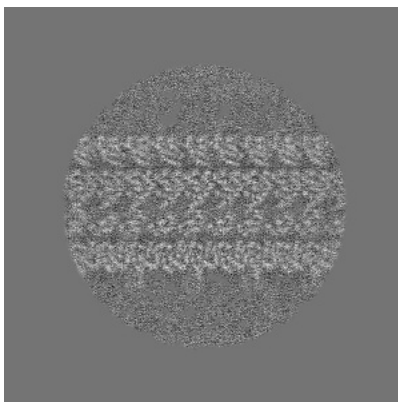


Z Index: 232

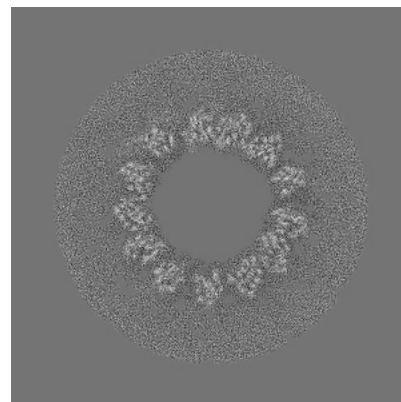
### 6.3.2 Raw map



X Index: 346



Y Index: 343

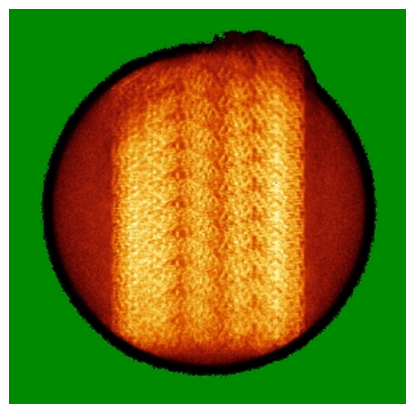


Z Index: 250

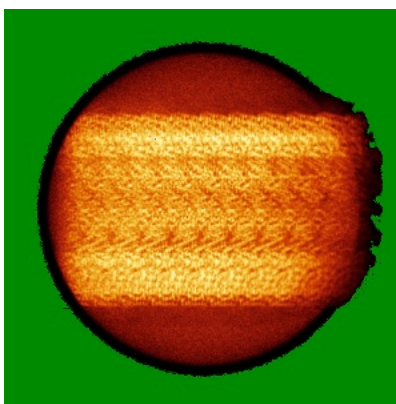
The images above show the largest variance slices of the map in three orthogonal directions.

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

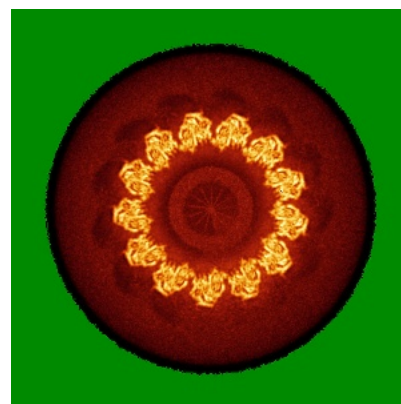
### 6.4.1 Primary map



X

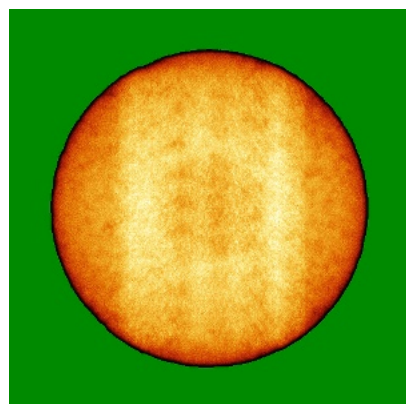


Y

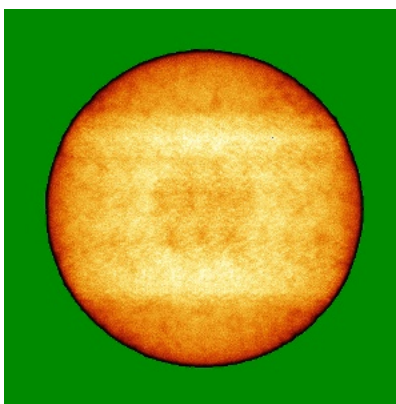


Z

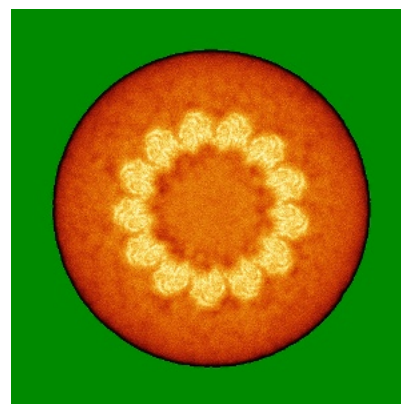
### 6.4.2 Raw map



X



Y



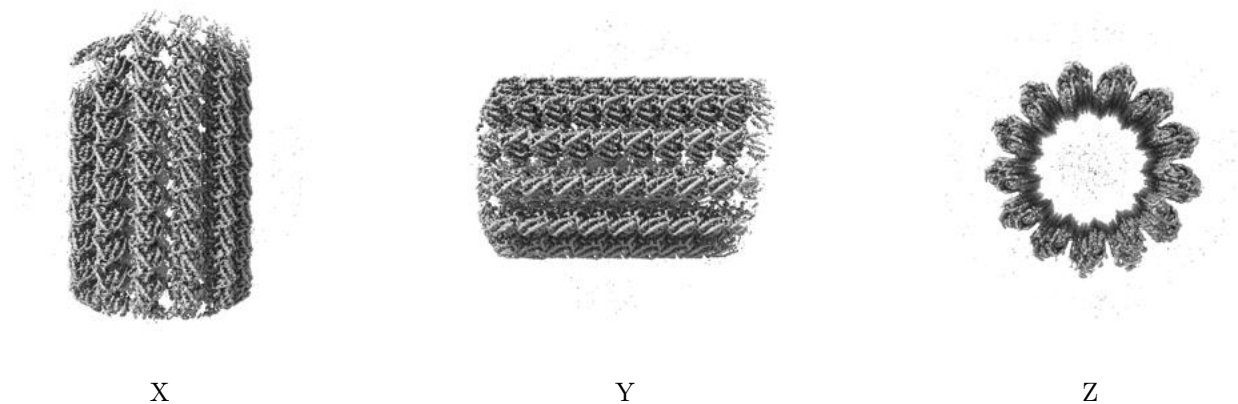
Z

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.



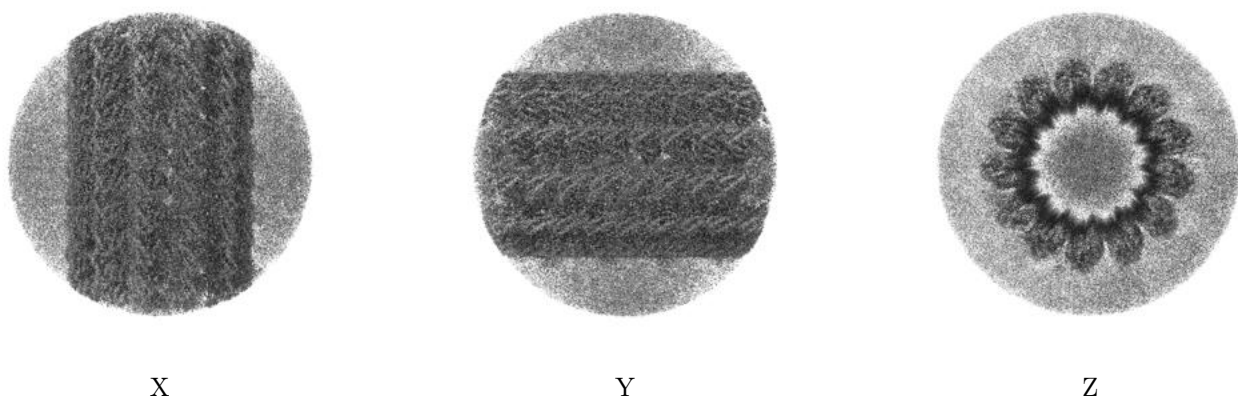
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

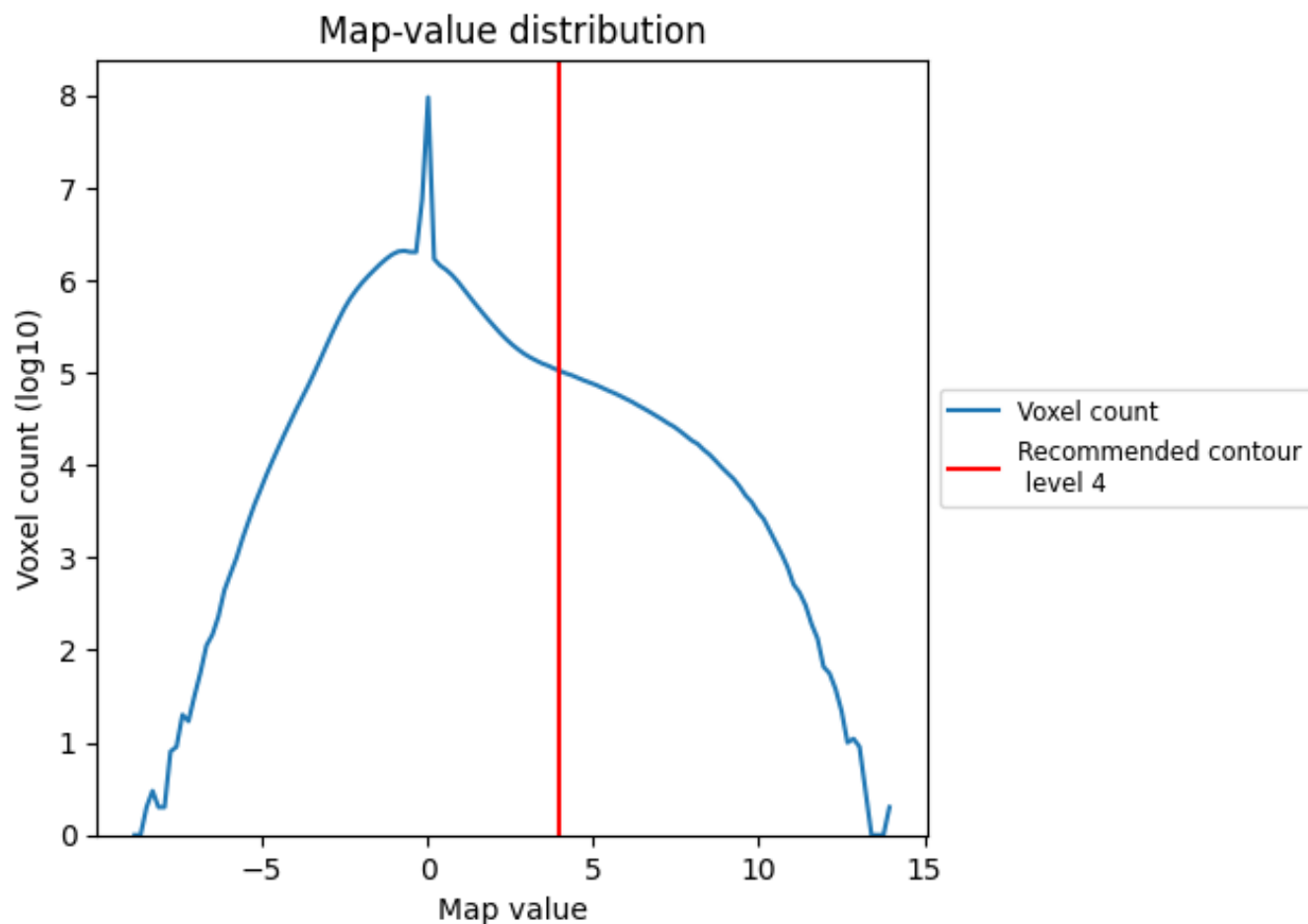
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

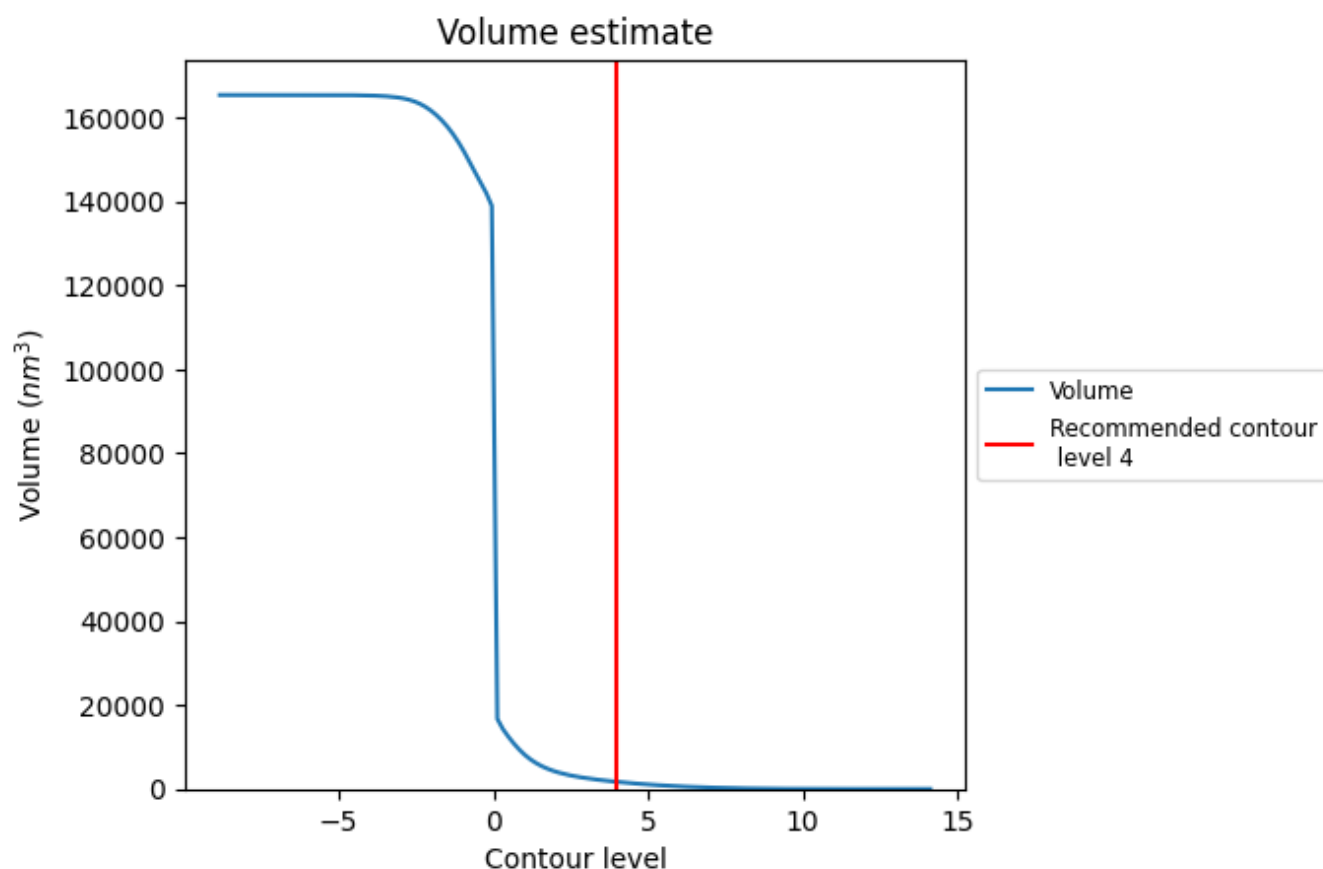
This section contains the results of statistical analysis of the map.

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



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

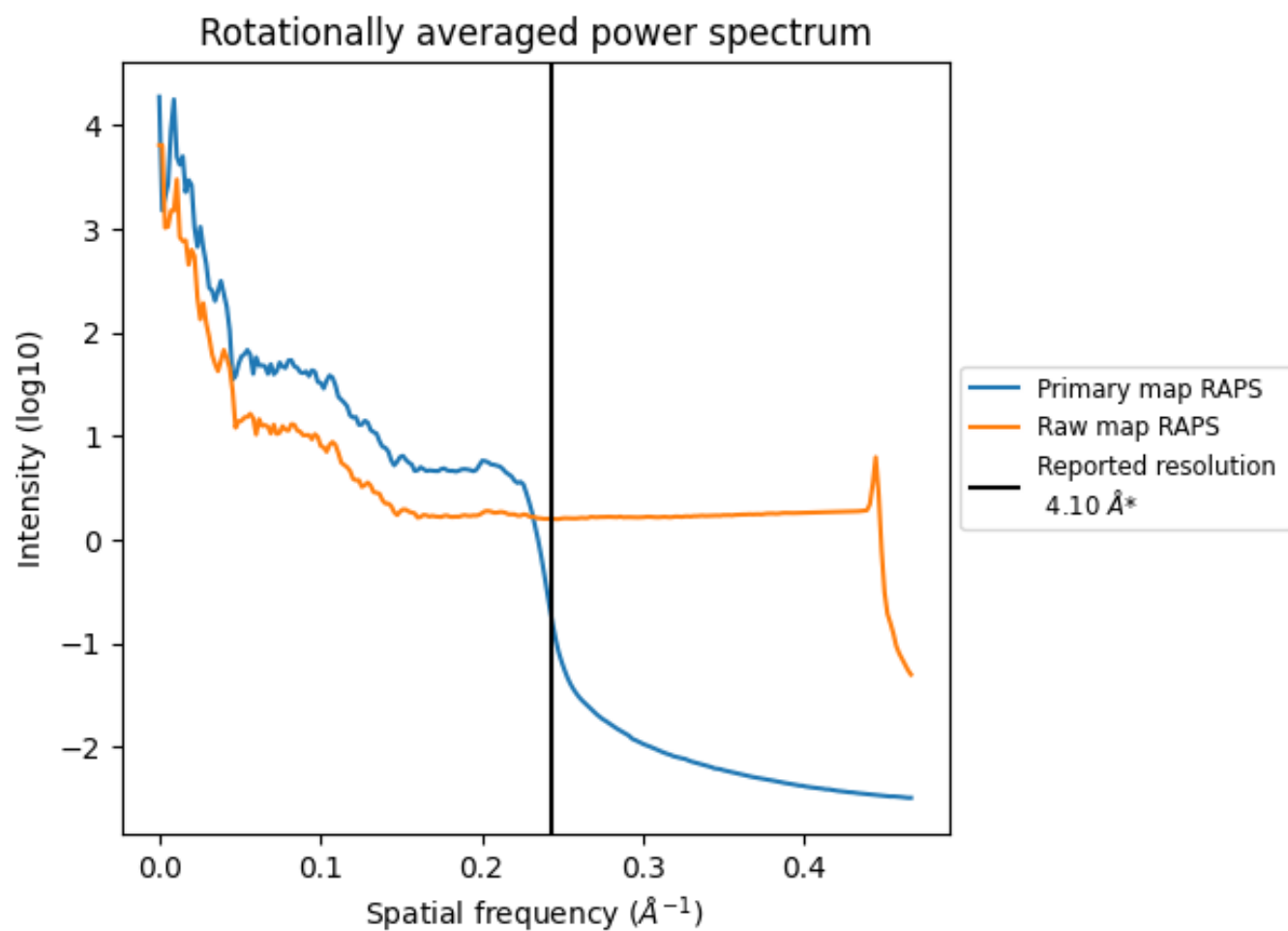
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1693 nm<sup>3</sup>; this corresponds to an approximate mass of 1529 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 ⓘ



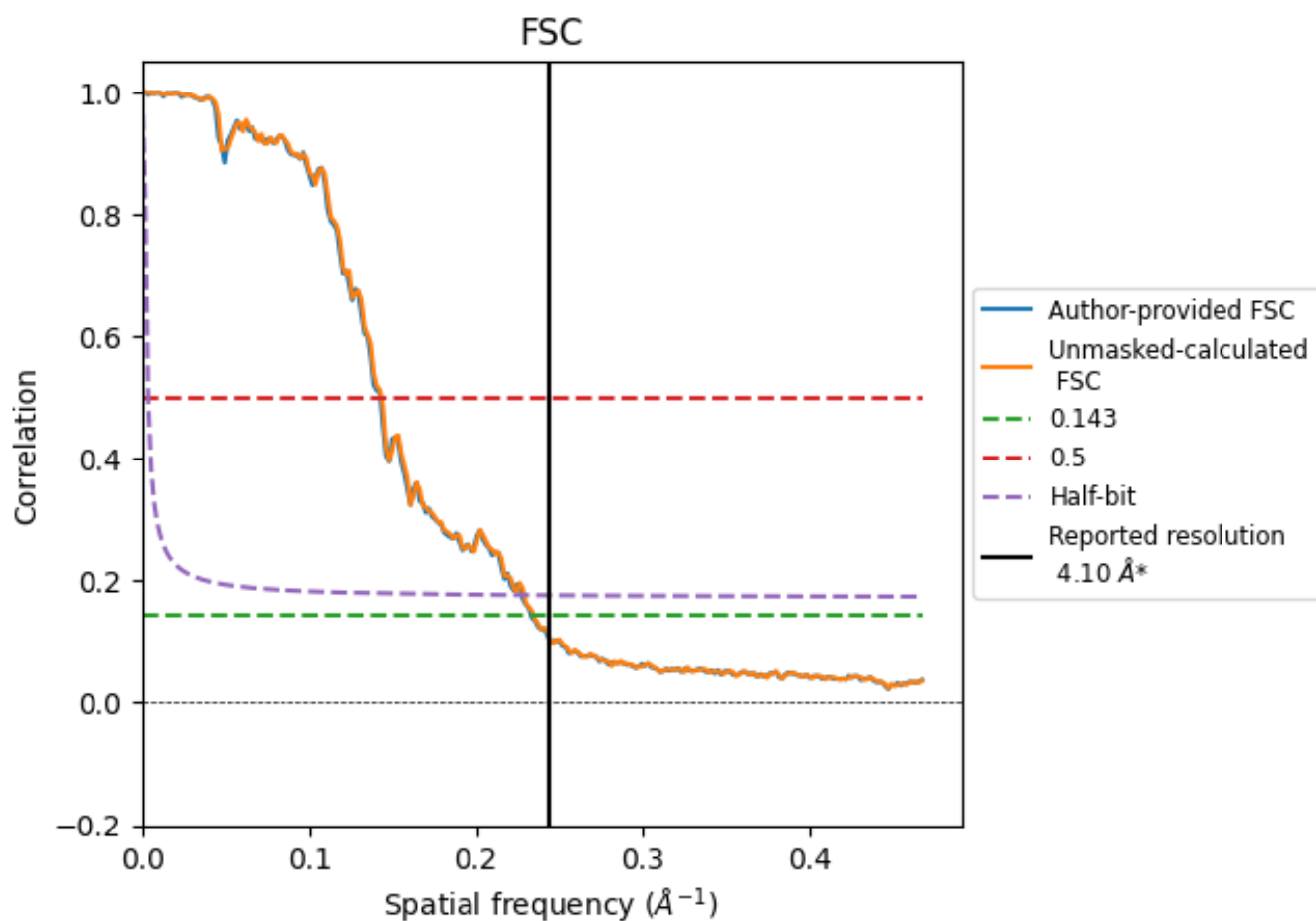
\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

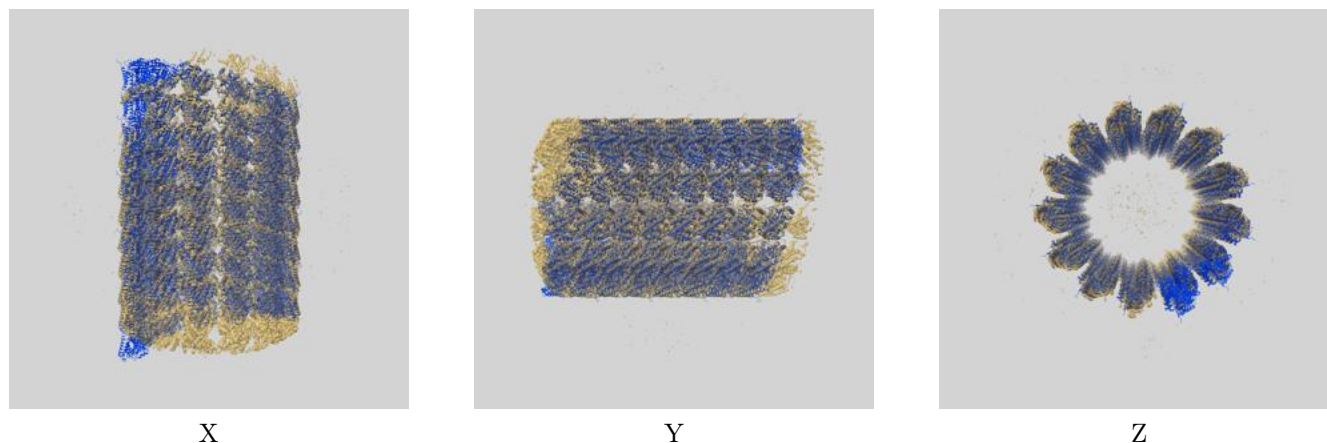
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.10                               | -    | -        |
| Author-provided FSC curve | 4.29                               | 7.01 | 4.39     |
| Unmasked-calculated*      | 4.26                               | 6.98 | 4.37     |

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

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

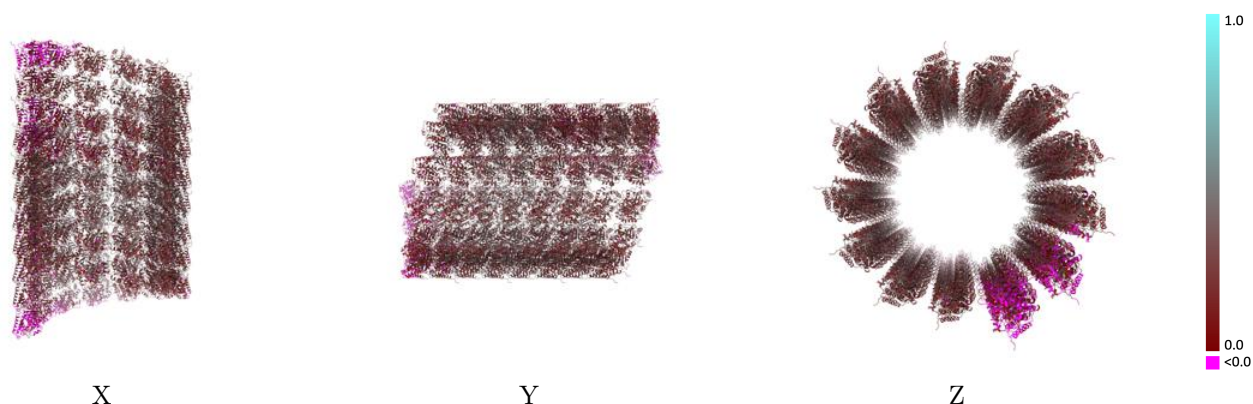
This section contains information regarding the fit between EMDB map EMD-0615 and PDB model 6O2T. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

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



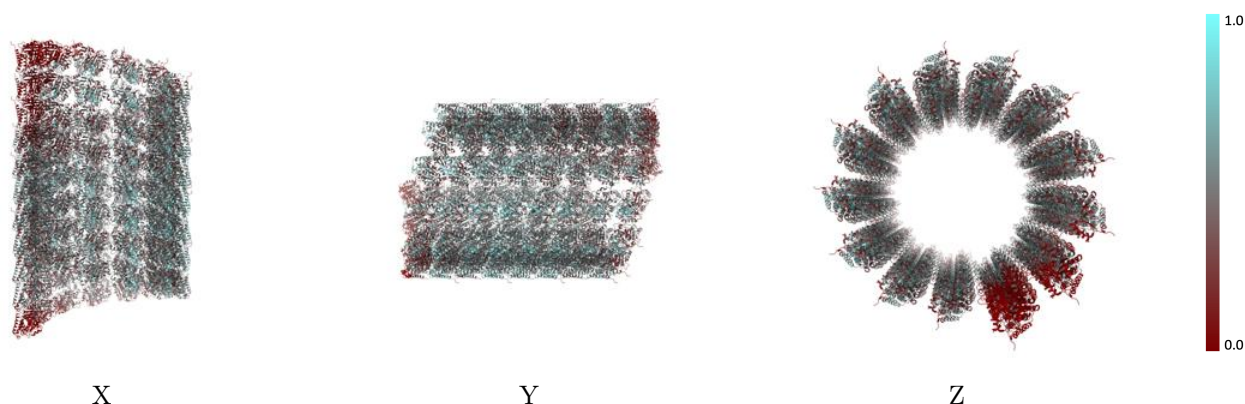
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



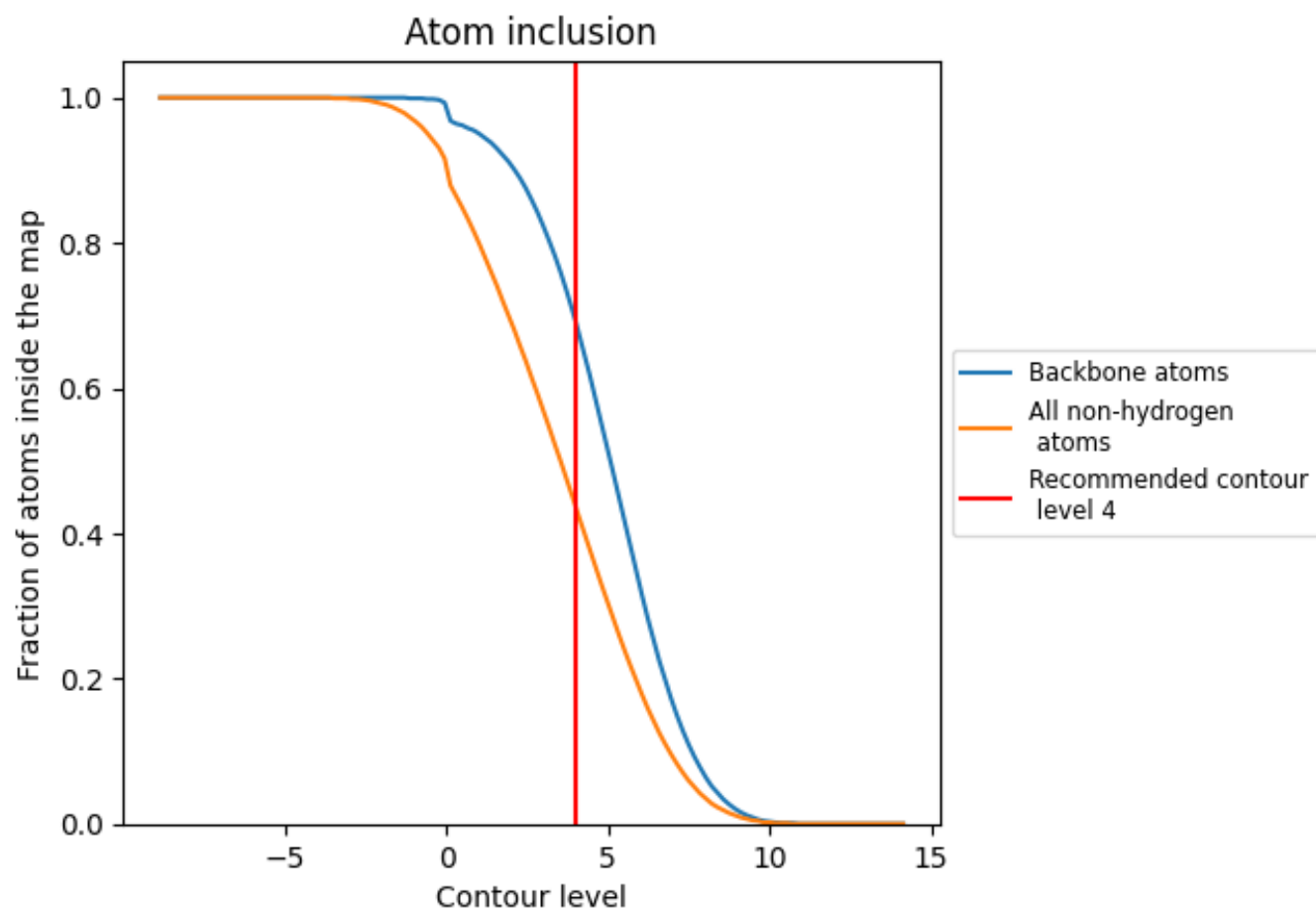
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 44% 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 (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4370   |  0.2520   |
| 1A    |  0.5330   |  0.3280   |
| 1B    |  0.5300   |  0.3240   |
| 1C    |  0.5270   |  0.3090   |
| 1D    |  0.5080   |  0.2960   |
| 1E    |  0.4940   |  0.2760   |
| 1F    |  0.4850   |  0.2680   |
| 1G    |  0.4730   |  0.2560   |
| 1H    |  0.5500   |  0.3230   |
| 1I    |  0.4500   |  0.2330   |
| 1J    |  0.4390   |  0.2160   |
| 1K    |  0.4240   |  0.2030   |
| 1L    |  0.3840   |  0.1670   |
| 1M    |  0.0980   |  0.0820   |
| 1N    |  0.5380  |  0.3080  |
| 1O    |  0.5400 |  0.3230 |
| 1P    |  0.5400 |  0.3190 |
| 1Q    |  0.5310 |  0.3080 |
| 1R    |  0.5030 |  0.2770 |
| 1S    |  0.4870 |  0.2560 |
| 1T    |  0.4600 |  0.2340 |
| 1U    |  0.4460 |  0.2200 |
| 1V    |  0.4340 |  0.2010 |
| 1W    |  0.4110 |  0.1800 |
| 1X    |  0.3930 |  0.1610 |
| 1Y    |  0.2960 |  0.0920 |
| 1Z    |  0.5450 |  0.2890 |
| 2A    |  0.5160 |  0.2910 |
| 2B    |  0.5270 |  0.3340 |
| 2C    |  0.5390 |  0.3360 |
| 2D    |  0.5220 |  0.3250 |
| 2E    |  0.5300 |  0.3340 |
| 2F    |  0.5240 |  0.3280 |
| 2G    |  0.5230 |  0.3270 |
| 2H    |  0.4840 |  0.2240 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 2I    |  0.5200   |  0.3190   |
| 2J    |  0.5090   |  0.3170   |
| 2K    |  0.5150   |  0.3160   |
| 2L    |  0.5150   |  0.3140   |
| 2M    |  0.4750   |  0.2600   |
| 2N    |  0.4560   |  0.2170   |
| 2O    |  0.5160   |  0.2870   |
| 2P    |  0.5230   |  0.3040   |
| 2Q    |  0.5020   |  0.2800   |
| 2R    |  0.5180   |  0.3030   |
| 2S    |  0.5200   |  0.3100   |
| 2T    |  0.5220   |  0.3180   |
| 2U    |  0.5220   |  0.3200   |
| 2V    |  0.5190   |  0.3170   |
| 2W    |  0.5000   |  0.2830   |
| 2X    |  0.5000   |  0.2970   |
| 2Y    |  0.4750   |  0.2530   |
| 2Z    |  0.4210  |  0.1820  |
| 3A    |  0.4260 |  0.2130 |
| 3B    |  0.4000 |  0.2530 |
| 3C    |  0.4380 |  0.2540 |
| 3D    |  0.4470 |  0.2550 |
| 3E    |  0.4760 |  0.2650 |
| 3F    |  0.4600 |  0.2550 |
| 3G    |  0.4720 |  0.2530 |
| 3H    |  0.1380 |  0.0620 |
| 3I    |  0.4590 |  0.2530 |
| 3J    |  0.4740 |  0.2550 |
| 3K    |  0.4650 |  0.2560 |
| 3L    |  0.4750 |  0.2600 |
| 3M    |  0.4580 |  0.2310 |
| 3N    |  0.3220 |  0.1580 |
| 3O    |  0.2000 |  0.1110 |
| 3P    |  0.2780 |  0.1480 |
| 3Q    |  0.3310 |  0.1770 |
| 3R    |  0.4000 |  0.2050 |
| 3S    |  0.4260 |  0.2250 |
| 3T    |  0.4380 |  0.2340 |
| 3U    |  0.4540 |  0.2530 |
| 3V    |  0.4780 |  0.2630 |
| 3W    |  0.4660 |  0.2660 |
| 3X    |  0.4490 |  0.2470 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 3Y    |  0.4310   |  0.2070   |
| 3Z    |  0.0640   |  0.0130   |
| 4A    |  0.3910   |  0.2670   |
| 4B    |  0.4050   |  0.2890   |
| 4C    |  0.4030   |  0.2790   |
| 4D    |  0.3890   |  0.2700   |
| 4E    |  0.3900   |  0.2670   |
| 4F    |  0.3920   |  0.2730   |
| 4G    |  0.3990   |  0.2810   |
| 4H    |  0.4720   |  0.2730   |
| 4I    |  0.3870   |  0.2670   |
| 4J    |  0.3750   |  0.2670   |
| 4K    |  0.3380   |  0.2440   |
| 4L    |  0.1220   |  0.0690   |
| 4M    |  0.0250   |  0.0010   |
| 4N    |  0.3510   |  0.2250   |
| 4O    |  0.4730   |  0.2770   |
| 4P    |  0.4680   |  0.2700   |
| 4Q    |  0.4620  |  0.2690  |
| 4R    |  0.4640 |  0.2760 |
| 4S    |  0.4660 |  0.2830 |
| 4T    |  0.4740 |  0.2930 |
| 4U    |  0.4740 |  0.2960 |
| 4V    |  0.4740 |  0.3020 |
| 4W    |  0.4680 |  0.2890 |
| 4X    |  0.3510 |  0.2370 |
| 4Y    |  0.0540 |  0.1630 |
| 4Z    |  0.4550 |  0.2530 |