



Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 09:26 PM EDT

PDB ID : 9NW3 / pdb_00009nw3
EMDB ID : EMD-49872
Title : Ciliary tip central pair
Authors : Legal, T.L.; Bui, K.H.
Deposited on : 2025-03-21
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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>.

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

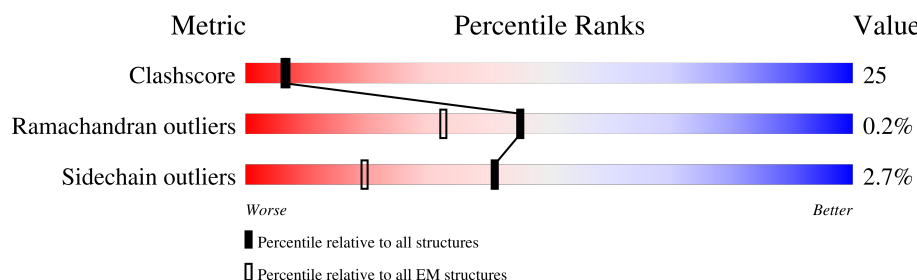
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 ≥ 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 | AA | 449 | <div> <div>21%</div> <div>73%</div> <div>23%</div> <div>.</div> </div> |
| 1 | AC | 449 | <div> <div>22%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 1 | AE | 449 | <div> <div>25%</div> <div>70%</div> <div>26%</div> <div>.</div> </div> |
| 1 | BA | 449 | <div> <div>15%</div> <div>72%</div> <div>24%</div> <div>.</div> </div> |
| 1 | BC | 449 | <div> <div>13%</div> <div>69%</div> <div>26%</div> <div>.</div> </div> |
| 1 | BE | 449 | <div> <div>13%</div> <div>69%</div> <div>26%</div> <div>.</div> </div> |
| 1 | CA | 449 | <div> <div>10%</div> <div>72%</div> <div>24%</div> <div>.</div> </div> |
| 1 | CC | 449 | <div> <div>8%</div> <div>69%</div> <div>26%</div> <div>.</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | CE | 449 | <div> <div>9%</div> <div>70%</div> <div>26%</div> <div>.</div> </div> |
| 1 | DA | 449 | <div> <div>18%</div> <div>70%</div> <div>25%</div> <div>.</div> </div> |
| 1 | DC | 449 | <div> <div>16%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 1 | DE | 449 | <div> <div>11%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 1 | EA | 449 | <div> <div>33%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 1 | EC | 449 | <div> <div>29%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 1 | EE | 449 | <div> <div>26%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |
| 1 | FA | 449 | <div> <div>46%</div> <div>68%</div> <div>27%</div> <div>.</div> </div> |
| 1 | FC | 449 | <div> <div>42%</div> <div>67%</div> <div>29%</div> <div>.</div> </div> |
| 1 | FE | 449 | <div> <div>39%</div> <div>67%</div> <div>28%</div> <div>.</div> </div> |
| 1 | GA | 449 | <div> <div>49%</div> <div>73%</div> <div>22%</div> <div>.</div> </div> |
| 1 | GC | 449 | <div> <div>49%</div> <div>70%</div> <div>25%</div> <div>.</div> </div> |
| 1 | GE | 449 | <div> <div>51%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 1 | HA | 449 | <div> <div>49%</div> <div>71%</div> <div>24%</div> <div>.</div> </div> |
| 1 | HC | 449 | <div> <div>47%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |
| 1 | HE | 449 | <div> <div>49%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |
| 1 | IA | 449 | <div> <div>49%</div> <div>71%</div> <div>24%</div> <div>.</div> </div> |
| 1 | IC | 449 | <div> <div>47%</div> <div>68%</div> <div>27%</div> <div>.</div> </div> |
| 1 | IE | 449 | <div> <div>49%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 1 | JA | 449 | <div> <div>50%</div> <div>73%</div> <div>23%</div> <div>.</div> </div> |
| 1 | JC | 449 | <div> <div>52%</div> <div>70%</div> <div>26%</div> <div>.</div> </div> |
| 1 | JE | 449 | <div> <div>55%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 1 | KA | 449 | <div> <div>56%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 1 | KC | 449 | <div> <div>56%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |
| 1 | KE | 449 | <div> <div>57%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | LA | 449 | |
| 1 | LC | 449 | |
| 1 | LE | 449 | |
| 1 | MA | 449 | |
| 1 | MC | 449 | |
| 1 | ME | 449 | |
| 2 | AB | 443 | |
| 2 | AD | 443 | |
| 2 | AF | 443 | |
| 2 | BB | 443 | |
| 2 | BD | 443 | |
| 2 | BF | 443 | |
| 2 | CB | 443 | |
| 2 | CD | 443 | |
| 2 | CF | 443 | |
| 2 | DB | 443 | |
| 2 | DD | 443 | |
| 2 | DF | 443 | |
| 2 | EB | 443 | |
| 2 | ED | 443 | |
| 2 | EF | 443 | |
| 2 | FB | 443 | |
| 2 | FD | 443 | |
| 2 | FF | 443 | |
| 2 | GB | 443 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | GD | 443 | <div> <div>50%</div> <div>68%</div> <div>28%</div> <div>.</div> </div> |
| 2 | GF | 443 | <div> <div>51%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 2 | HB | 443 | <div> <div>48%</div> <div>70%</div> <div>26%</div> <div>.</div> </div> |
| 2 | HD | 443 | <div> <div>49%</div> <div>70%</div> <div>27%</div> <div>.</div> </div> |
| 2 | HF | 443 | <div> <div>52%</div> <div>72%</div> <div>24%</div> <div>.</div> </div> |
| 2 | IB | 443 | <div> <div>50%</div> <div>69%</div> <div>27%</div> <div>.</div> </div> |
| 2 | ID | 443 | <div> <div>50%</div> <div>70%</div> <div>27%</div> <div>.</div> </div> |
| 2 | IF | 443 | <div> <div>49%</div> <div>72%</div> <div>24%</div> <div>.</div> </div> |
| 2 | JB | 443 | <div> <div>53%</div> <div>70%</div> <div>27%</div> <div>.</div> </div> |
| 2 | JD | 443 | <div> <div>55%</div> <div>70%</div> <div>26%</div> <div>.</div> </div> |
| 2 | JF | 443 | <div> <div>61%</div> <div>73%</div> <div>24%</div> <div>.</div> </div> |
| 2 | KB | 443 | <div> <div>54%</div> <div>65%</div> <div>32%</div> <div>.</div> </div> |
| 2 | KD | 443 | <div> <div>53%</div> <div>66%</div> <div>31%</div> <div>.</div> </div> |
| 2 | KF | 443 | <div> <div>51%</div> <div>68%</div> <div>28%</div> <div>..</div> </div> |
| 2 | LB | 443 | <div> <div>45%</div> <div>64%</div> <div>33%</div> <div>.</div> </div> |
| 2 | LD | 443 | <div> <div>43%</div> <div>65%</div> <div>32%</div> <div>.</div> </div> |
| 2 | LF | 443 | <div> <div>42%</div> <div>66%</div> <div>30%</div> <div>.</div> </div> |
| 2 | MB | 443 | <div> <div>37%</div> <div>68%</div> <div>29%</div> <div>.</div> </div> |
| 2 | MD | 443 | <div> <div>35%</div> <div>69%</div> <div>28%</div> <div>.</div> </div> |
| 2 | MF | 443 | <div> <div>35%</div> <div>71%</div> <div>25%</div> <div>.</div> </div> |
| 3 | 1A | 213 | <div> <div>45%</div> <div>60%</div> <div>6%</div> <div>34%</div> </div> |
| 3 | 1B | 213 | <div> <div>44%</div> <div>61%</div> <div>5%</div> <div>34%</div> </div> |
| 3 | 1C | 213 | <div> <div>44%</div> <div>61%</div> <div>5%</div> <div>34%</div> </div> |
| 4 | 2A | 742 | <div> <div>14%</div> <div>17%</div> <div>6%</div> <div>74%</div> </div> |
| 4 | 2B | 742 | <div> <div>13%</div> <div>17%</div> <div>7%</div> <div>74%</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | 2C | 742 | |
| 5 | 3A | 495 | |
| 5 | 3B | 495 | |
| 5 | 3C | 495 | |
| 6 | 4A | 317 | |
| 6 | 4B | 317 | |
| 6 | 4C | 317 | |
| 6 | 4D | 317 | |
| 7 | 5A | 1754 | |
| 7 | 5B | 1754 | |
| 7 | 5C | 1754 | |
| 8 | 6A | 346 | |
| 8 | 6B | 346 | |
| 8 | 6C | 346 | |
| 9 | 7A | 101 | |
| 9 | 7B | 101 | |
| 9 | 7C | 101 | |
| 9 | 7D | 101 | |
| 9 | 7E | 101 | |
| 9 | 7F | 101 | |
| 10 | 8A | 38 | |
| 10 | 8B | 38 | |
| 10 | 8C | 38 | |
| 10 | 8D | 38 | |
| 10 | 8E | 38 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 10 | 8F | 38 | <div> <div>26%</div> <div>82%</div> <div>18%</div> </div> |
| 10 | 8G | 38 | <div> <div>39%</div> <div>79%</div> <div>21%</div> </div> |
| 10 | 8H | 38 | <div> <div>37%</div> <div>79%</div> <div>21%</div> </div> |
| 10 | 8I | 38 | <div> <div>29%</div> <div>82%</div> <div>18%</div> </div> |
| 10 | 8J | 38 | <div> <div>26%</div> <div>76%</div> <div>24%</div> </div> |
| 10 | 8K | 38 | <div> <div>37%</div> <div>76%</div> <div>24%</div> </div> |
| 10 | 8L | 38 | <div> <div>34%</div> <div>79%</div> <div>21%</div> </div> |
| 10 | 8M | 38 | <div> <div>34%</div> <div>79%</div> <div>21%</div> </div> |
| 10 | 8N | 38 | <div> <div>29%</div> <div>79%</div> <div>21%</div> </div> |
| 10 | 8O | 38 | <div> <div>34%</div> <div>82%</div> <div>18%</div> </div> |
| 10 | 8P | 38 | <div> <div>32%</div> <div>76%</div> <div>24%</div> </div> |
| 10 | 8Q | 38 | <div> <div>24%</div> <div>82%</div> <div>18%</div> </div> |
| 10 | 8R | 38 | <div> <div>26%</div> <div>82%</div> <div>18%</div> </div> |
| 10 | 8S | 38 | <div> <div>58%</div> <div>71%</div> <div>29%</div> </div> |
| 10 | 8T | 38 | <div> <div>53%</div> <div>71%</div> <div>29%</div> </div> |
| 10 | 8U | 38 | <div> <div>47%</div> <div>71%</div> <div>29%</div> </div> |
| 10 | 8V | 38 | <div> <div>63%</div> <div>68%</div> <div>32%</div> </div> |
| 10 | 8W | 38 | <div> <div>68%</div> <div>74%</div> <div>26%</div> </div> |
| 10 | 8X | 38 | <div> <div>71%</div> <div>76%</div> <div>24%</div> </div> |
| 10 | 8Y | 38 | <div> <div>84%</div> <div>74%</div> <div>26%</div> </div> |
| 10 | 8Z | 38 | <div> <div>63%</div> <div>76%</div> <div>24%</div> </div> |
| 10 | 9A | 38 | <div> <div>58%</div> <div>76%</div> <div>24%</div> </div> |

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 318666 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 chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | AA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | AC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | AE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | BA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | BC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | BE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | CA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | CC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | CE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | DA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | DC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | DE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | EA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | EC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | EE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | FA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |
| 1 | FC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1 | FE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | GA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | GC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | GE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | HA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | HC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | HE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | IA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | IC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | IE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | JA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | JC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | JE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | KA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | KC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | KE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | LA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | LC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | LE | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | MA | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |
| 1 | MC | 430 | Total 3350 | C 2122 | N 569 | O 637 | S 22 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | ME | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3350 | 2122 | 569 | 637 | 22 | | |

- Molecule 2 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | AB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | AD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | AF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | BB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | BD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | BF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | CB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | CD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | CF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | DB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | DD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | DF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | EB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | ED | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | EF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | FB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | FD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | FF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | GB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | GD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | GF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | HB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | HD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | HF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | IB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | ID | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | IF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | JB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | JD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | JF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | KB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | KD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | KF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | LB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | LD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | LF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | MB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | MD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |
| 2 | MF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3366 | 2115 | 577 | 646 | 28 | | |

- Molecule 3 is a protein called Sperm flagellar protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 1A | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 717 | 200 | 215 | 9 | | |
| 3 | 1B | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 717 | 200 | 215 | 9 | | |
| 3 | 1C | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1141 | 717 | 200 | 215 | 9 | | |

- Molecule 4 is a protein called TLP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | 2A | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1615 | 1046 | 279 | 283 | 7 | | |
| 4 | 2B | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1615 | 1046 | 279 | 283 | 7 | | |
| 4 | 2C | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1615 | 1046 | 279 | 283 | 7 | | |

- Molecule 5 is a protein called C2 domain protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | 3A | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2752 | 1754 | 470 | 518 | 10 | | |
| 5 | 3B | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2752 | 1754 | 470 | 518 | 10 | | |
| 5 | 3C | 335 | Total | C | N | O | S | 0 | 0 |
| | | | 2752 | 1754 | 470 | 518 | 10 | | |

- Molecule 6 is a protein called CFAP213.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | 4A | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 981 | 298 | 303 | 5 | | |
| 6 | 4B | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 981 | 298 | 303 | 5 | | |
| 6 | 4C | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 981 | 298 | 303 | 5 | | |
| 6 | 4D | 189 | Total | C | N | O | S | 0 | 0 |
| | | | 1587 | 981 | 298 | 303 | 5 | | |

- Molecule 7 is a protein called TLP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 7 | 5A | 705 | Total | C | N | O | S | 0 | 0 |
| | | | 5953 | 3778 | 1021 | 1141 | 13 | | |
| 7 | 5B | 705 | Total | C | N | O | S | 0 | 0 |
| | | | 5953 | 3778 | 1021 | 1141 | 13 | | |
| 7 | 5C | 705 | Total | C | N | O | S | 0 | 0 |
| | | | 5953 | 3778 | 1021 | 1141 | 13 | | |

- Molecule 8 is a protein called Cation channel family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | 6A | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2077 | 1352 | 338 | 380 | 7 | | |
| 8 | 6B | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2077 | 1352 | 338 | 380 | 7 | | |
| 8 | 6C | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2077 | 1352 | 338 | 380 | 7 | | |

- Molecule 9 is a protein called Dpy-30 motif protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9 | 7A | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |
| 9 | 7B | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |
| 9 | 7C | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |
| 9 | 7D | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |
| 9 | 7E | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |
| 9 | 7F | 46 | Total | C | N | O | 0 | 0 |
| | | | 383 | 247 | 66 | 70 | | |

- Molecule 10 is a protein called Unknown.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | 8A | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8B | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8C | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |

Continued on next page...

Continued from previous page...

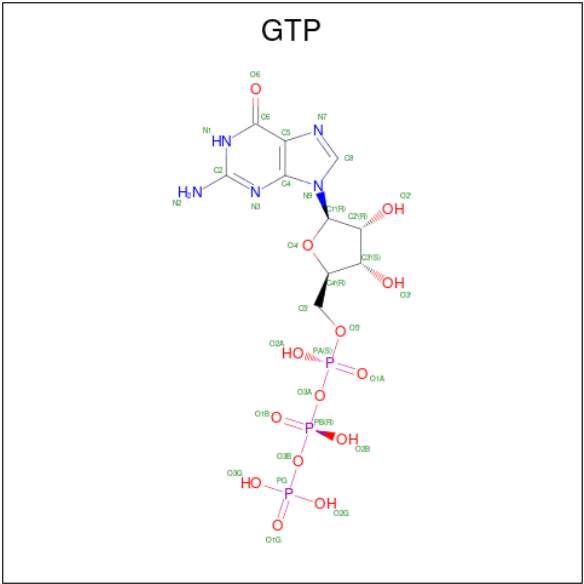
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | 8D | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8E | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8F | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8G | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8H | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8I | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8J | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8K | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8L | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8M | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8N | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8O | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8P | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8Q | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8R | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8S | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8T | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8U | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8V | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8W | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8X | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10 | 8Y | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 8Z | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |
| 10 | 9A | 38 | Total | C | N | O | 0 | 0 |
| | | | 189 | 114 | 38 | 37 | | |

- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 11 | CE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | DA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | DC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | DE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | EA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | EC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | EE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | FA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | FC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | FE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | GA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | GC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | GE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | HA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | HC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | HE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | IA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | IC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | IE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | JA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 11 | JC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 11 | JE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | KA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | KC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | KE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | LA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | LC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | LE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | MA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | MC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 11 | ME | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 12 | AA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | AC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | AE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | BA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | BC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | BE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | CA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | CC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | CE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

Continued on next page...

Continued from previous page...

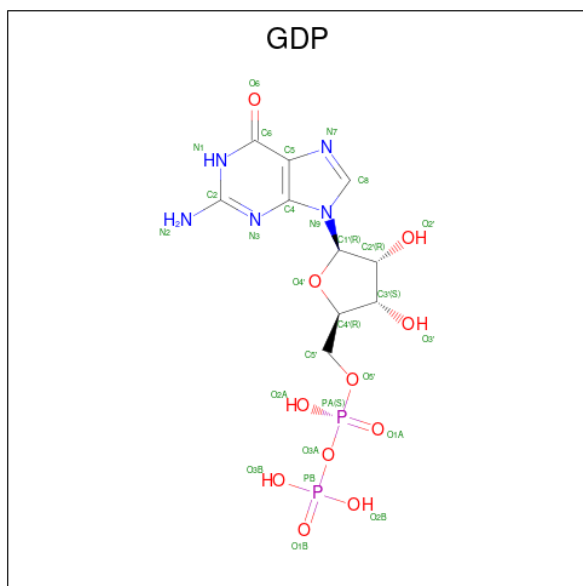
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 12 | DA | 1 | Total 1 | Mg 1 | 0 |
| 12 | DC | 1 | Total 1 | Mg 1 | 0 |
| 12 | DE | 1 | Total 1 | Mg 1 | 0 |
| 12 | EA | 1 | Total 1 | Mg 1 | 0 |
| 12 | ED | 1 | Total 1 | Mg 1 | 0 |
| 12 | EE | 1 | Total 1 | Mg 1 | 0 |
| 12 | FB | 1 | Total 1 | Mg 1 | 0 |
| 12 | FD | 1 | Total 1 | Mg 1 | 0 |
| 12 | FE | 1 | Total 1 | Mg 1 | 0 |
| 12 | GA | 1 | Total 1 | Mg 1 | 0 |
| 12 | GC | 1 | Total 1 | Mg 1 | 0 |
| 12 | GE | 1 | Total 1 | Mg 1 | 0 |
| 12 | HA | 1 | Total 1 | Mg 1 | 0 |
| 12 | HC | 1 | Total 1 | Mg 1 | 0 |
| 12 | HE | 1 | Total 1 | Mg 1 | 0 |
| 12 | IA | 1 | Total 1 | Mg 1 | 0 |
| 12 | IC | 1 | Total 1 | Mg 1 | 0 |
| 12 | IE | 1 | Total 1 | Mg 1 | 0 |
| 12 | JA | 1 | Total 1 | Mg 1 | 0 |
| 12 | JC | 1 | Total 1 | Mg 1 | 0 |
| 12 | JE | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 12 | KA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | KC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | KE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | LA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | LC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | LE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | MB | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | MD | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 12 | MF | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 13 | AF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | BB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | BD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | BF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | CB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | CD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | CF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | DB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | DD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | DF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | EB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | ED | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | EF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | FB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | FD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | FF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | GB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | GD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | GF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | HB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 13 | HD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |

Continued on next page...

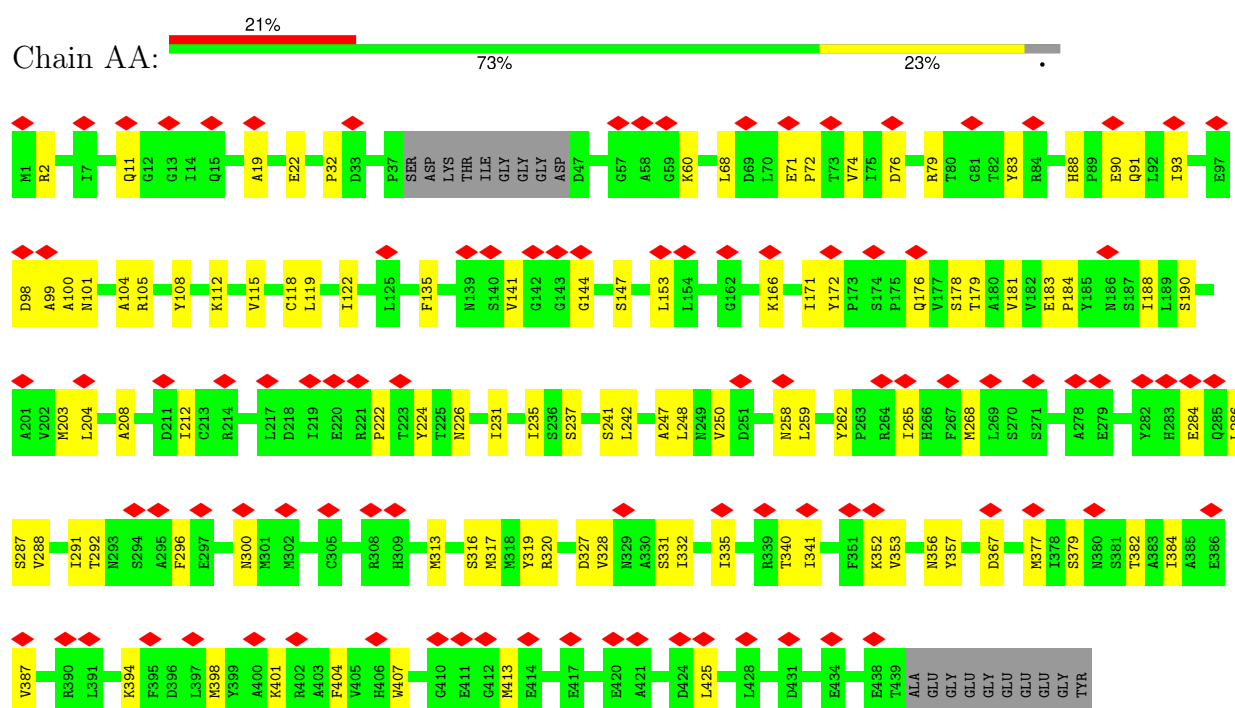
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 13 | HF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | IB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | ID | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | IF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | JB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | JD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | JF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | KB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | KD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | KF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | LB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | LD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | LF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | MB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | MD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 13 | MF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

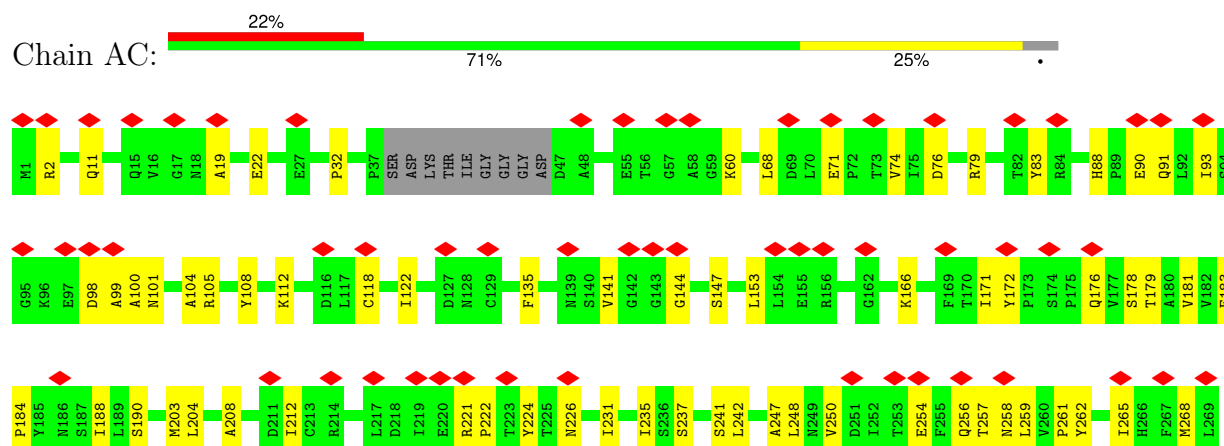
3 Residue-property plots [i](#)

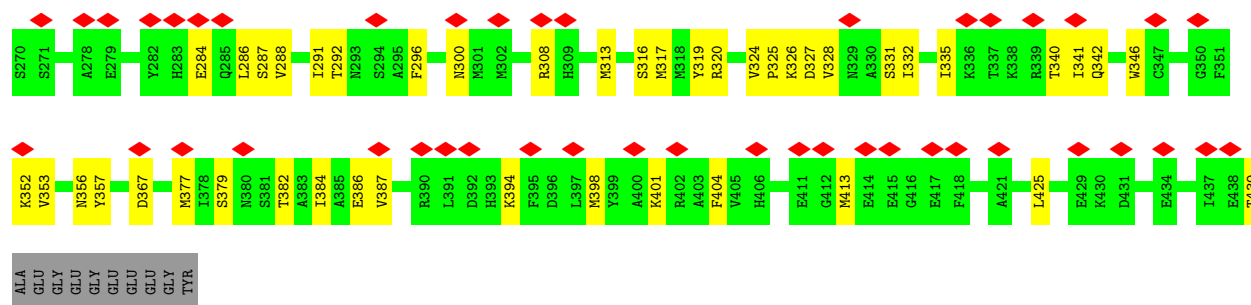
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain

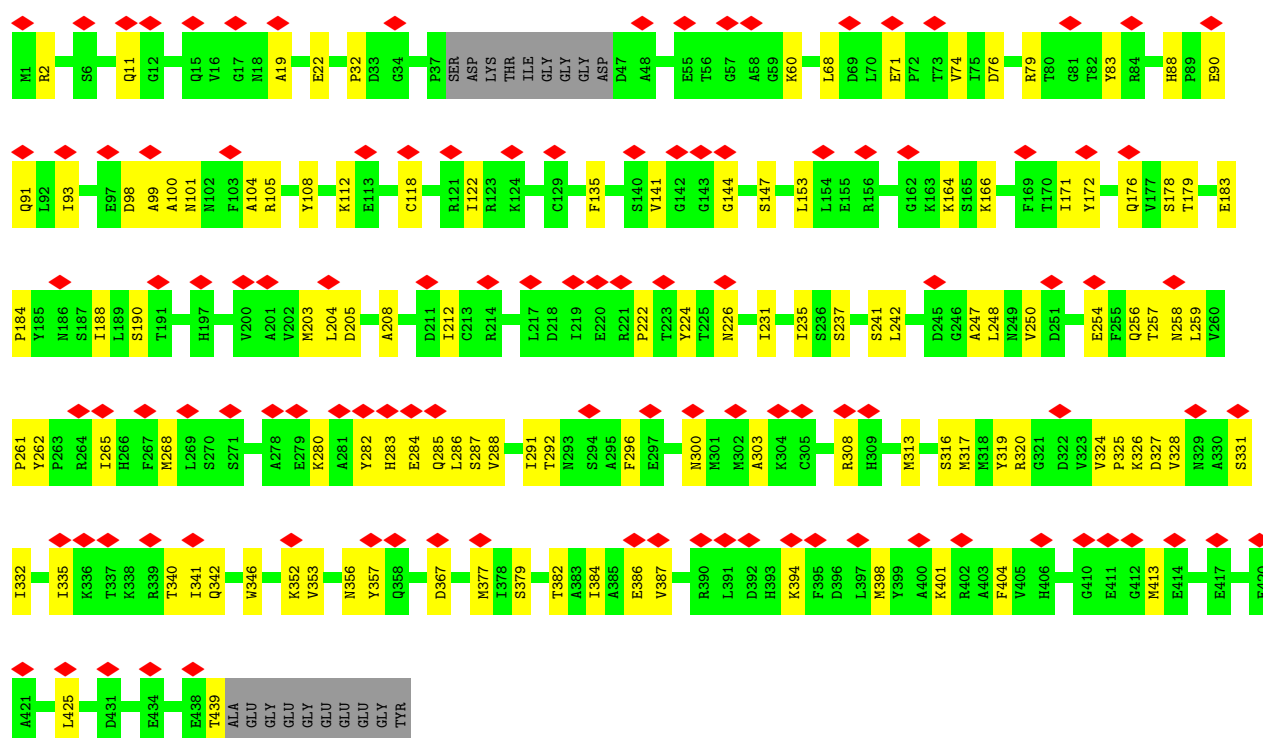


• Molecule 1: Tubulin alpha chain

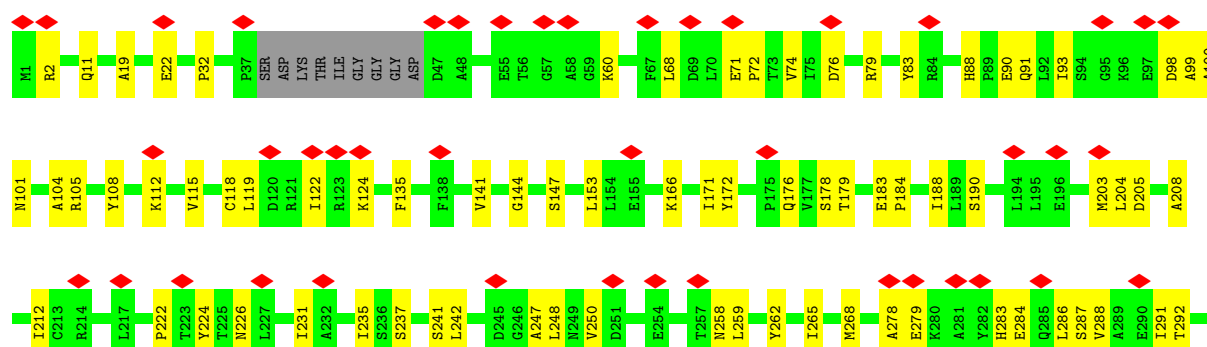
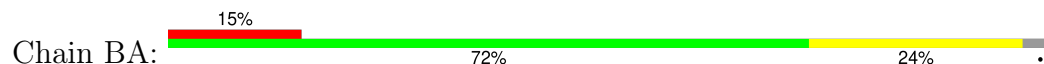


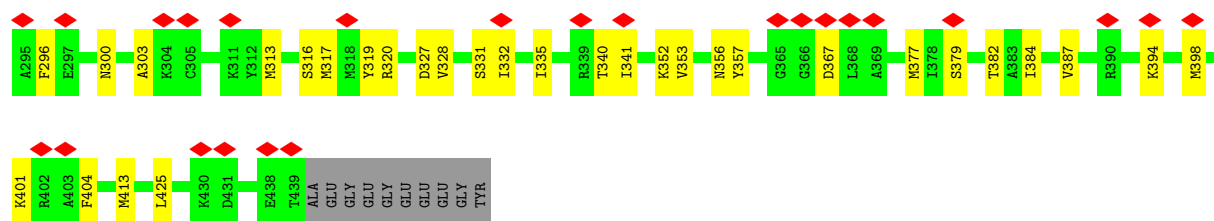


• Molecule 1: Tubulin alpha chain

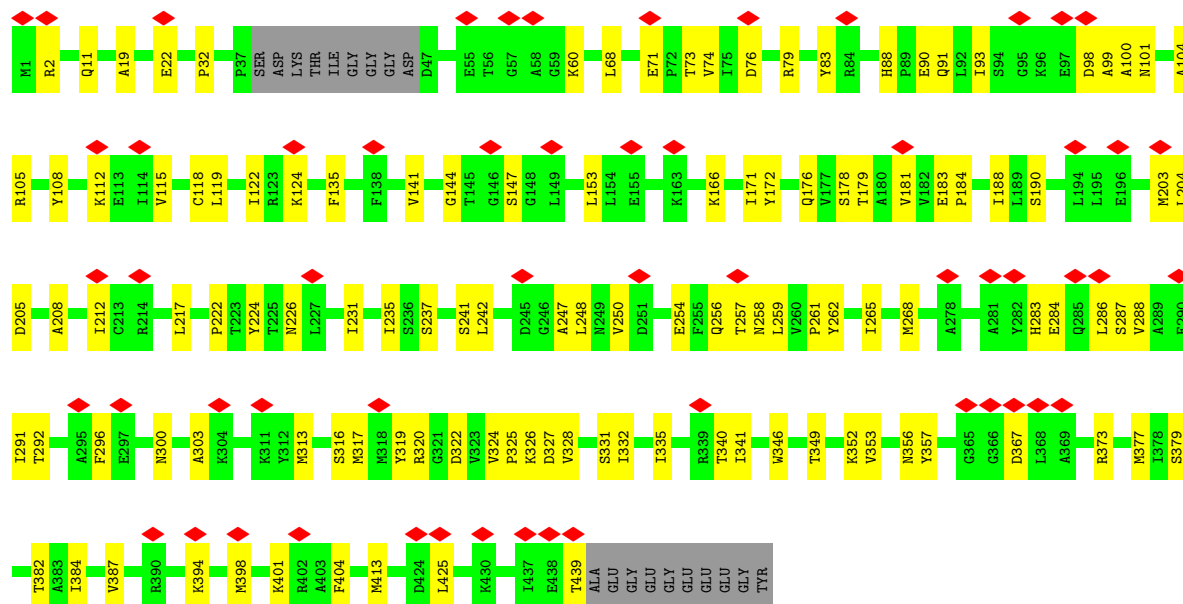


• Molecule 1: Tubulin alpha chain

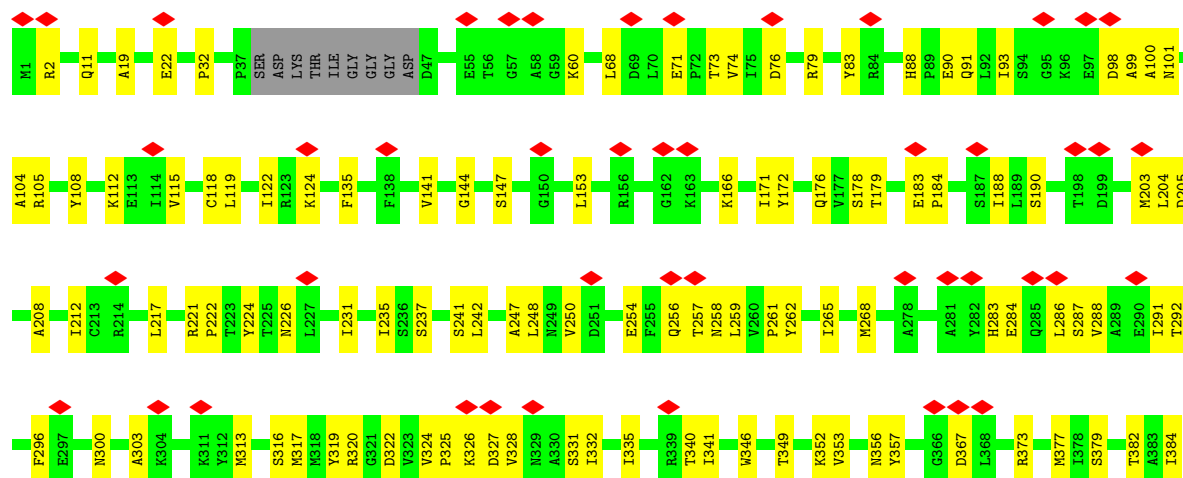


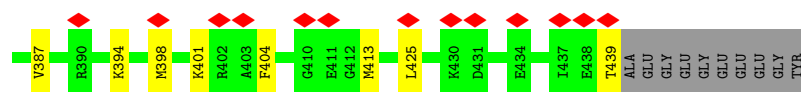


• Molecule 1: Tubulin alpha chain

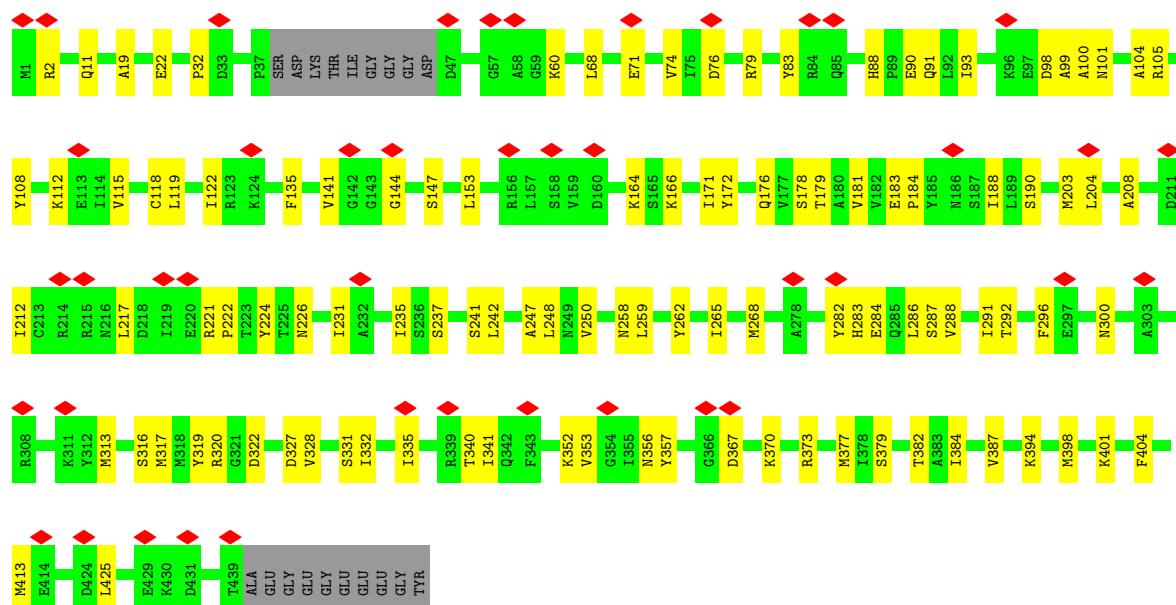
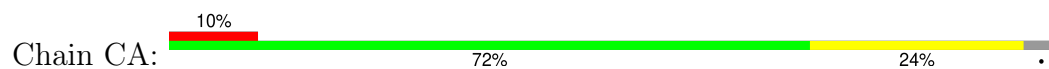


• Molecule 1: Tubulin alpha chain

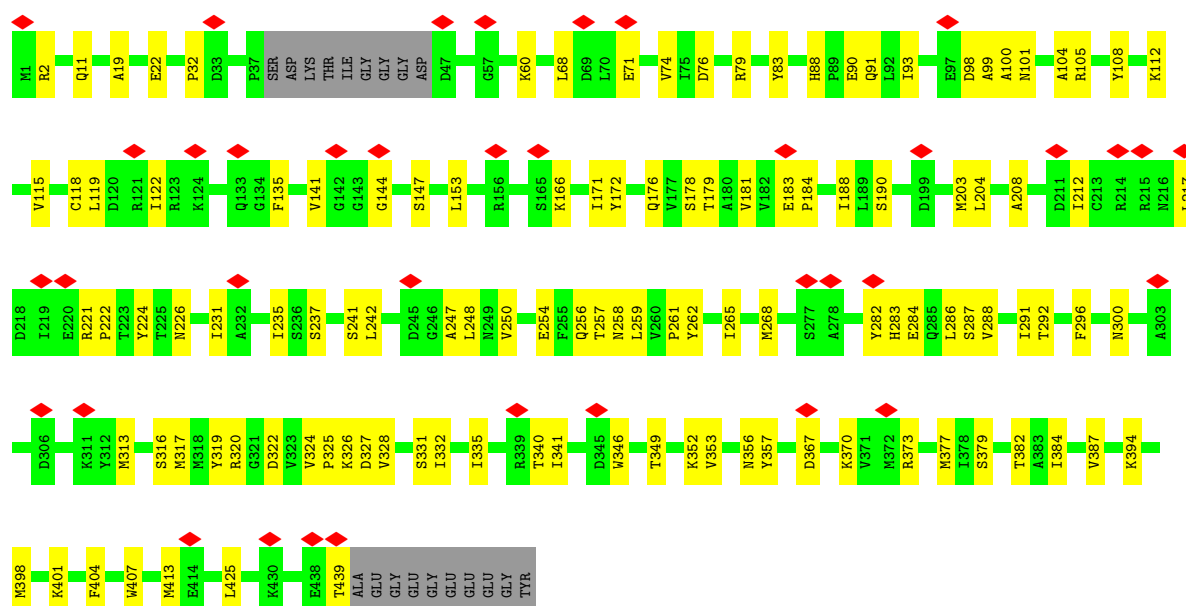




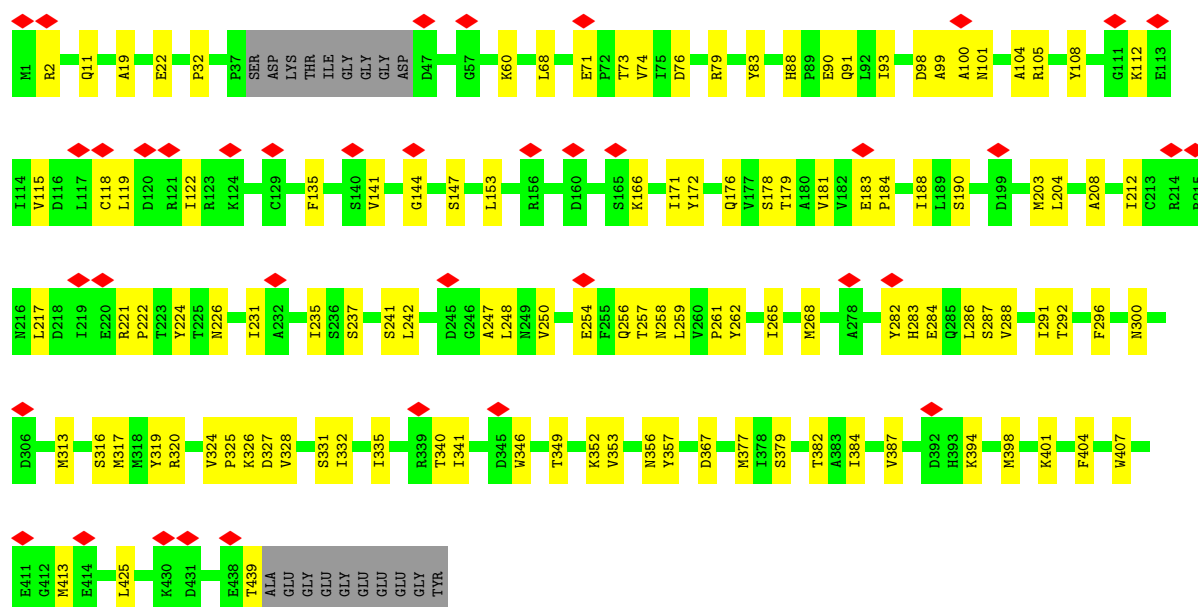
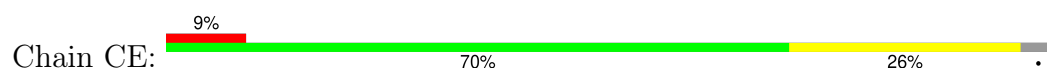
• Molecule 1: Tubulin alpha chain



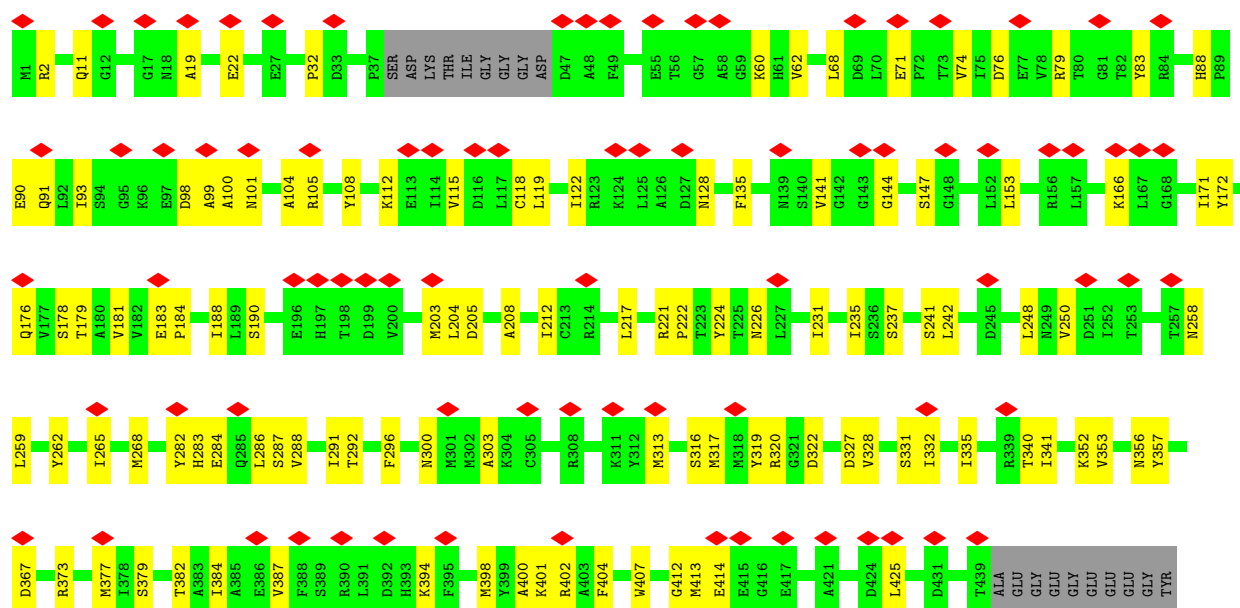
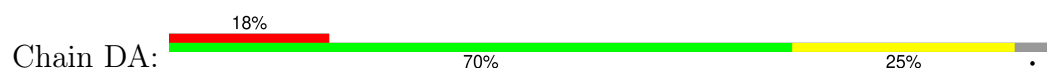
• Molecule 1: Tubulin alpha chain



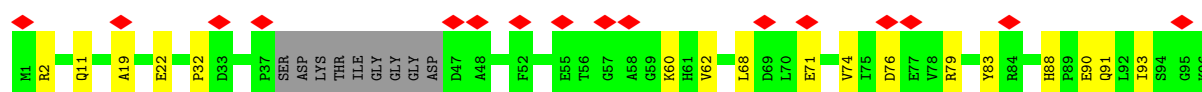
• Molecule 1: Tubulin alpha chain

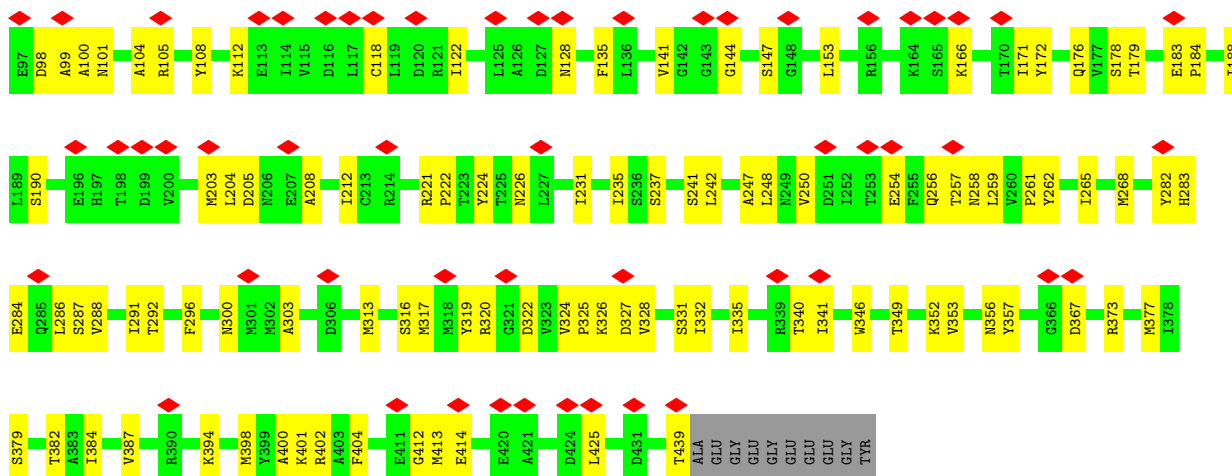


• Molecule 1: Tubulin alpha chain

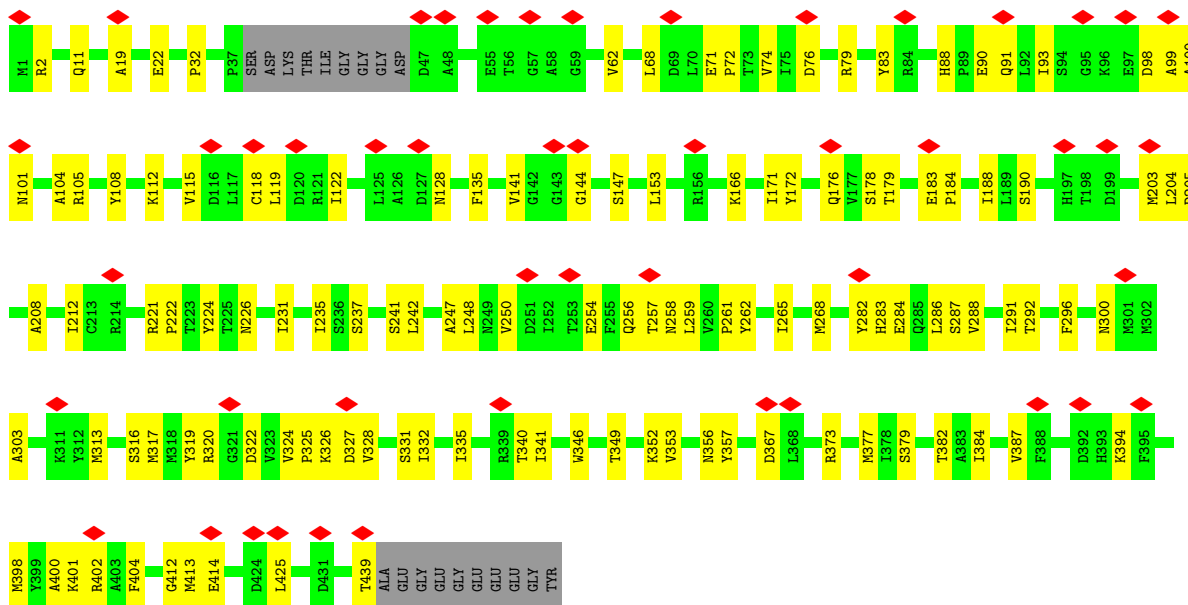


• Molecule 1: Tubulin alpha chain

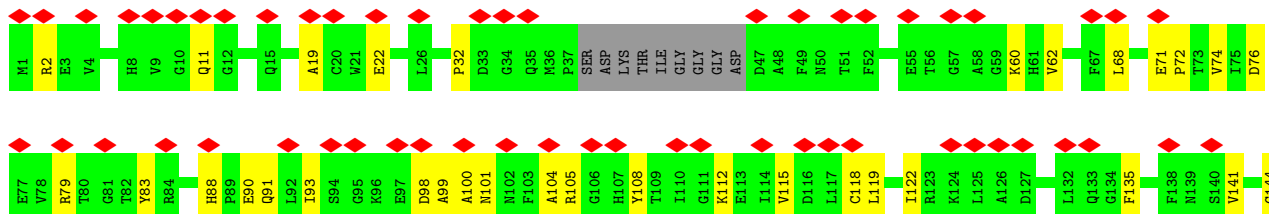
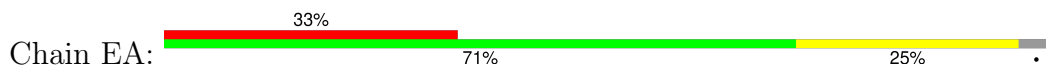


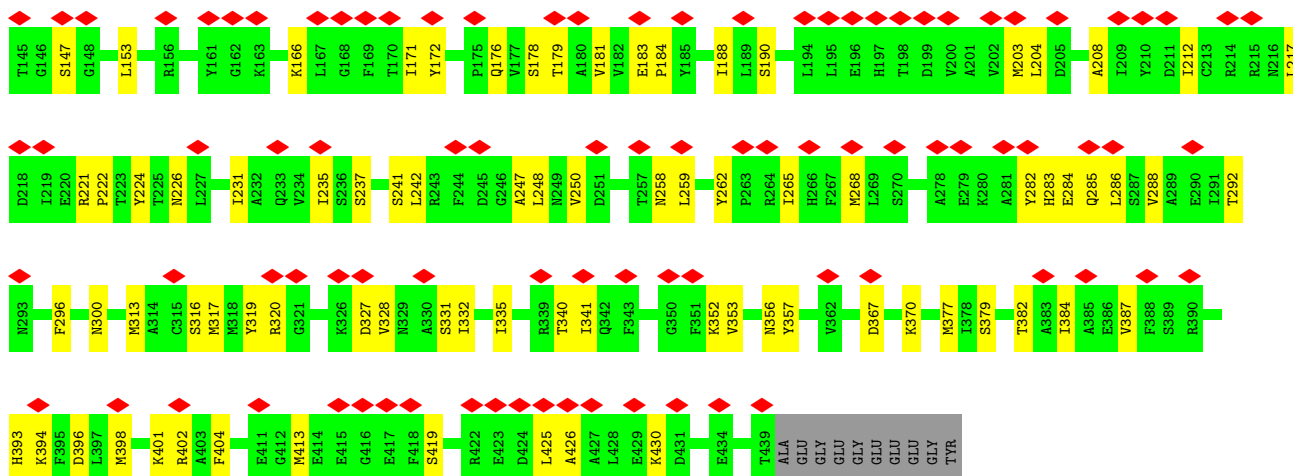


• Molecule 1: Tubulin alpha chain

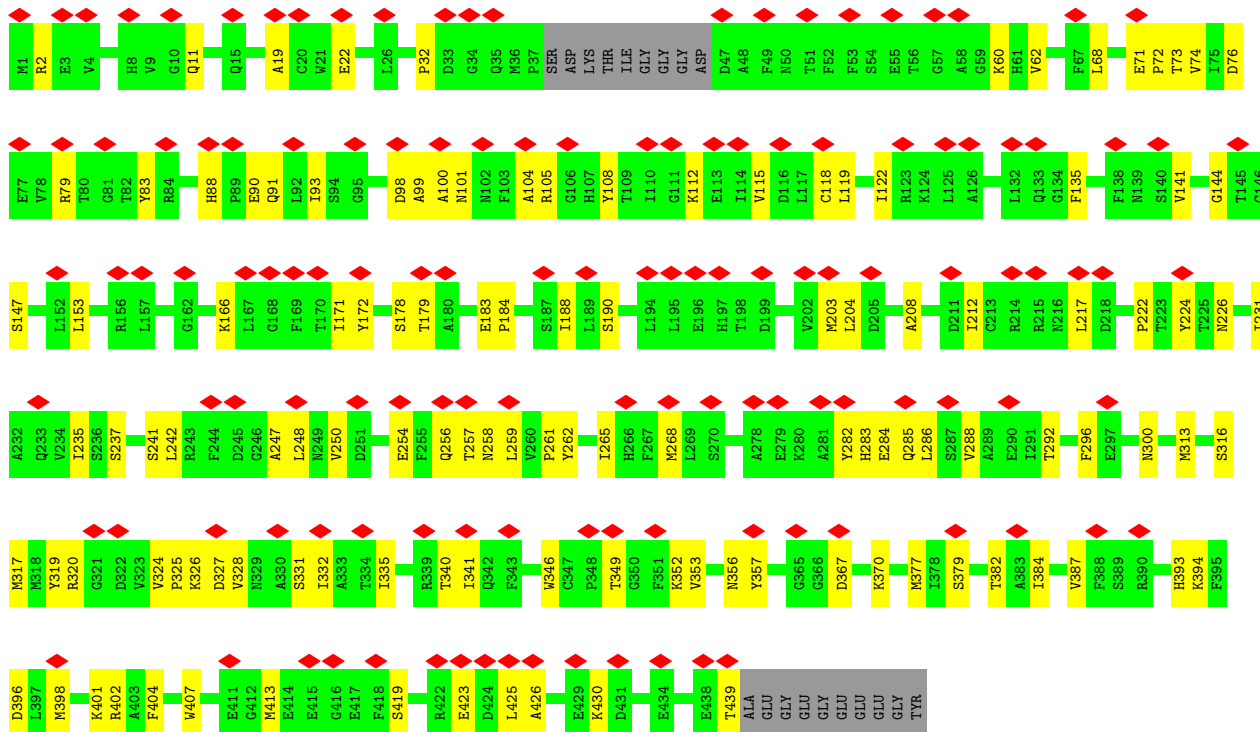


• Molecule 1: Tubulin alpha chain

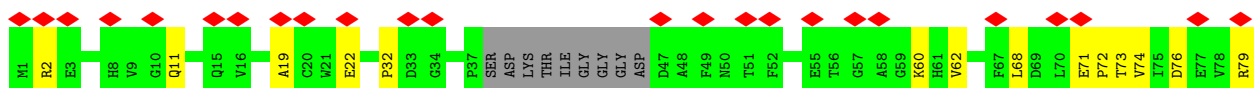


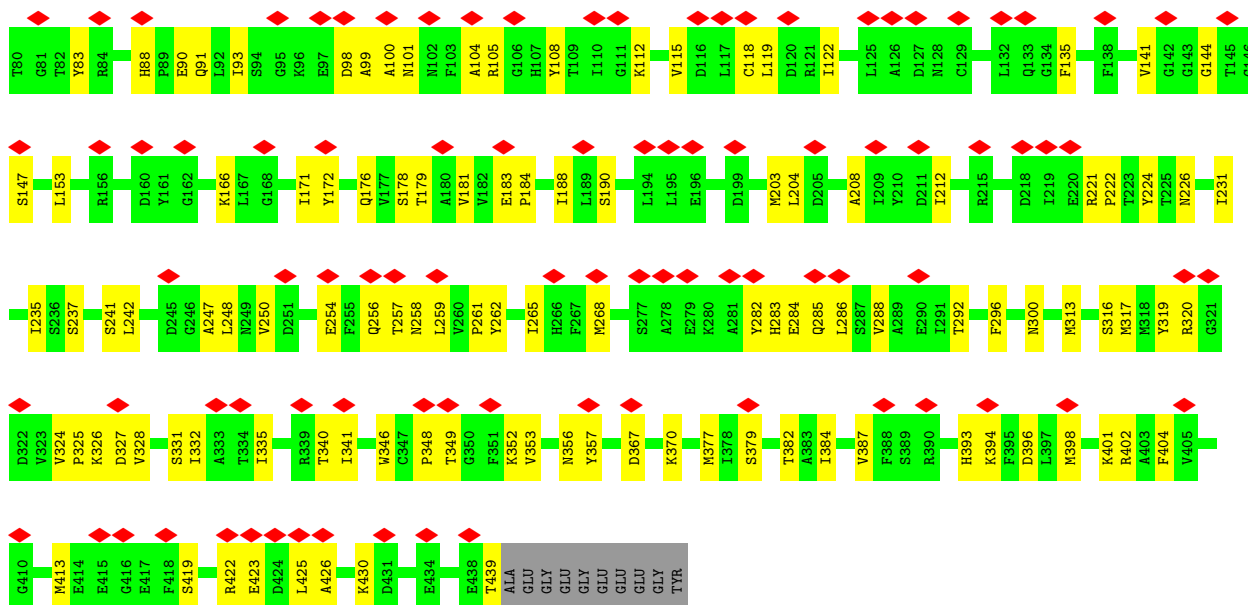


• Molecule 1: Tubulin alpha chain

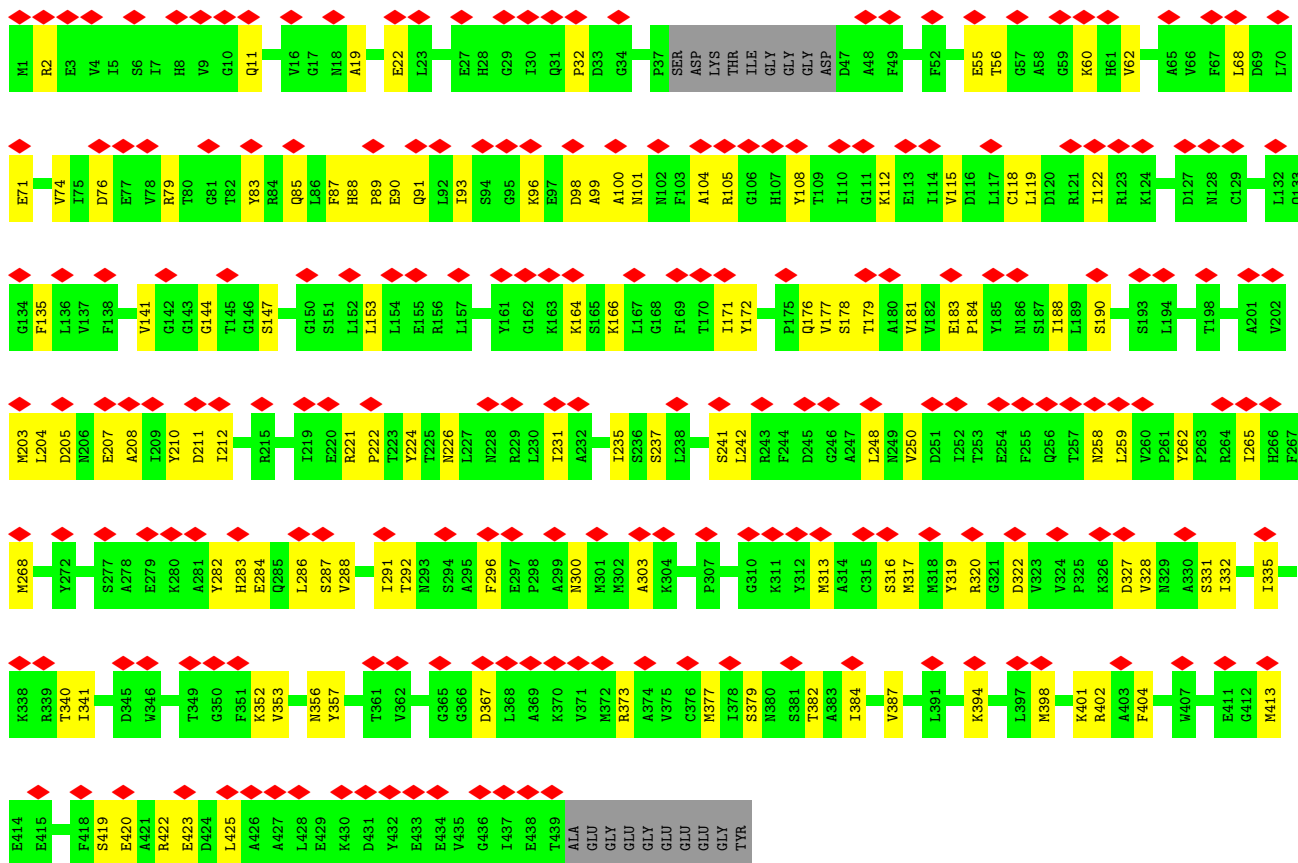


• Molecule 1: Tubulin alpha chain

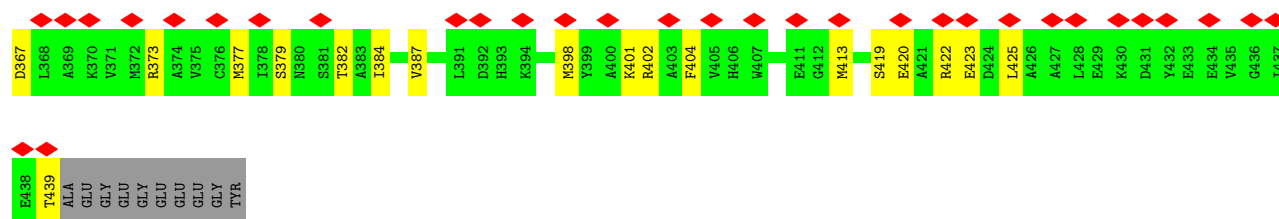




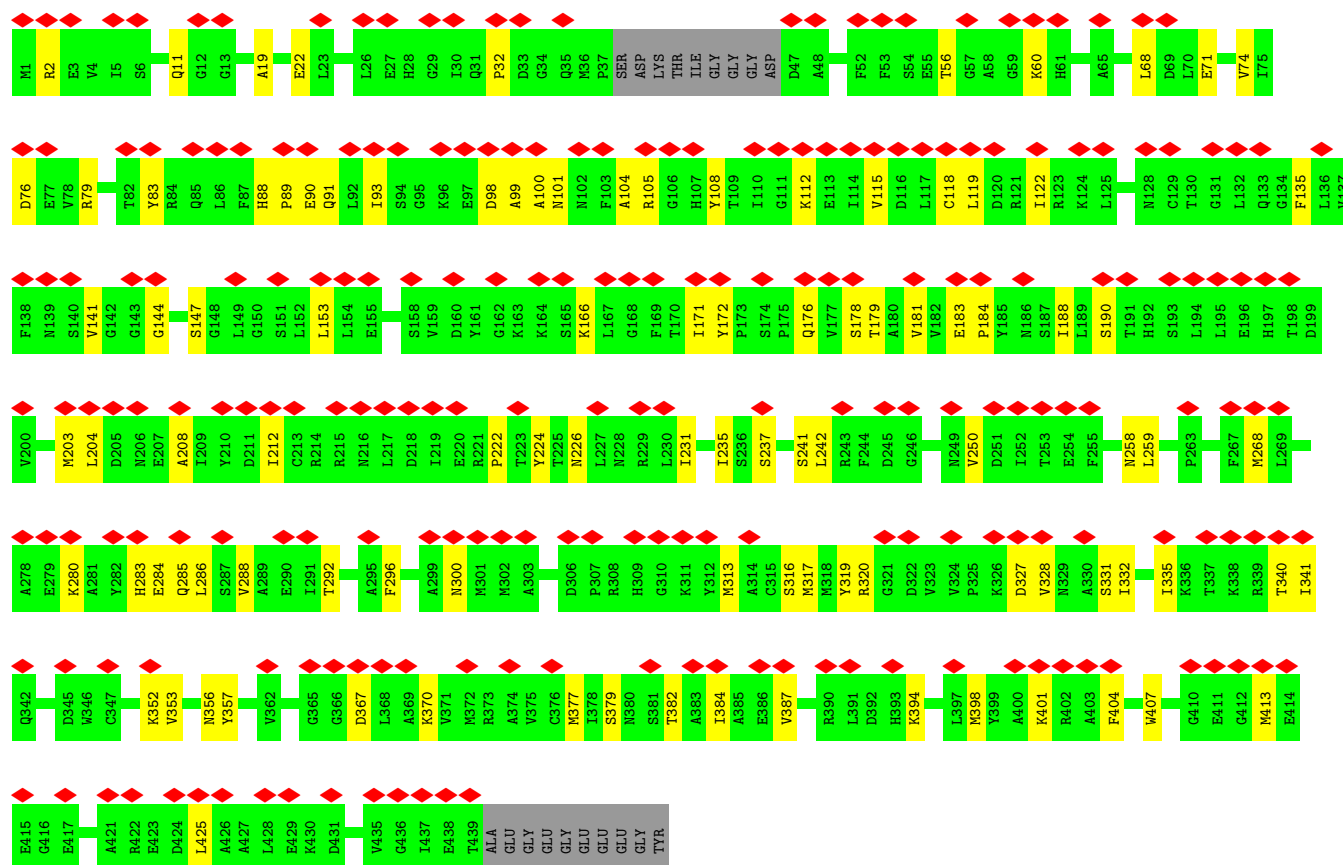
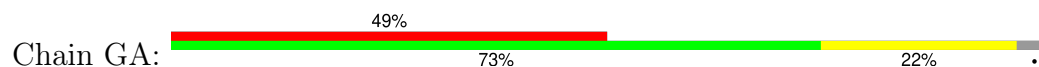
• Molecule 1: Tubulin alpha chain



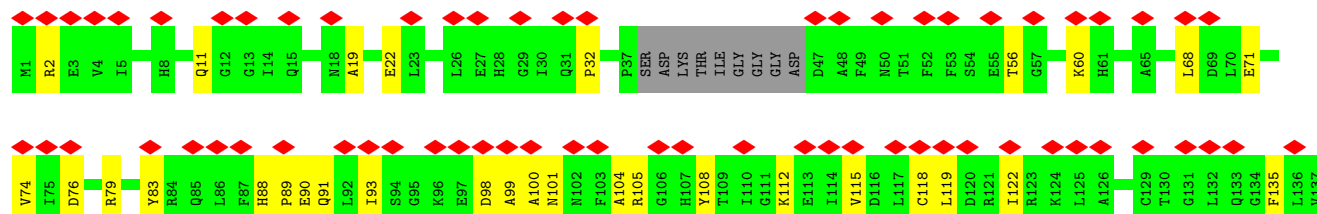
• Molecule 1: Tubulin alpha chain

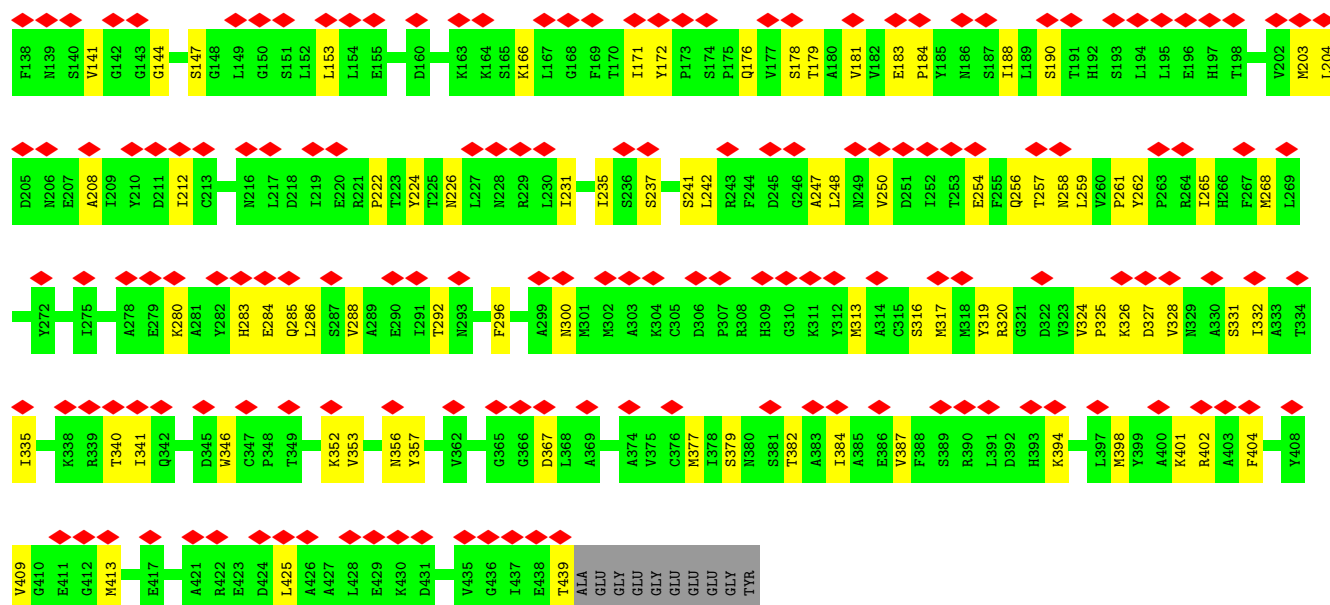


• Molecule 1: Tubulin alpha chain

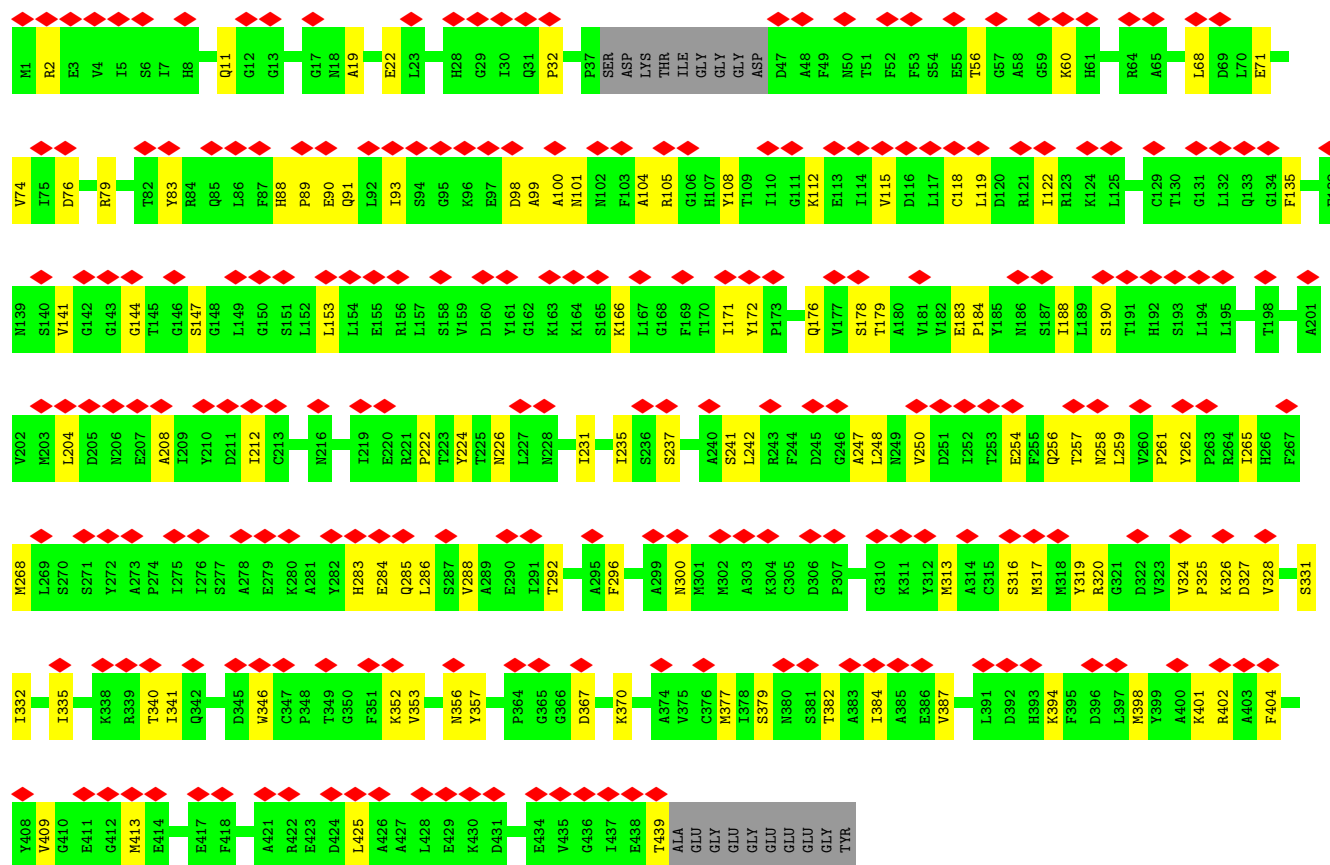
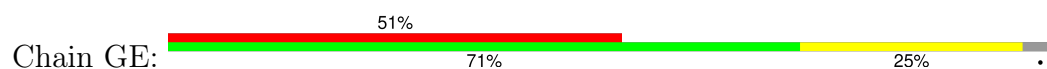


• Molecule 1: Tubulin alpha chain

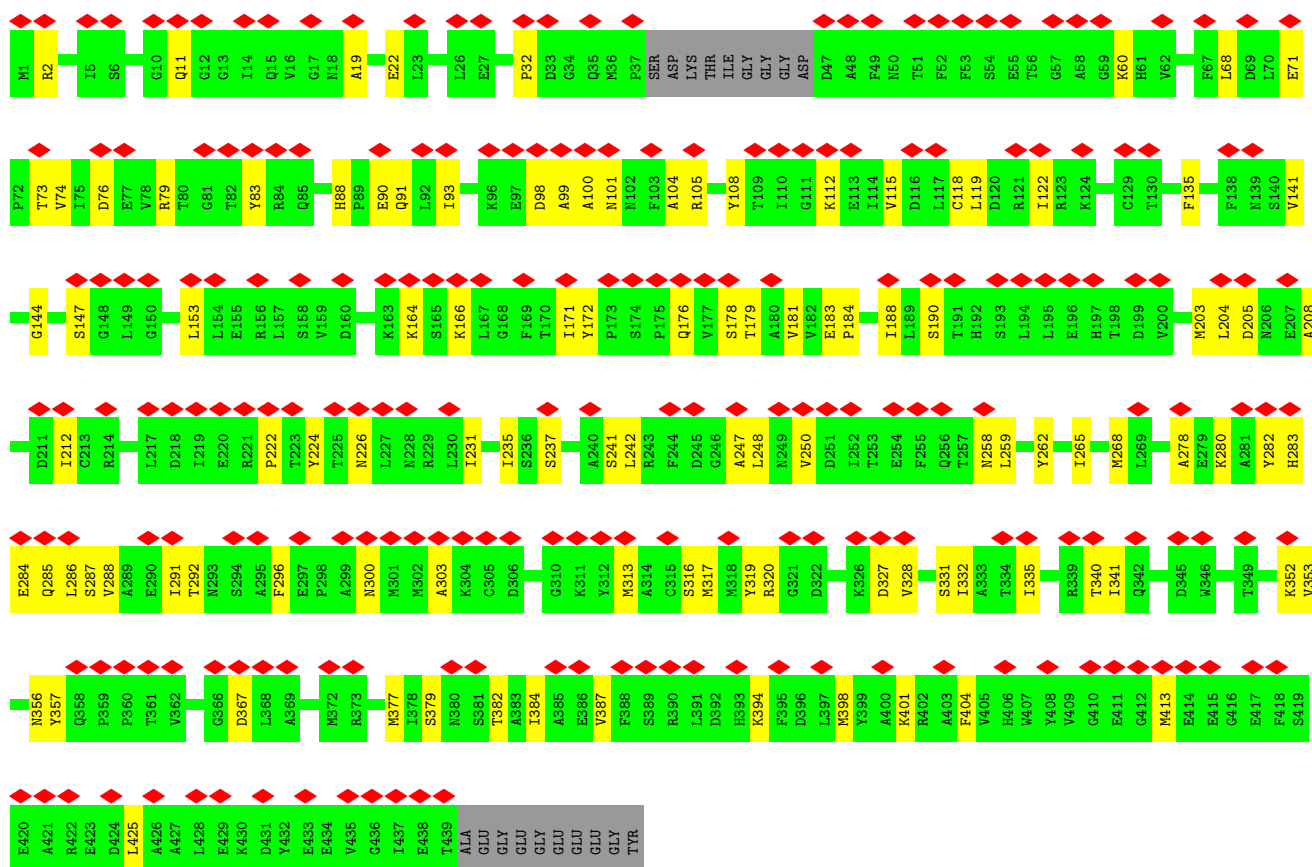
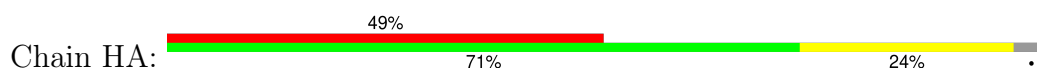


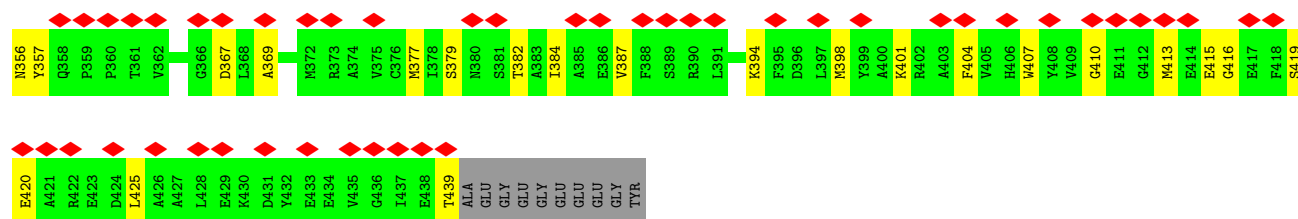


• Molecule 1: Tubulin alpha chain

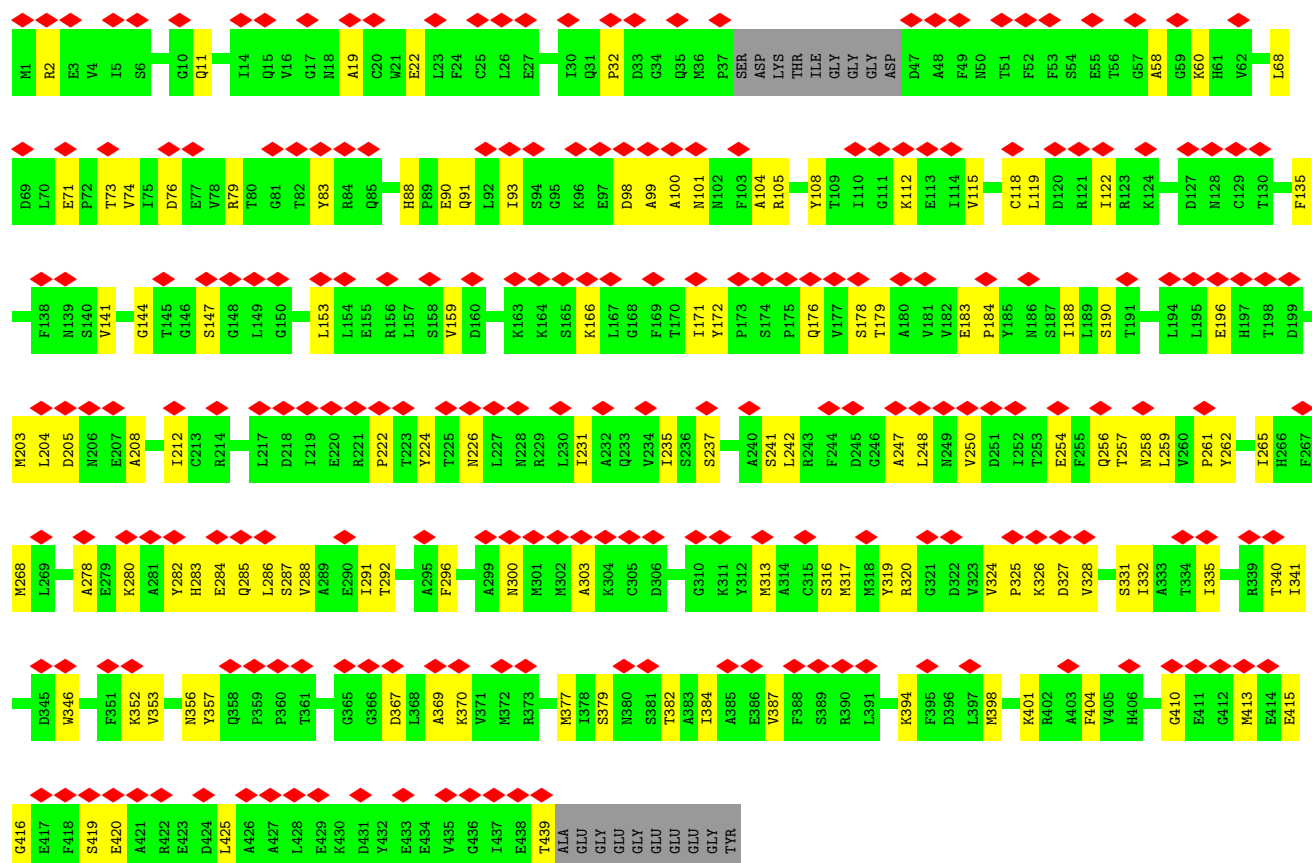


• Molecule 1: Tubulin alpha chain

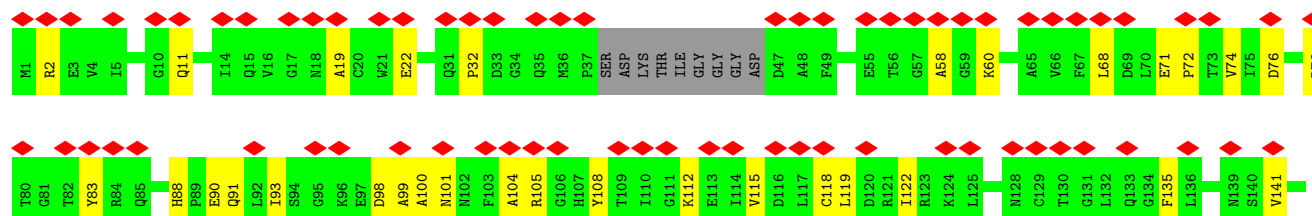
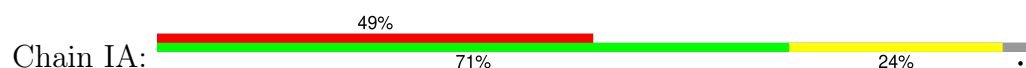


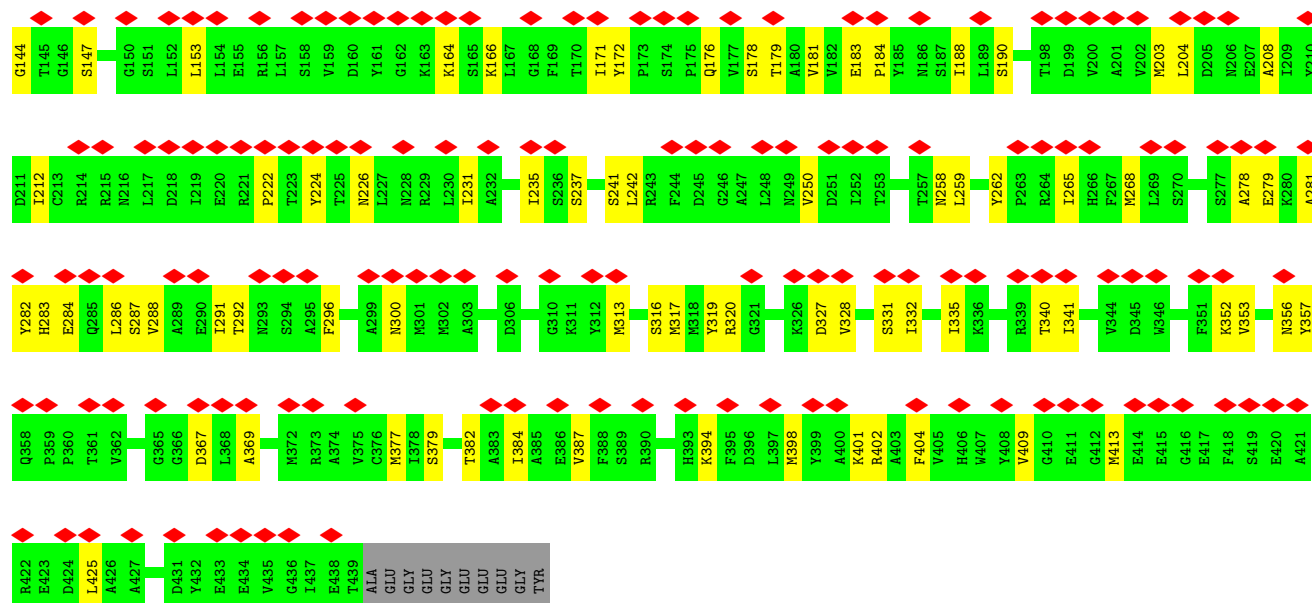


• Molecule 1: Tubulin alpha chain

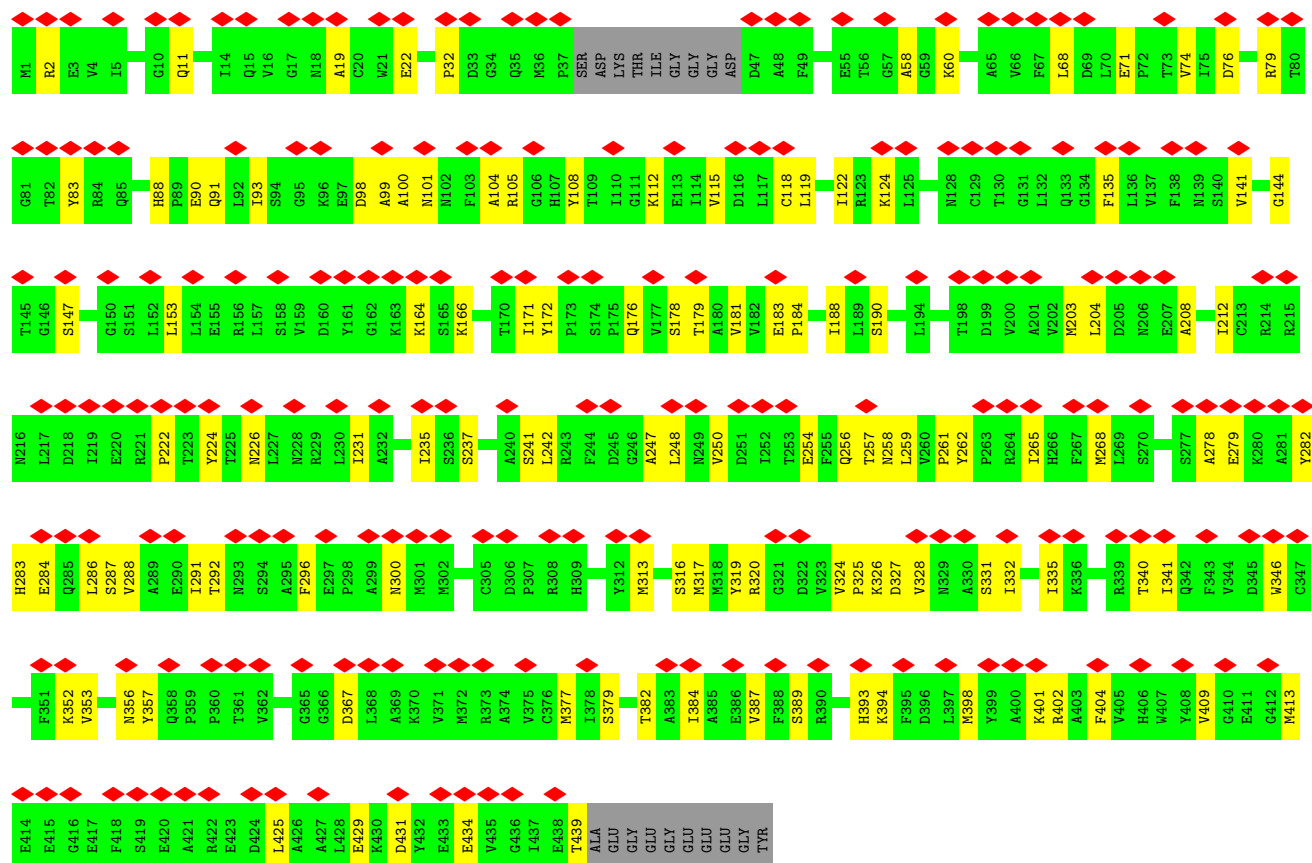


• Molecule 1: Tubulin alpha chain

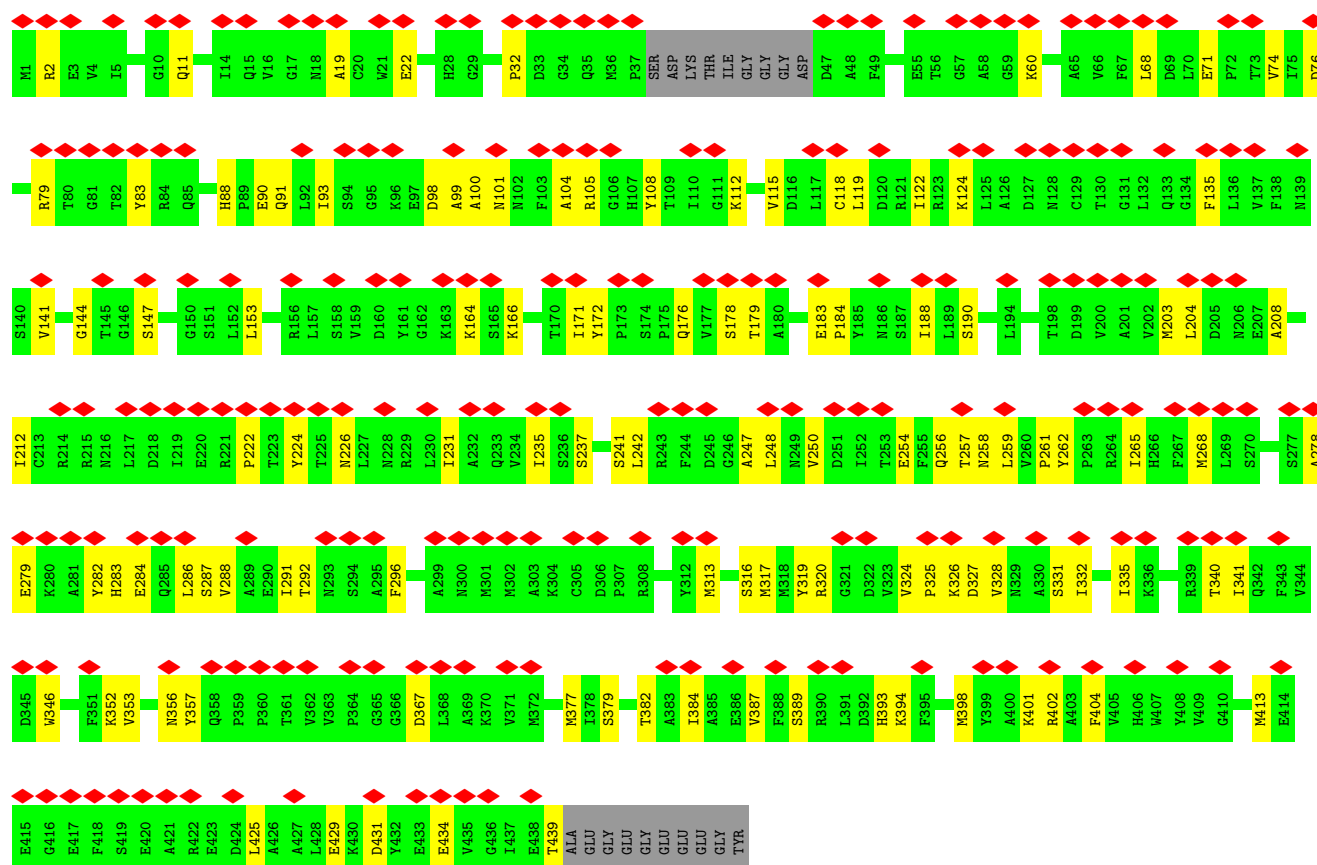




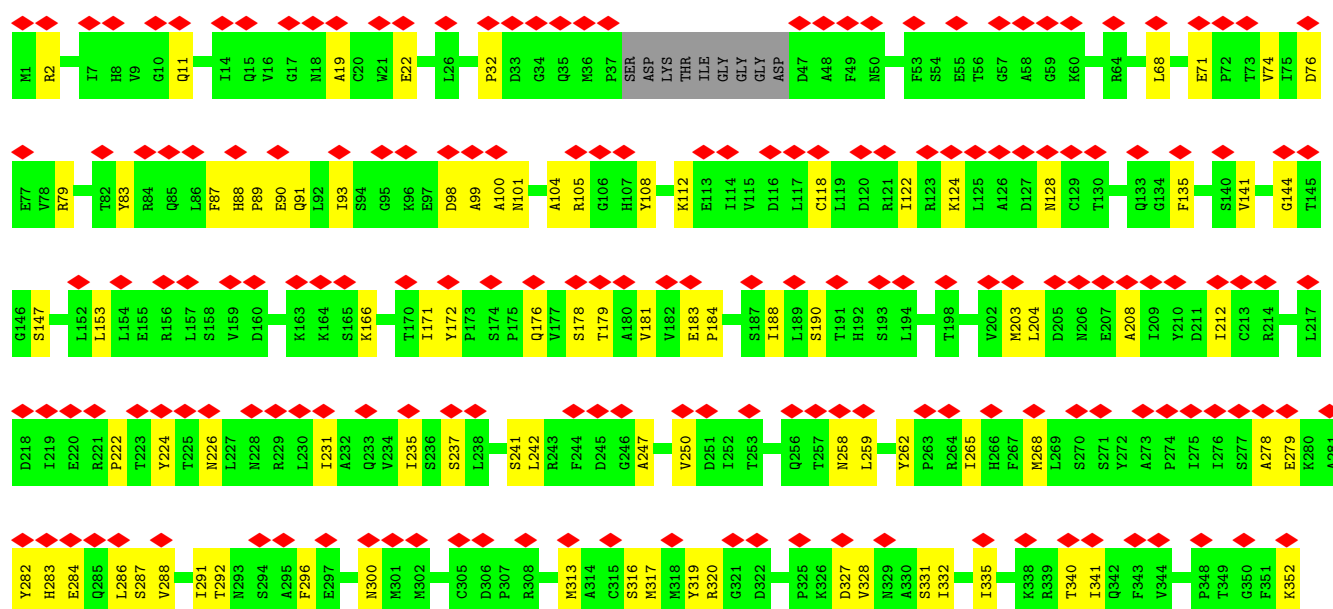
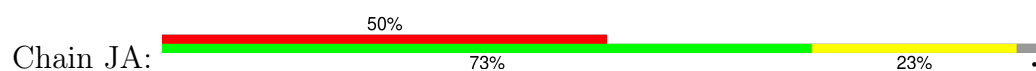
• Molecule 1: Tubulin alpha chain

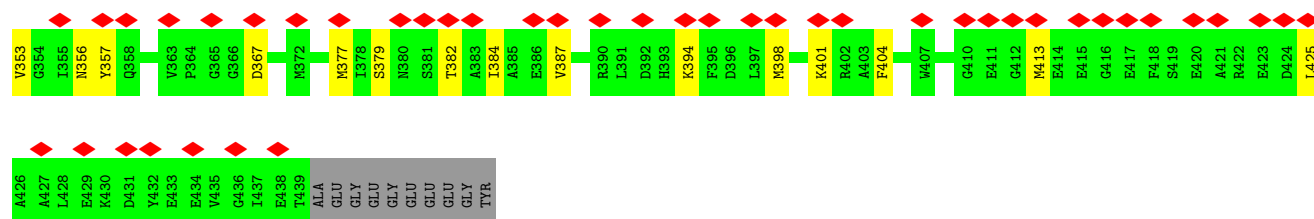


• Molecule 1: Tubulin alpha chain

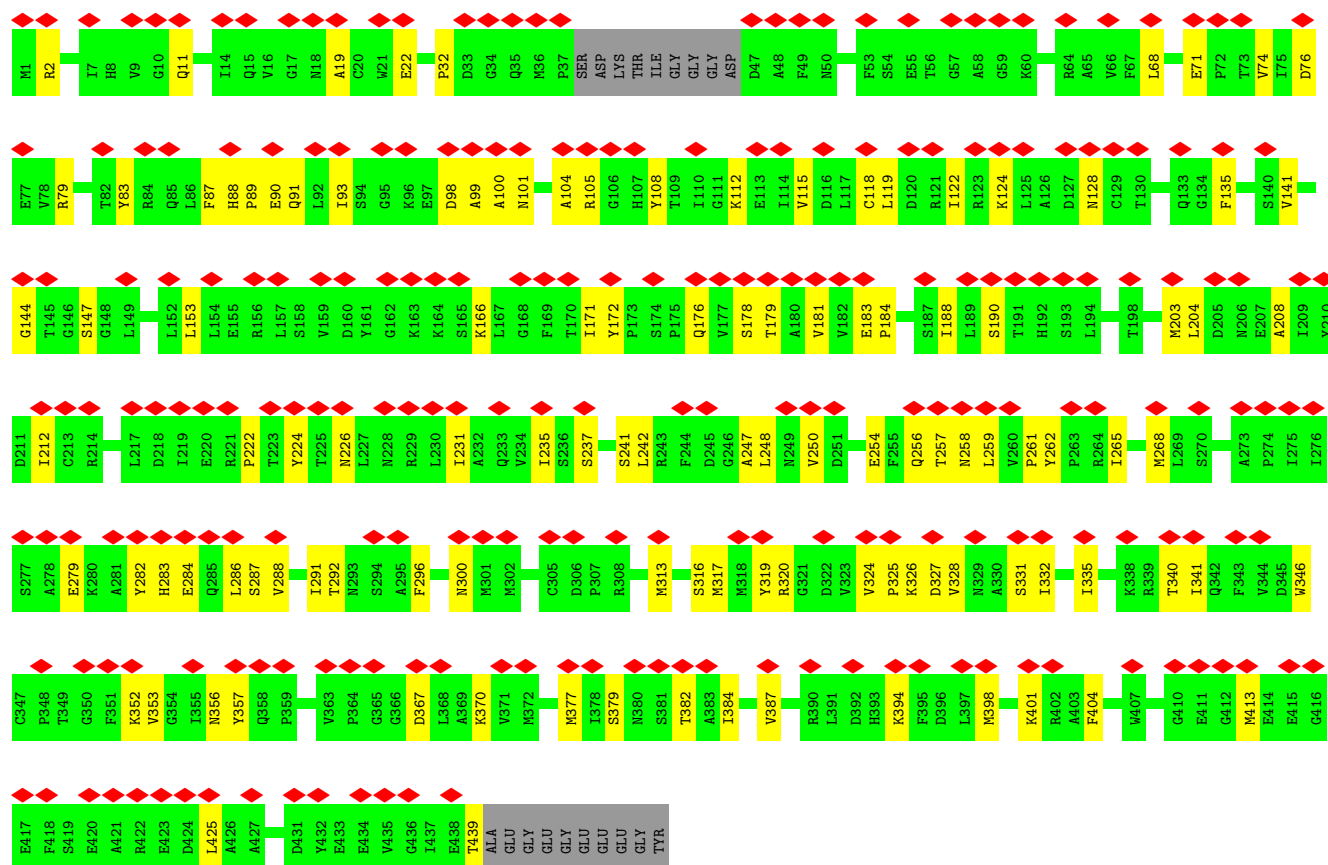
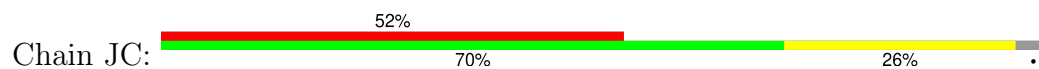


• Molecule 1: Tubulin alpha chain

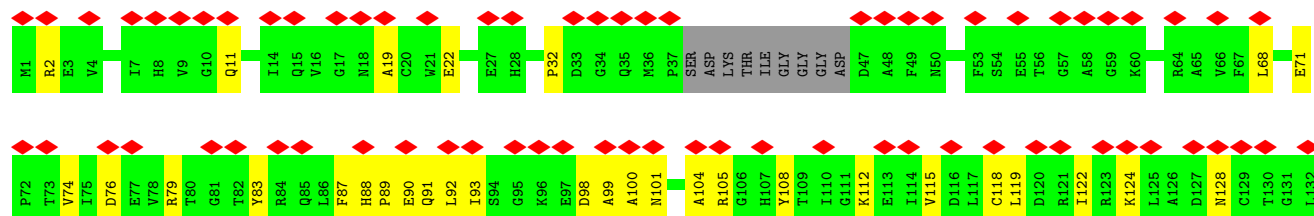


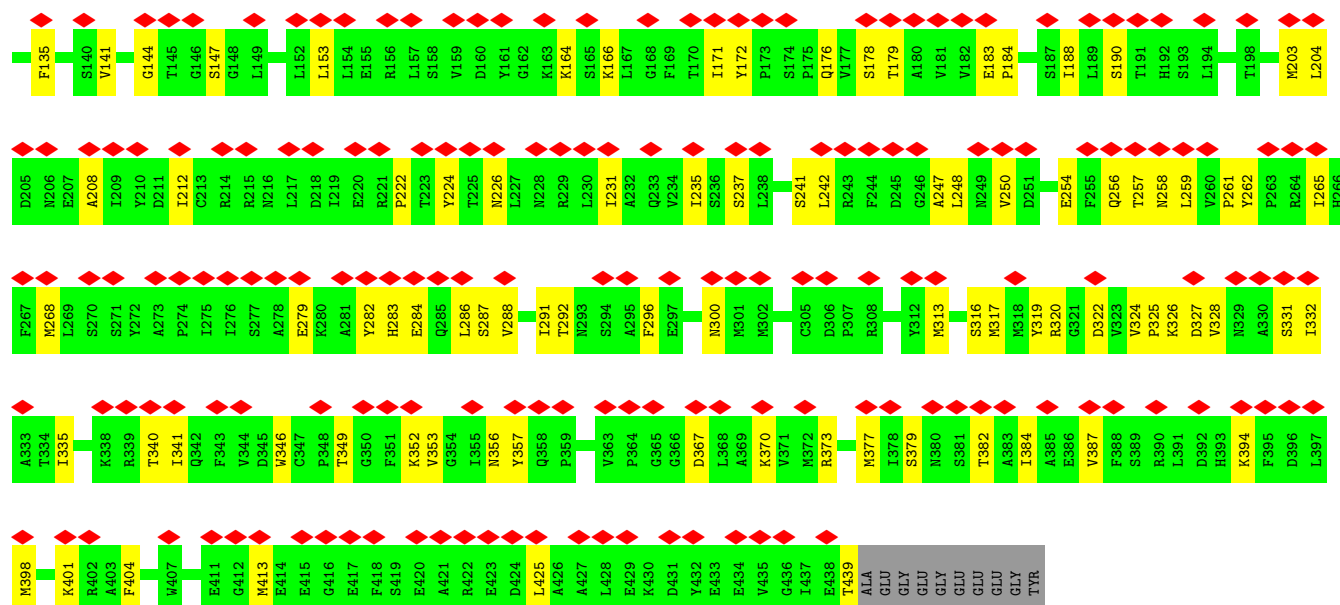


• Molecule 1: Tubulin alpha chain

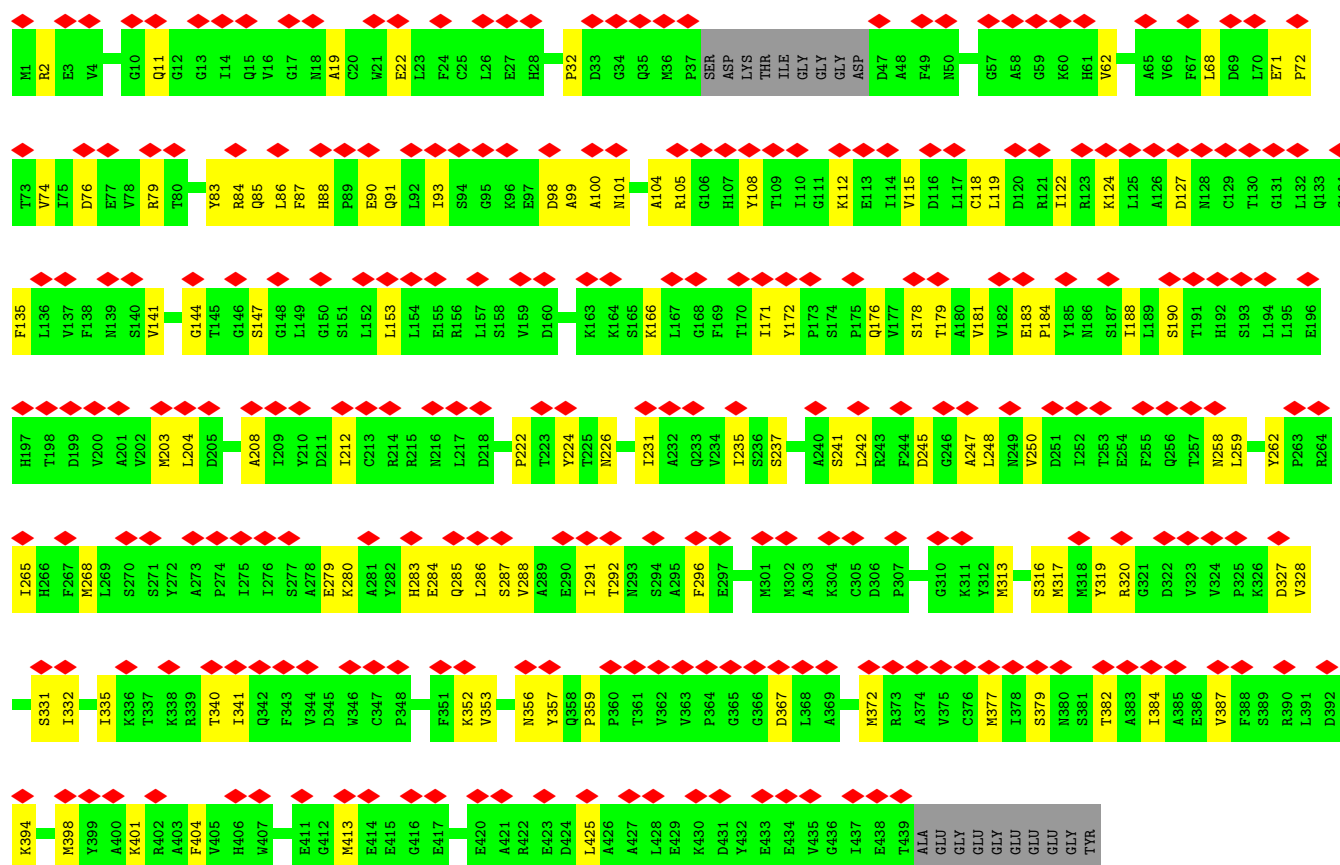
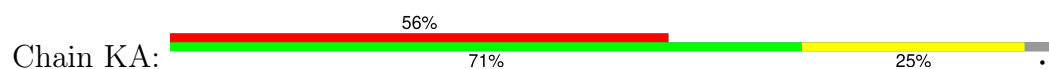


• Molecule 1: Tubulin alpha chain

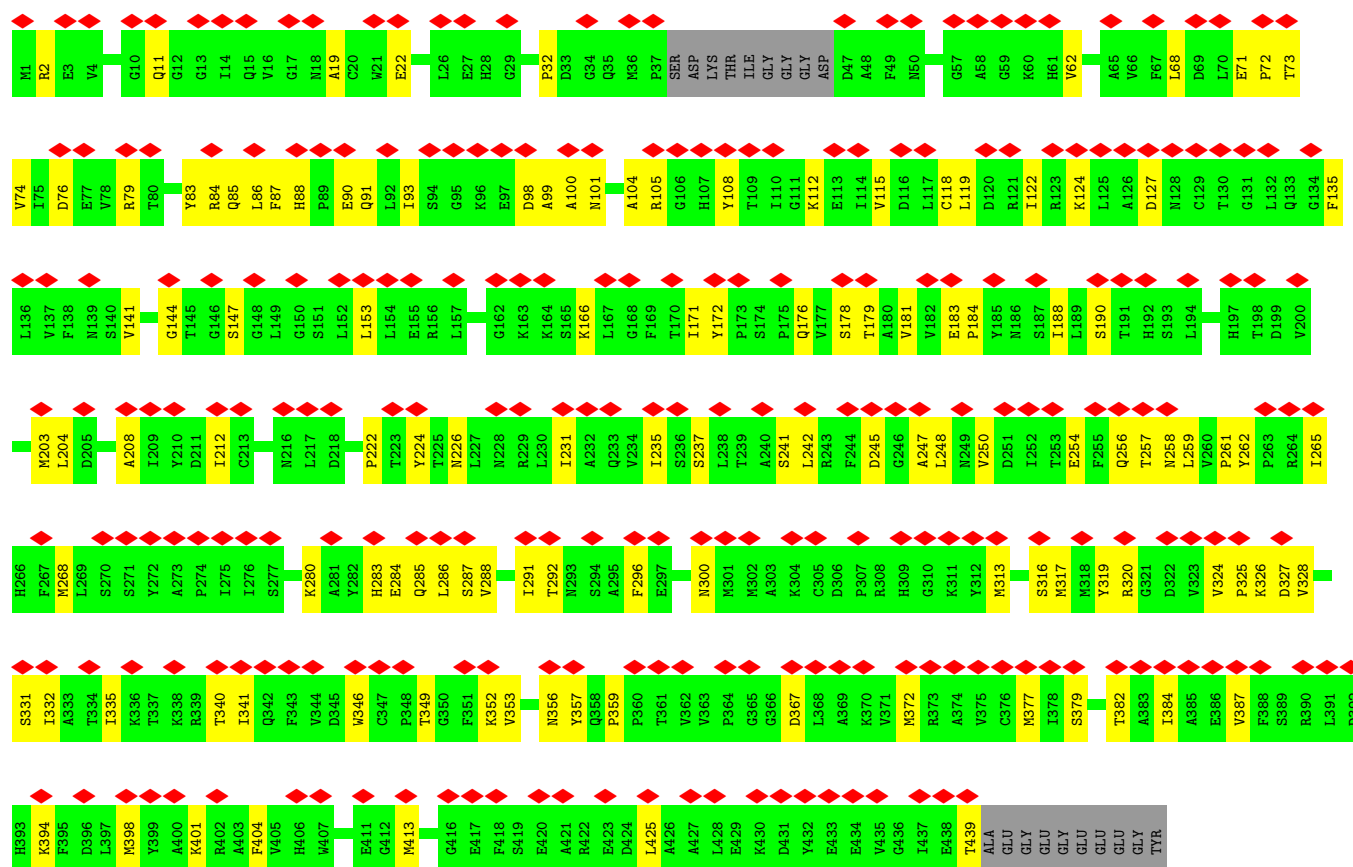




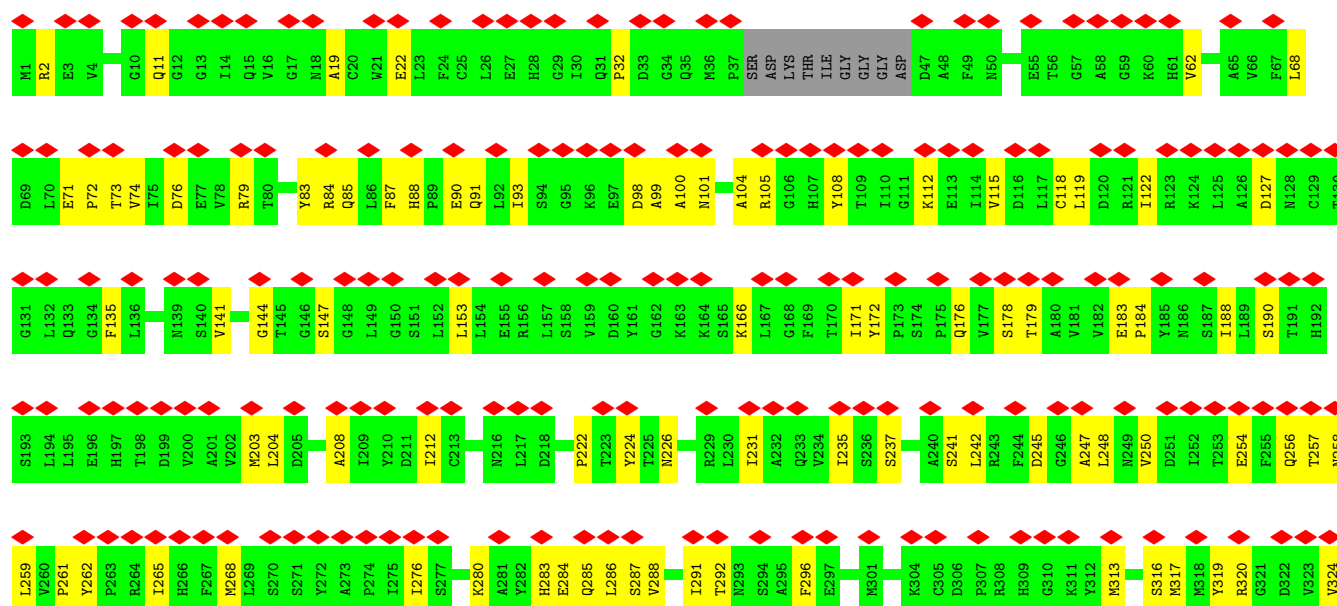
• Molecule 1: Tubulin alpha chain

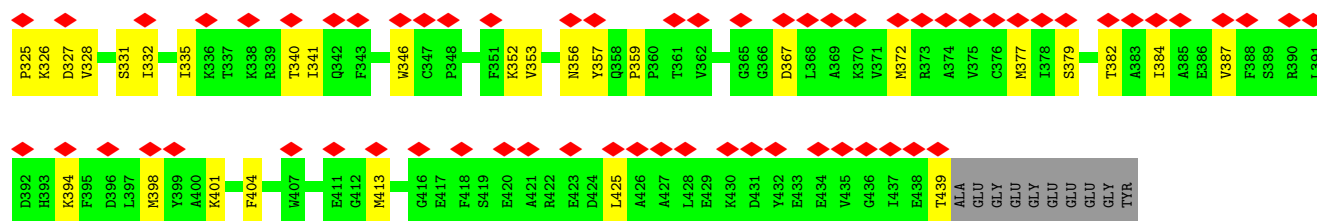


• Molecule 1: Tubulin alpha chain

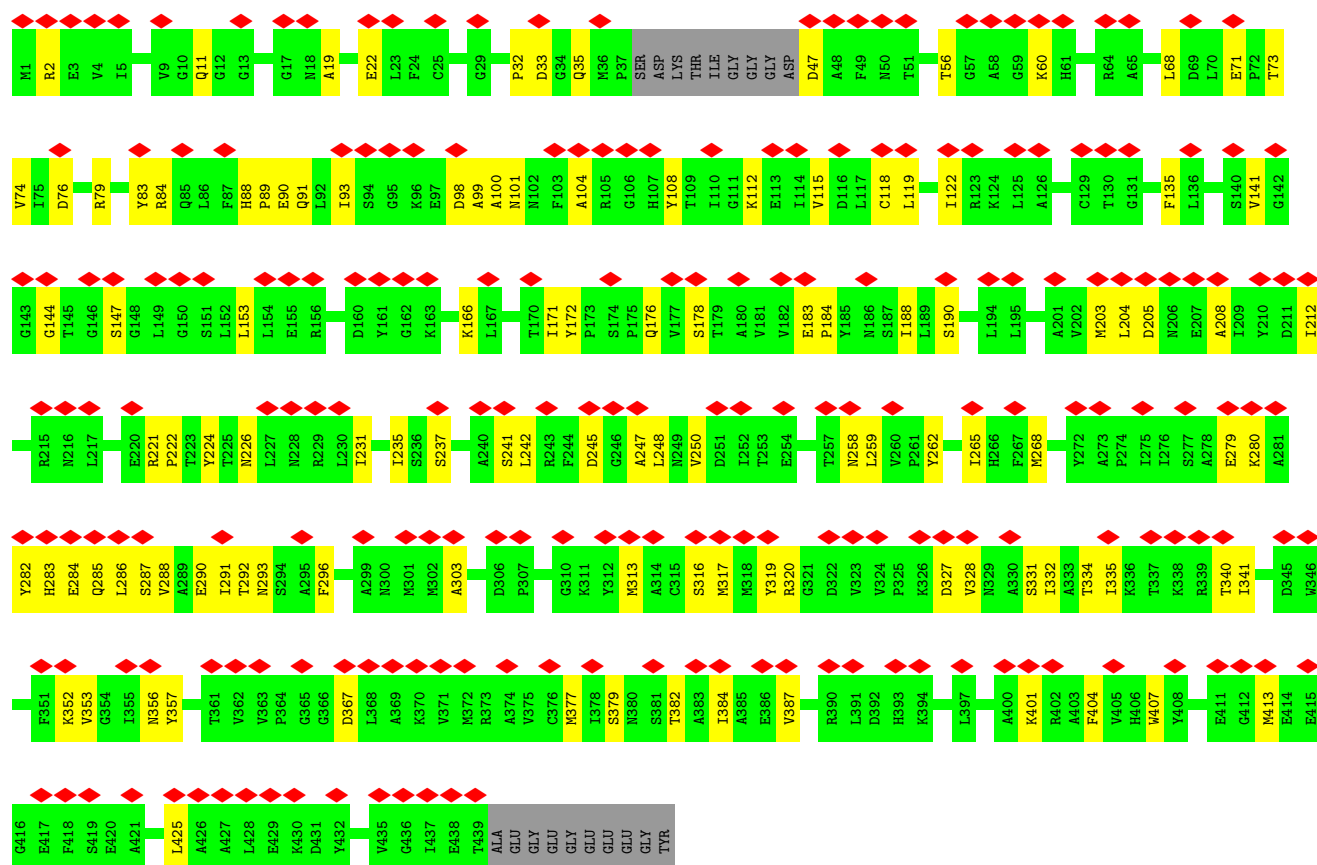
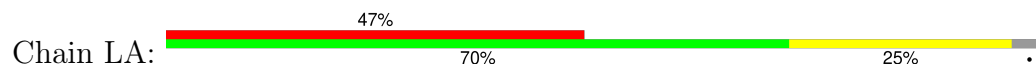


• Molecule 1: Tubulin alpha chain

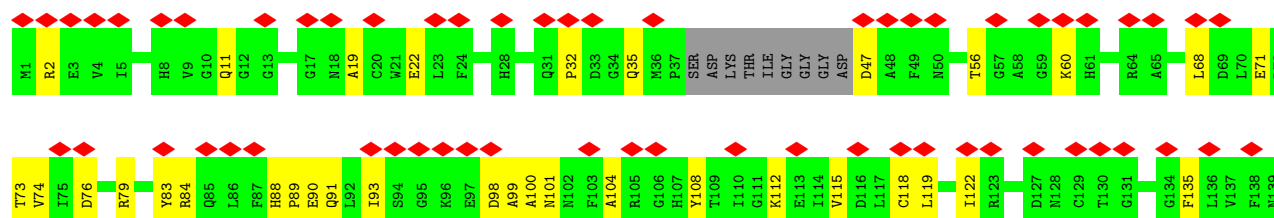


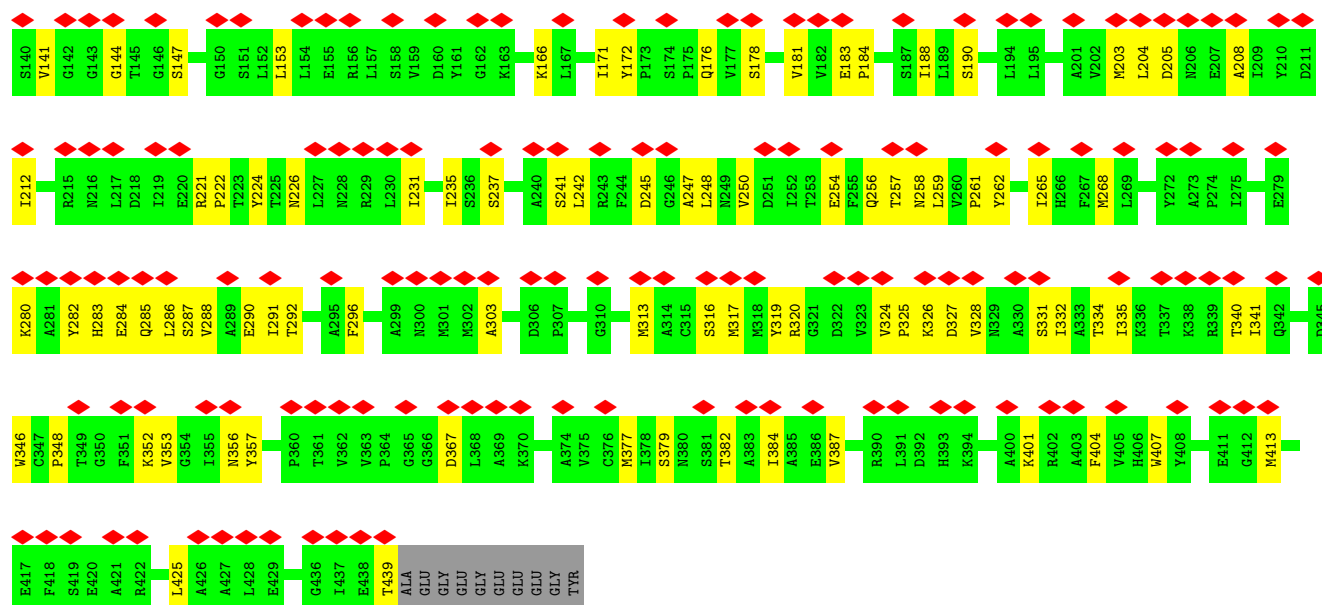


• Molecule 1: Tubulin alpha chain

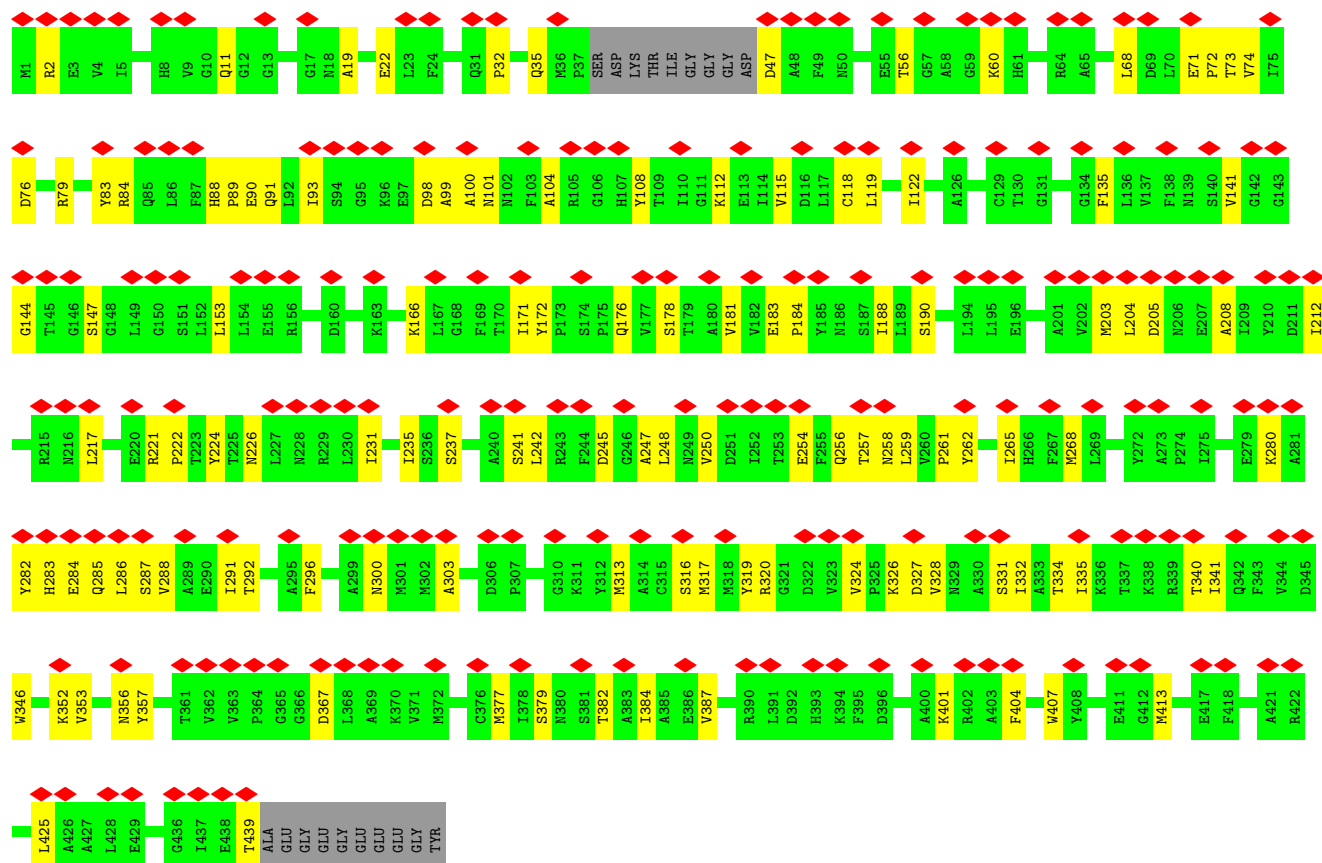


• Molecule 1: Tubulin alpha chain





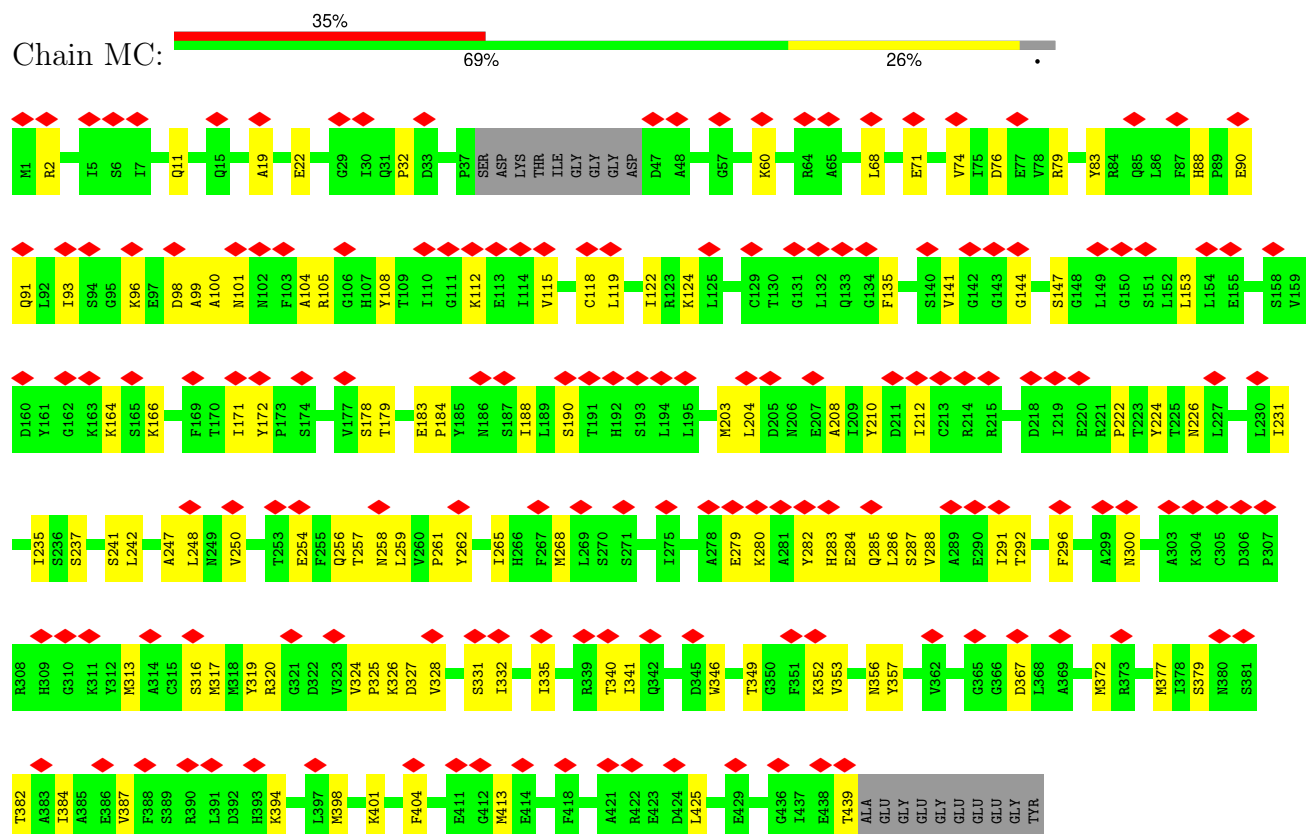
• Molecule 1: Tubulin alpha chain



• Molecule 1: Tubulin alpha chain



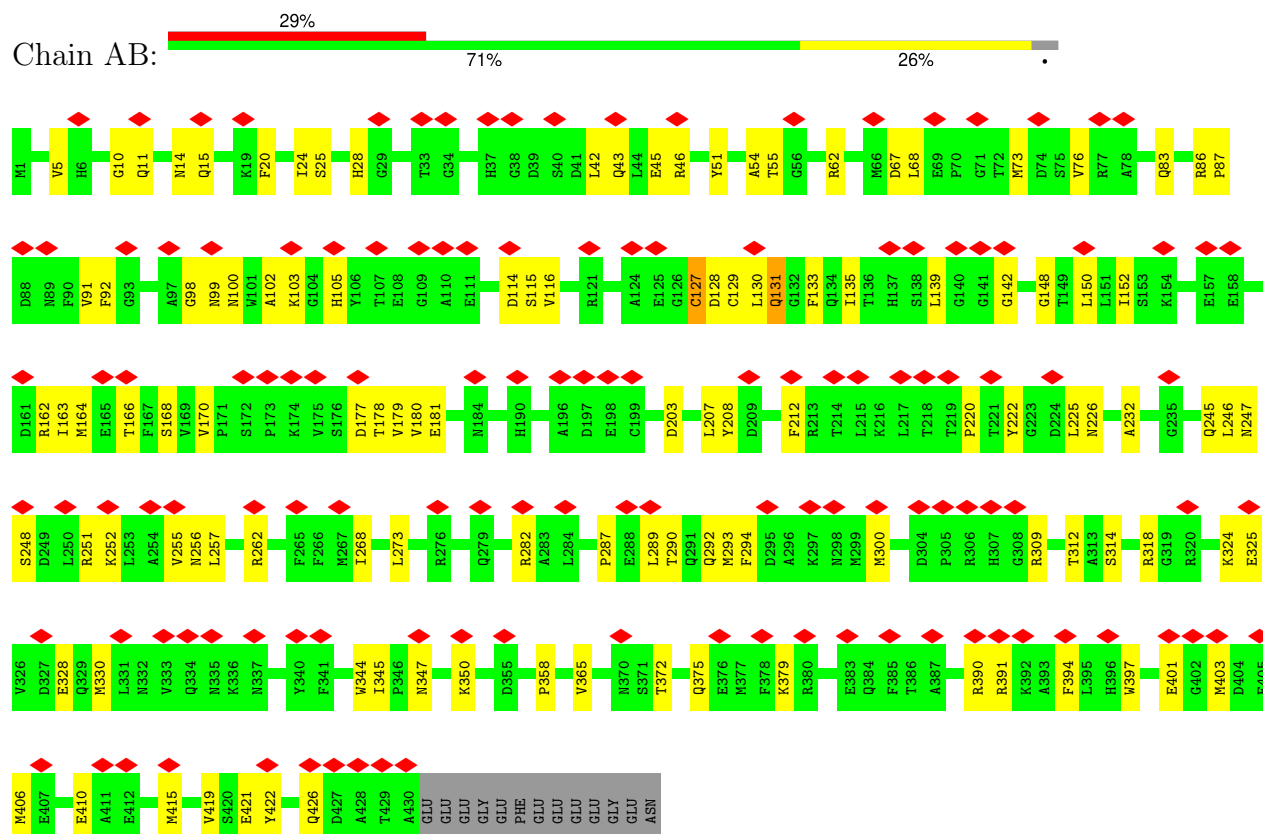
• Molecule 1: Tubulin alpha chain



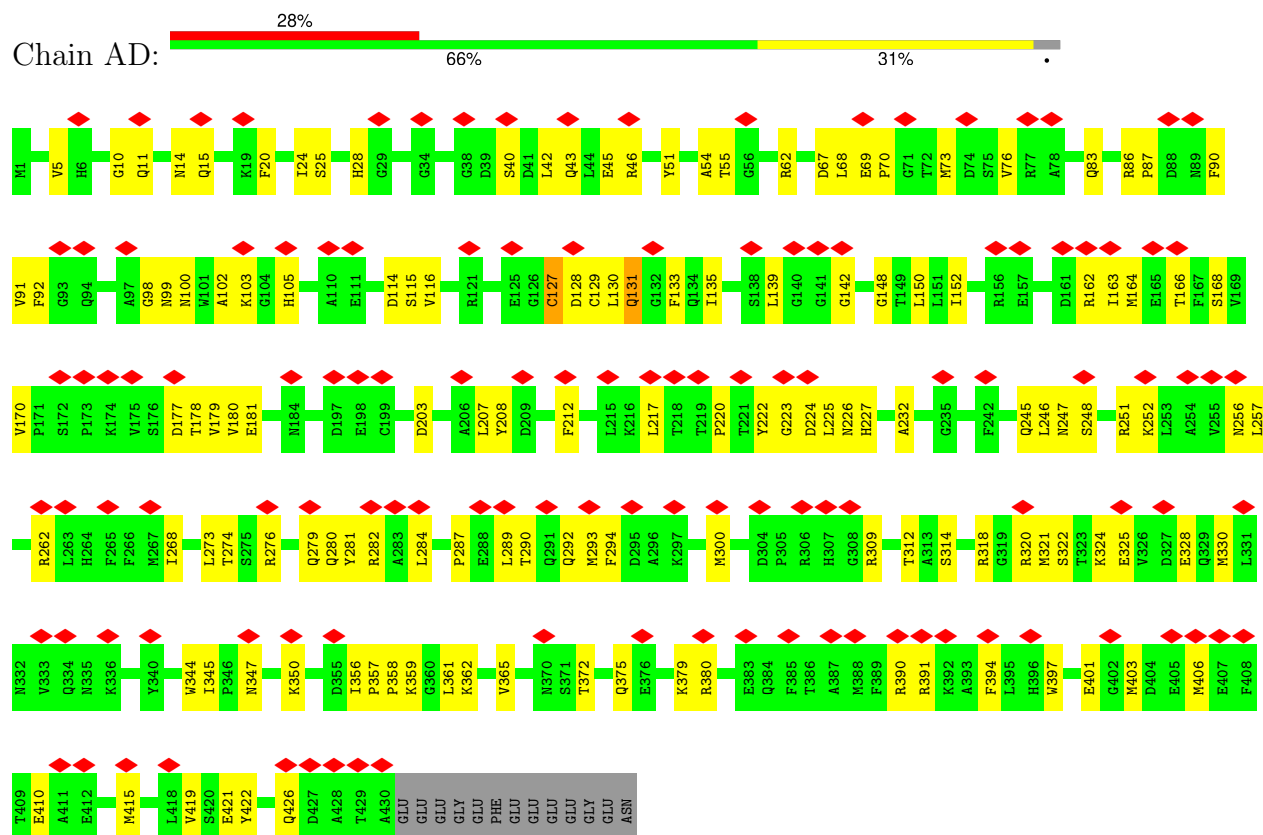
- Molecule 1: Tubulin alpha chain



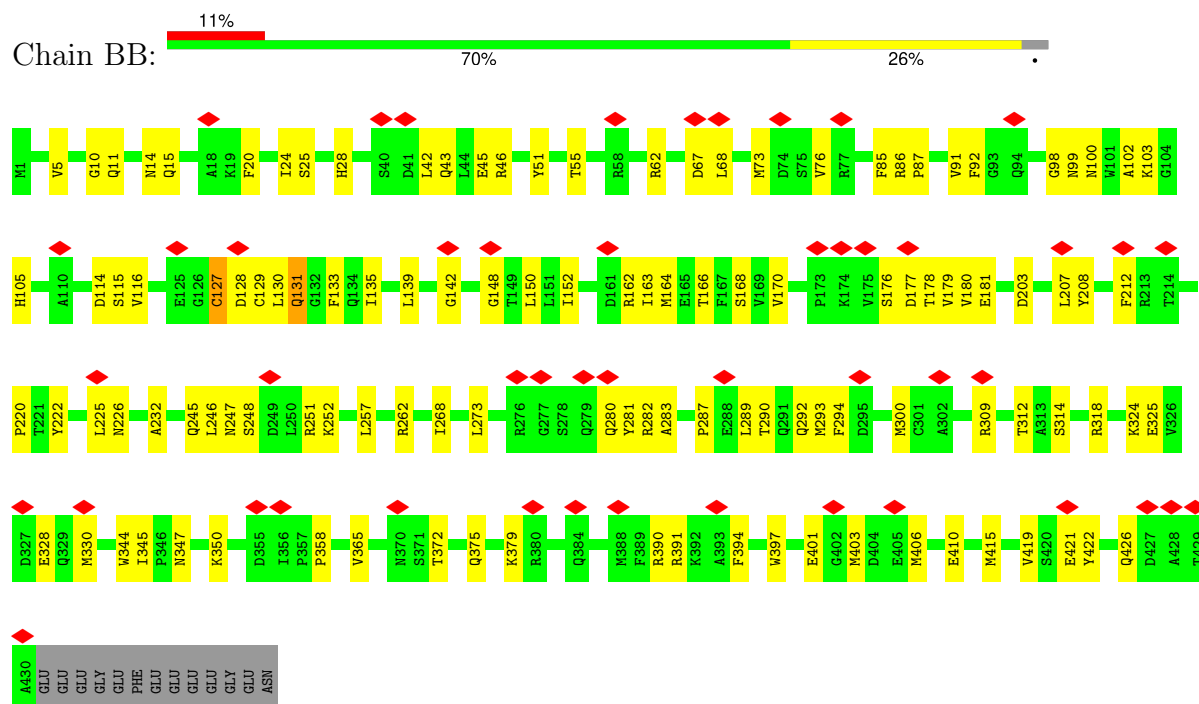
- Molecule 2: Tubulin beta chain



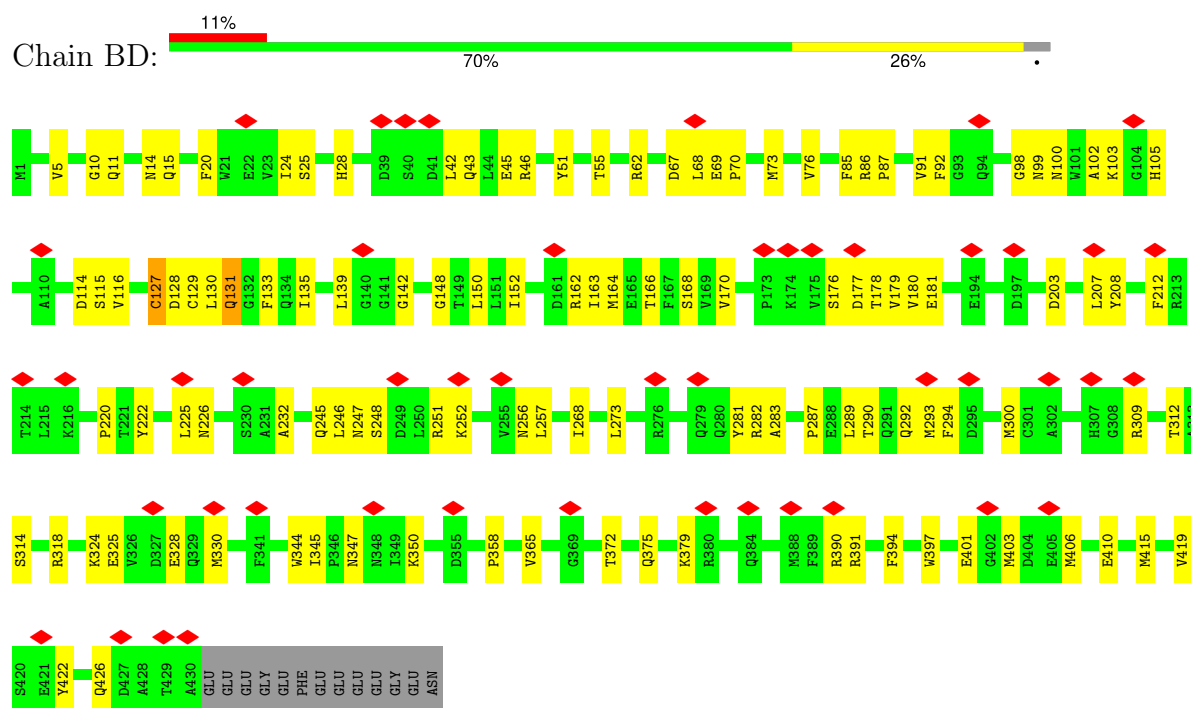
- Molecule 2: Tubulin beta chain



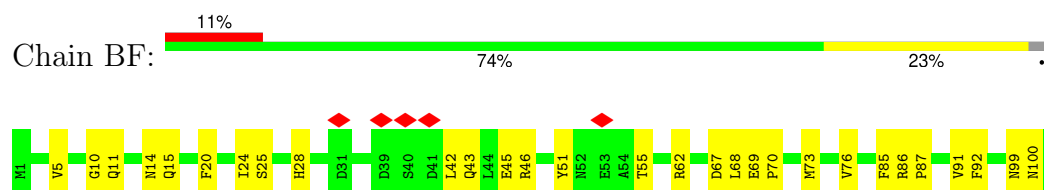
- Molecule 2: Tubulin beta chain

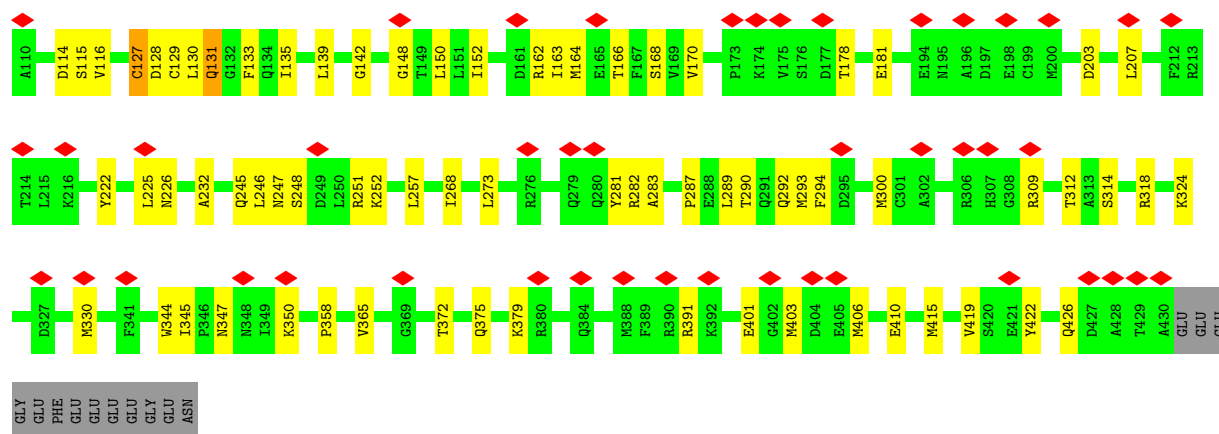


- Molecule 2: Tubulin beta chain

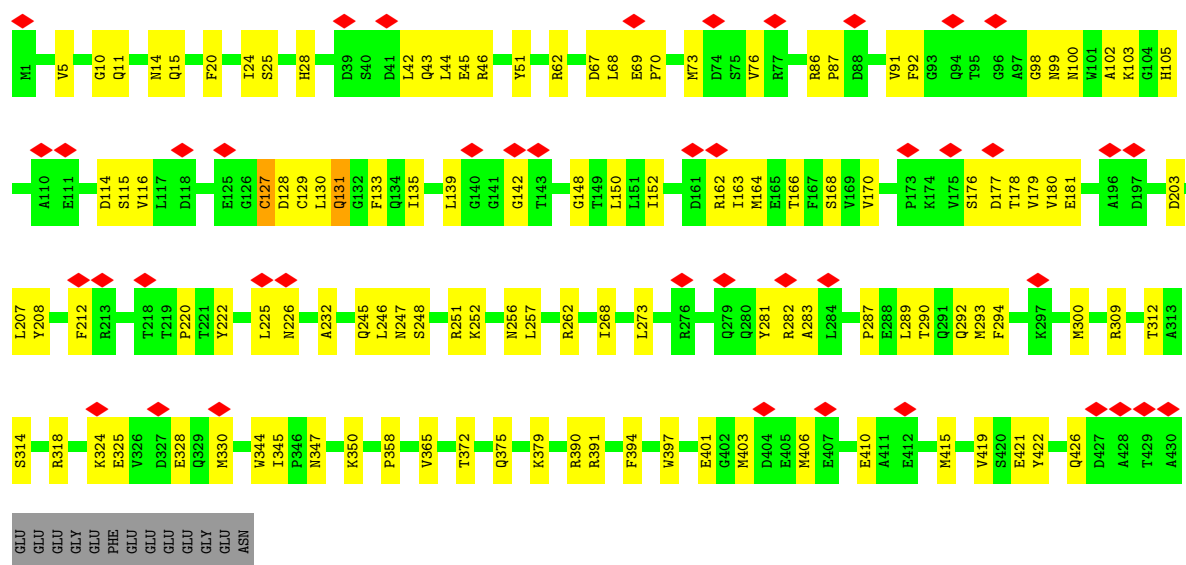
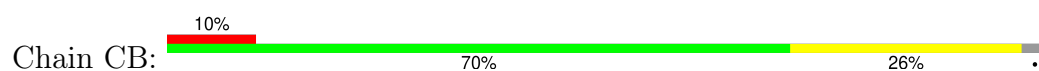


- Molecule 2: Tubulin beta chain

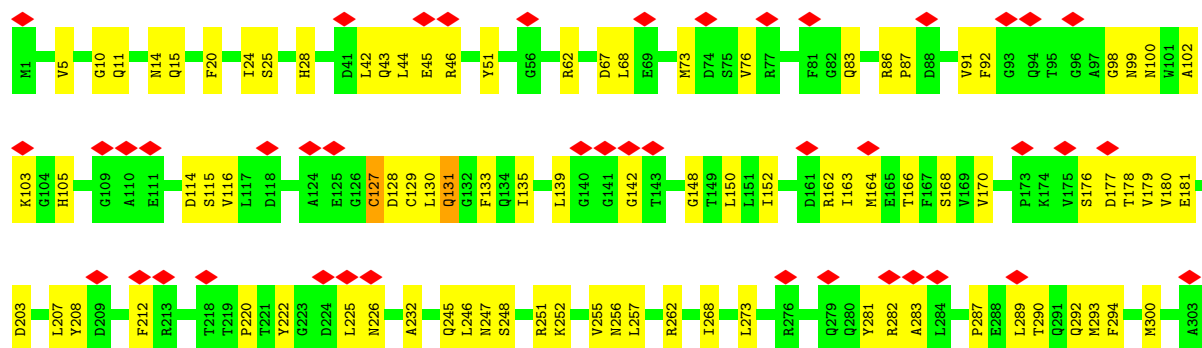
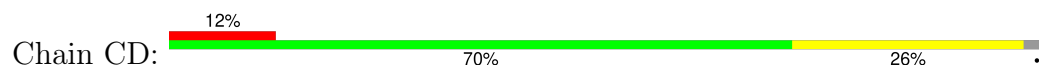


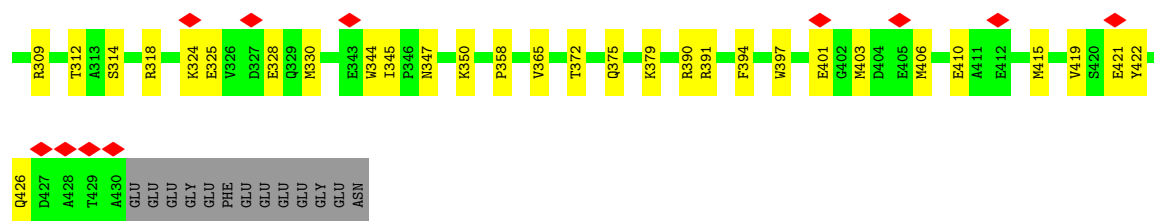


• Molecule 2: Tubulin beta chain

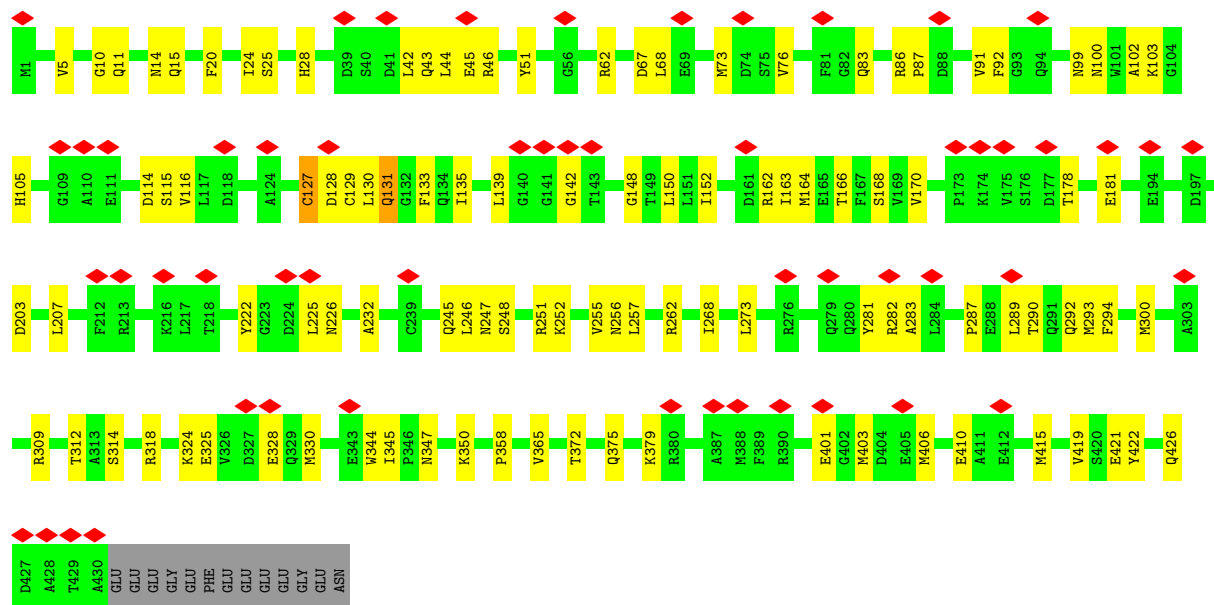
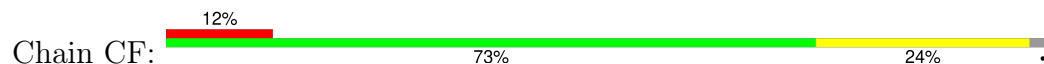


• Molecule 2: Tubulin beta chain

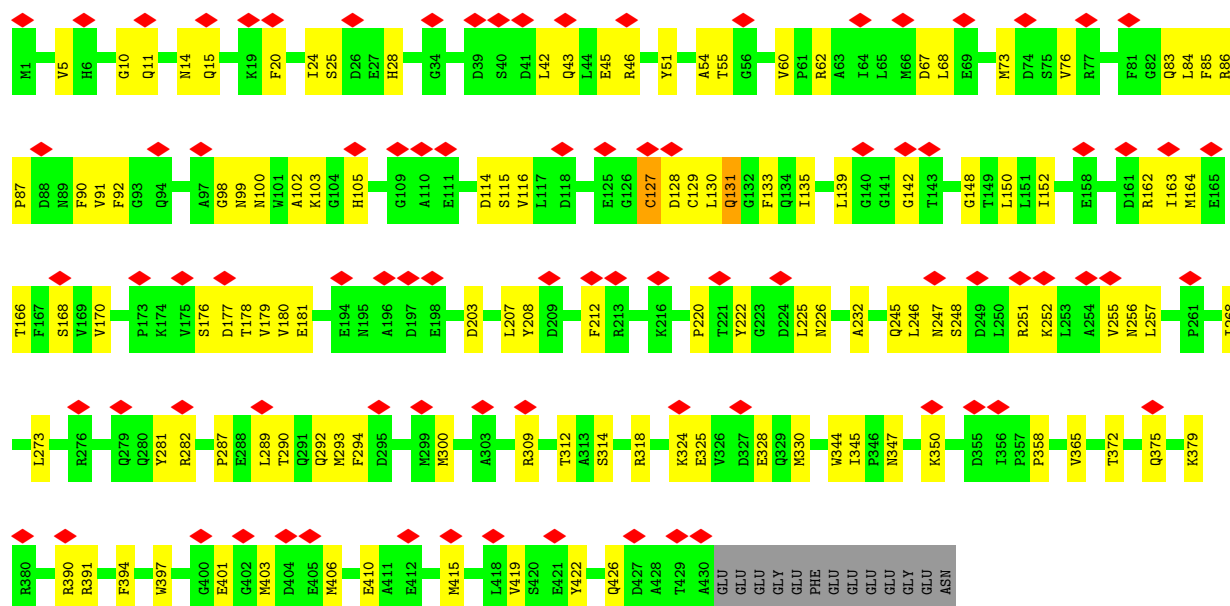




• Molecule 2: Tubulin beta chain

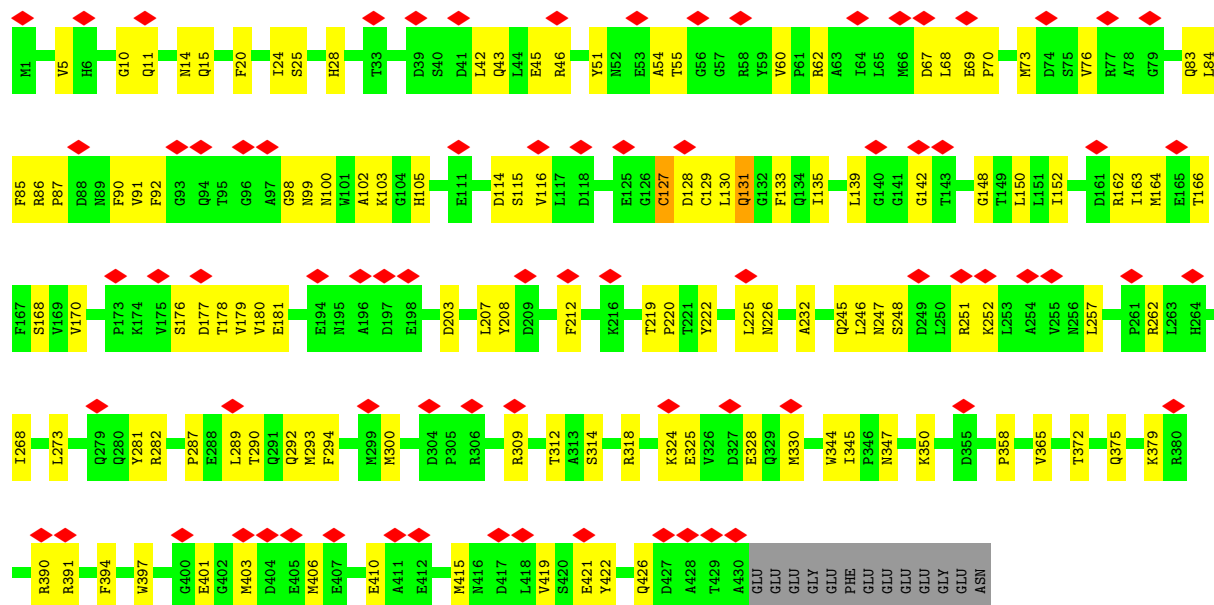


• Molecule 2: Tubulin beta chain




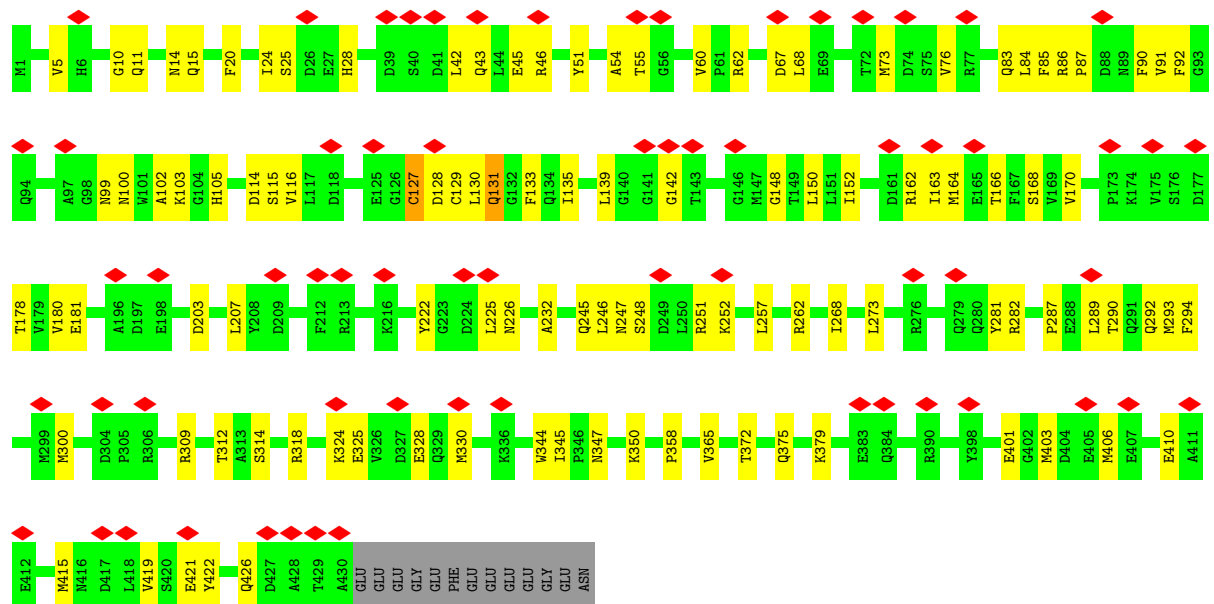
- Molecule 2: Tubulin beta chain

Chain DD: 



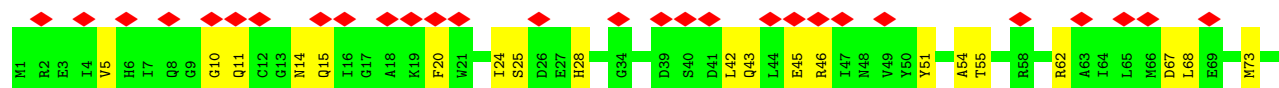
- Molecule 2: Tubulin beta chain

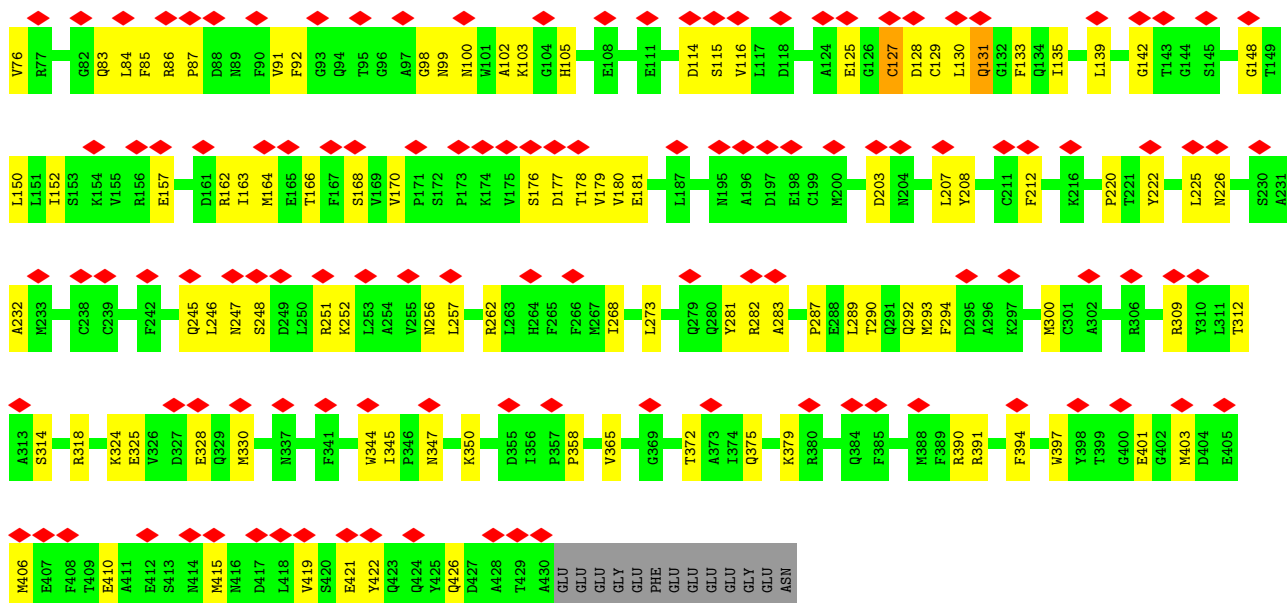
Chain DF: 



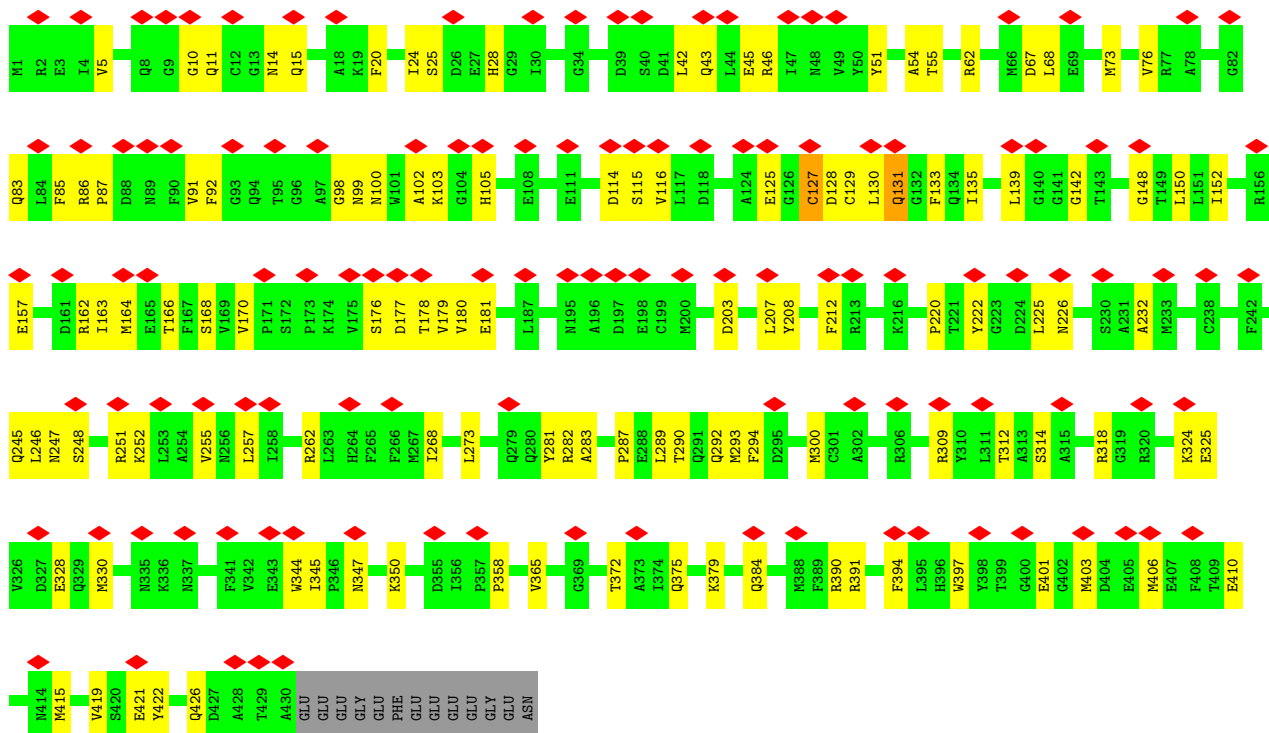
- Molecule 2: Tubulin beta chain

Chain EB: 



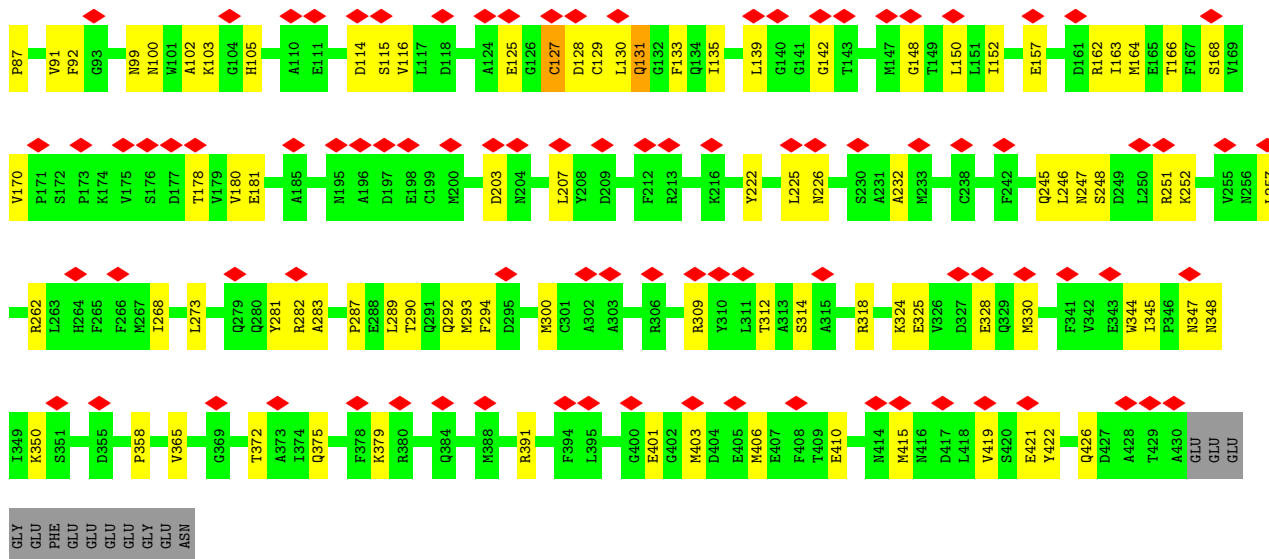


• Molecule 2: Tubulin beta chain

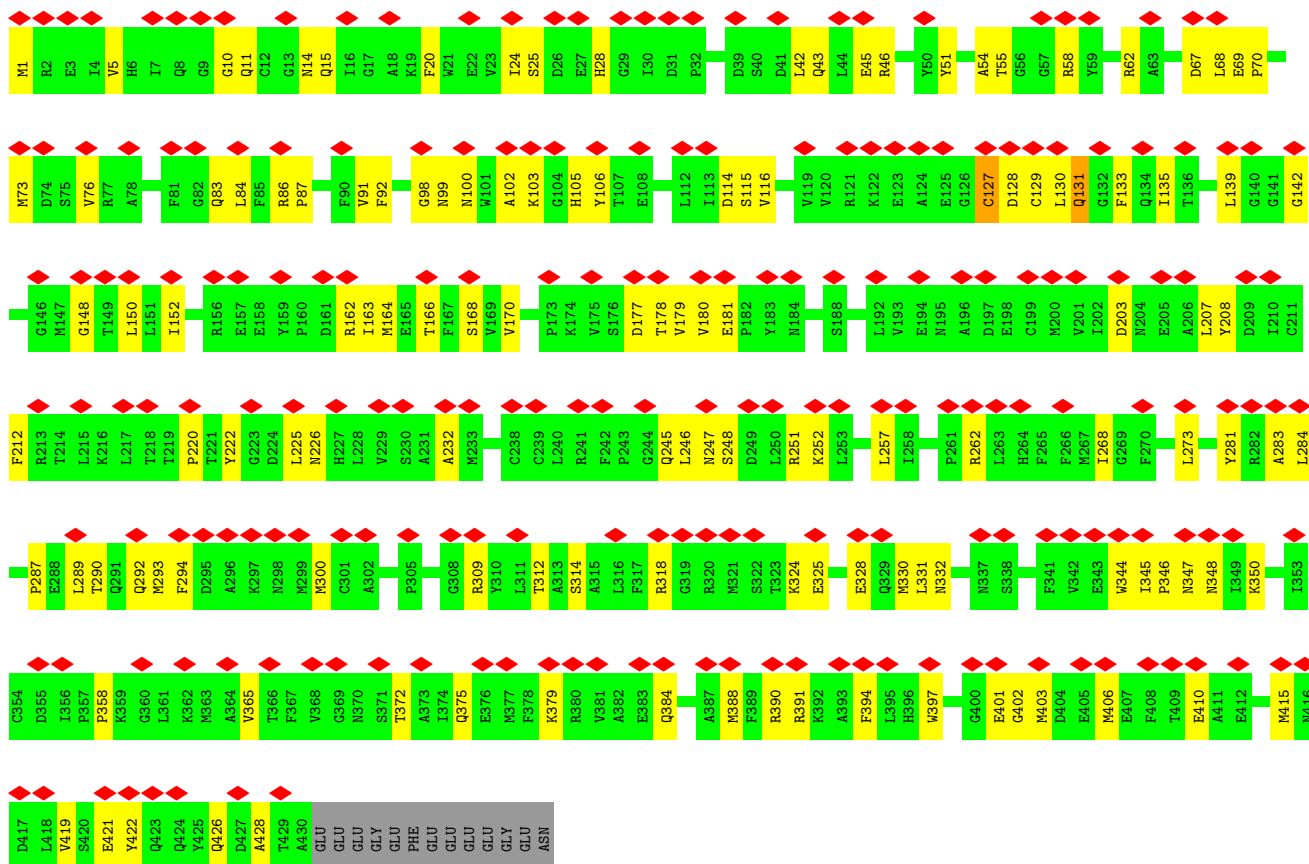


• Molecule 2: Tubulin beta chain



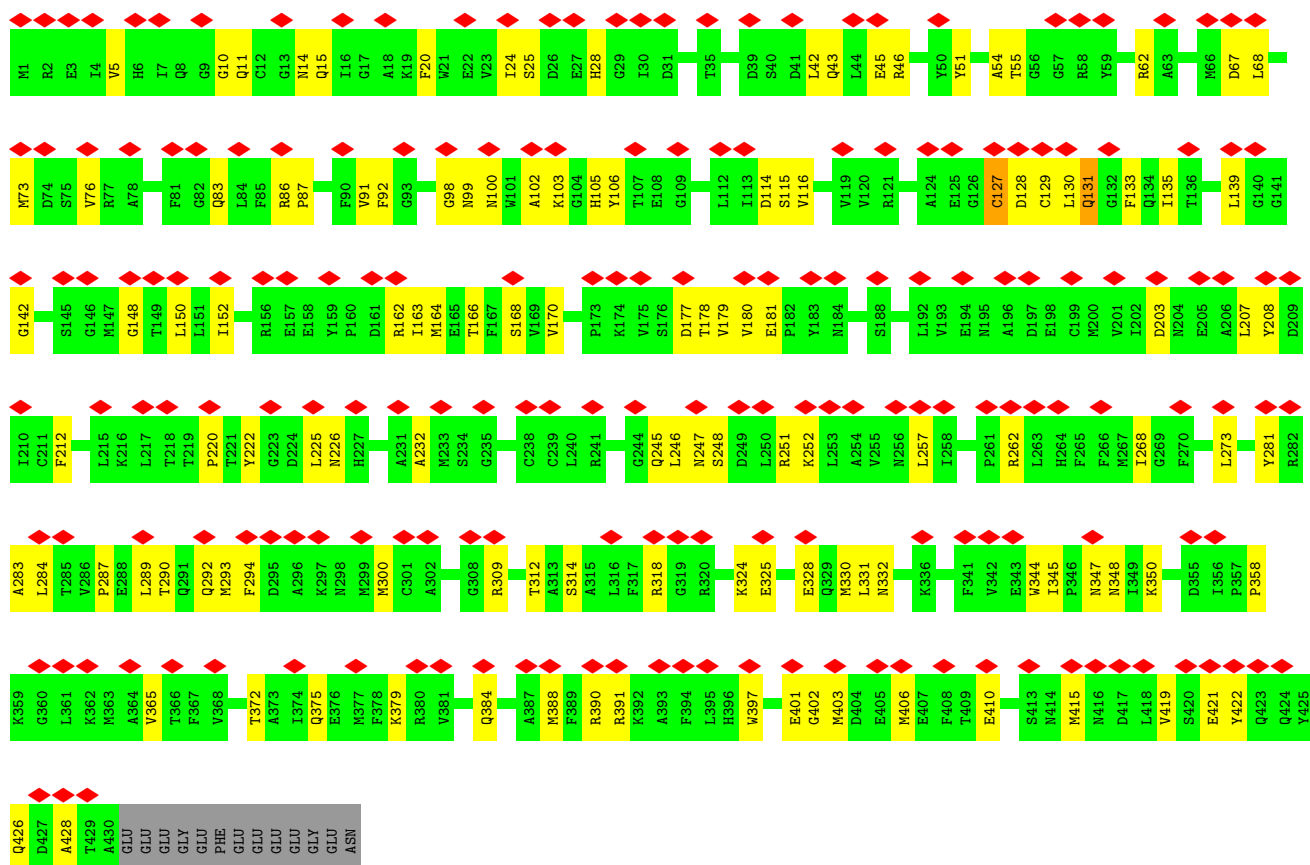


• Molecule 2: Tubulin beta chain

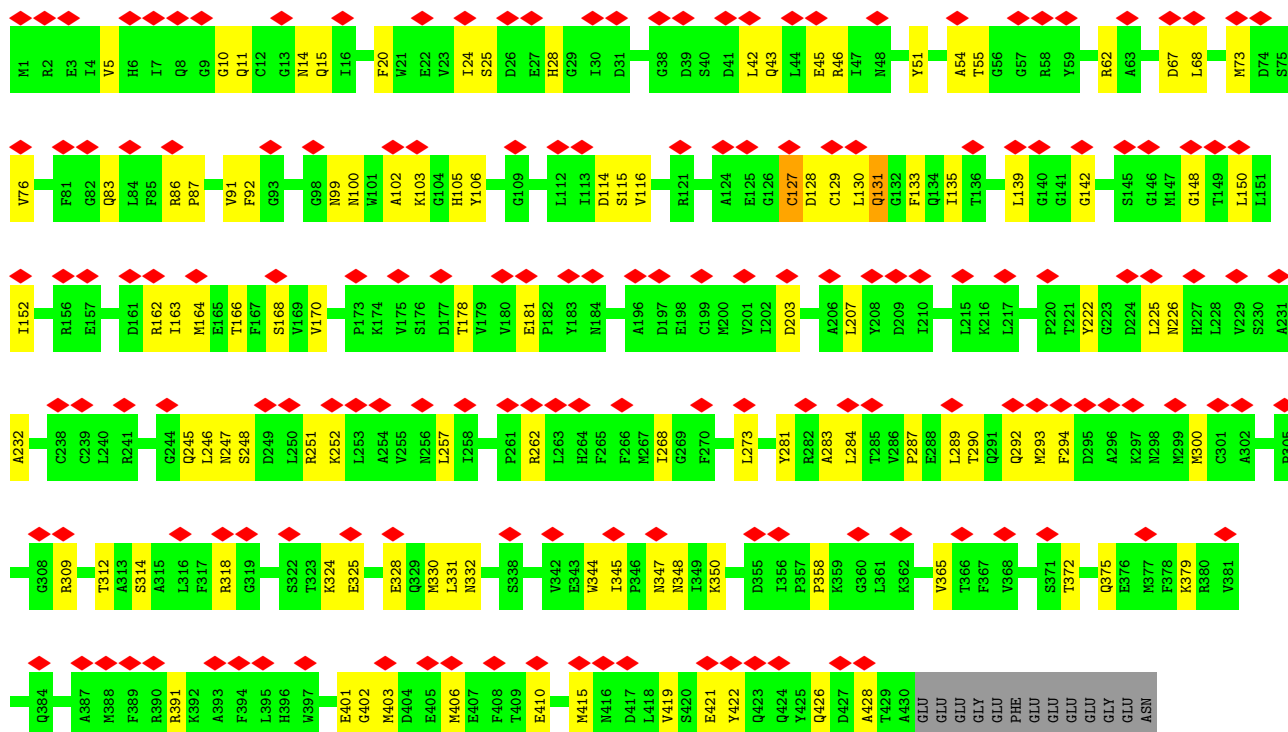
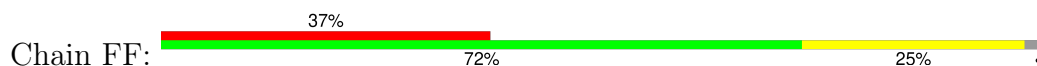


• Molecule 2: Tubulin beta chain

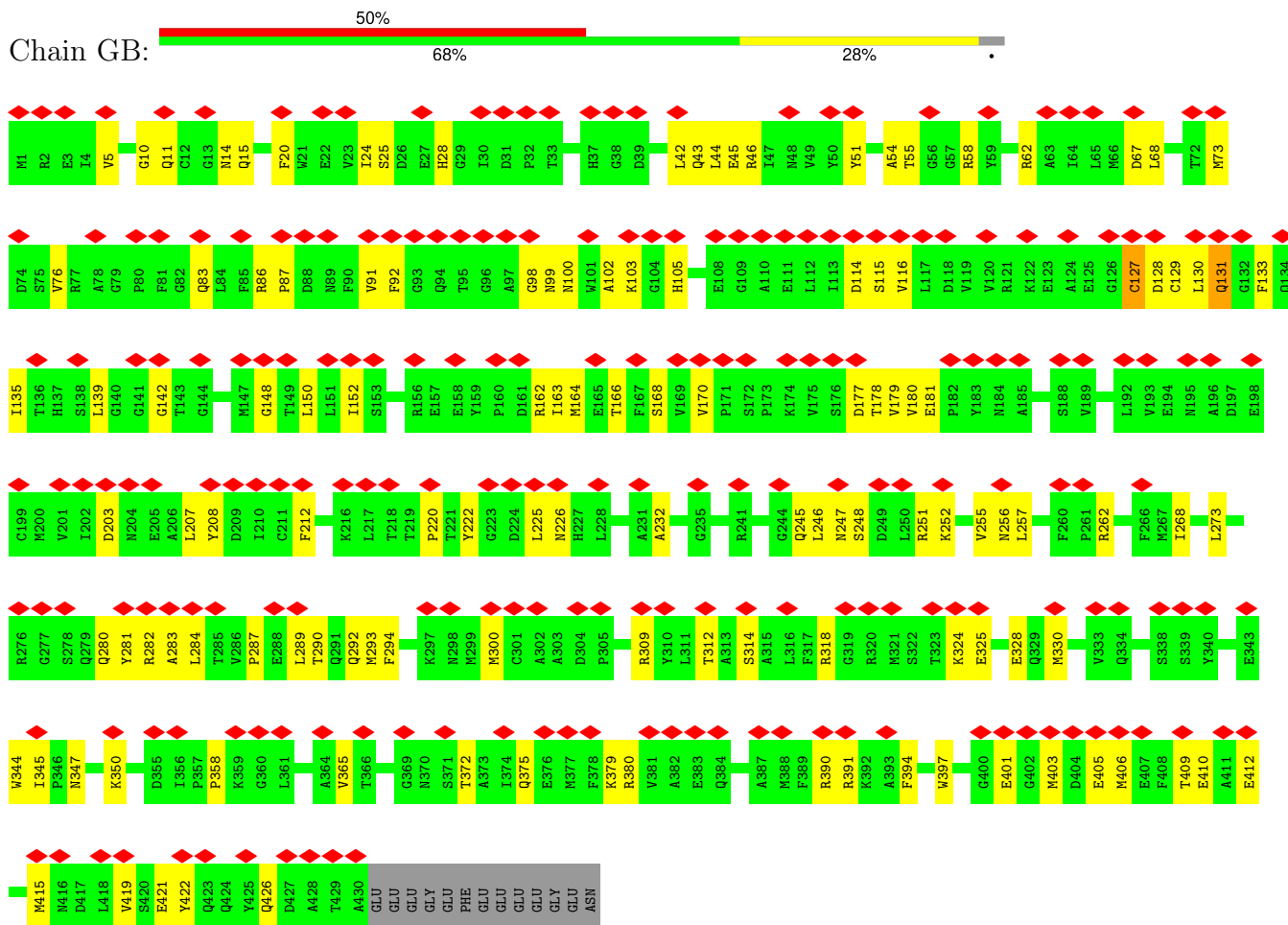




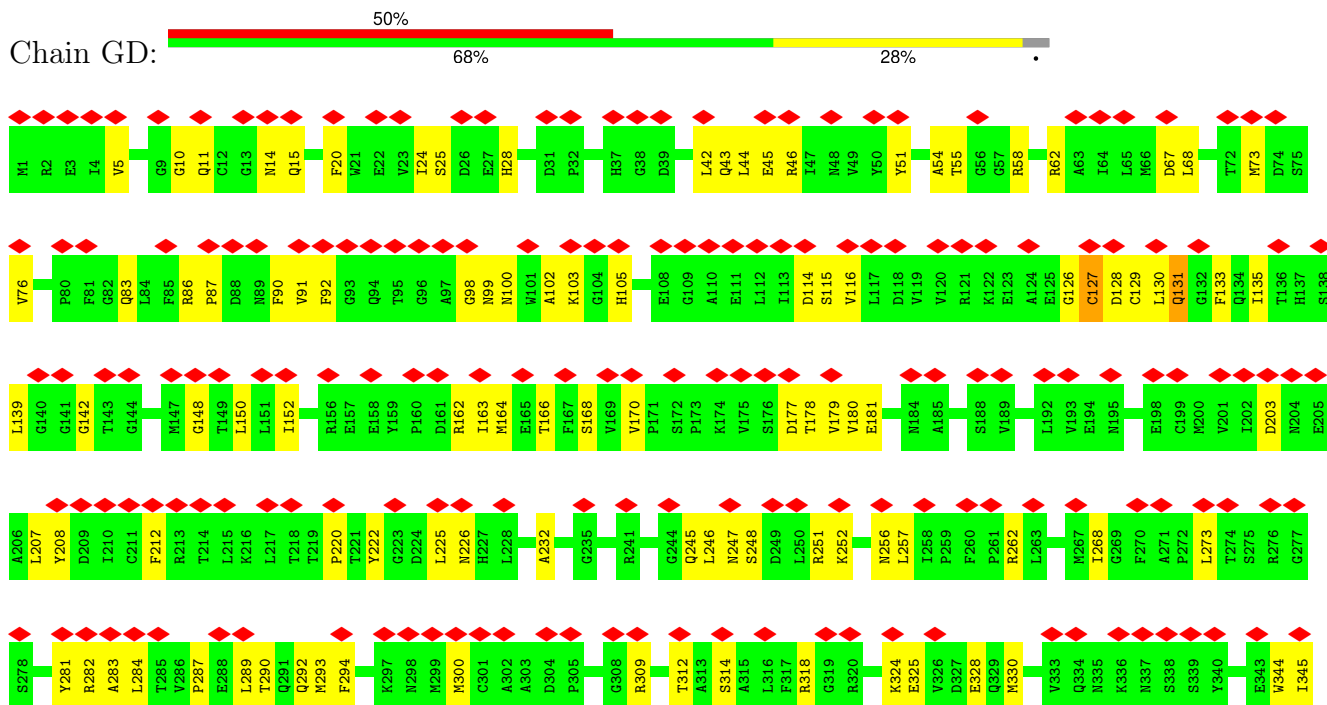
• Molecule 2: Tubulin beta chain

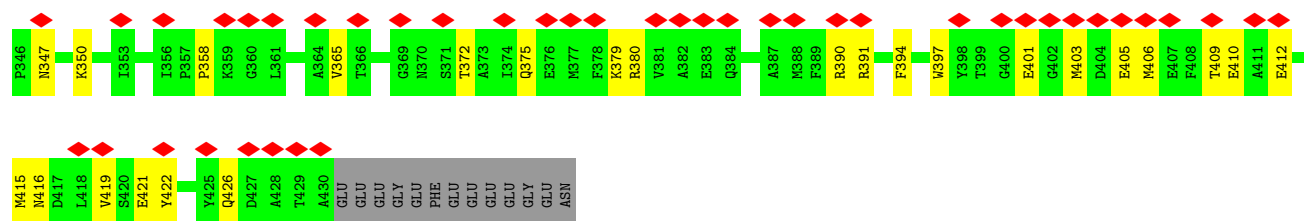


- Molecule 2: Tubulin beta chain

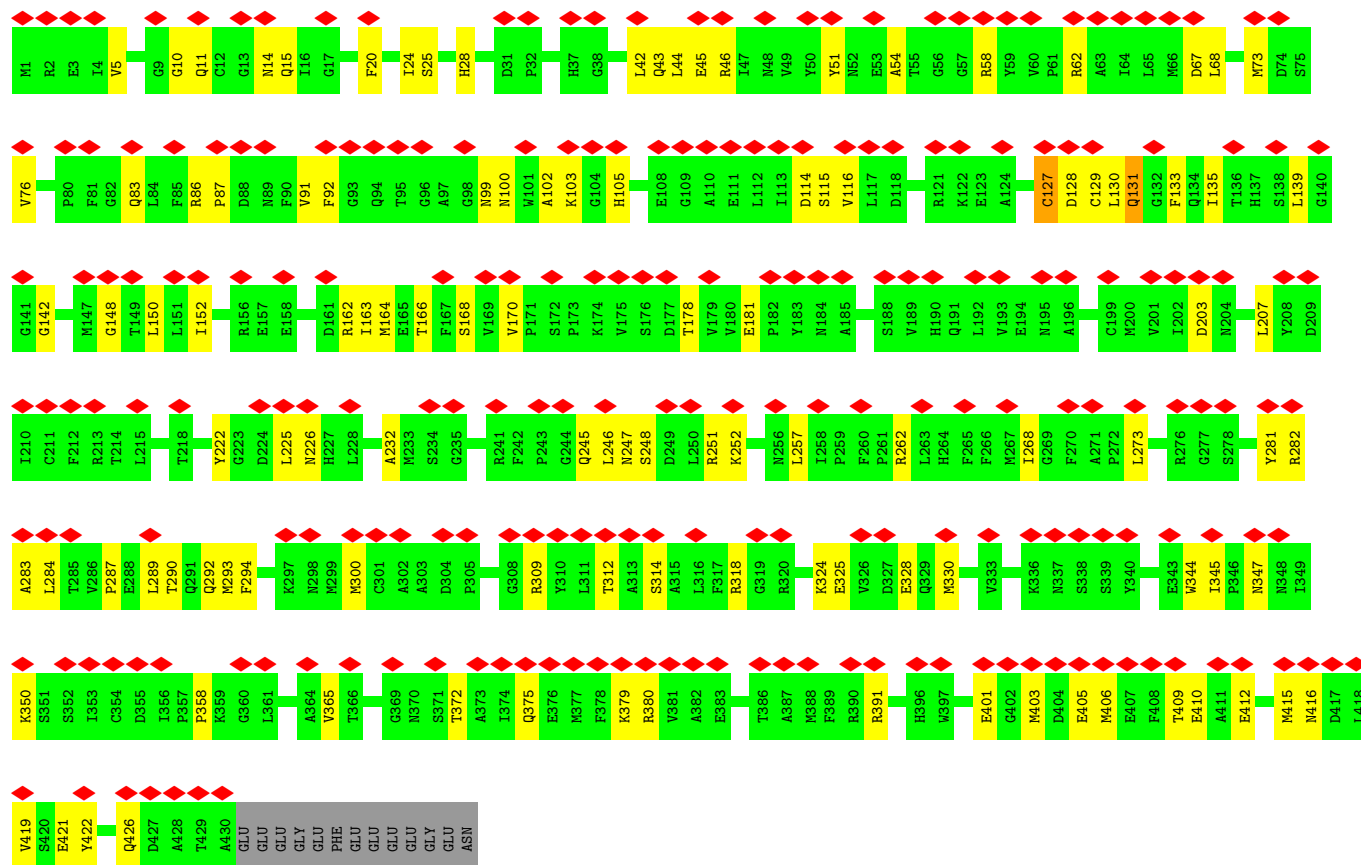


- Molecule 2: Tubulin beta chain



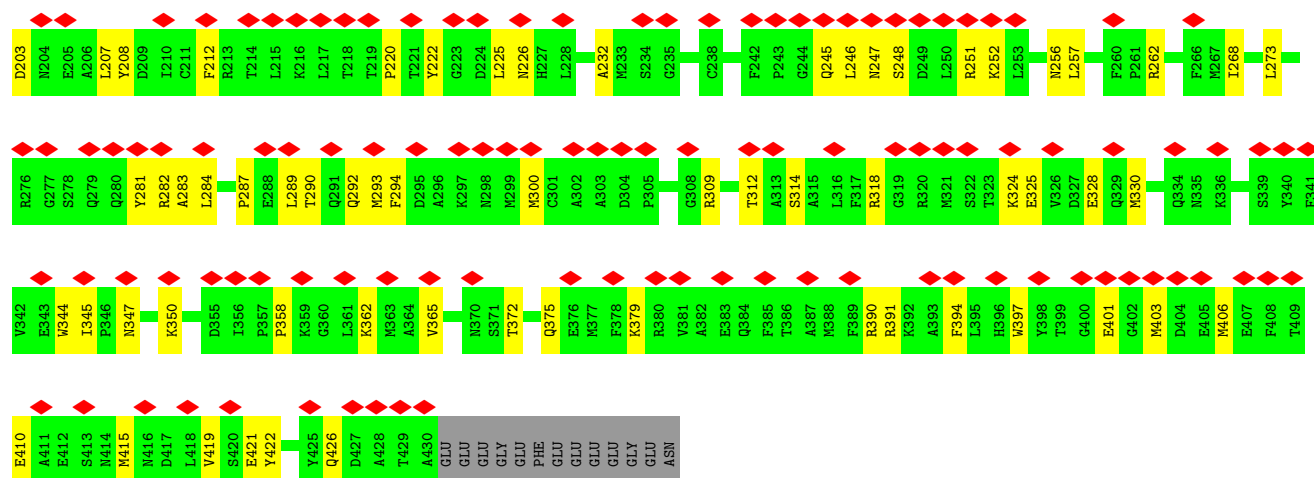


• Molecule 2: Tubulin beta chain

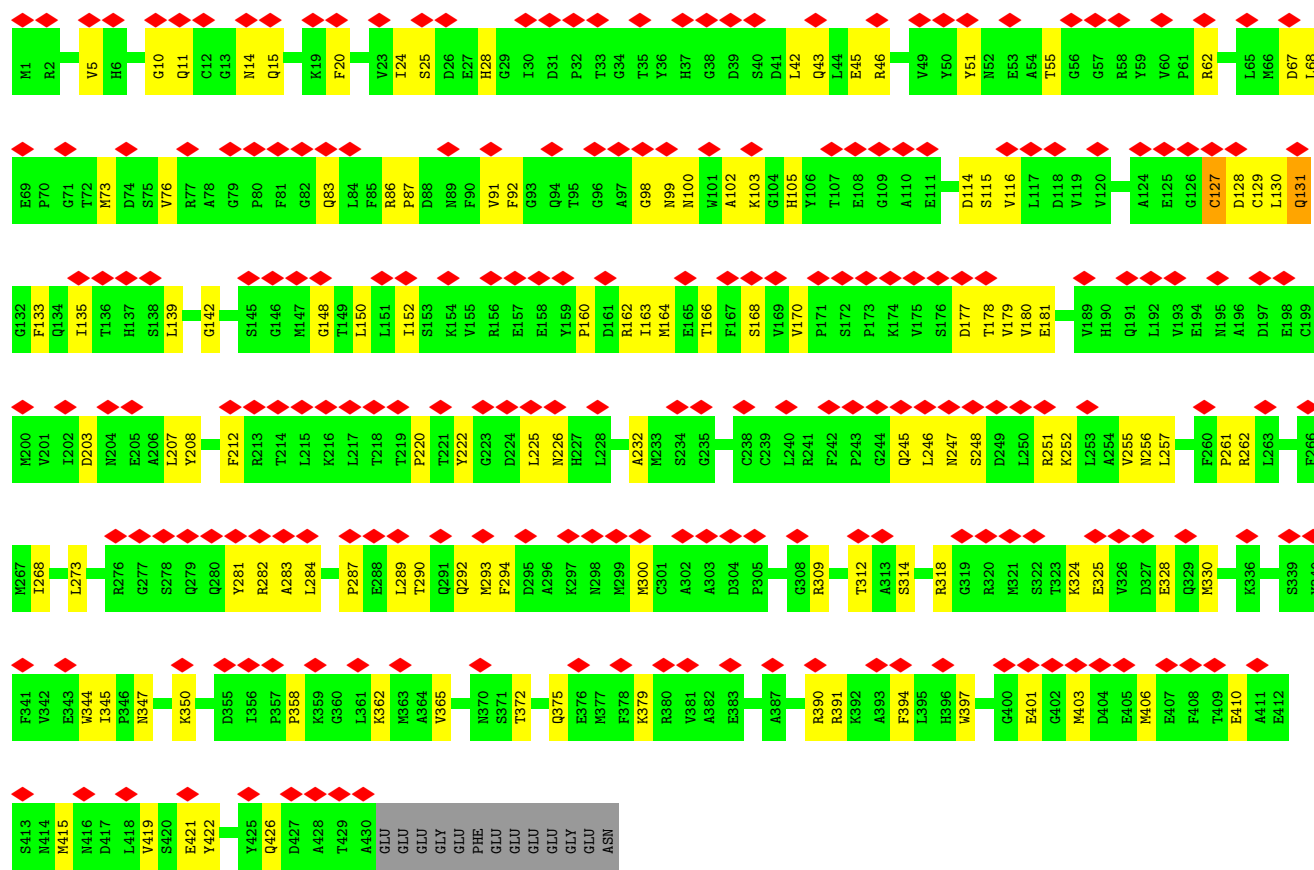
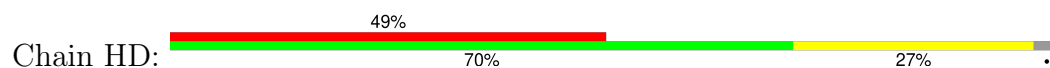


• Molecule 2: Tubulin beta chain

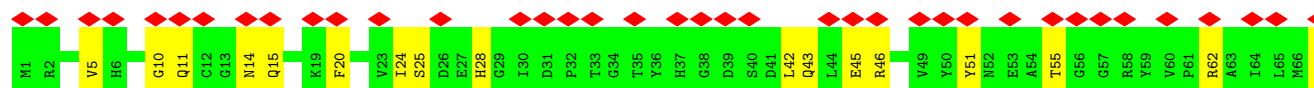
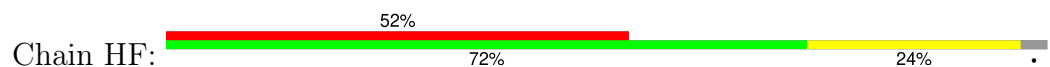


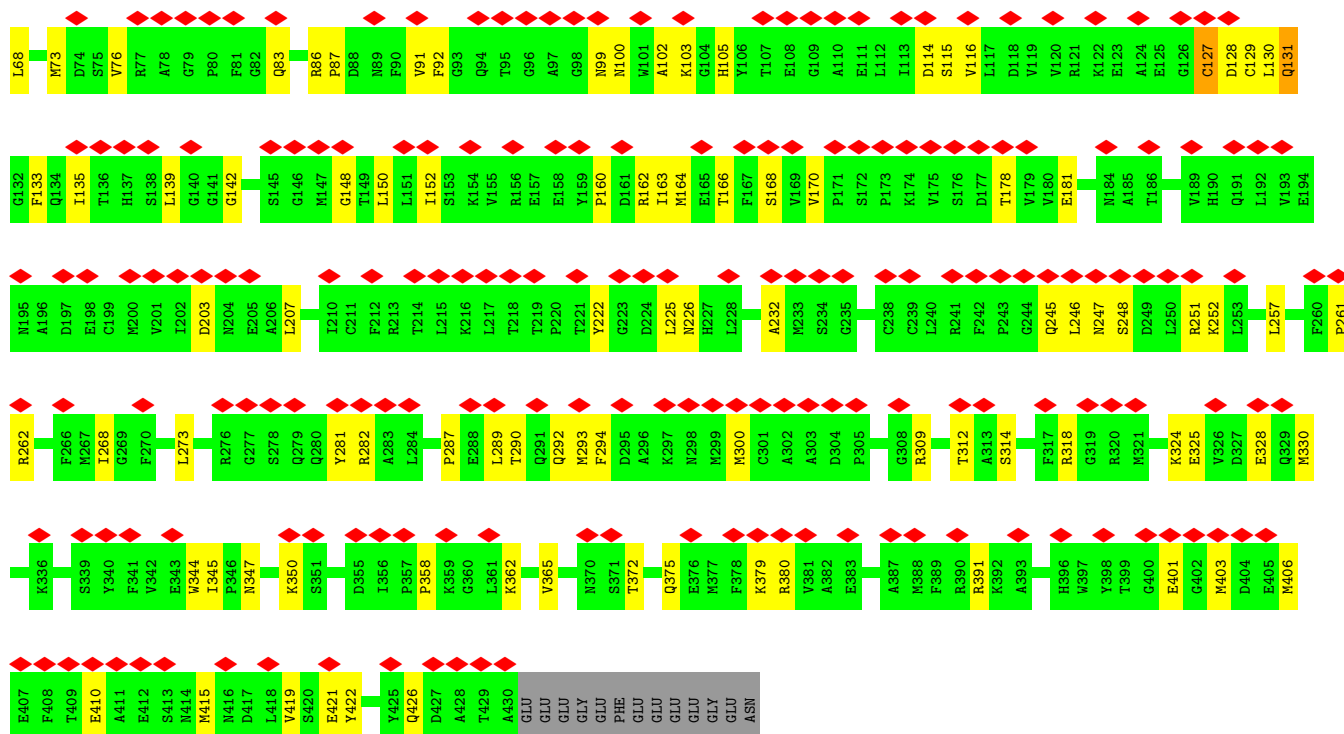


• Molecule 2: Tubulin beta chain

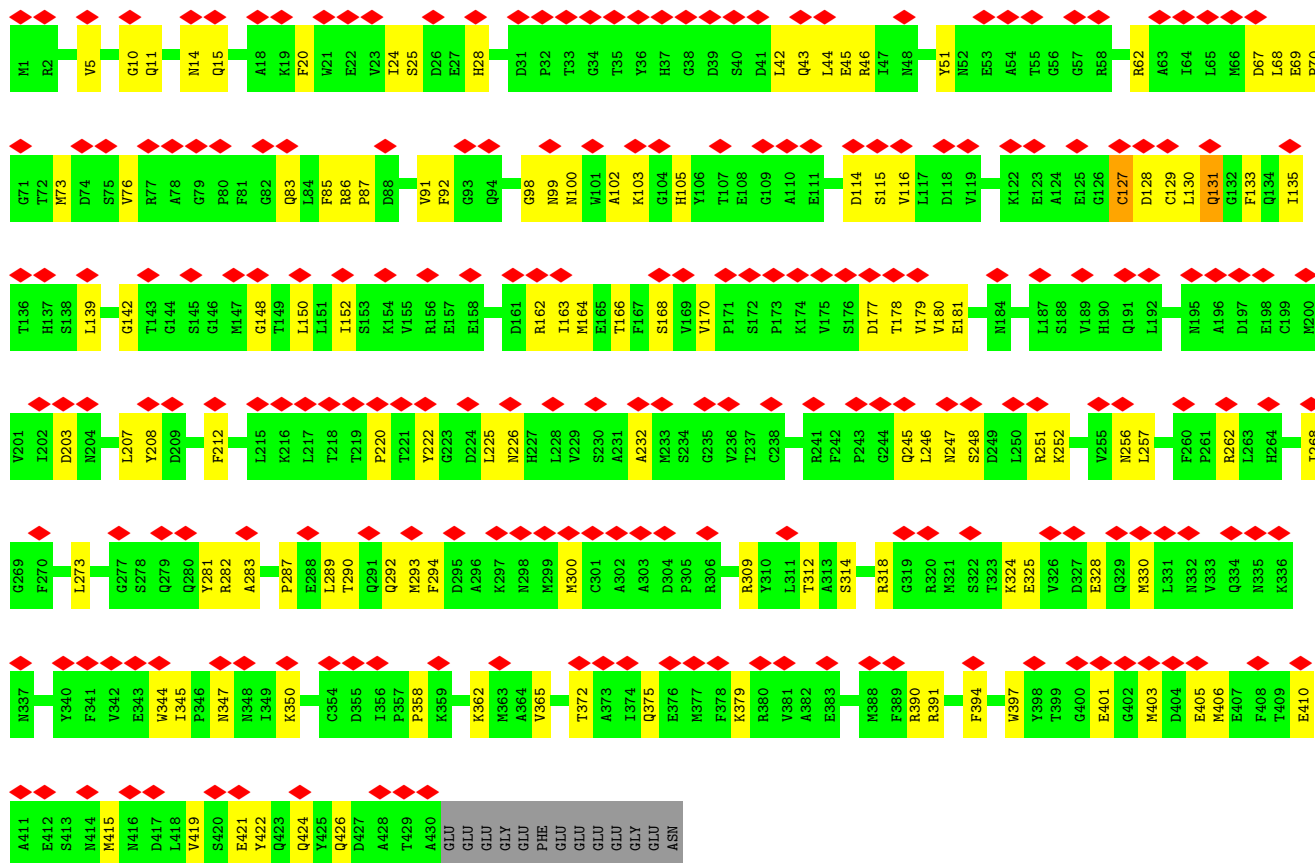


• Molecule 2: Tubulin beta chain

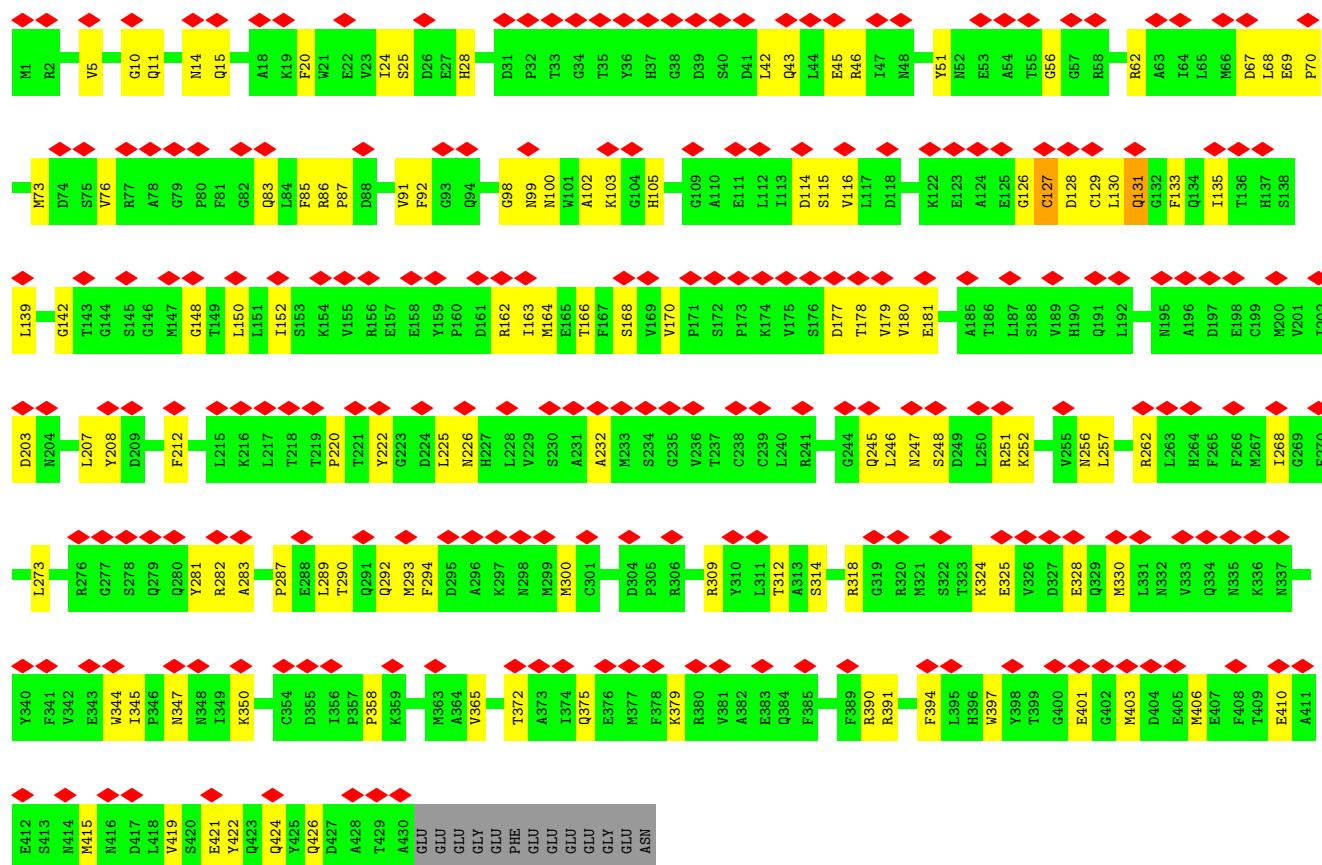




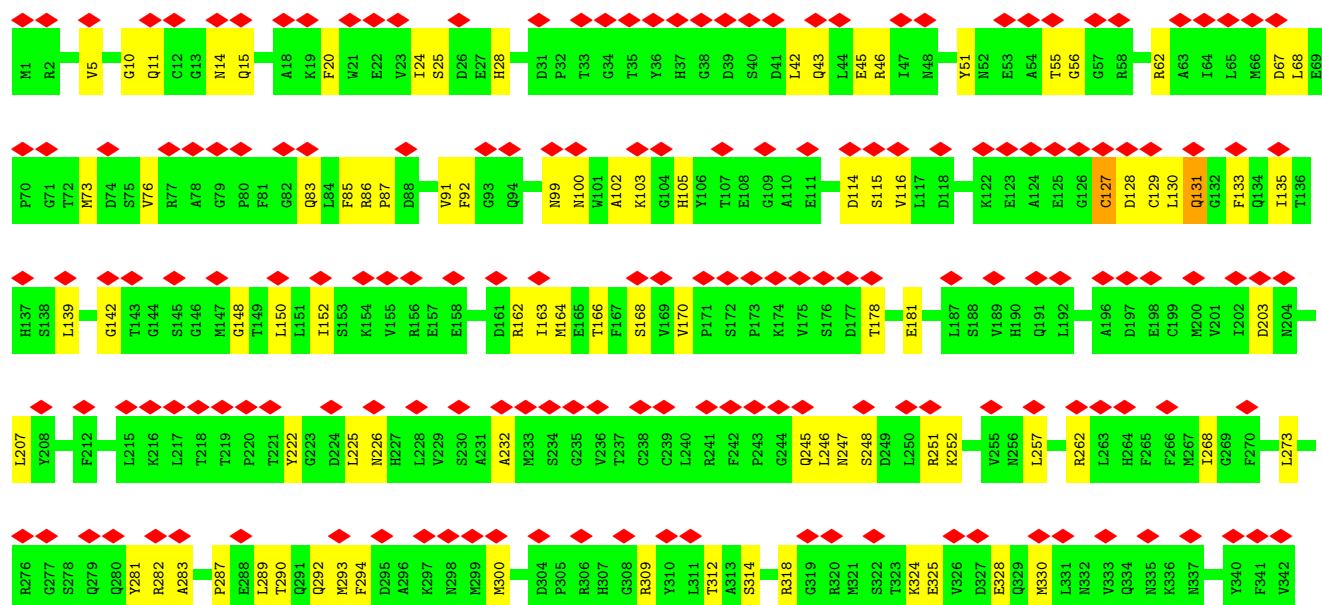
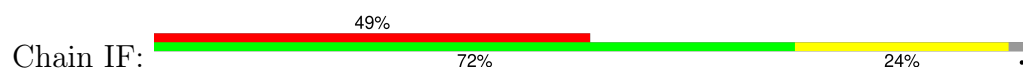
• Molecule 2: Tubulin beta chain

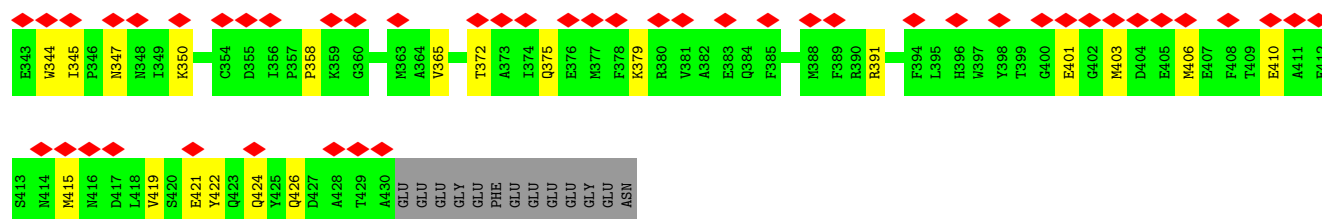


- Molecule 2: Tubulin beta chain

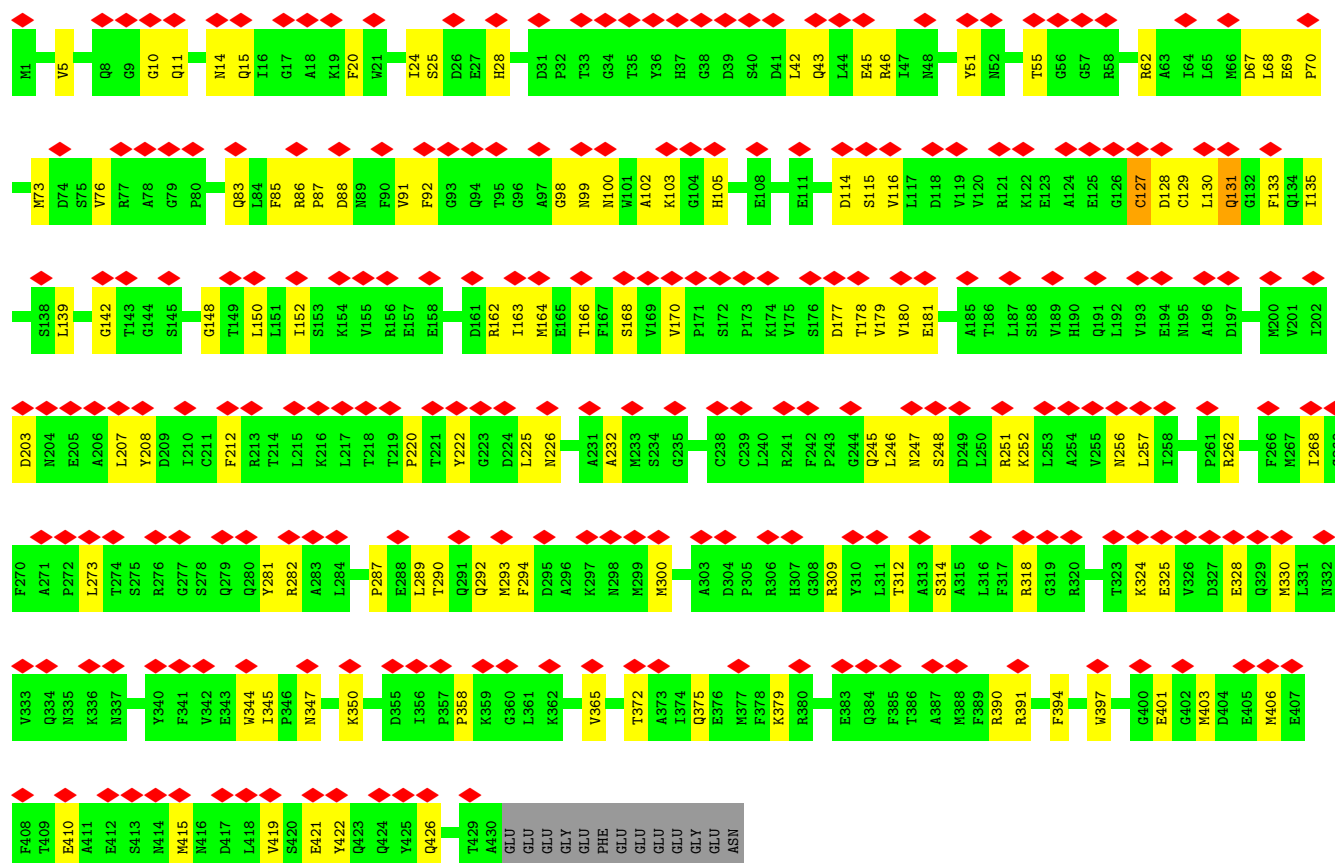


- Molecule 2: Tubulin beta chain

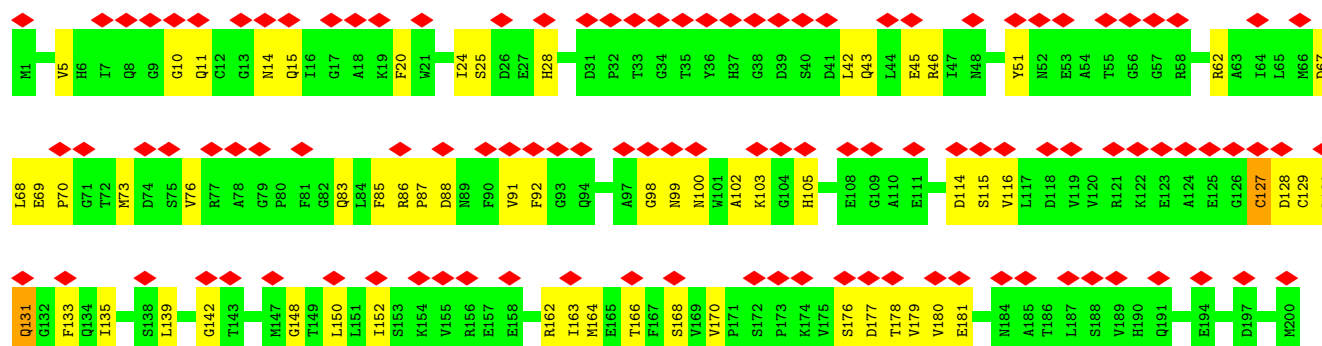
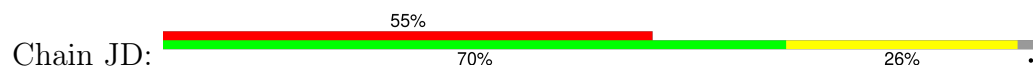


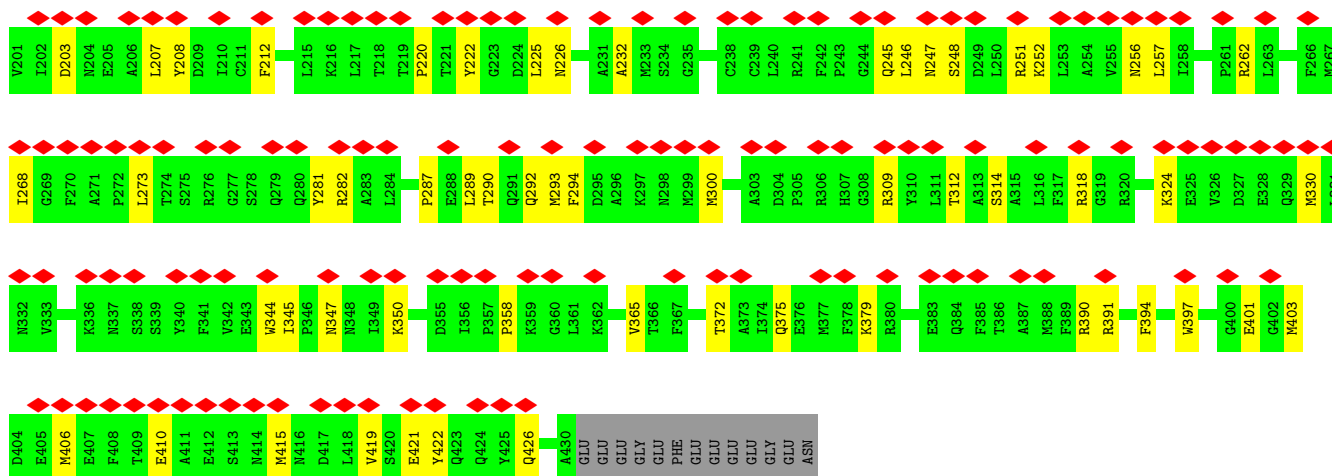


• Molecule 2: Tubulin beta chain

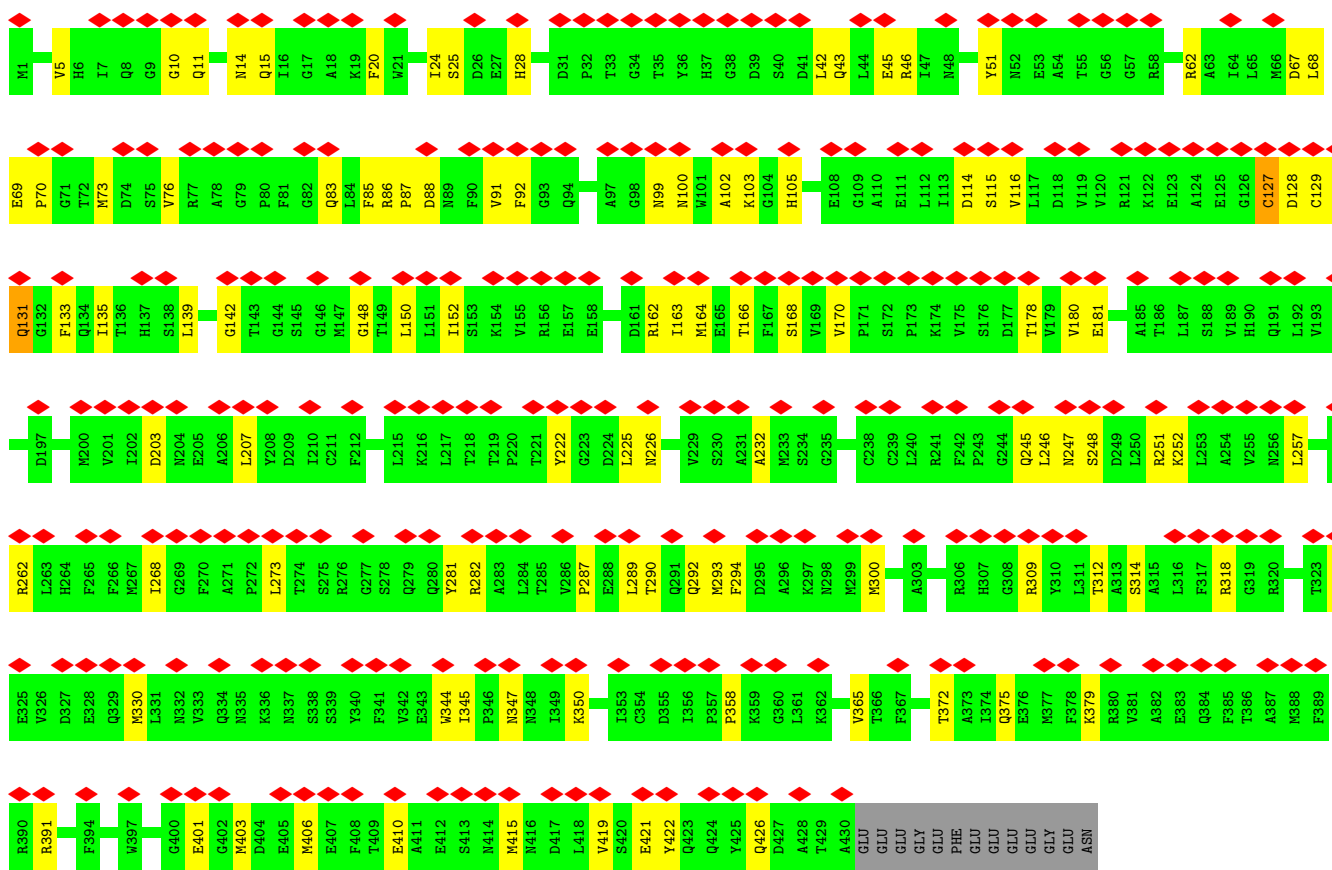
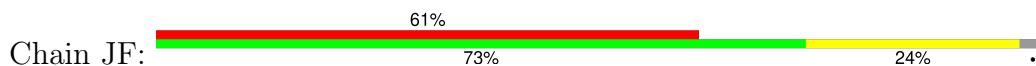


• Molecule 2: Tubulin beta chain

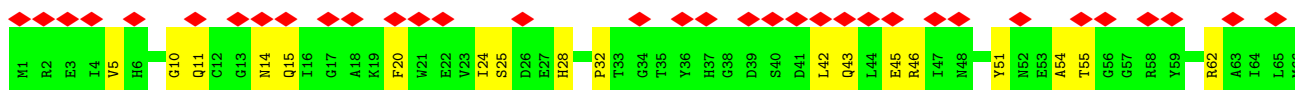


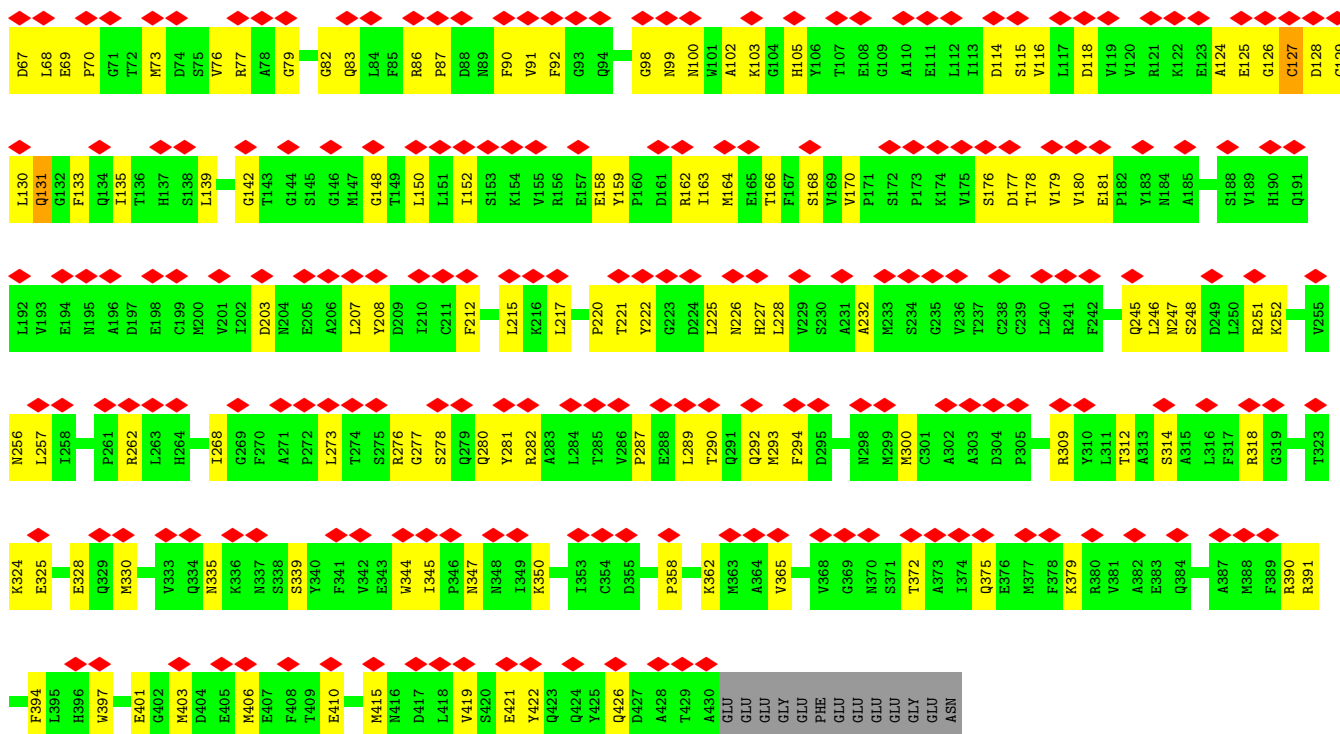


• Molecule 2: Tubulin beta chain

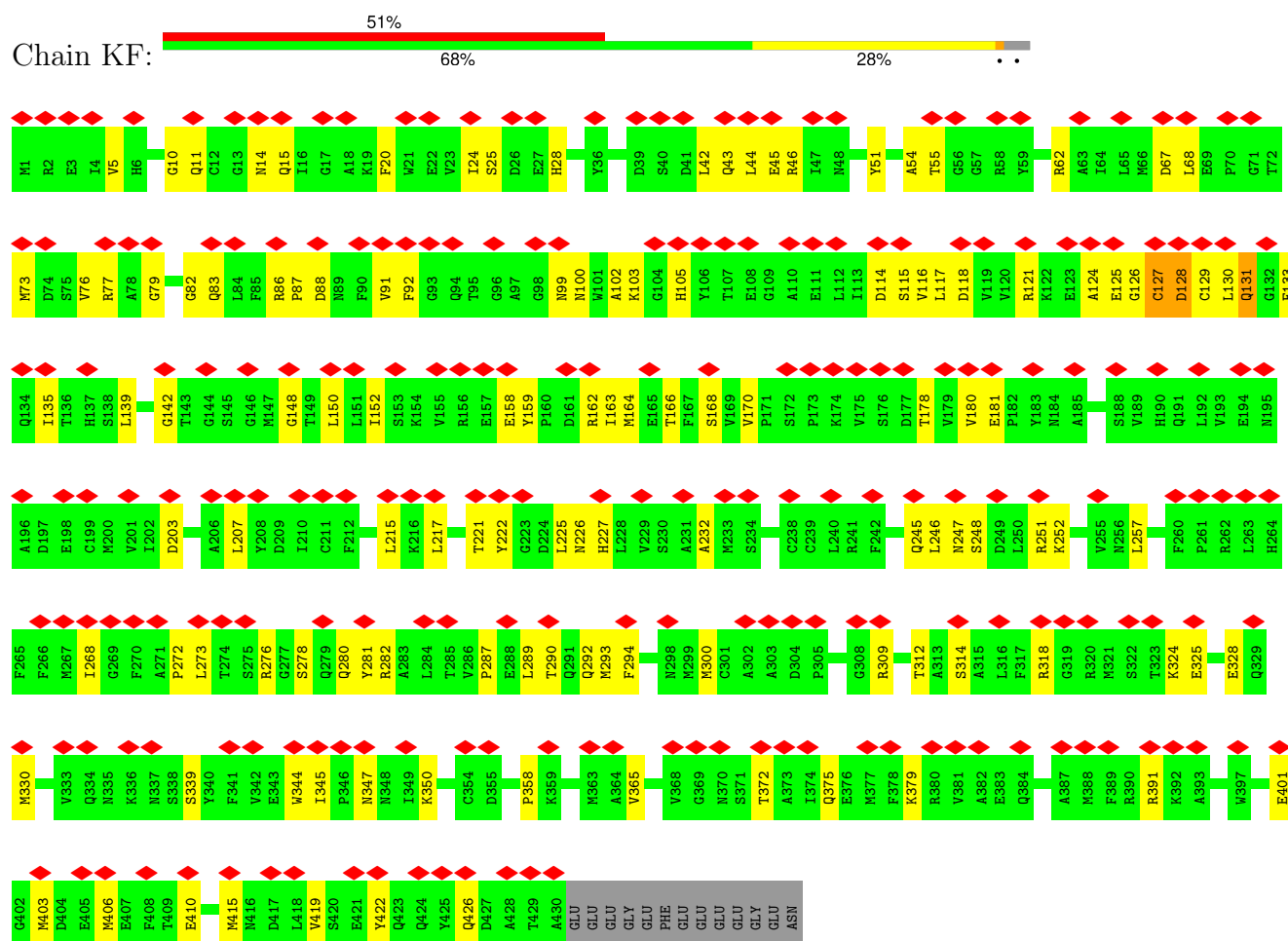


• Molecule 2: Tubulin beta chain

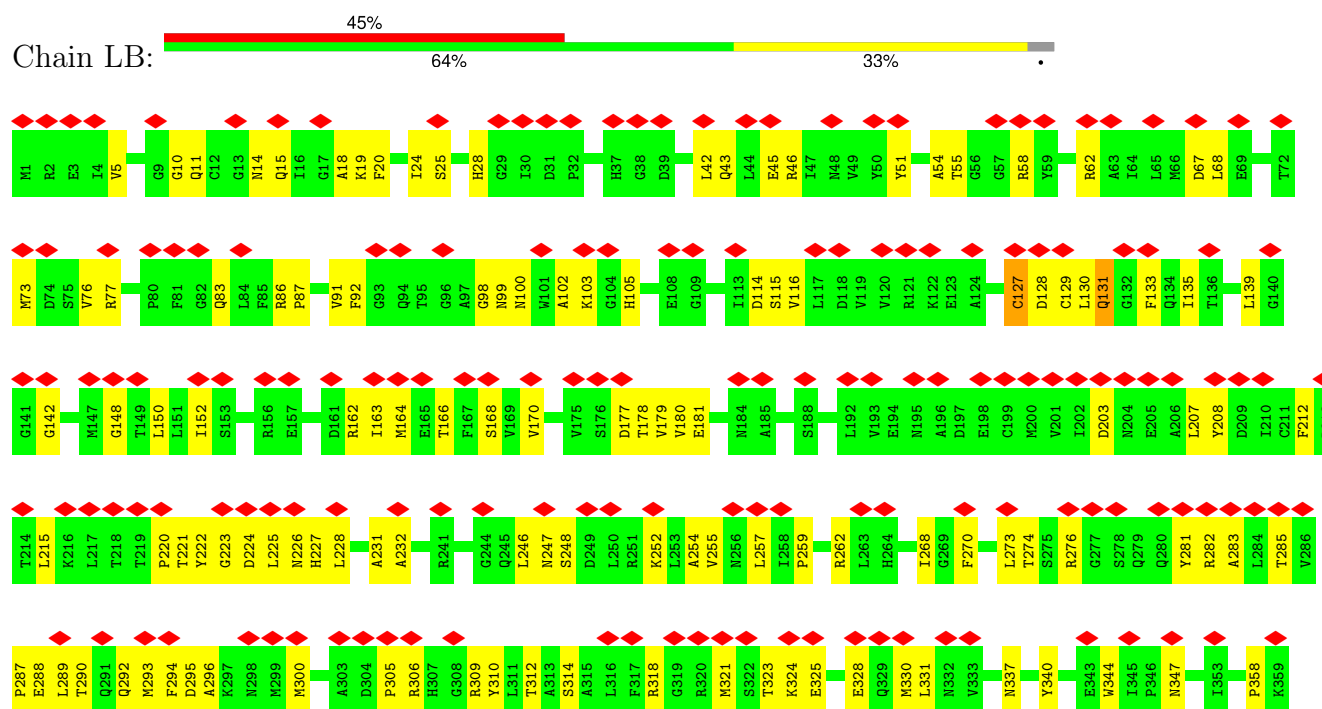


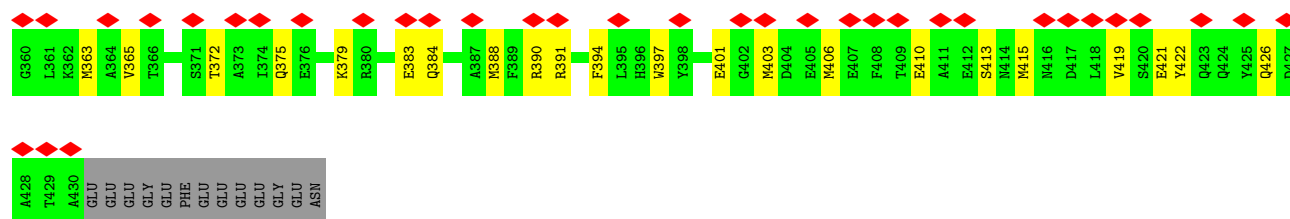


- Molecule 2: Tubulin beta chain

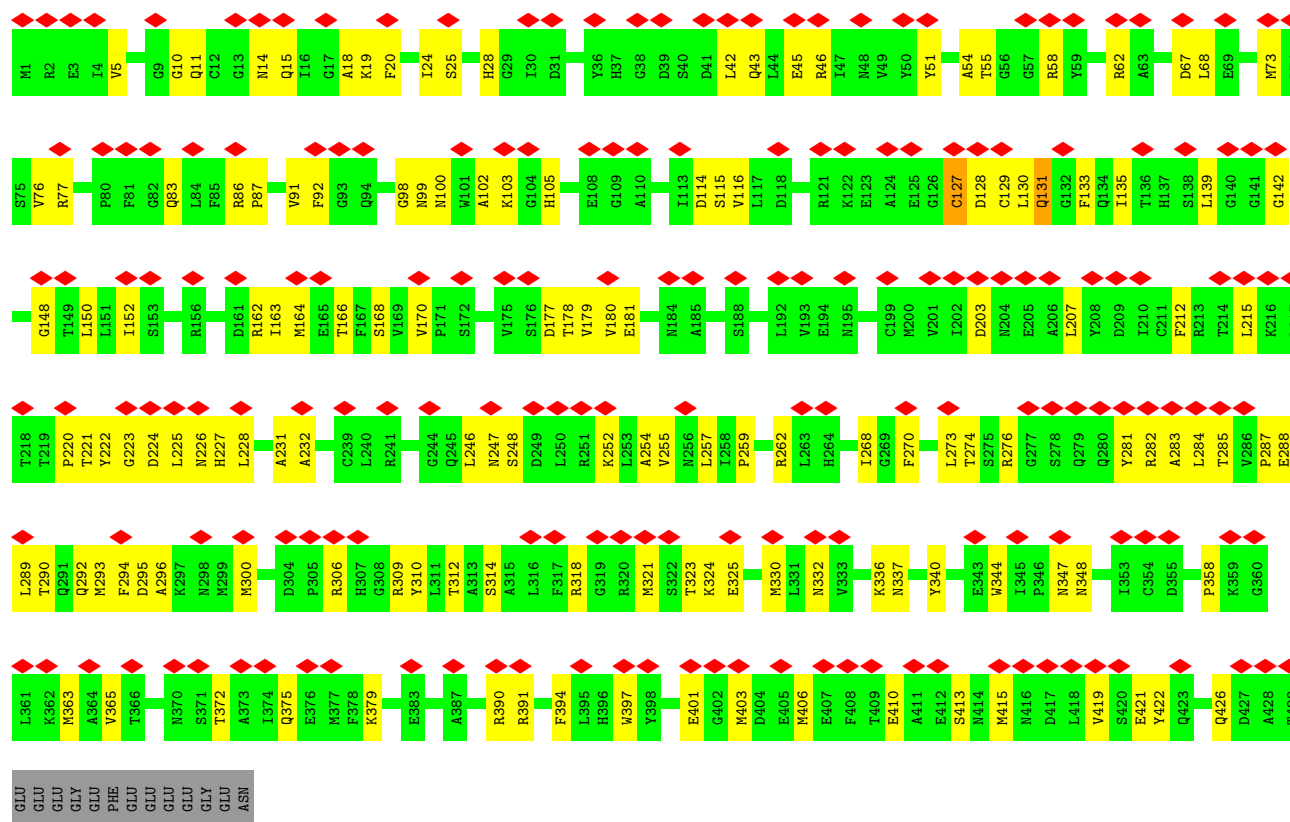
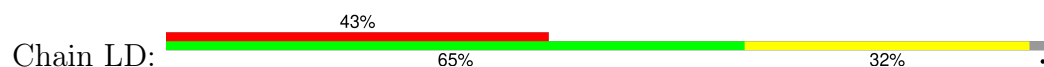


- Molecule 2: Tubulin beta chain

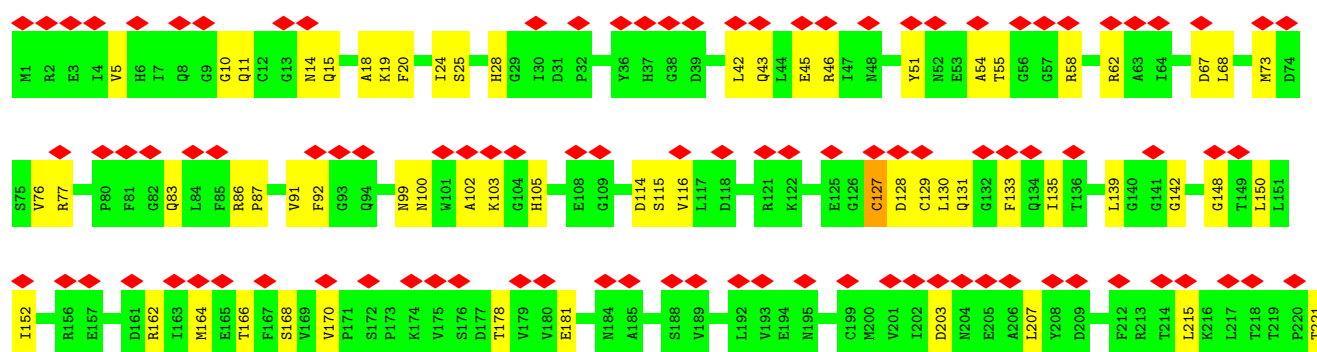
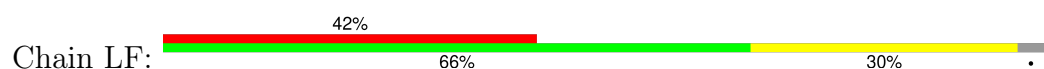


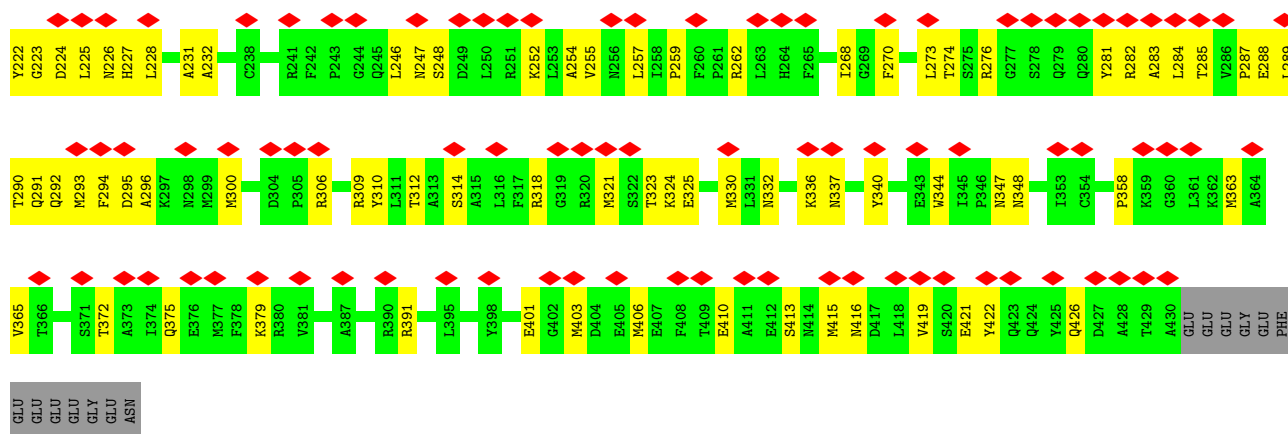


• Molecule 2: Tubulin beta chain

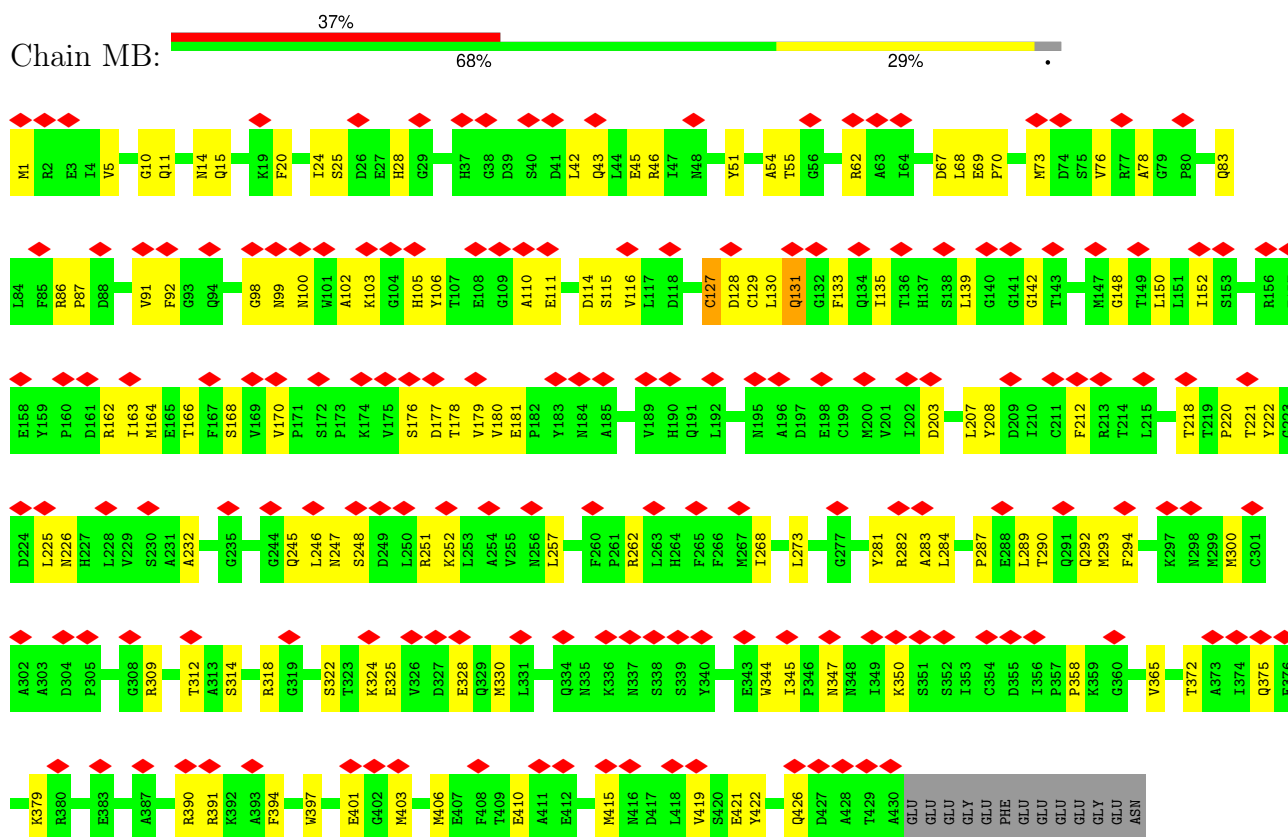


• Molecule 2: Tubulin beta chain

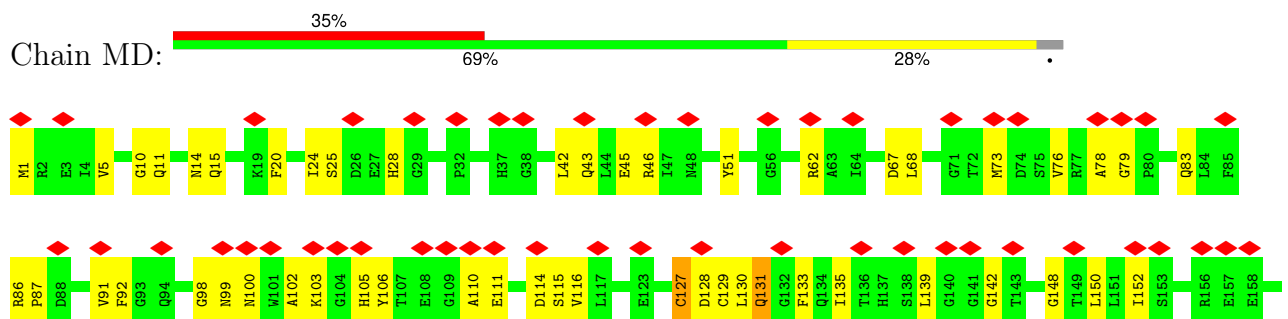


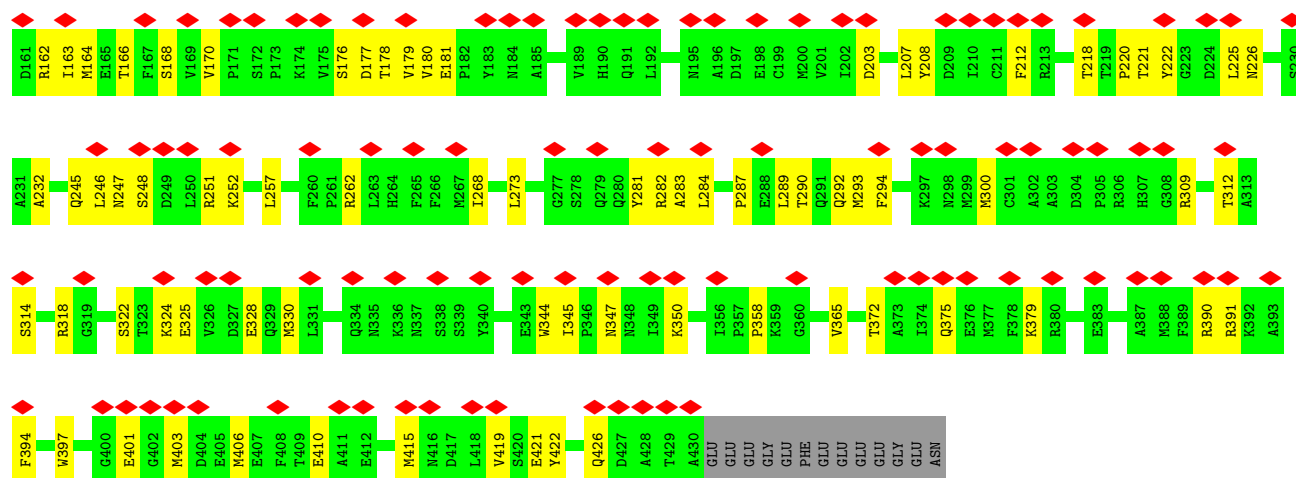


• Molecule 2: Tubulin beta chain

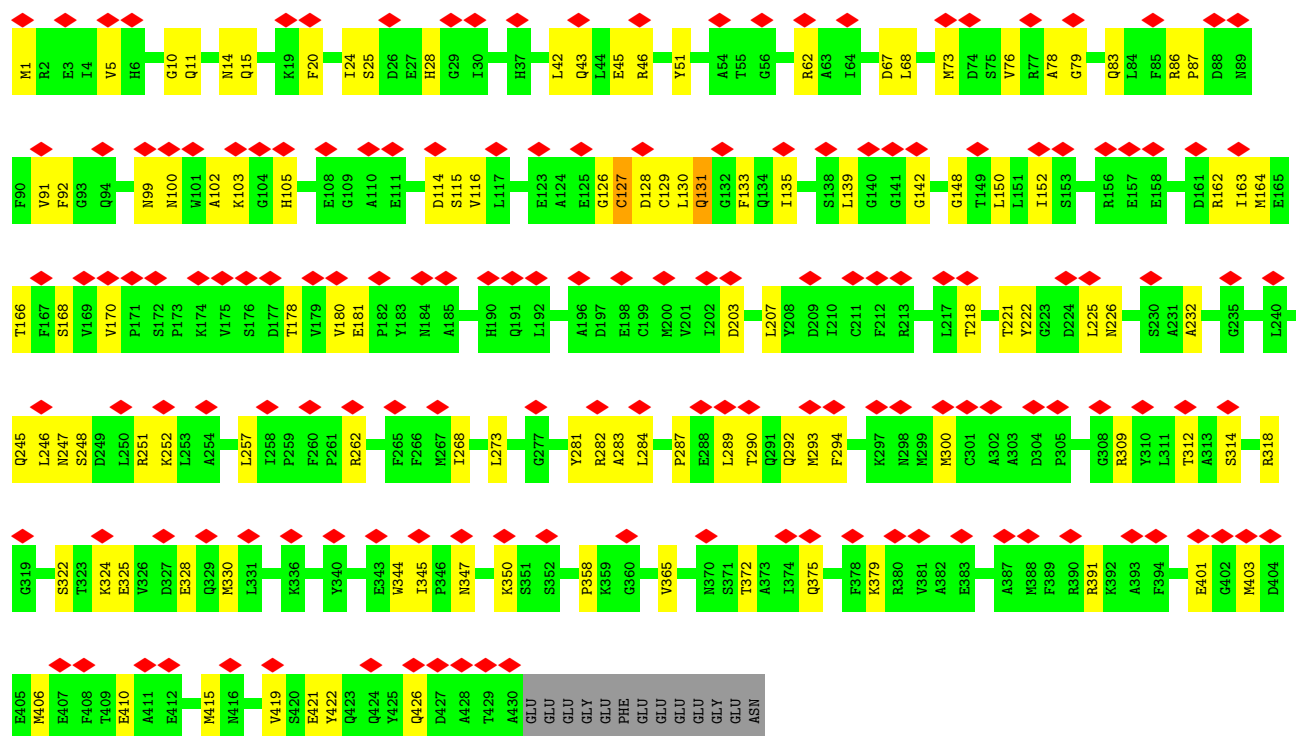
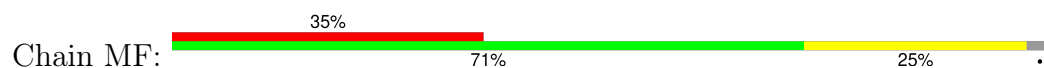


• Molecule 2: Tubulin beta chain

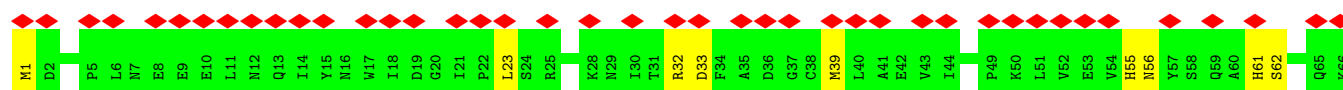


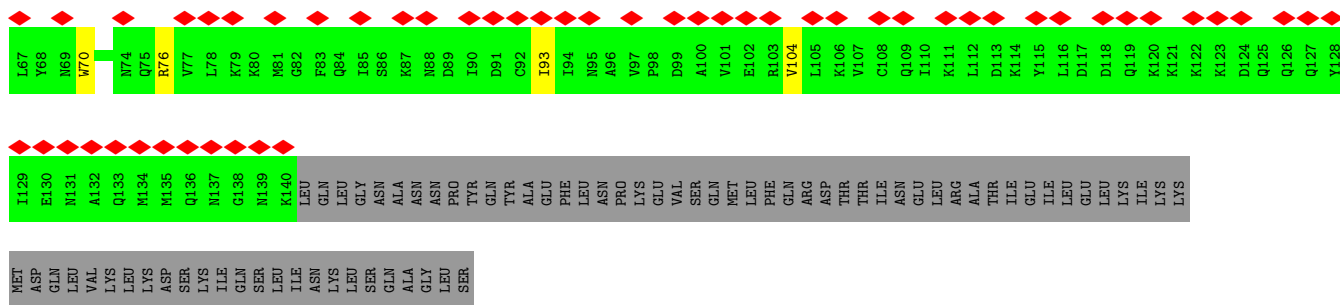


• Molecule 2: Tubulin beta chain

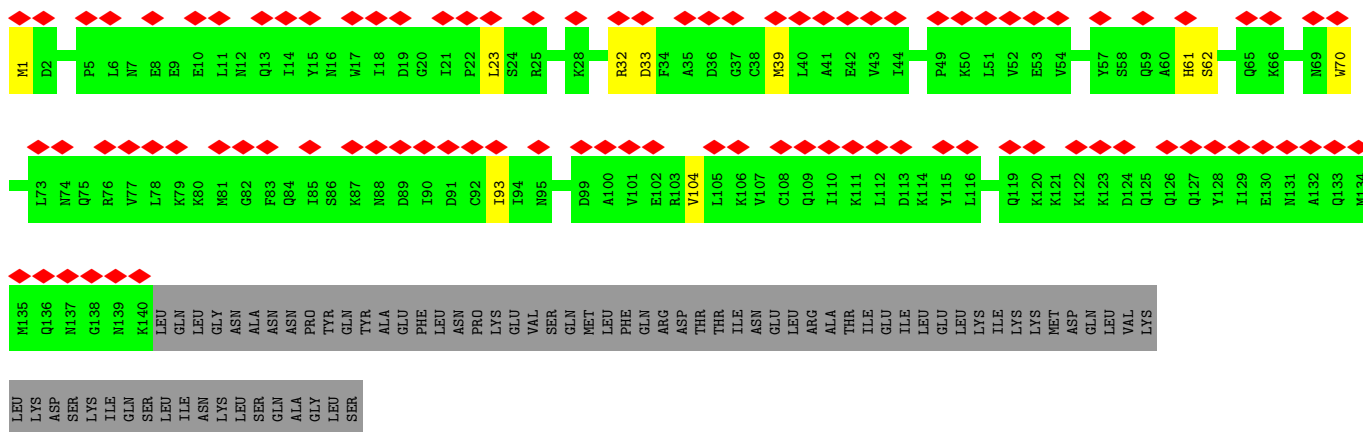


• Molecule 3: Sperm flagellar protein

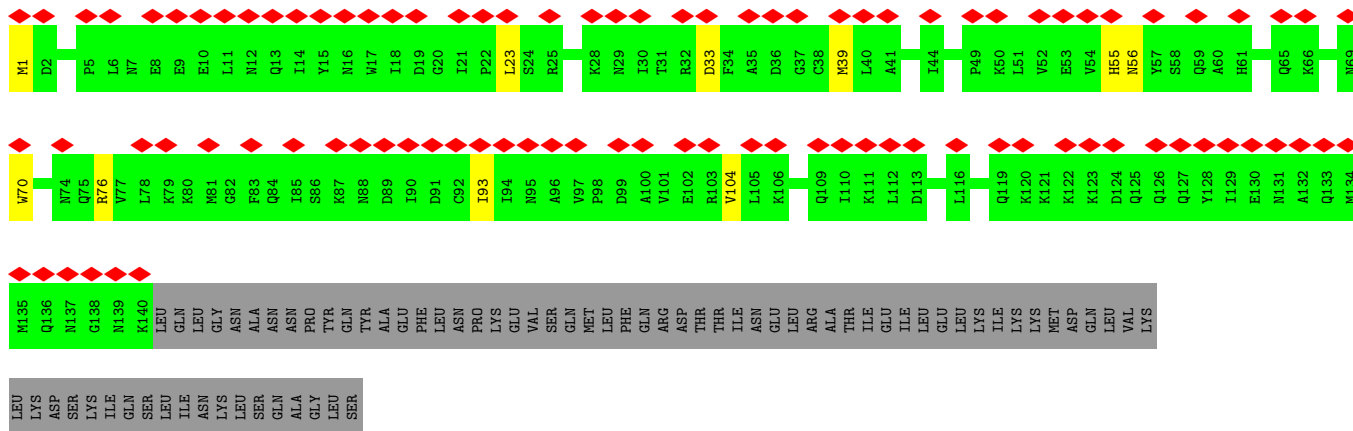




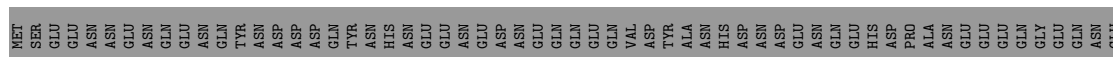
- Molecule 3: Sperm flagellar protein



- Molecule 3: Sperm flagellar protein



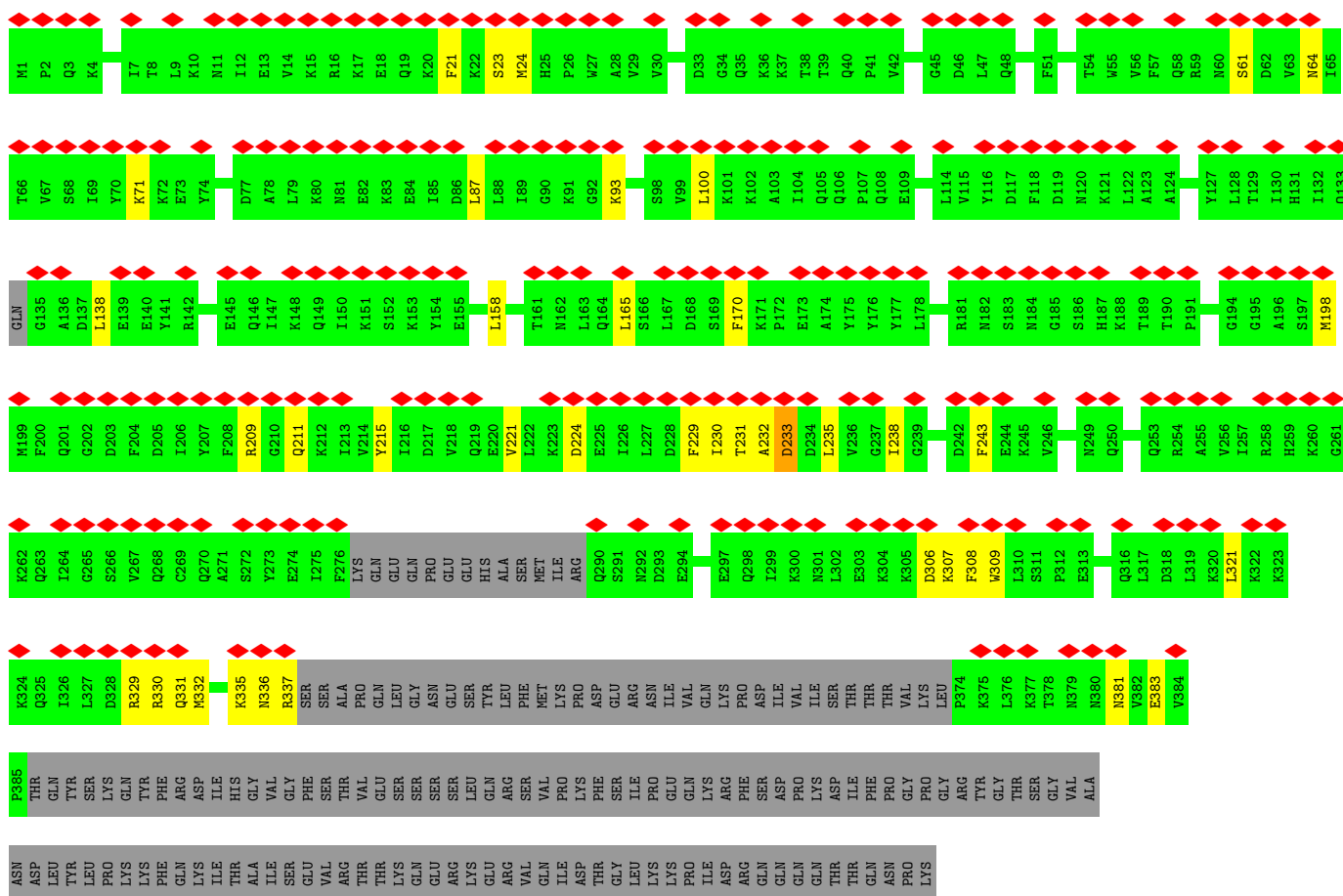
- Molecule 4: TLP1





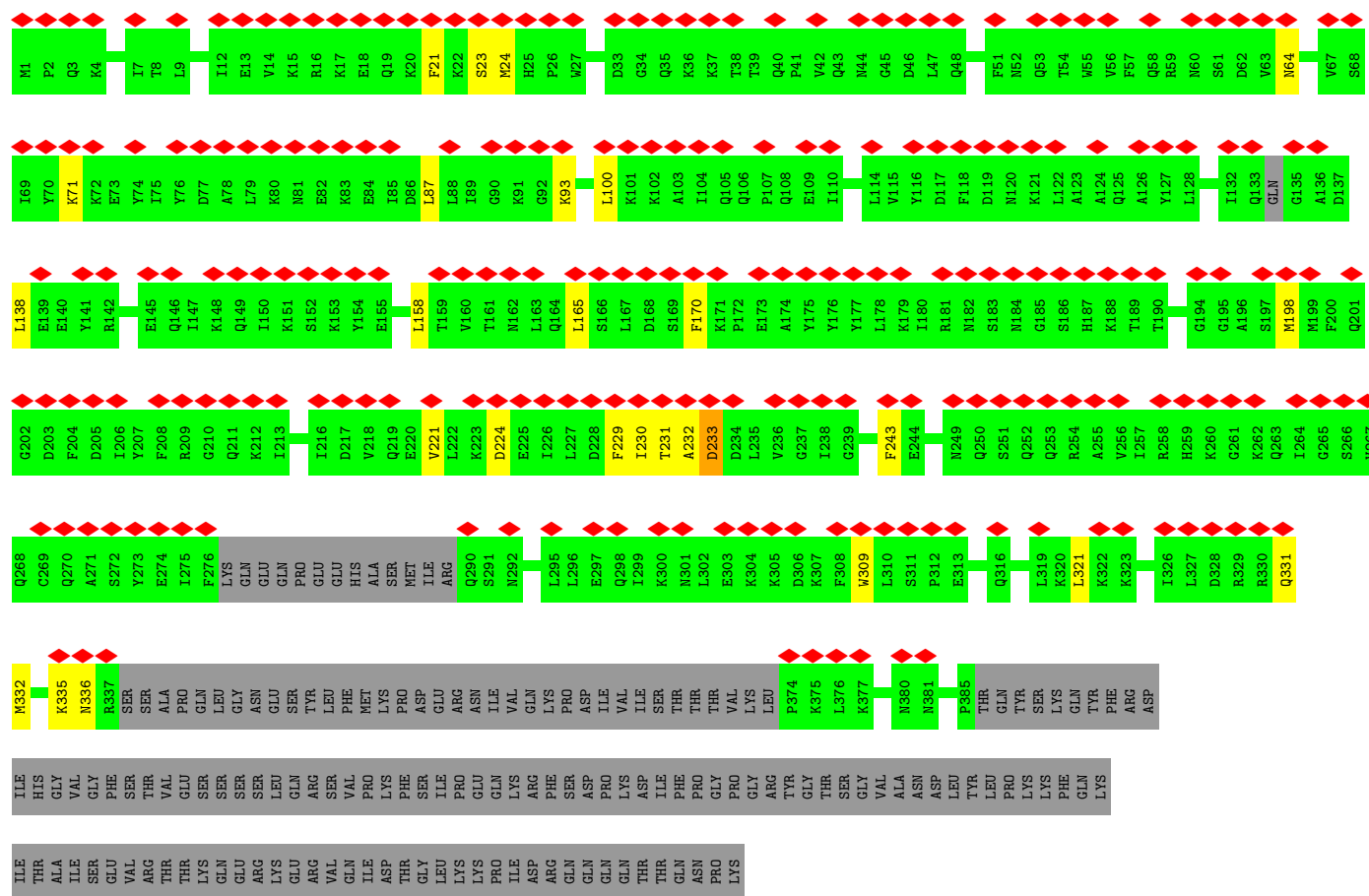


- Molecule 5: C2 domain protein

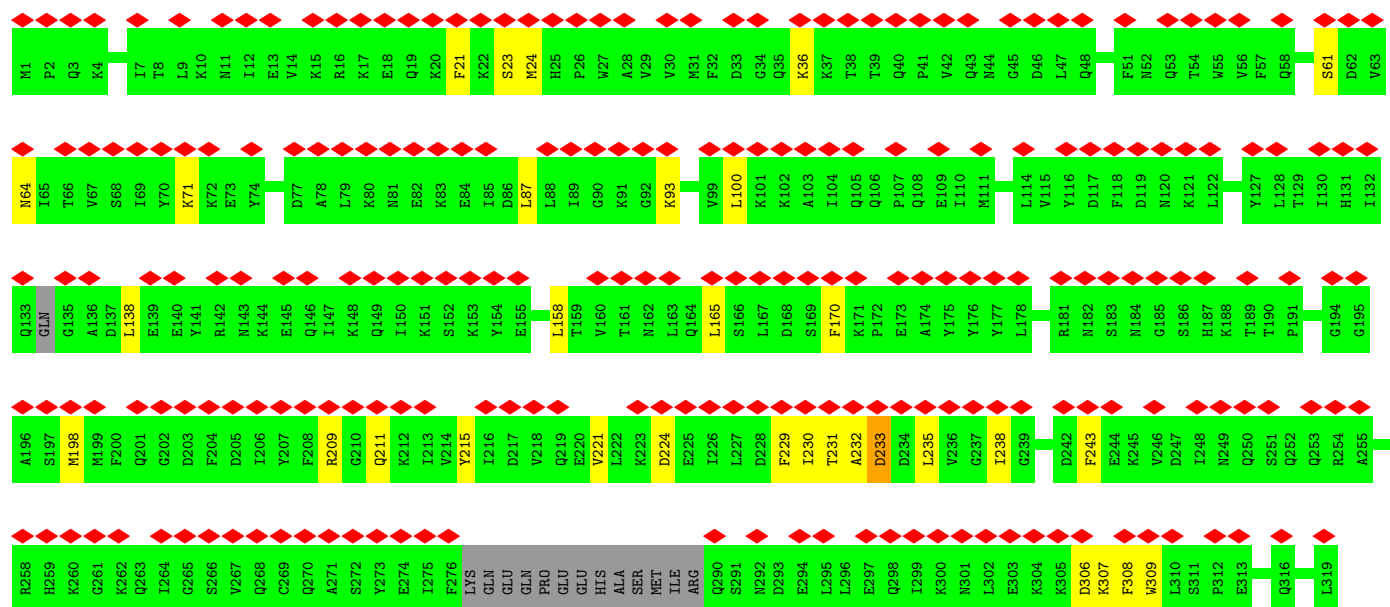


- Molecule 5: C2 domain protein



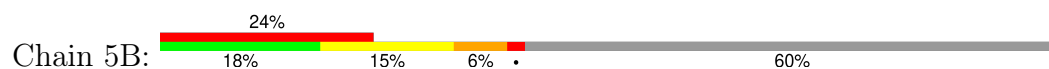


● Molecule 5: C2 domain protein



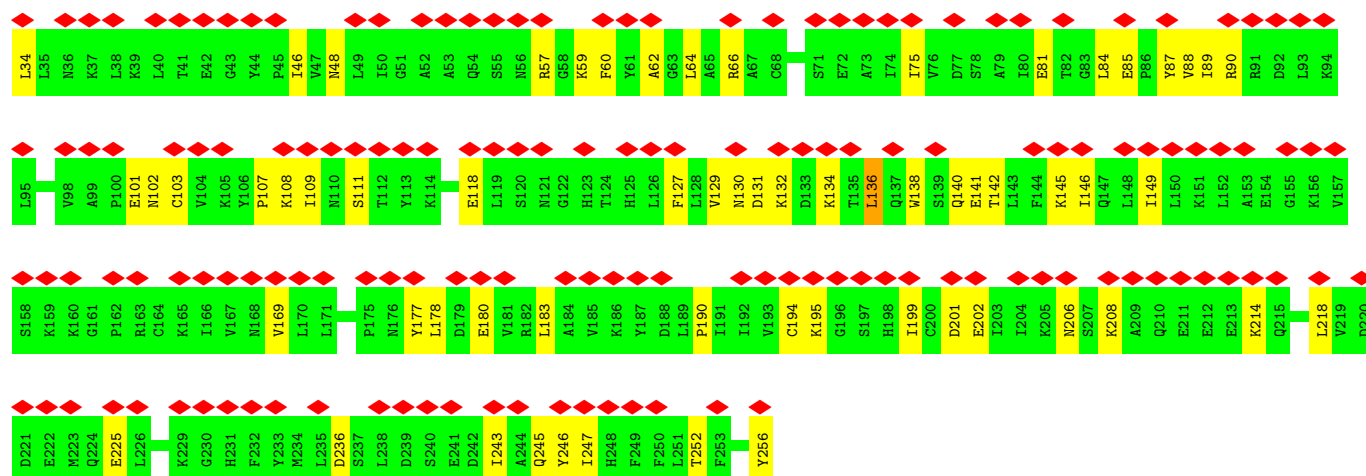




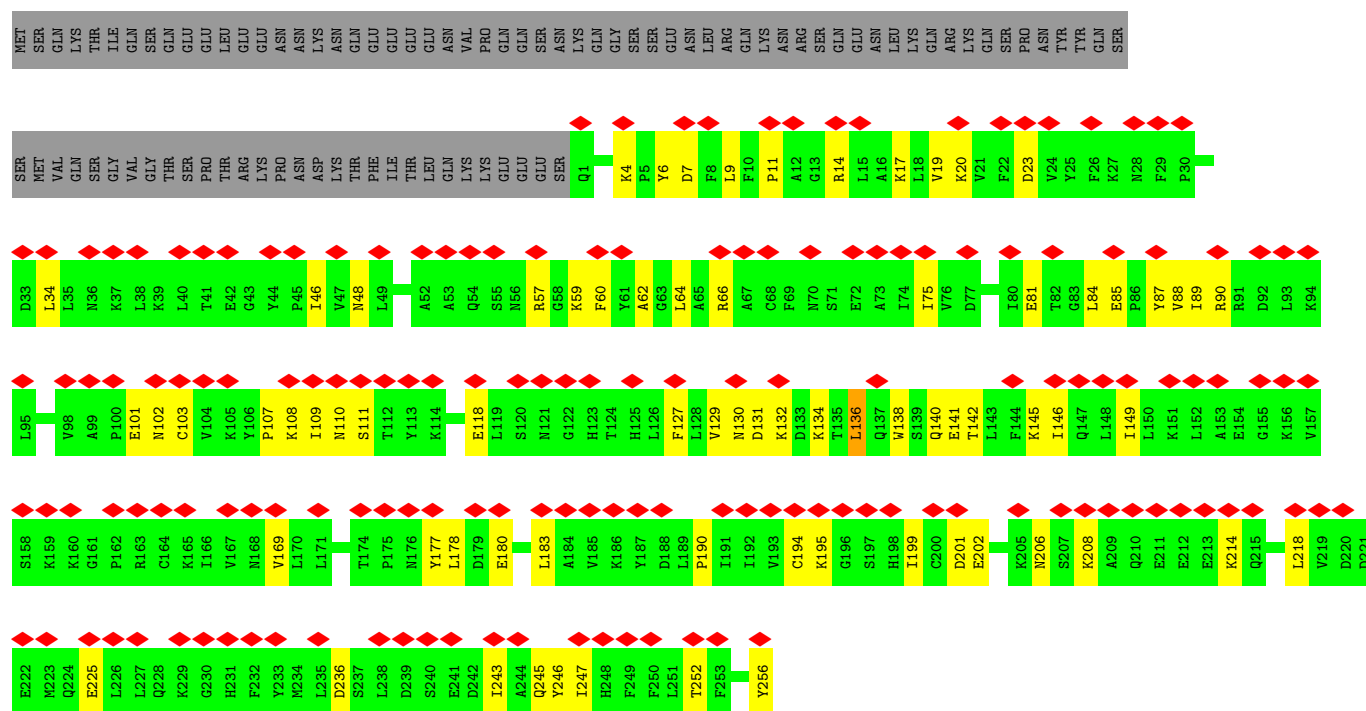




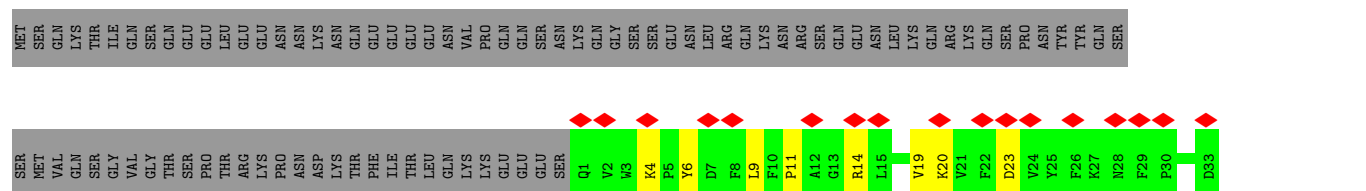


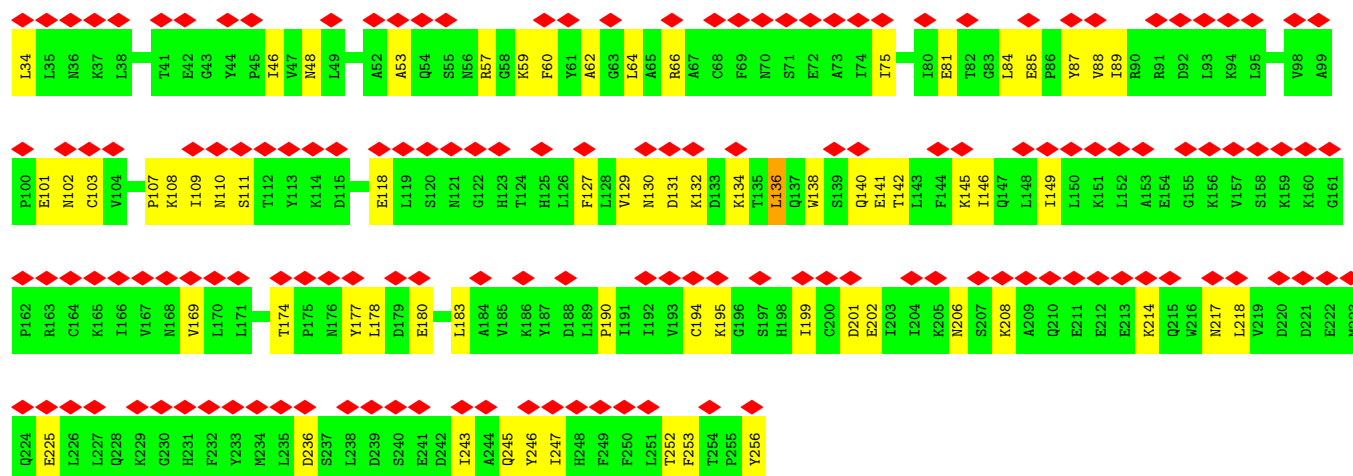


• Molecule 8: Cation channel family protein

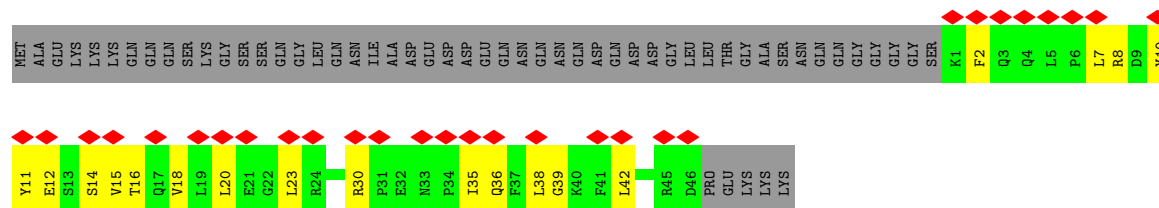
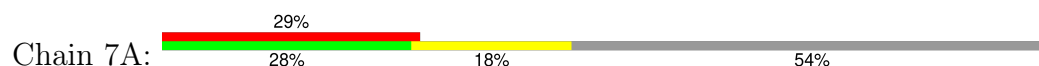


• Molecule 8: Cation channel family protein

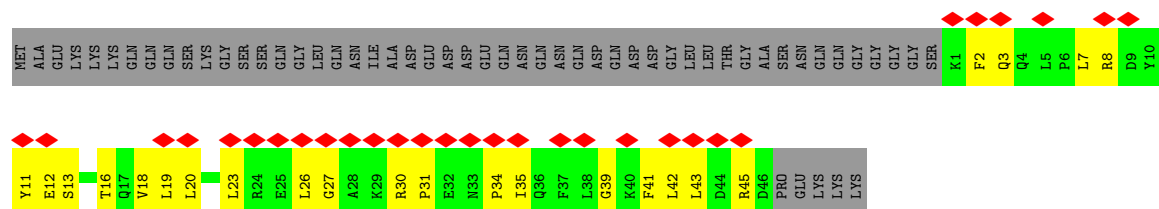
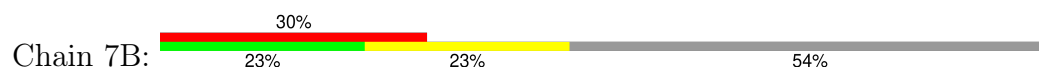




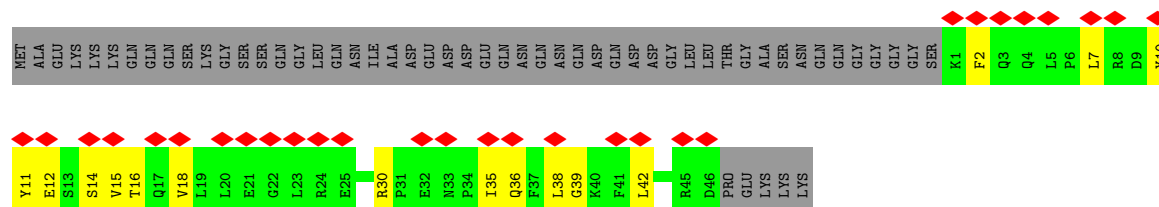
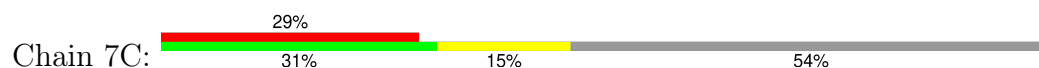
• Molecule 9: Dpy-30 motif protein



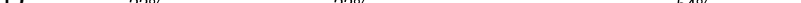
• Molecule 9: Dpy-30 motif protein

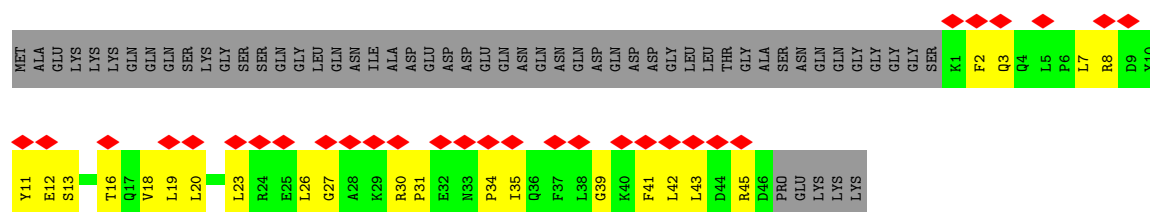


• Molecule 9: Dpy-30 motif protein

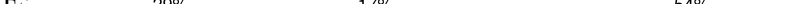


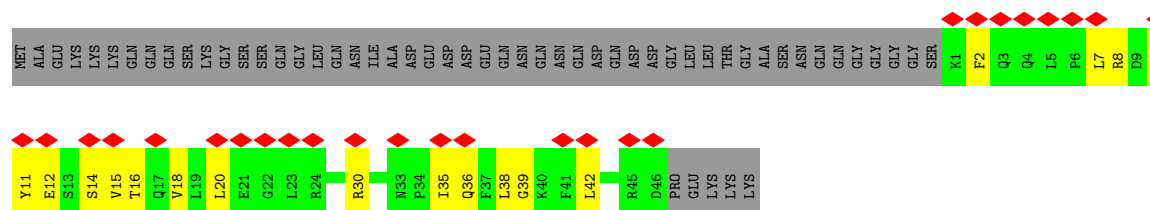
• Molecule 9: Dpy-30 motif protein

Chain 7D: 

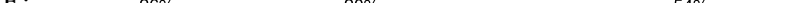


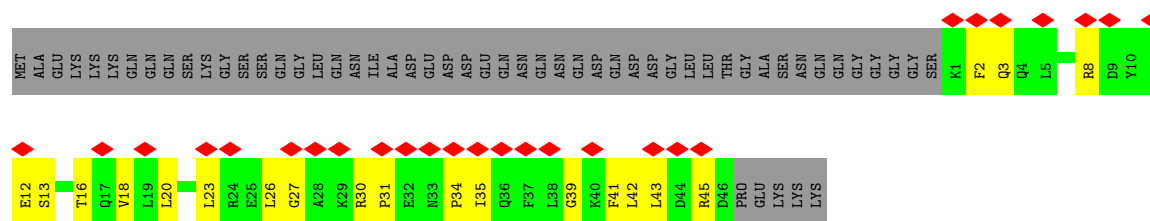
- Molecule 9: Dpy-30 motif protein

Chain 7E: 

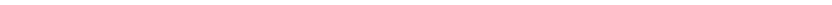


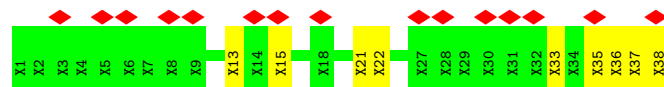
- Molecule 9: Dpy-30 motif protein

Chain 7F: 




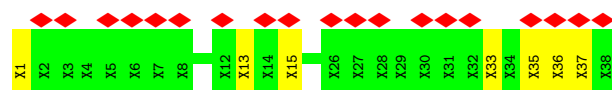
- Molecule 10: Unknown

Chain 8A:  39% 76% 24%




- Molecule 10: Unknown

Chain 8B: 

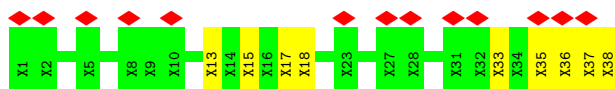
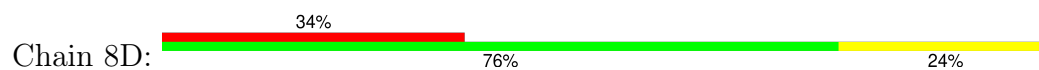


- Molecule 10: Unknown

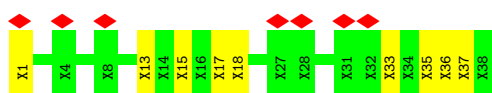
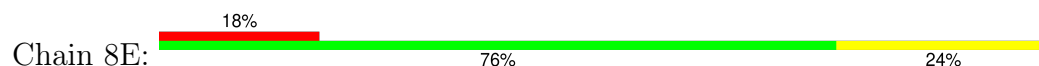
Chain 8C: 



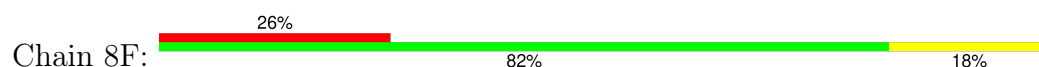
- Molecule 10: Unknown



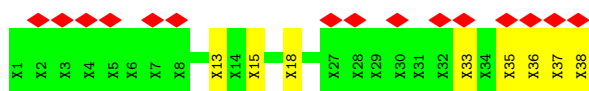
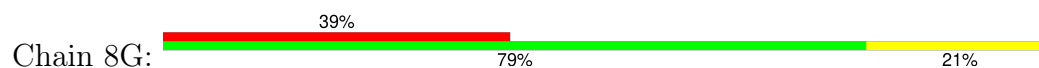
- Molecule 10: Unknown



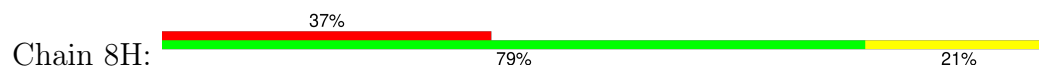
- Molecule 10: Unknown



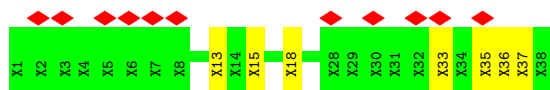
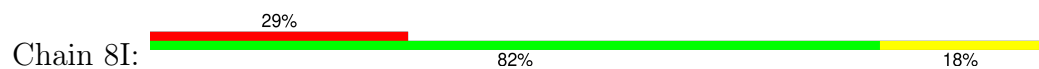
- Molecule 10: Unknown



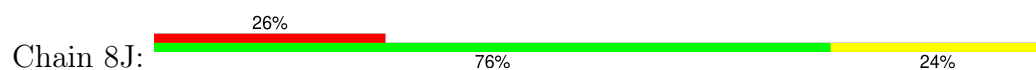
- Molecule 10: Unknown



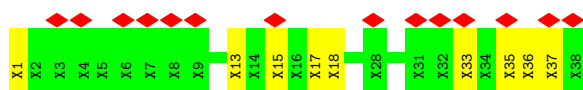
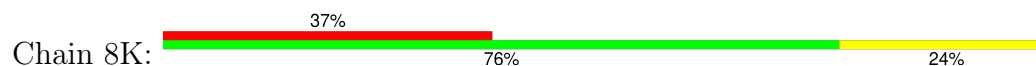
- Molecule 10: Unknown



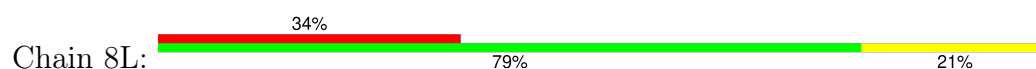
- Molecule 10: Unknown



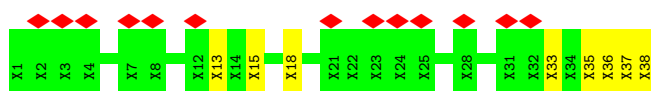
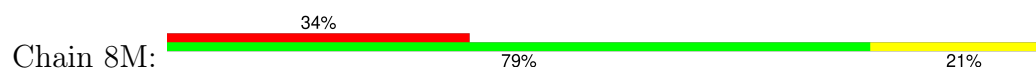
• Molecule 10: Unknown



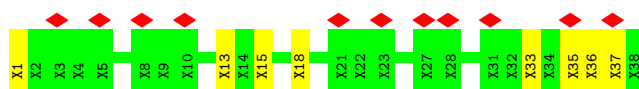
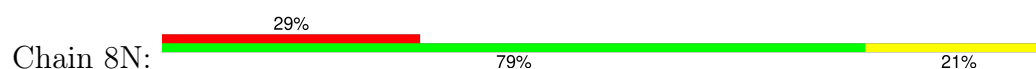
• Molecule 10: Unknown



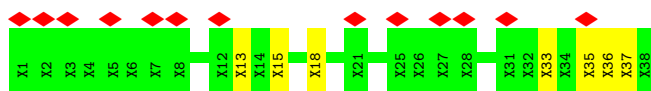
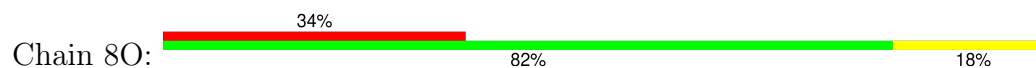
• Molecule 10: Unknown



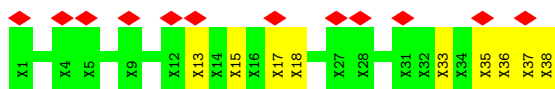
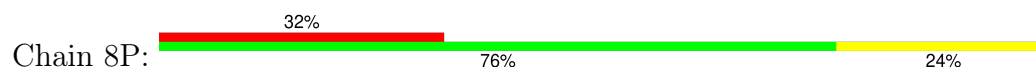
• Molecule 10: Unknown



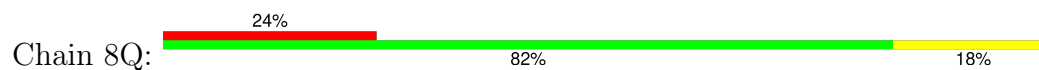
• Molecule 10: Unknown



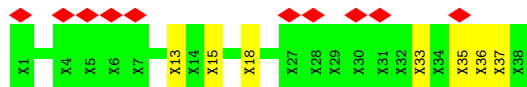
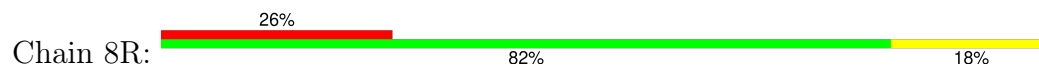
• Molecule 10: Unknown



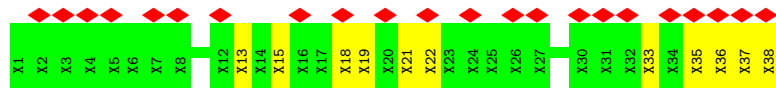
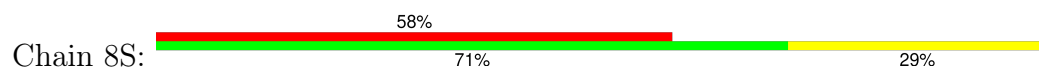
• Molecule 10: Unknown



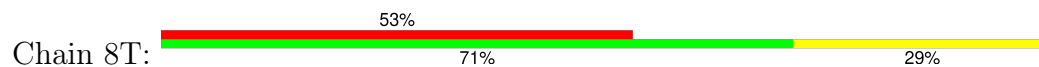
• Molecule 10: Unknown



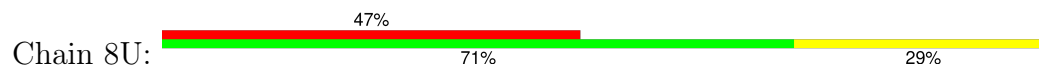
• Molecule 10: Unknown



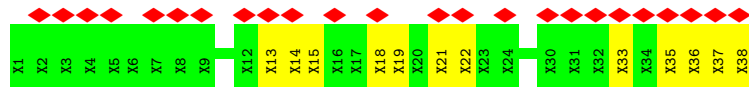
• Molecule 10: Unknown



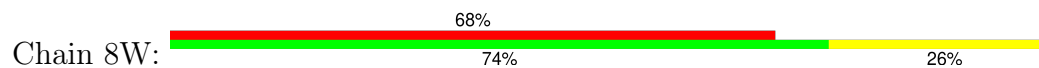
• Molecule 10: Unknown



• Molecule 10: Unknown

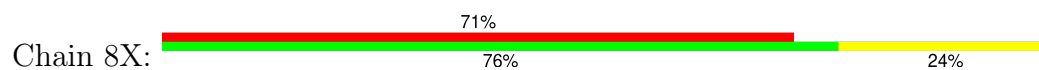


• Molecule 10: Unknown

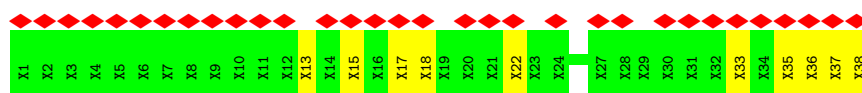
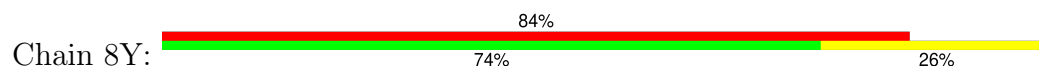




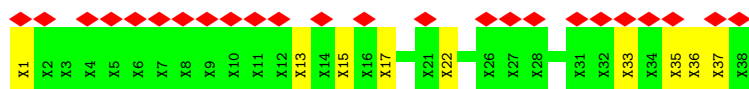
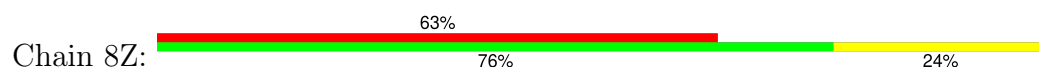
• Molecule 10: Unknown



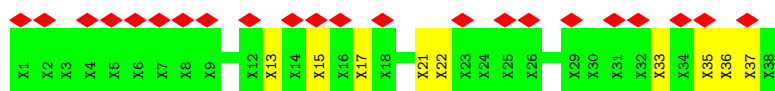
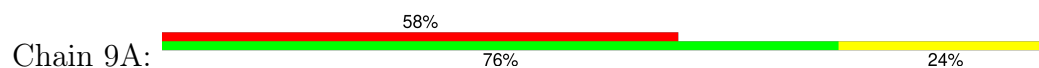
• Molecule 10: Unknown



• Molecule 10: Unknown



• Molecule 10: Unknown



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 66174 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 45 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 2.798 | Depositor |
| Minimum map value | -0.007 | Depositor |
| Average map value | 0.006 | Depositor |
| Map value standard deviation | 0.056 | Depositor |
| Recommended contour level | 0.17 | Depositor |
| Map size (Å) | 931.6, 931.6, 931.6 | wwPDB |
| Map dimensions | 680, 680, 680 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.37, 1.37, 1.37 | Depositor |

5 Model quality

5.1 Standard geometry

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

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 | AA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | AC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | AE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | BA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | BC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | BE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | CA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | CC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | CE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | DA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | DC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | DE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | EA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | EC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | EE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | FA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | FC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | FE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | GA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | GC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | GE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | HA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | HC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | HE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | IA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | IC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | IE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | JA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | JC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | JE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | KA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | KC | 0.19 | 0/3421 | 0.45 | 0/4636 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | KE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | LA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | LC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | LE | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | MA | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | MC | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 1 | ME | 0.19 | 0/3421 | 0.45 | 0/4636 |
| 2 | AB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | AD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | AF | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | BB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | BD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | BF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | CB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | CD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | CF | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | DB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | DD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | DF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | EB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | ED | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | EF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | FB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | FD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | FF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | GB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | GD | 0.21 | 0/3439 | 0.47 | 5/4655 (0.1%) |
| 2 | GF | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | HB | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | HD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | HF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | IB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | ID | 0.21 | 0/3439 | 0.47 | 5/4655 (0.1%) |
| 2 | IF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | JB | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | JD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | JF | 0.21 | 0/3439 | 0.46 | 4/4655 (0.1%) |
| 2 | KB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | KD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | KF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | LB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | LD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | LF | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | MB | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | MD | 0.21 | 0/3439 | 0.47 | 4/4655 (0.1%) |
| 2 | MF | 0.21 | 0/3439 | 0.46 | 5/4655 (0.1%) |
| 3 | 1A | 0.68 | 0/1161 | 1.23 | 0/1566 |
| 3 | 1B | 0.68 | 0/1161 | 1.23 | 0/1566 |
| 3 | 1C | 0.68 | 0/1161 | 1.23 | 0/1566 |
| 4 | 2A | 0.76 | 1/1642 (0.1%) | 1.29 | 13/2193 (0.6%) |
| 4 | 2B | 0.76 | 1/1642 (0.1%) | 1.29 | 13/2193 (0.6%) |
| 4 | 2C | 0.76 | 1/1642 (0.1%) | 1.29 | 13/2193 (0.6%) |
| 5 | 3A | 0.65 | 0/2795 | 1.13 | 1/3751 (0.0%) |
| 5 | 3B | 0.65 | 0/2795 | 1.13 | 1/3751 (0.0%) |
| 5 | 3C | 0.65 | 0/2795 | 1.13 | 1/3751 (0.0%) |
| 6 | 4A | 0.99 | 2/1610 (0.1%) | 1.50 | 35/2151 (1.6%) |
| 6 | 4B | 0.99 | 2/1610 (0.1%) | 1.50 | 35/2151 (1.6%) |
| 6 | 4C | 0.99 | 2/1610 (0.1%) | 1.50 | 35/2151 (1.6%) |
| 6 | 4D | 0.99 | 2/1610 (0.1%) | 1.50 | 35/2151 (1.6%) |
| 7 | 5A | 1.02 | 31/6042 (0.5%) | 1.37 | 68/8049 (0.8%) |
| 7 | 5B | 1.02 | 31/6042 (0.5%) | 1.37 | 68/8049 (0.8%) |
| 7 | 5C | 1.02 | 31/6042 (0.5%) | 1.37 | 68/8049 (0.8%) |
| 8 | 6A | 0.71 | 0/2126 | 1.03 | 0/2877 |
| 8 | 6B | 0.71 | 0/2126 | 1.03 | 0/2877 |
| 8 | 6C | 0.71 | 0/2126 | 1.03 | 0/2877 |
| 9 | 7A | 0.58 | 0/390 | 0.66 | 0/524 |
| 9 | 7B | 0.59 | 0/390 | 0.68 | 0/524 |
| 9 | 7C | 0.58 | 0/390 | 0.67 | 0/524 |
| 9 | 7D | 0.59 | 0/390 | 0.68 | 0/524 |
| 9 | 7E | 0.58 | 0/390 | 0.66 | 0/524 |
| 9 | 7F | 0.59 | 0/390 | 0.68 | 0/524 |
| All | All | 0.39 | 104/317618 (0.0%) | 0.65 | 545/429405 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4 | 2A | 0 | 1 |
| 4 | 2B | 0 | 1 |
| 4 | 2C | 0 | 2 |
| 7 | 5A | 0 | 7 |
| 7 | 5B | 0 | 7 |
| 7 | 5C | 0 | 7 |
| All | All | 0 | 25 |

All (104) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 7 | 5C | 1372 | VAL | CA-C | 14.89 | 1.71 | 1.52 |
| 7 | 5B | 1372 | VAL | CA-C | 14.89 | 1.71 | 1.52 |
| 7 | 5A | 1372 | VAL | CA-C | 14.88 | 1.71 | 1.52 |
| 7 | 5B | 1372 | VAL | N-CA | 14.51 | 1.64 | 1.46 |
| 7 | 5C | 1372 | VAL | N-CA | 14.50 | 1.64 | 1.46 |
| 7 | 5A | 1372 | VAL | N-CA | 14.49 | 1.64 | 1.46 |
| 7 | 5C | 1471 | ILE | N-CA | 10.94 | 1.60 | 1.46 |
| 7 | 5A | 1471 | ILE | N-CA | 10.93 | 1.60 | 1.46 |
| 7 | 5B | 1471 | ILE | N-CA | 10.93 | 1.60 | 1.46 |
| 7 | 5A | 1372 | VAL | C-O | 9.87 | 1.35 | 1.24 |
| 7 | 5C | 1372 | VAL | C-O | 9.87 | 1.35 | 1.24 |
| 7 | 5B | 1372 | VAL | C-O | 9.84 | 1.35 | 1.24 |
| 7 | 5A | 1467 | SER | C-O | 9.73 | 1.35 | 1.24 |
| 7 | 5C | 1467 | SER | C-O | 9.73 | 1.35 | 1.24 |
| 7 | 5B | 1467 | SER | C-O | 9.71 | 1.35 | 1.24 |
| 7 | 5C | 1250 | VAL | C-N | 8.71 | 1.46 | 1.33 |
| 7 | 5B | 1250 | VAL | C-N | 8.71 | 1.46 | 1.33 |
| 7 | 5A | 1250 | VAL | C-N | 8.70 | 1.46 | 1.33 |
| 7 | 5A | 1471 | ILE | CA-C | 8.23 | 1.63 | 1.52 |
| 7 | 5B | 1471 | ILE | CA-C | 8.22 | 1.63 | 1.52 |
| 7 | 5C | 1471 | ILE | CA-C | 8.19 | 1.63 | 1.52 |
| 7 | 5B | 1283 | ALA | C-N | 8.12 | 1.45 | 1.33 |
| 7 | 5A | 1283 | ALA | C-N | 8.10 | 1.45 | 1.33 |
| 7 | 5C | 1283 | ALA | C-N | 8.08 | 1.45 | 1.33 |
| 7 | 5B | 1380 | LEU | C-O | 7.69 | 1.33 | 1.24 |
| 7 | 5A | 1380 | LEU | C-O | 7.63 | 1.33 | 1.24 |
| 7 | 5C | 1380 | LEU | C-O | 7.61 | 1.33 | 1.24 |
| 7 | 5A | 1377 | LYS | C-O | 6.71 | 1.31 | 1.24 |
| 7 | 5C | 1377 | LYS | C-O | 6.69 | 1.31 | 1.24 |
| 7 | 5B | 1377 | LYS | C-O | 6.67 | 1.31 | 1.24 |
| 7 | 5A | 1431 | GLU | C-O | 6.46 | 1.31 | 1.24 |
| 7 | 5B | 1431 | GLU | C-O | 6.44 | 1.31 | 1.24 |
| 7 | 5C | 1431 | GLU | C-O | 6.44 | 1.31 | 1.24 |
| 7 | 5A | 1315 | ARG | C-O | -6.30 | 1.16 | 1.24 |
| 7 | 5C | 1315 | ARG | C-O | -6.30 | 1.16 | 1.24 |
| 7 | 5B | 1252 | THR | C-N | 6.24 | 1.41 | 1.33 |
| 7 | 5A | 1252 | THR | C-N | 6.22 | 1.41 | 1.33 |
| 7 | 5B | 1315 | ARG | C-O | -6.22 | 1.16 | 1.24 |
| 7 | 5C | 1252 | THR | C-N | 6.19 | 1.41 | 1.33 |
| 7 | 5C | 1322 | VAL | C-O | -6.17 | 1.17 | 1.24 |
| 7 | 5A | 1322 | VAL | C-O | -6.17 | 1.17 | 1.24 |
| 7 | 5B | 1322 | VAL | C-O | -6.10 | 1.17 | 1.24 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 7 | 5C | 1377 | LYS | CA-C | 5.95 | 1.60 | 1.52 |
| 7 | 5B | 1377 | LYS | CA-C | 5.94 | 1.60 | 1.52 |
| 7 | 5A | 1377 | LYS | CA-C | 5.93 | 1.60 | 1.52 |
| 7 | 5B | 1254 | GLY | C-N | 5.91 | 1.42 | 1.33 |
| 7 | 5A | 1254 | GLY | C-N | 5.88 | 1.41 | 1.33 |
| 7 | 5A | 799 | LYS | CA-C | 5.84 | 1.60 | 1.52 |
| 7 | 5B | 1376 | GLN | C-O | 5.84 | 1.30 | 1.24 |
| 7 | 5C | 1254 | GLY | C-N | 5.83 | 1.41 | 1.33 |
| 7 | 5B | 799 | LYS | CA-C | 5.83 | 1.60 | 1.52 |
| 7 | 5C | 799 | LYS | CA-C | 5.83 | 1.60 | 1.52 |
| 7 | 5C | 1376 | GLN | C-O | 5.82 | 1.30 | 1.24 |
| 7 | 5A | 1375 | GLN | C-O | 5.82 | 1.30 | 1.24 |
| 7 | 5A | 1376 | GLN | C-O | 5.82 | 1.30 | 1.24 |
| 7 | 5B | 1375 | GLN | C-O | 5.82 | 1.30 | 1.24 |
| 7 | 5C | 1428 | GLU | C-O | 5.80 | 1.30 | 1.24 |
| 7 | 5C | 1375 | GLN | C-O | 5.80 | 1.30 | 1.24 |
| 7 | 5A | 1428 | GLU | C-O | 5.75 | 1.30 | 1.24 |
| 7 | 5B | 1428 | GLU | C-O | 5.75 | 1.30 | 1.24 |
| 7 | 5A | 1379 | LYS | C-O | 5.73 | 1.30 | 1.24 |
| 7 | 5C | 1379 | LYS | C-O | 5.72 | 1.30 | 1.24 |
| 7 | 5B | 1379 | LYS | C-O | 5.70 | 1.30 | 1.24 |
| 7 | 5B | 1343 | LYS | C-O | 5.59 | 1.30 | 1.24 |
| 7 | 5B | 1248 | LEU | C-N | 5.58 | 1.42 | 1.33 |
| 7 | 5C | 1343 | LYS | C-O | 5.58 | 1.30 | 1.24 |
| 7 | 5A | 1248 | LEU | C-N | 5.56 | 1.42 | 1.33 |
| 7 | 5C | 1248 | LEU | C-N | 5.55 | 1.42 | 1.33 |
| 6 | 4D | 108 | LYS | N-CA | 5.55 | 1.53 | 1.46 |
| 7 | 5A | 1343 | LYS | C-O | 5.53 | 1.30 | 1.24 |
| 6 | 4B | 108 | LYS | N-CA | 5.51 | 1.53 | 1.46 |
| 6 | 4A | 108 | LYS | N-CA | 5.47 | 1.53 | 1.46 |
| 6 | 4C | 108 | LYS | N-CA | 5.46 | 1.53 | 1.46 |
| 6 | 4C | 160 | ASP | CA-C | -5.45 | 1.45 | 1.52 |
| 6 | 4B | 160 | ASP | CA-C | -5.44 | 1.45 | 1.52 |
| 6 | 4D | 160 | ASP | CA-C | -5.43 | 1.45 | 1.52 |
| 6 | 4A | 160 | ASP | CA-C | -5.42 | 1.45 | 1.52 |
| 7 | 5B | 1407 | GLN | CA-C | -5.32 | 1.45 | 1.52 |
| 7 | 5C | 1407 | GLN | CA-C | -5.28 | 1.46 | 1.52 |
| 7 | 5A | 1407 | GLN | CA-C | -5.28 | 1.46 | 1.52 |
| 7 | 5C | 1440 | GLU | C-O | 5.19 | 1.30 | 1.24 |
| 7 | 5A | 1336 | LYS | C-O | 5.18 | 1.30 | 1.24 |
| 4 | 2B | 17 | ILE | CA-C | -5.17 | 1.46 | 1.52 |
| 7 | 5A | 1432 | ALA | C-O | 5.17 | 1.30 | 1.24 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 7 | 5A | 1440 | GLU | C-O | 5.16 | 1.30 | 1.24 |
| 7 | 5B | 1440 | GLU | C-O | 5.16 | 1.30 | 1.24 |
| 7 | 5B | 1336 | LYS | C-O | 5.16 | 1.30 | 1.24 |
| 7 | 5C | 1336 | LYS | C-O | 5.15 | 1.30 | 1.24 |
| 7 | 5B | 1432 | ALA | C-O | 5.15 | 1.30 | 1.24 |
| 7 | 5C | 1307 | ALA | C-O | -5.13 | 1.18 | 1.24 |
| 7 | 5C | 1443 | LYS | C-O | 5.13 | 1.30 | 1.24 |
| 7 | 5C | 1432 | ALA | C-O | 5.12 | 1.30 | 1.24 |
| 7 | 5A | 1443 | LYS | C-O | 5.12 | 1.30 | 1.24 |
| 4 | 2A | 17 | ILE | CA-C | -5.10 | 1.46 | 1.52 |
| 7 | 5B | 1443 | LYS | C-O | 5.09 | 1.30 | 1.24 |
| 7 | 5B | 1307 | ALA | C-O | -5.08 | 1.18 | 1.24 |
| 7 | 5B | 1464 | GLU | C-O | 5.08 | 1.30 | 1.24 |
| 7 | 5A | 1307 | ALA | C-O | -5.07 | 1.18 | 1.24 |
| 4 | 2C | 17 | ILE | CA-C | -5.06 | 1.47 | 1.52 |
| 7 | 5C | 1464 | GLU | C-O | 5.06 | 1.30 | 1.24 |
| 7 | 5A | 1464 | GLU | C-O | 5.04 | 1.30 | 1.24 |
| 7 | 5B | 1371 | GLU | CA-C | 5.03 | 1.59 | 1.52 |
| 7 | 5C | 1371 | GLU | CA-C | 5.03 | 1.59 | 1.52 |
| 7 | 5A | 1371 | GLU | CA-C | 5.01 | 1.59 | 1.52 |

All (545) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 7 | 5A | 1283 | ALA | O-C-N | -18.60 | 96.86 | 121.97 |
| 7 | 5B | 1283 | ALA | O-C-N | -18.59 | 96.87 | 121.97 |
| 7 | 5C | 1283 | ALA | O-C-N | -18.55 | 96.93 | 121.97 |
| 4 | 2C | 17 | ILE | N-CA-C | -15.81 | 94.97 | 110.30 |
| 4 | 2A | 17 | ILE | N-CA-C | -15.75 | 95.02 | 110.30 |
| 4 | 2B | 17 | ILE | N-CA-C | -15.73 | 95.04 | 110.30 |
| 6 | 4C | 107 | MET | N-CA-C | 15.43 | 129.46 | 111.71 |
| 6 | 4A | 107 | MET | N-CA-C | 15.42 | 129.44 | 111.71 |
| 6 | 4B | 107 | MET | N-CA-C | 15.38 | 129.40 | 111.71 |
| 6 | 4D | 107 | MET | N-CA-C | 15.36 | 129.38 | 111.71 |
| 7 | 5B | 1373 | PHE | N-CA-C | 13.55 | 126.05 | 111.28 |
| 7 | 5A | 1373 | PHE | N-CA-C | 13.54 | 126.04 | 111.28 |
| 7 | 5C | 1373 | PHE | N-CA-C | 13.50 | 126.00 | 111.28 |
| 7 | 5C | 1254 | GLY | CA-C-N | 11.84 | 139.54 | 120.60 |
| 7 | 5C | 1254 | GLY | C-N-CA | 11.84 | 139.54 | 120.60 |
| 7 | 5B | 1254 | GLY | CA-C-N | 11.84 | 139.54 | 120.60 |
| 7 | 5B | 1254 | GLY | C-N-CA | 11.84 | 139.54 | 120.60 |
| 7 | 5A | 1254 | GLY | CA-C-N | 11.81 | 139.50 | 120.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 7 | 5A | 1254 | GLY | C-N-CA | 11.81 | 139.50 | 120.60 |
| 7 | 5C | 1407 | GLN | N-CA-C | -11.42 | 98.84 | 111.28 |
| 7 | 5A | 1407 | GLN | N-CA-C | -11.39 | 98.87 | 111.28 |
| 7 | 5B | 1407 | GLN | N-CA-C | -11.38 | 98.87 | 111.28 |
| 7 | 5C | 1278 | GLY | O-C-N | -10.64 | 108.87 | 122.70 |
| 7 | 5A | 1278 | GLY | O-C-N | -10.63 | 108.88 | 122.70 |
| 7 | 5B | 1278 | GLY | O-C-N | -10.61 | 108.91 | 122.70 |
| 6 | 4B | 259 | THR | N-CA-C | 10.55 | 122.86 | 111.36 |
| 6 | 4A | 259 | THR | N-CA-C | 10.53 | 122.84 | 111.36 |
| 6 | 4D | 259 | THR | N-CA-C | 10.53 | 122.84 | 111.36 |
| 6 | 4C | 259 | THR | N-CA-C | 10.53 | 122.83 | 111.36 |
| 7 | 5A | 773 | ARG | N-CA-C | 10.32 | 123.68 | 109.54 |
| 7 | 5C | 773 | ARG | N-CA-C | 10.32 | 123.67 | 109.54 |
| 7 | 5B | 773 | ARG | N-CA-C | 10.31 | 123.66 | 109.54 |
| 7 | 5A | 1280 | SER | O-C-N | -9.89 | 109.43 | 122.59 |
| 7 | 5C | 1280 | SER | O-C-N | -9.89 | 109.44 | 122.59 |
| 7 | 5C | 842 | LEU | N-CA-C | 9.88 | 126.00 | 113.55 |
| 7 | 5B | 1280 | SER | O-C-N | -9.87 | 109.47 | 122.59 |
| 4 | 2C | 145 | GLN | N-CA-C | 9.85 | 117.09 | 108.22 |
| 7 | 5B | 842 | LEU | N-CA-C | 9.85 | 125.97 | 113.55 |
| 4 | 2B | 145 | GLN | N-CA-C | 9.85 | 117.08 | 108.22 |
| 7 | 5A | 842 | LEU | N-CA-C | 9.85 | 125.95 | 113.55 |
| 4 | 2A | 145 | GLN | N-CA-C | 9.84 | 117.08 | 108.22 |
| 7 | 5C | 1471 | ILE | N-CA-C | 9.51 | 129.11 | 109.34 |
| 7 | 5B | 1471 | ILE | N-CA-C | 9.49 | 129.09 | 109.34 |
| 7 | 5A | 1471 | ILE | N-CA-C | 9.49 | 129.08 | 109.34 |
| 6 | 4C | 132 | LYS | N-CA-C | 9.36 | 121.56 | 111.36 |
| 6 | 4A | 132 | LYS | N-CA-C | 9.36 | 121.56 | 111.36 |
| 6 | 4B | 132 | LYS | N-CA-C | 9.35 | 121.56 | 111.36 |
| 6 | 4D | 132 | LYS | N-CA-C | 9.35 | 121.55 | 111.36 |
| 7 | 5B | 1254 | GLY | O-C-N | -9.34 | 110.56 | 122.70 |
| 7 | 5C | 1254 | GLY | O-C-N | -9.33 | 110.57 | 122.70 |
| 7 | 5A | 1254 | GLY | O-C-N | -9.32 | 110.59 | 122.70 |
| 7 | 5C | 1372 | VAL | N-CA-C | 8.93 | 127.92 | 109.34 |
| 7 | 5A | 1372 | VAL | N-CA-C | 8.93 | 127.92 | 109.34 |
| 7 | 5B | 1372 | VAL | N-CA-C | 8.93 | 127.90 | 109.34 |
| 7 | 5A | 1270 | ASP | N-CA-C | 8.87 | 120.72 | 111.14 |
| 7 | 5C | 1270 | ASP | N-CA-C | 8.86 | 120.71 | 111.14 |
| 7 | 5B | 1270 | ASP | N-CA-C | 8.85 | 120.70 | 111.14 |
| 4 | 2A | 147 | PHE | N-CA-C | -8.54 | 92.62 | 110.80 |
| 4 | 2B | 147 | PHE | N-CA-C | -8.53 | 92.63 | 110.80 |
| 4 | 2C | 147 | PHE | N-CA-C | -8.51 | 92.67 | 110.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 6 | 4B | 256 | ASN | N-CA-C | 8.40 | 120.51 | 111.36 |
| 6 | 4A | 256 | ASN | N-CA-C | 8.39 | 120.51 | 111.36 |
| 6 | 4C | 256 | ASN | N-CA-C | 8.38 | 120.49 | 111.36 |
| 6 | 4D | 256 | ASN | N-CA-C | 8.36 | 120.48 | 111.36 |
| 6 | 4D | 252 | VAL | N-CA-C | 8.07 | 118.17 | 110.42 |
| 6 | 4B | 252 | VAL | N-CA-C | 8.05 | 118.15 | 110.42 |
| 6 | 4A | 252 | VAL | N-CA-C | 8.04 | 118.14 | 110.42 |
| 6 | 4C | 252 | VAL | N-CA-C | 8.04 | 118.14 | 110.42 |
| 7 | 5B | 1565 | GLU | N-CA-C | 7.90 | 122.38 | 112.03 |
| 7 | 5C | 1565 | GLU | N-CA-C | 7.90 | 122.38 | 112.03 |
| 7 | 5A | 1565 | GLU | N-CA-C | 7.88 | 122.35 | 112.03 |
| 4 | 2C | 16 | GLN | N-CA-C | 7.84 | 119.90 | 111.36 |
| 4 | 2C | 146 | PRO | CA-C-N | 7.84 | 136.51 | 121.54 |
| 4 | 2C | 146 | PRO | C-N-CA | 7.84 | 136.51 | 121.54 |
| 4 | 2B | 146 | PRO | CA-C-N | 7.83 | 136.50 | 121.54 |
| 4 | 2B | 146 | PRO | C-N-CA | 7.83 | 136.50 | 121.54 |
| 7 | 5C | 1492 | SER | CA-C-O | -7.83 | 112.78 | 121.00 |
| 4 | 2A | 146 | PRO | CA-C-N | 7.83 | 136.49 | 121.54 |
| 4 | 2A | 146 | PRO | C-N-CA | 7.83 | 136.49 | 121.54 |
| 7 | 5A | 1492 | SER | CA-C-O | -7.82 | 112.80 | 121.00 |
| 4 | 2B | 16 | GLN | N-CA-C | 7.80 | 119.86 | 111.36 |
| 7 | 5B | 1492 | SER | CA-C-O | -7.79 | 112.81 | 121.00 |
| 4 | 2A | 16 | GLN | N-CA-C | 7.77 | 119.83 | 111.36 |
| 7 | 5C | 1253 | ILE | O-C-N | -7.71 | 112.79 | 122.97 |
| 7 | 5A | 1253 | ILE | O-C-N | -7.71 | 112.79 | 122.97 |
| 7 | 5B | 1253 | ILE | O-C-N | -7.71 | 112.80 | 122.97 |
| 7 | 5A | 1282 | GLN | O-C-N | -7.61 | 112.01 | 122.20 |
| 7 | 5C | 1282 | GLN | O-C-N | -7.60 | 112.02 | 122.20 |
| 7 | 5B | 1282 | GLN | O-C-N | -7.59 | 112.03 | 122.20 |
| 7 | 5B | 1269 | ASP | N-CA-C | -7.57 | 103.14 | 112.38 |
| 7 | 5A | 1269 | ASP | N-CA-C | -7.55 | 103.17 | 112.38 |
| 7 | 5C | 1269 | ASP | N-CA-C | -7.55 | 103.17 | 112.38 |
| 4 | 2A | 175 | VAL | N-CA-C | 7.48 | 118.28 | 110.72 |
| 4 | 2B | 175 | VAL | N-CA-C | 7.47 | 118.26 | 110.72 |
| 7 | 5C | 1260 | THR | CA-C-N | 7.46 | 131.66 | 120.31 |
| 7 | 5C | 1260 | THR | C-N-CA | 7.46 | 131.66 | 120.31 |
| 7 | 5B | 1260 | THR | CA-C-N | 7.46 | 131.65 | 120.31 |
| 7 | 5B | 1260 | THR | C-N-CA | 7.46 | 131.65 | 120.31 |
| 7 | 5A | 1260 | THR | CA-C-N | 7.45 | 131.64 | 120.31 |
| 7 | 5A | 1260 | THR | C-N-CA | 7.45 | 131.64 | 120.31 |
| 4 | 2C | 175 | VAL | N-CA-C | 7.43 | 118.23 | 110.72 |
| 7 | 5C | 1357 | LYS | O-C-N | 7.42 | 129.71 | 122.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 7 | 5A | 1357 | LYS | O-C-N | 7.41 | 129.70 | 122.07 |
| 4 | 2A | 143 | LEU | N-CA-C | -7.41 | 95.02 | 110.80 |
| 7 | 5B | 1357 | LYS | O-C-N | 7.41 | 129.70 | 122.07 |
| 4 | 2B | 143 | LEU | N-CA-C | -7.40 | 95.04 | 110.80 |
| 4 | 2C | 143 | LEU | N-CA-C | -7.40 | 95.05 | 110.80 |
| 6 | 4B | 152 | PHE | N-CA-C | 7.28 | 122.27 | 112.88 |
| 6 | 4A | 152 | PHE | N-CA-C | 7.27 | 122.26 | 112.88 |
| 6 | 4D | 152 | PHE | N-CA-C | 7.27 | 122.26 | 112.88 |
| 6 | 4C | 152 | PHE | N-CA-C | 7.26 | 122.25 | 112.88 |
| 6 | 4D | 97 | GLN | CA-C-N | 7.26 | 128.92 | 119.84 |
| 6 | 4D | 97 | GLN | C-N-CA | 7.26 | 128.92 | 119.84 |
| 6 | 4D | 190 | TRP | CA-CB-CG | 7.26 | 127.39 | 113.60 |
| 7 | 5C | 1294 | ILE | N-CA-C | 7.25 | 118.02 | 110.62 |
| 7 | 5B | 1294 | ILE | N-CA-C | 7.25 | 118.02 | 110.62 |
| 7 | 5A | 1294 | ILE | N-CA-C | 7.25 | 118.01 | 110.62 |
| 6 | 4A | 97 | GLN | CA-C-N | 7.24 | 128.89 | 119.84 |
| 6 | 4A | 97 | GLN | C-N-CA | 7.24 | 128.89 | 119.84 |
| 6 | 4C | 190 | TRP | CA-CB-CG | 7.24 | 127.35 | 113.60 |
| 6 | 4A | 190 | TRP | CA-CB-CG | 7.23 | 127.34 | 113.60 |
| 6 | 4B | 97 | GLN | CA-C-N | 7.23 | 128.88 | 119.84 |
| 6 | 4B | 97 | GLN | C-N-CA | 7.23 | 128.88 | 119.84 |
| 6 | 4B | 190 | TRP | CA-CB-CG | 7.23 | 127.34 | 113.60 |
| 6 | 4C | 97 | GLN | CA-C-N | 7.22 | 128.87 | 119.84 |
| 6 | 4C | 97 | GLN | C-N-CA | 7.22 | 128.87 | 119.84 |
| 6 | 4D | 145 | PHE | N-CA-C | 7.21 | 119.53 | 109.15 |
| 2 | FB | 127 | CYS | N-CA-C | 7.19 | 120.13 | 110.35 |
| 2 | CB | 127 | CYS | N-CA-C | 7.18 | 120.12 | 110.35 |
| 2 | CD | 127 | CYS | N-CA-C | 7.18 | 120.12 | 110.35 |
| 2 | MB | 127 | CYS | N-CA-C | 7.18 | 120.11 | 110.35 |
| 2 | MD | 127 | CYS | N-CA-C | 7.18 | 120.11 | 110.35 |
| 6 | 4B | 145 | PHE | N-CA-C | 7.18 | 119.48 | 109.15 |
| 7 | 5B | 1279 | ASP | CA-C-N | 7.18 | 135.25 | 121.54 |
| 7 | 5B | 1279 | ASP | C-N-CA | 7.18 | 135.25 | 121.54 |
| 2 | FD | 127 | CYS | N-CA-C | 7.17 | 120.11 | 110.35 |
| 2 | FF | 127 | CYS | N-CA-C | 7.17 | 120.11 | 110.35 |
| 2 | EB | 127 | CYS | N-CA-C | 7.17 | 120.10 | 110.35 |
| 2 | CF | 127 | CYS | N-CA-C | 7.17 | 120.10 | 110.35 |
| 2 | LD | 127 | CYS | N-CA-C | 7.17 | 120.09 | 110.35 |
| 7 | 5A | 1278 | GLY | CA-C-N | 7.17 | 133.27 | 122.95 |
| 7 | 5A | 1278 | GLY | C-N-CA | 7.17 | 133.27 | 122.95 |
| 6 | 4C | 145 | PHE | N-CA-C | 7.16 | 119.47 | 109.15 |
| 2 | KD | 127 | CYS | N-CA-C | 7.16 | 120.09 | 110.35 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2 | ED | 127 | CYS | N-CA-C | 7.16 | 120.09 | 110.35 |
| 2 | ID | 127 | CYS | N-CA-C | 7.16 | 120.09 | 110.35 |
| 7 | 5C | 1278 | GLY | CA-C-N | 7.16 | 133.26 | 122.95 |
| 7 | 5C | 1278 | GLY | C-N-CA | 7.16 | 133.26 | 122.95 |
| 2 | MB | 131 | GLN | N-CA-C | -7.16 | 103.16 | 112.68 |
| 6 | 4C | 134 | LEU | N-CA-C | -7.16 | 104.81 | 113.97 |
| 7 | 5A | 1279 | ASP | CA-C-N | 7.16 | 135.21 | 121.54 |
| 7 | 5A | 1279 | ASP | C-N-CA | 7.16 | 135.21 | 121.54 |
| 2 | EB | 131 | GLN | N-CA-C | -7.15 | 103.17 | 112.68 |
| 2 | CD | 131 | GLN | N-CA-C | -7.15 | 103.17 | 112.68 |
| 4 | 2A | 151 | VAL | N-CA-C | 7.15 | 124.22 | 109.34 |
| 4 | 2C | 151 | VAL | N-CA-C | 7.15 | 124.21 | 109.34 |
| 2 | AD | 127 | CYS | N-CA-C | 7.15 | 120.07 | 110.35 |
| 2 | HB | 127 | CYS | N-CA-C | 7.15 | 120.07 | 110.35 |
| 2 | MF | 127 | CYS | N-CA-C | 7.15 | 120.07 | 110.35 |
| 2 | KF | 131 | GLN | N-CA-C | -7.15 | 103.17 | 112.68 |
| 7 | 5B | 1278 | GLY | CA-C-N | 7.15 | 133.24 | 122.95 |
| 7 | 5B | 1278 | GLY | C-N-CA | 7.15 | 133.24 | 122.95 |
| 2 | AB | 127 | CYS | N-CA-C | 7.15 | 120.07 | 110.35 |
| 2 | LF | 127 | CYS | N-CA-C | 7.15 | 120.07 | 110.35 |
| 7 | 5C | 1279 | ASP | CA-C-N | 7.15 | 135.19 | 121.54 |
| 7 | 5C | 1279 | ASP | C-N-CA | 7.15 | 135.19 | 121.54 |
| 2 | KD | 131 | GLN | N-CA-C | -7.14 | 103.18 | 112.68 |
| 2 | LD | 131 | GLN | N-CA-C | -7.14 | 103.18 | 112.68 |
| 4 | 2B | 151 | VAL | N-CA-C | 7.14 | 124.20 | 109.34 |
| 6 | 4A | 145 | PHE | N-CA-C | 7.14 | 119.44 | 109.15 |
| 6 | 4A | 134 | LEU | N-CA-C | -7.14 | 104.83 | 113.97 |
| 2 | DF | 131 | GLN | N-CA-C | -7.14 | 103.18 | 112.68 |
| 2 | KB | 127 | CYS | N-CA-C | 7.14 | 120.06 | 110.35 |
| 2 | GD | 131 | GLN | N-CA-C | -7.14 | 103.19 | 112.68 |
| 2 | IB | 127 | CYS | N-CA-C | 7.14 | 120.06 | 110.35 |
| 6 | 4B | 134 | LEU | N-CA-C | -7.14 | 104.83 | 113.97 |
| 6 | 4D | 134 | LEU | N-CA-C | -7.13 | 104.84 | 113.97 |
| 2 | GD | 127 | CYS | N-CA-C | 7.13 | 120.05 | 110.35 |
| 2 | GF | 127 | CYS | N-CA-C | 7.13 | 120.05 | 110.35 |
| 2 | AD | 131 | GLN | N-CA-C | -7.13 | 103.19 | 112.68 |
| 2 | GF | 131 | GLN | N-CA-C | -7.13 | 103.19 | 112.68 |
| 2 | IB | 131 | GLN | N-CA-C | -7.13 | 103.19 | 112.68 |
| 2 | JB | 127 | CYS | N-CA-C | 7.13 | 120.05 | 110.35 |
| 2 | LB | 127 | CYS | N-CA-C | 7.13 | 120.05 | 110.35 |
| 2 | BB | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | BD | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2 | DB | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | HD | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | HF | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |
| 2 | IF | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |
| 2 | MF | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |
| 2 | AF | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |
| 2 | DD | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | FF | 131 | GLN | N-CA-C | -7.13 | 103.20 | 112.68 |
| 2 | GB | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | JD | 127 | CYS | N-CA-C | 7.13 | 120.04 | 110.35 |
| 2 | EF | 127 | CYS | N-CA-C | 7.12 | 120.04 | 110.35 |
| 2 | HD | 131 | GLN | N-CA-C | -7.12 | 103.21 | 112.68 |
| 2 | MD | 131 | GLN | N-CA-C | -7.12 | 103.21 | 112.68 |
| 2 | ID | 131 | GLN | N-CA-C | -7.12 | 103.21 | 112.68 |
| 2 | JD | 131 | GLN | N-CA-C | -7.12 | 103.21 | 112.68 |
| 2 | CB | 131 | GLN | N-CA-C | -7.12 | 103.22 | 112.68 |
| 2 | ED | 131 | GLN | N-CA-C | -7.12 | 103.22 | 112.68 |
| 2 | BB | 131 | GLN | N-CA-C | -7.11 | 103.22 | 112.68 |
| 2 | BF | 131 | GLN | N-CA-C | -7.11 | 103.22 | 112.68 |
| 2 | CF | 131 | GLN | N-CA-C | -7.11 | 103.22 | 112.68 |
| 2 | JF | 131 | GLN | N-CA-C | -7.11 | 103.22 | 112.68 |
| 2 | LB | 131 | GLN | N-CA-C | -7.11 | 103.23 | 112.68 |
| 2 | IF | 127 | CYS | N-CA-C | 7.11 | 120.01 | 110.35 |
| 2 | JB | 131 | GLN | N-CA-C | -7.11 | 103.23 | 112.68 |
| 2 | DB | 131 | GLN | N-CA-C | -7.10 | 103.23 | 112.68 |
| 2 | FD | 131 | GLN | N-CA-C | -7.10 | 103.23 | 112.68 |
| 2 | AB | 131 | GLN | N-CA-C | -7.10 | 103.23 | 112.68 |
| 2 | BF | 127 | CYS | N-CA-C | 7.10 | 120.01 | 110.35 |
| 2 | EF | 131 | GLN | N-CA-C | -7.10 | 103.24 | 112.68 |
| 2 | HB | 131 | GLN | N-CA-C | -7.10 | 103.24 | 112.68 |
| 2 | JF | 127 | CYS | N-CA-C | 7.10 | 120.00 | 110.35 |
| 2 | AF | 127 | CYS | N-CA-C | 7.10 | 120.00 | 110.35 |
| 2 | LF | 131 | GLN | N-CA-C | -7.09 | 103.25 | 112.68 |
| 2 | BD | 127 | CYS | N-CA-C | 7.09 | 120.00 | 110.35 |
| 2 | KB | 131 | GLN | N-CA-C | -7.09 | 103.25 | 112.68 |
| 2 | DF | 127 | CYS | N-CA-C | 7.09 | 119.99 | 110.35 |
| 2 | FB | 131 | GLN | N-CA-C | -7.09 | 103.25 | 112.68 |
| 2 | DD | 131 | GLN | N-CA-C | -7.08 | 103.27 | 112.68 |
| 2 | HF | 127 | CYS | N-CA-C | 7.08 | 119.97 | 110.35 |
| 2 | GB | 131 | GLN | N-CA-C | -7.07 | 103.28 | 112.68 |
| 2 | KF | 127 | CYS | N-CA-C | 7.06 | 119.95 | 110.35 |
| 7 | 5C | 1483 | VAL | O-C-N | 7.05 | 128.71 | 121.87 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7 | 5B | 1483 | VAL | O-C-N | 7.04 | 128.70 | 121.87 |
| 7 | 5A | 1483 | VAL | O-C-N | 7.04 | 128.70 | 121.87 |
| 6 | 4B | 153 | ASP | N-CA-C | -7.01 | 99.45 | 109.96 |
| 6 | 4A | 153 | ASP | N-CA-C | -7.00 | 99.45 | 109.96 |
| 7 | 5A | 843 | LEU | N-CA-C | 7.00 | 121.08 | 108.48 |
| 7 | 5B | 843 | LEU | N-CA-C | 7.00 | 121.08 | 108.48 |
| 6 | 4C | 153 | ASP | N-CA-C | -7.00 | 99.47 | 109.96 |
| 7 | 5C | 843 | LEU | N-CA-C | 6.99 | 121.06 | 108.48 |
| 6 | 4D | 153 | ASP | N-CA-C | -6.99 | 99.48 | 109.96 |
| 4 | 2C | 147 | PHE | N-CA-CB | 6.97 | 122.27 | 110.49 |
| 7 | 5A | 1319 | HIS | N-CA-C | -6.96 | 103.62 | 111.14 |
| 7 | 5C | 1319 | HIS | N-CA-C | -6.96 | 103.63 | 111.14 |
| 7 | 5B | 1319 | HIS | N-CA-C | -6.95 | 103.63 | 111.14 |
| 4 | 2A | 147 | PHE | N-CA-CB | 6.95 | 122.23 | 110.49 |
| 4 | 2B | 147 | PHE | N-CA-CB | 6.93 | 122.21 | 110.49 |
| 6 | 4D | 230 | TYR | N-CA-C | 6.92 | 120.87 | 110.14 |
| 6 | 4B | 230 | TYR | N-CA-C | 6.92 | 120.86 | 110.14 |
| 6 | 4A | 230 | TYR | N-CA-C | 6.92 | 120.86 | 110.14 |
| 6 | 4C | 230 | TYR | N-CA-C | 6.90 | 120.84 | 110.14 |
| 7 | 5A | 1577 | LYS | N-CA-C | -6.86 | 98.76 | 109.25 |
| 7 | 5B | 1577 | LYS | N-CA-C | -6.85 | 98.77 | 109.25 |
| 7 | 5C | 1577 | LYS | N-CA-C | -6.84 | 98.78 | 109.25 |
| 6 | 4A | 262 | ASN | N-CA-C | 6.79 | 120.33 | 110.28 |
| 6 | 4B | 262 | ASN | N-CA-C | 6.77 | 120.30 | 110.28 |
| 6 | 4D | 262 | ASN | N-CA-C | 6.77 | 120.30 | 110.28 |
| 7 | 5C | 798 | LYS | O-C-N | -6.76 | 114.31 | 122.22 |
| 7 | 5B | 798 | LYS | O-C-N | -6.75 | 114.32 | 122.22 |
| 6 | 4C | 262 | ASN | N-CA-C | 6.75 | 120.27 | 110.28 |
| 7 | 5A | 798 | LYS | O-C-N | -6.74 | 114.33 | 122.22 |
| 7 | 5A | 1565 | GLU | CA-C-O | -6.69 | 113.68 | 119.97 |
| 7 | 5B | 1565 | GLU | CA-C-O | -6.68 | 113.69 | 119.97 |
| 7 | 5C | 799 | LYS | N-CA-C | 6.68 | 118.25 | 110.97 |
| 7 | 5B | 799 | LYS | N-CA-C | 6.66 | 118.23 | 110.97 |
| 7 | 5B | 1488 | GLU | N-CA-C | -6.66 | 104.10 | 111.36 |
| 7 | 5C | 1565 | GLU | CA-C-O | -6.66 | 113.71 | 119.97 |
| 7 | 5A | 799 | LYS | N-CA-C | 6.65 | 118.22 | 110.97 |
| 7 | 5A | 1488 | GLU | N-CA-C | -6.64 | 104.12 | 111.36 |
| 7 | 5C | 1488 | GLU | N-CA-C | -6.62 | 104.14 | 111.36 |
| 7 | 5B | 1371 | GLU | N-CA-C | 6.61 | 124.89 | 110.80 |
| 7 | 5A | 1371 | GLU | N-CA-C | 6.61 | 124.88 | 110.80 |
| 7 | 5C | 1371 | GLU | N-CA-C | 6.59 | 124.84 | 110.80 |
| 7 | 5C | 1565 | GLU | CA-C-N | -6.55 | 110.85 | 120.28 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 7 | 5C | 1565 | GLU | C-N-CA | -6.55 | 110.85 | 120.28 |
| 7 | 5A | 1253 | ILE | CA-C-N | 6.55 | 134.24 | 121.41 |
| 7 | 5A | 1253 | ILE | C-N-CA | 6.55 | 134.24 | 121.41 |
| 7 | 5B | 1253 | ILE | CA-C-N | 6.54 | 134.22 | 121.41 |
| 7 | 5B | 1253 | ILE | C-N-CA | 6.54 | 134.22 | 121.41 |
| 7 | 5C | 1253 | ILE | CA-C-N | 6.54 | 134.22 | 121.41 |
| 7 | 5C | 1253 | ILE | C-N-CA | 6.54 | 134.22 | 121.41 |
| 7 | 5A | 1565 | GLU | CA-C-N | -6.51 | 110.90 | 120.28 |
| 7 | 5A | 1565 | GLU | C-N-CA | -6.51 | 110.90 | 120.28 |
| 7 | 5B | 1565 | GLU | CA-C-N | -6.50 | 110.91 | 120.28 |
| 7 | 5B | 1565 | GLU | C-N-CA | -6.50 | 110.91 | 120.28 |
| 5 | 3A | 233 | ASP | CA-CB-CG | 6.36 | 118.96 | 112.60 |
| 5 | 3C | 233 | ASP | CA-CB-CG | 6.36 | 118.95 | 112.60 |
| 6 | 4B | 232 | LYS | N-CA-C | 6.34 | 119.47 | 109.96 |
| 6 | 4A | 232 | LYS | N-CA-C | 6.33 | 119.46 | 109.96 |
| 6 | 4D | 232 | LYS | N-CA-C | 6.33 | 119.45 | 109.96 |
| 6 | 4C | 232 | LYS | N-CA-C | 6.32 | 119.44 | 109.96 |
| 5 | 3B | 233 | ASP | CA-CB-CG | 6.32 | 118.92 | 112.60 |
| 7 | 5C | 1427 | LYS | CA-C-N | 6.29 | 129.00 | 120.38 |
| 7 | 5C | 1427 | LYS | C-N-CA | 6.29 | 129.00 | 120.38 |
| 7 | 5A | 1427 | LYS | CA-C-N | 6.29 | 129.00 | 120.38 |
| 7 | 5A | 1427 | LYS | C-N-CA | 6.29 | 129.00 | 120.38 |
| 7 | 5B | 1427 | LYS | CA-C-N | 6.27 | 128.97 | 120.38 |
| 7 | 5B | 1427 | LYS | C-N-CA | 6.27 | 128.97 | 120.38 |
| 7 | 5B | 1492 | SER | CA-C-N | -6.24 | 109.62 | 121.54 |
| 7 | 5B | 1492 | SER | C-N-CA | -6.24 | 109.62 | 121.54 |
| 7 | 5A | 1492 | SER | CA-C-N | -6.24 | 109.63 | 121.54 |
| 7 | 5A | 1492 | SER | C-N-CA | -6.24 | 109.63 | 121.54 |
| 7 | 5C | 1492 | SER | CA-C-N | -6.24 | 109.63 | 121.54 |
| 7 | 5C | 1492 | SER | C-N-CA | -6.24 | 109.63 | 121.54 |
| 4 | 2B | 171 | VAL | N-CA-C | -6.07 | 96.72 | 109.34 |
| 4 | 2C | 171 | VAL | N-CA-C | -6.06 | 96.74 | 109.34 |
| 4 | 2A | 171 | VAL | N-CA-C | -6.05 | 96.75 | 109.34 |
| 7 | 5A | 1281 | ASN | O-C-N | -5.98 | 114.07 | 122.26 |
| 6 | 4D | 133 | GLN | N-CA-C | 5.97 | 119.80 | 111.74 |
| 6 | 4A | 133 | GLN | N-CA-C | 5.95 | 119.78 | 111.74 |
| 6 | 4B | 133 | GLN | N-CA-C | 5.95 | 119.77 | 111.74 |
| 7 | 5B | 1491 | LEU | N-CA-C | -5.95 | 104.87 | 111.36 |
| 6 | 4B | 278 | TYR | N-CA-C | 5.94 | 117.76 | 111.28 |
| 6 | 4A | 278 | TYR | N-CA-C | 5.94 | 117.76 | 111.28 |
| 6 | 4C | 133 | GLN | N-CA-C | 5.94 | 119.76 | 111.74 |
| 7 | 5C | 1281 | ASN | O-C-N | -5.94 | 114.13 | 122.26 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7 | 5A | 1491 | LEU | N-CA-C | -5.93 | 104.89 | 111.36 |
| 7 | 5C | 1491 | LEU | N-CA-C | -5.93 | 104.89 | 111.36 |
| 7 | 5B | 1281 | ASN | O-C-N | -5.93 | 114.14 | 122.26 |
| 6 | 4A | 137 | ASN | CA-C-N | 5.92 | 125.82 | 119.85 |
| 6 | 4A | 137 | ASN | C-N-CA | 5.92 | 125.82 | 119.85 |
| 6 | 4C | 278 | TYR | N-CA-C | 5.91 | 117.72 | 111.28 |
| 6 | 4C | 137 | ASN | CA-C-N | 5.90 | 125.81 | 119.85 |
| 6 | 4C | 137 | ASN | C-N-CA | 5.90 | 125.81 | 119.85 |
| 6 | 4D | 278 | TYR | N-CA-C | 5.90 | 117.71 | 111.28 |
| 6 | 4B | 137 | ASN | CA-C-N | 5.89 | 125.80 | 119.85 |
| 6 | 4B | 137 | ASN | C-N-CA | 5.89 | 125.80 | 119.85 |
| 6 | 4D | 137 | ASN | CA-C-N | 5.88 | 125.79 | 119.85 |
| 6 | 4D | 137 | ASN | C-N-CA | 5.88 | 125.79 | 119.85 |
| 6 | 4D | 155 | ASP | N-CA-C | 5.82 | 118.20 | 108.02 |
| 6 | 4A | 155 | ASP | N-CA-C | 5.81 | 118.19 | 108.02 |
| 4 | 2A | 144 | ASN | N-CA-C | 5.80 | 118.92 | 108.48 |
| 6 | 4B | 155 | ASP | N-CA-C | 5.79 | 118.15 | 108.02 |
| 7 | 5C | 1245 | GLY | O-C-N | -5.79 | 115.17 | 122.70 |
| 6 | 4C | 155 | ASP | N-CA-C | 5.79 | 118.15 | 108.02 |
| 4 | 2B | 144 | ASN | N-CA-C | 5.78 | 118.89 | 108.48 |
| 7 | 5B | 1245 | GLY | O-C-N | -5.78 | 115.18 | 122.70 |
| 4 | 2C | 144 | ASN | N-CA-C | 5.78 | 118.88 | 108.48 |
| 7 | 5A | 1245 | GLY | O-C-N | -5.78 | 115.19 | 122.70 |
| 7 | 5C | 1580 | LYS | N-CA-C | 5.77 | 123.09 | 110.80 |
| 7 | 5B | 1485 | LYS | N-CA-C | -5.77 | 105.07 | 111.36 |
| 7 | 5A | 1580 | LYS | N-CA-C | 5.76 | 123.08 | 110.80 |
| 7 | 5B | 1580 | LYS | N-CA-C | 5.75 | 123.06 | 110.80 |
| 7 | 5A | 1485 | LYS | N-CA-C | -5.75 | 105.09 | 111.36 |
| 7 | 5A | 1282 | GLN | CA-C-N | 5.75 | 131.74 | 123.17 |
| 7 | 5A | 1282 | GLN | C-N-CA | 5.75 | 131.74 | 123.17 |
| 7 | 5C | 1282 | GLN | CA-C-N | 5.75 | 131.73 | 123.17 |
| 7 | 5C | 1282 | GLN | C-N-CA | 5.75 | 131.73 | 123.17 |
| 7 | 5B | 1282 | GLN | CA-C-N | 5.74 | 131.73 | 123.17 |
| 7 | 5B | 1282 | GLN | C-N-CA | 5.74 | 131.73 | 123.17 |
| 7 | 5C | 833 | PHE | N-CA-C | -5.74 | 101.78 | 110.28 |
| 7 | 5C | 1485 | LYS | N-CA-C | -5.73 | 105.12 | 111.36 |
| 7 | 5A | 833 | PHE | N-CA-C | -5.72 | 101.81 | 110.28 |
| 7 | 5C | 1470 | LYS | N-CA-C | 5.71 | 117.50 | 111.28 |
| 6 | 4D | 279 | LEU | N-CA-C | 5.69 | 117.48 | 111.28 |
| 7 | 5B | 833 | PHE | N-CA-C | -5.69 | 101.86 | 110.28 |
| 7 | 5A | 1470 | LYS | N-CA-C | 5.68 | 117.47 | 111.28 |
| 6 | 4C | 279 | LEU | N-CA-C | 5.67 | 117.46 | 111.28 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | 4B | 279 | LEU | N-CA-C | 5.67 | 117.46 | 111.28 |
| 6 | 4A | 110 | LYS | N-CA-C | 5.66 | 118.66 | 110.28 |
| 6 | 4B | 110 | LYS | N-CA-C | 5.66 | 118.66 | 110.28 |
| 7 | 5B | 1470 | LYS | N-CA-C | 5.66 | 117.45 | 111.28 |
| 6 | 4D | 110 | LYS | N-CA-C | 5.66 | 118.66 | 110.28 |
| 2 | HB | 129 | CYS | N-CA-CB | -5.66 | 101.89 | 110.77 |
| 2 | HF | 129 | CYS | N-CA-CB | -5.66 | 101.89 | 110.77 |
| 2 | ID | 129 | CYS | N-CA-CB | -5.65 | 101.90 | 110.77 |
| 6 | 4A | 279 | LEU | N-CA-C | 5.65 | 117.44 | 111.28 |
| 6 | 4C | 110 | LYS | N-CA-C | 5.65 | 118.64 | 110.28 |
| 2 | BD | 129 | CYS | N-CA-CB | -5.64 | 101.91 | 110.77 |
| 2 | AF | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | FD | 129 | CYS | N-CA-CB | -5.64 | 101.91 | 110.77 |
| 2 | GB | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | GD | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | JD | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | IF | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | AD | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | CD | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | GF | 129 | CYS | N-CA-CB | -5.64 | 101.92 | 110.77 |
| 2 | DD | 129 | CYS | N-CA-CB | -5.63 | 101.93 | 110.77 |
| 2 | CF | 129 | CYS | N-CA-CB | -5.63 | 101.93 | 110.77 |
| 2 | HD | 129 | CYS | N-CA-CB | -5.63 | 101.93 | 110.77 |
| 2 | EB | 129 | CYS | N-CA-CB | -5.63 | 101.94 | 110.77 |
| 2 | IB | 129 | CYS | N-CA-CB | -5.63 | 101.94 | 110.77 |
| 2 | JB | 129 | CYS | N-CA-CB | -5.63 | 101.94 | 110.77 |
| 2 | KF | 129 | CYS | N-CA-CB | -5.62 | 101.94 | 110.77 |
| 2 | BF | 129 | CYS | N-CA-CB | -5.62 | 101.95 | 110.77 |
| 6 | 4C | 139 | ASP | CA-C-N | 5.62 | 126.86 | 119.84 |
| 6 | 4C | 139 | ASP | C-N-CA | 5.62 | 126.86 | 119.84 |
| 2 | AB | 129 | CYS | N-CA-CB | -5.62 | 101.95 | 110.77 |
| 2 | KD | 129 | CYS | N-CA-CB | -5.62 | 101.95 | 110.77 |
| 2 | BB | 129 | CYS | N-CA-CB | -5.61 | 101.96 | 110.77 |
| 2 | JF | 129 | CYS | N-CA-CB | -5.61 | 101.96 | 110.77 |
| 6 | 4C | 264 | GLY | N-CA-C | -5.61 | 107.30 | 114.37 |
| 2 | EF | 129 | CYS | N-CA-CB | -5.61 | 101.97 | 110.77 |
| 6 | 4A | 139 | ASP | CA-C-N | 5.60 | 126.84 | 119.84 |
| 6 | 4A | 139 | ASP | C-N-CA | 5.60 | 126.84 | 119.84 |
| 2 | KB | 129 | CYS | N-CA-CB | -5.60 | 101.97 | 110.77 |
| 6 | 4B | 139 | ASP | CA-C-N | 5.60 | 126.84 | 119.84 |
| 6 | 4B | 139 | ASP | C-N-CA | 5.60 | 126.84 | 119.84 |
| 6 | 4A | 264 | GLY | N-CA-C | -5.60 | 107.31 | 114.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | 4D | 264 | GLY | N-CA-C | -5.60 | 107.32 | 114.37 |
| 2 | CB | 129 | CYS | N-CA-CB | -5.59 | 101.99 | 110.77 |
| 2 | FB | 129 | CYS | N-CA-CB | -5.59 | 101.99 | 110.77 |
| 2 | FF | 129 | CYS | N-CA-CB | -5.59 | 101.99 | 110.77 |
| 6 | 4B | 169 | ALA | N-CA-C | 5.59 | 117.38 | 111.28 |
| 6 | 4B | 264 | GLY | N-CA-C | -5.59 | 107.33 | 114.37 |
| 2 | DB | 129 | CYS | N-CA-CB | -5.59 | 102.00 | 110.77 |
| 2 | ED | 129 | CYS | N-CA-CB | -5.58 | 102.00 | 110.77 |
| 6 | 4D | 139 | ASP | CA-C-N | 5.58 | 126.82 | 119.84 |
| 6 | 4D | 139 | ASP | C-N-CA | 5.58 | 126.82 | 119.84 |
| 2 | DF | 129 | CYS | N-CA-CB | -5.58 | 102.01 | 110.77 |
| 2 | LB | 129 | CYS | N-CA-CB | -5.58 | 102.01 | 110.77 |
| 6 | 4D | 169 | ALA | N-CA-C | 5.58 | 117.36 | 111.28 |
| 7 | 5B | 1470 | LYS | CA-C-N | -5.58 | 111.93 | 121.97 |
| 7 | 5B | 1470 | LYS | C-N-CA | -5.58 | 111.93 | 121.97 |
| 2 | MB | 129 | CYS | N-CA-CB | -5.58 | 102.02 | 110.77 |
| 2 | LF | 129 | CYS | N-CA-CB | -5.57 | 102.03 | 110.77 |
| 6 | 4A | 169 | ALA | N-CA-C | 5.57 | 117.35 | 111.28 |
| 2 | MD | 129 | CYS | N-CA-CB | -5.57 | 102.03 | 110.77 |
| 6 | 4C | 169 | ALA | N-CA-C | 5.56 | 117.34 | 111.28 |
| 2 | LD | 129 | CYS | N-CA-CB | -5.55 | 102.05 | 110.77 |
| 2 | MF | 129 | CYS | N-CA-CB | -5.55 | 102.05 | 110.77 |
| 7 | 5A | 1470 | LYS | CA-C-N | -5.55 | 111.98 | 121.97 |
| 7 | 5A | 1470 | LYS | C-N-CA | -5.55 | 111.98 | 121.97 |
| 7 | 5C | 1470 | LYS | CA-C-N | -5.54 | 112.00 | 121.97 |
| 7 | 5C | 1470 | LYS | C-N-CA | -5.54 | 112.00 | 121.97 |
| 4 | 2C | 149 | ILE | O-C-N | -5.52 | 115.67 | 122.57 |
| 6 | 4B | 139 | ASP | N-CA-C | 5.48 | 116.61 | 109.64 |
| 6 | 4A | 139 | ASP | N-CA-C | 5.47 | 116.59 | 109.64 |
| 6 | 4C | 139 | ASP | N-CA-C | 5.46 | 116.58 | 109.64 |
| 4 | 2A | 149 | ILE | O-C-N | -5.45 | 115.76 | 122.57 |
| 6 | 4D | 139 | ASP | N-CA-C | 5.45 | 116.56 | 109.64 |
| 4 | 2B | 149 | ILE | O-C-N | -5.43 | 115.78 | 122.57 |
| 6 | 4D | 277 | GLU | N-CA-C | 5.41 | 117.93 | 111.71 |
| 6 | 4B | 277 | GLU | N-CA-C | 5.38 | 117.89 | 111.71 |
| 6 | 4C | 277 | GLU | N-CA-C | 5.37 | 117.89 | 111.71 |
| 6 | 4A | 277 | GLU | N-CA-C | 5.36 | 117.87 | 111.71 |
| 7 | 5B | 1315 | ARG | CA-C-N | 5.34 | 127.87 | 120.29 |
| 7 | 5B | 1315 | ARG | C-N-CA | 5.34 | 127.87 | 120.29 |
| 7 | 5C | 1257 | ASP | CA-C-N | 5.32 | 128.40 | 120.31 |
| 7 | 5C | 1257 | ASP | C-N-CA | 5.32 | 128.40 | 120.31 |
| 7 | 5C | 1315 | ARG | CA-C-N | 5.32 | 127.84 | 120.29 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 7 | 5C | 1315 | ARG | C-N-CA | 5.32 | 127.84 | 120.29 |
| 7 | 5A | 1315 | ARG | CA-C-N | 5.31 | 127.83 | 120.29 |
| 7 | 5A | 1315 | ARG | C-N-CA | 5.31 | 127.83 | 120.29 |
| 7 | 5A | 1257 | ASP | CA-C-N | 5.31 | 128.38 | 120.31 |
| 7 | 5A | 1257 | ASP | C-N-CA | 5.31 | 128.38 | 120.31 |
| 7 | 5B | 1257 | ASP | CA-C-N | 5.30 | 128.36 | 120.31 |
| 7 | 5B | 1257 | ASP | C-N-CA | 5.30 | 128.36 | 120.31 |
| 7 | 5C | 1245 | GLY | CA-C-N | 5.30 | 131.26 | 121.52 |
| 7 | 5C | 1245 | GLY | C-N-CA | 5.30 | 131.26 | 121.52 |
| 7 | 5A | 1245 | GLY | CA-C-N | 5.28 | 131.23 | 121.52 |
| 7 | 5A | 1245 | GLY | C-N-CA | 5.28 | 131.23 | 121.52 |
| 7 | 5B | 1245 | GLY | CA-C-N | 5.27 | 131.22 | 121.52 |
| 7 | 5B | 1245 | GLY | C-N-CA | 5.27 | 131.22 | 121.52 |
| 7 | 5B | 1391 | GLN | N-CA-C | -5.27 | 105.45 | 111.14 |
| 2 | EF | 128 | ASP | N-CA-C | 5.25 | 121.99 | 110.80 |
| 7 | 5C | 1391 | GLN | N-CA-C | -5.25 | 105.47 | 111.14 |
| 7 | 5A | 1391 | GLN | N-CA-C | -5.25 | 105.47 | 111.14 |
| 2 | EB | 128 | ASP | N-CA-C | 5.24 | 121.97 | 110.80 |
| 2 | MD | 128 | ASP | N-CA-C | 5.24 | 121.97 | 110.80 |
| 2 | GB | 128 | ASP | N-CA-C | 5.24 | 121.96 | 110.80 |
| 2 | DD | 128 | ASP | N-CA-C | 5.24 | 121.96 | 110.80 |
| 2 | KB | 128 | ASP | N-CA-C | 5.24 | 121.96 | 110.80 |
| 2 | FB | 128 | ASP | N-CA-C | 5.24 | 121.96 | 110.80 |
| 2 | BD | 128 | ASP | N-CA-C | 5.24 | 121.95 | 110.80 |
| 2 | DB | 128 | ASP | N-CA-C | 5.24 | 121.95 | 110.80 |
| 2 | JF | 128 | ASP | N-CA-C | 5.24 | 121.95 | 110.80 |
| 2 | DF | 128 | ASP | N-CA-C | 5.23 | 121.94 | 110.80 |
| 2 | IB | 128 | ASP | N-CA-C | 5.23 | 121.94 | 110.80 |
| 2 | ED | 128 | ASP | N-CA-C | 5.23 | 121.93 | 110.80 |
| 2 | HB | 128 | ASP | N-CA-C | 5.22 | 121.93 | 110.80 |
| 2 | KF | 128 | ASP | N-CA-C | 5.22 | 121.93 | 110.80 |
| 2 | BB | 128 | ASP | N-CA-C | 5.22 | 121.92 | 110.80 |
| 2 | FD | 128 | ASP | N-CA-C | 5.22 | 121.93 | 110.80 |
| 2 | KD | 128 | ASP | N-CA-C | 5.22 | 121.92 | 110.80 |
| 2 | AF | 128 | ASP | N-CA-C | 5.22 | 121.92 | 110.80 |
| 2 | FF | 128 | ASP | N-CA-C | 5.22 | 121.92 | 110.80 |
| 2 | JD | 128 | ASP | N-CA-C | 5.22 | 121.92 | 110.80 |
| 2 | CF | 128 | ASP | N-CA-C | 5.22 | 121.91 | 110.80 |
| 2 | AB | 128 | ASP | N-CA-C | 5.22 | 121.91 | 110.80 |
| 2 | BF | 128 | ASP | N-CA-C | 5.22 | 121.91 | 110.80 |
| 2 | GF | 128 | ASP | N-CA-C | 5.22 | 121.91 | 110.80 |
| 2 | MF | 128 | ASP | N-CA-C | 5.22 | 121.91 | 110.80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2 | HF | 128 | ASP | N-CA-C | 5.21 | 121.91 | 110.80 |
| 7 | 5B | 811 | GLN | CA-C-N | 5.21 | 131.50 | 121.54 |
| 7 | 5B | 811 | GLN | C-N-CA | 5.21 | 131.50 | 121.54 |
| 2 | IF | 128 | ASP | N-CA-C | 5.21 | 121.90 | 110.80 |
| 7 | 5A | 811 | GLN | CA-C-N | 5.21 | 131.50 | 121.54 |
| 7 | 5A | 811 | GLN | C-N-CA | 5.21 | 131.50 | 121.54 |
| 2 | CD | 128 | ASP | N-CA-C | 5.21 | 121.89 | 110.80 |
| 2 | JB | 128 | ASP | N-CA-C | 5.21 | 121.89 | 110.80 |
| 2 | LB | 128 | ASP | N-CA-C | 5.21 | 121.89 | 110.80 |
| 2 | CB | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | LD | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | GD | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | ID | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | LF | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 7 | 5C | 1396 | GLN | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | AD | 128 | ASP | N-CA-C | 5.20 | 121.87 | 110.80 |
| 2 | HD | 128 | ASP | N-CA-C | 5.20 | 121.88 | 110.80 |
| 2 | MB | 128 | ASP | N-CA-C | 5.20 | 121.87 | 110.80 |
| 7 | 5B | 1396 | GLN | N-CA-C | 5.19 | 121.86 | 110.80 |
| 7 | 5C | 811 | GLN | CA-C-N | 5.19 | 131.46 | 121.54 |
| 7 | 5C | 811 | GLN | C-N-CA | 5.19 | 131.46 | 121.54 |
| 7 | 5A | 1396 | GLN | N-CA-C | 5.19 | 121.85 | 110.80 |
| 7 | 5B | 800 | LYS | N-CA-C | 5.19 | 116.93 | 111.28 |
| 7 | 5A | 800 | LYS | N-CA-C | 5.18 | 116.92 | 111.28 |
| 6 | 4A | 234 | SER | N-CA-C | 5.17 | 116.92 | 111.28 |
| 6 | 4D | 234 | SER | N-CA-C | 5.16 | 116.91 | 111.28 |
| 6 | 4A | 106 | ALA | CA-C-N | 5.15 | 127.70 | 120.28 |
| 6 | 4A | 106 | ALA | C-N-CA | 5.15 | 127.70 | 120.28 |
| 6 | 4B | 234 | SER | N-CA-C | 5.15 | 116.89 | 111.28 |
| 6 | 4C | 234 | SER | N-CA-C | 5.14 | 116.88 | 111.28 |
| 6 | 4D | 106 | ALA | CA-C-N | 5.14 | 127.68 | 120.28 |
| 6 | 4D | 106 | ALA | C-N-CA | 5.14 | 127.68 | 120.28 |
| 7 | 5C | 800 | LYS | N-CA-C | 5.13 | 116.88 | 111.28 |
| 6 | 4B | 106 | ALA | CA-C-N | 5.13 | 127.67 | 120.28 |
| 6 | 4B | 106 | ALA | C-N-CA | 5.13 | 127.67 | 120.28 |
| 7 | 5B | 1470 | LYS | CA-C-O | -5.13 | 115.11 | 120.55 |
| 6 | 4C | 106 | ALA | CA-C-N | 5.12 | 127.66 | 120.28 |
| 6 | 4C | 106 | ALA | C-N-CA | 5.12 | 127.66 | 120.28 |
| 7 | 5A | 1470 | LYS | CA-C-O | -5.12 | 115.13 | 120.55 |
| 7 | 5C | 1470 | LYS | CA-C-O | -5.12 | 115.13 | 120.55 |
| 6 | 4C | 232 | LYS | CA-C-N | 5.11 | 131.29 | 121.54 |
| 6 | 4C | 232 | LYS | C-N-CA | 5.11 | 131.29 | 121.54 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 6 | 4B | 232 | LYS | CA-C-N | 5.11 | 131.29 | 121.54 |
| 6 | 4B | 232 | LYS | C-N-CA | 5.11 | 131.29 | 121.54 |
| 6 | 4D | 111 | GLU | N-CA-C | -5.11 | 105.95 | 113.61 |
| 6 | 4B | 217 | ASN | N-CA-C | 5.10 | 119.49 | 113.16 |
| 6 | 4A | 232 | LYS | CA-C-N | 5.10 | 131.28 | 121.54 |
| 6 | 4A | 232 | LYS | C-N-CA | 5.10 | 131.28 | 121.54 |
| 6 | 4D | 217 | ASN | N-CA-C | 5.10 | 119.48 | 113.16 |
| 6 | 4B | 111 | GLU | N-CA-C | -5.09 | 105.97 | 113.61 |
| 6 | 4D | 232 | LYS | CA-C-N | 5.09 | 131.26 | 121.54 |
| 6 | 4D | 232 | LYS | C-N-CA | 5.09 | 131.26 | 121.54 |
| 6 | 4A | 111 | GLU | N-CA-C | -5.08 | 106.00 | 113.61 |
| 6 | 4C | 111 | GLU | N-CA-C | -5.07 | 106.00 | 113.61 |
| 6 | 4C | 217 | ASN | N-CA-C | 5.07 | 119.45 | 113.16 |
| 6 | 4A | 217 | ASN | N-CA-C | 5.07 | 119.44 | 113.16 |
| 2 | GD | 126 | GLY | N-CA-C | 5.03 | 118.76 | 112.73 |
| 7 | 5C | 1407 | GLN | CA-C-N | -5.02 | 113.17 | 120.29 |
| 7 | 5C | 1407 | GLN | C-N-CA | -5.02 | 113.17 | 120.29 |
| 7 | 5B | 1407 | GLN | CA-C-N | -5.01 | 113.17 | 120.29 |
| 7 | 5B | 1407 | GLN | C-N-CA | -5.01 | 113.17 | 120.29 |
| 7 | 5A | 1407 | GLN | CA-C-N | -5.01 | 113.17 | 120.29 |
| 7 | 5A | 1407 | GLN | C-N-CA | -5.01 | 113.17 | 120.29 |
| 2 | ID | 126 | GLY | N-CA-C | 5.01 | 118.74 | 112.73 |
| 2 | MF | 126 | GLY | N-CA-C | 5.01 | 118.74 | 112.73 |

There are no chirality outliers.

All (25) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 4 | 2A | 142 | LEU | Mainchain |
| 4 | 2B | 142 | LEU | Mainchain |
| 4 | 2C | 142 | LEU | Mainchain |
| 4 | 2C | 144 | ASN | Peptide |
| 7 | 5A | 1253 | ILE | Mainchain |
| 7 | 5A | 1278 | GLY | Mainchain |
| 7 | 5A | 1279 | ASP | Mainchain |
| 7 | 5A | 1280 | SER | Mainchain |
| 7 | 5A | 1281 | ASN | Mainchain |
| 7 | 5A | 1282 | GLN | Mainchain |
| 7 | 5A | 1283 | ALA | Mainchain |
| 7 | 5B | 1253 | ILE | Mainchain |
| 7 | 5B | 1278 | GLY | Mainchain |
| 7 | 5B | 1279 | ASP | Mainchain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 7 | 5B | 1280 | SER | Mainchain |
| 7 | 5B | 1281 | ASN | Mainchain |
| 7 | 5B | 1282 | GLN | Mainchain |
| 7 | 5B | 1283 | ALA | Mainchain |
| 7 | 5C | 1253 | ILE | Mainchain |
| 7 | 5C | 1278 | GLY | Mainchain |
| 7 | 5C | 1279 | ASP | Mainchain |
| 7 | 5C | 1280 | SER | Mainchain |
| 7 | 5C | 1281 | ASN | Mainchain |
| 7 | 5C | 1282 | GLN | Mainchain |
| 7 | 5C | 1283 | ALA | Mainchain |

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 | AA | 3350 | 0 | 3287 | 97 | 0 |
| 1 | AC | 3350 | 0 | 3284 | 169 | 0 |
| 1 | AE | 3350 | 0 | 3282 | 192 | 0 |
| 1 | BA | 3350 | 0 | 3285 | 101 | 0 |
| 1 | BC | 3350 | 0 | 3282 | 168 | 0 |
| 1 | BE | 3350 | 0 | 3281 | 171 | 0 |
| 1 | CA | 3350 | 0 | 3284 | 117 | 0 |
| 1 | CC | 3350 | 0 | 3280 | 189 | 0 |
| 1 | CE | 3350 | 0 | 3280 | 190 | 0 |
| 1 | DA | 3350 | 0 | 3278 | 138 | 0 |
| 1 | DC | 3350 | 0 | 3276 | 211 | 0 |
| 1 | DE | 3350 | 0 | 3275 | 212 | 0 |
| 1 | EA | 3350 | 0 | 3281 | 157 | 0 |
| 1 | EC | 3350 | 0 | 3279 | 216 | 0 |
| 1 | EE | 3350 | 0 | 3279 | 226 | 0 |
| 1 | FA | 3350 | 0 | 3277 | 235 | 0 |
| 1 | FC | 3350 | 0 | 3274 | 277 | 0 |
| 1 | FE | 3350 | 0 | 3276 | 269 | 0 |
| 1 | GA | 3350 | 0 | 3284 | 181 | 0 |
| 1 | GC | 3350 | 0 | 3279 | 234 | 0 |
| 1 | GE | 3350 | 0 | 3278 | 227 | 0 |
| 1 | HA | 3350 | 0 | 3286 | 144 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | HC | 3350 | 0 | 3283 | 243 | 0 |
| 1 | HE | 3350 | 0 | 3283 | 259 | 0 |
| 1 | IA | 3350 | 0 | 3282 | 169 | 0 |
| 1 | IC | 3350 | 0 | 3279 | 247 | 0 |
| 1 | IE | 3350 | 0 | 3279 | 215 | 0 |
| 1 | JA | 3350 | 0 | 3283 | 158 | 0 |
| 1 | JC | 3350 | 0 | 3278 | 221 | 0 |
| 1 | JE | 3350 | 0 | 3278 | 231 | 0 |
| 1 | KA | 3350 | 0 | 3283 | 219 | 0 |
| 1 | KC | 3350 | 0 | 3282 | 283 | 0 |
| 1 | KE | 3350 | 0 | 3281 | 266 | 0 |
| 1 | LA | 3350 | 0 | 3281 | 234 | 0 |
| 1 | LC | 3350 | 0 | 3277 | 315 | 0 |
| 1 | LE | 3350 | 0 | 3277 | 275 | 0 |
| 1 | MA | 3350 | 0 | 3286 | 176 | 0 |
| 1 | MC | 3350 | 0 | 3283 | 235 | 0 |
| 1 | ME | 3350 | 0 | 3283 | 231 | 0 |
| 2 | AB | 3366 | 0 | 3252 | 166 | 0 |
| 2 | AD | 3366 | 0 | 3246 | 262 | 0 |
| 2 | AF | 3366 | 0 | 3248 | 182 | 0 |
| 2 | BB | 3366 | 0 | 3254 | 182 | 0 |
| 2 | BD | 3366 | 0 | 3254 | 181 | 0 |
| 2 | BF | 3366 | 0 | 3254 | 109 | 0 |
| 2 | CB | 3366 | 0 | 3255 | 204 | 0 |
| 2 | CD | 3366 | 0 | 3255 | 205 | 0 |
| 2 | CF | 3366 | 0 | 3255 | 129 | 0 |
| 2 | DB | 3366 | 0 | 3252 | 214 | 0 |
| 2 | DD | 3366 | 0 | 3252 | 221 | 0 |
| 2 | DF | 3366 | 0 | 3252 | 137 | 0 |
| 2 | EB | 3366 | 0 | 3253 | 240 | 0 |
| 2 | ED | 3366 | 0 | 3252 | 242 | 0 |
| 2 | EF | 3366 | 0 | 3252 | 165 | 0 |
| 2 | FB | 3366 | 0 | 3250 | 254 | 0 |
| 2 | FD | 3366 | 0 | 3250 | 242 | 0 |
| 2 | FF | 3366 | 0 | 3250 | 170 | 0 |
| 2 | GB | 3366 | 0 | 3251 | 242 | 0 |
| 2 | GD | 3366 | 0 | 3251 | 220 | 0 |
| 2 | GF | 3366 | 0 | 3252 | 147 | 0 |
| 2 | HB | 3366 | 0 | 3255 | 197 | 0 |
| 2 | HD | 3366 | 0 | 3255 | 190 | 0 |
| 2 | HF | 3366 | 0 | 3255 | 120 | 0 |
| 2 | IB | 3366 | 0 | 3254 | 194 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | ID | 3366 | 0 | 3254 | 185 | 0 |
| 2 | IF | 3366 | 0 | 3255 | 123 | 0 |
| 2 | JB | 3366 | 0 | 3254 | 209 | 0 |
| 2 | JD | 3366 | 0 | 3254 | 198 | 0 |
| 2 | JF | 3366 | 0 | 3254 | 138 | 0 |
| 2 | KB | 3366 | 0 | 3248 | 356 | 0 |
| 2 | KD | 3366 | 0 | 3246 | 348 | 0 |
| 2 | KF | 3366 | 0 | 3246 | 290 | 0 |
| 2 | LB | 3366 | 0 | 3241 | 435 | 0 |
| 2 | LD | 3366 | 0 | 3244 | 399 | 0 |
| 2 | LF | 3366 | 0 | 3249 | 355 | 0 |
| 2 | MB | 3366 | 0 | 3255 | 242 | 0 |
| 2 | MD | 3366 | 0 | 3256 | 225 | 0 |
| 2 | MF | 3366 | 0 | 3256 | 145 | 0 |
| 3 | 1A | 1141 | 0 | 1144 | 37 | 0 |
| 3 | 1B | 1141 | 0 | 1145 | 23 | 0 |
| 3 | 1C | 1141 | 0 | 1144 | 14 | 0 |
| 4 | 2A | 1615 | 0 | 1664 | 170 | 0 |
| 4 | 2B | 1615 | 0 | 1665 | 183 | 0 |
| 4 | 2C | 1615 | 0 | 1662 | 215 | 0 |
| 5 | 3A | 2752 | 0 | 2802 | 129 | 0 |
| 5 | 3B | 2752 | 0 | 2807 | 46 | 0 |
| 5 | 3C | 2752 | 0 | 2802 | 129 | 0 |
| 6 | 4A | 1587 | 0 | 1558 | 487 | 0 |
| 6 | 4B | 1587 | 0 | 1561 | 408 | 0 |
| 6 | 4C | 1587 | 0 | 1562 | 349 | 0 |
| 6 | 4D | 1587 | 0 | 1569 | 339 | 0 |
| 7 | 5A | 5953 | 0 | 6017 | 966 | 0 |
| 7 | 5B | 5953 | 0 | 6016 | 943 | 0 |
| 7 | 5C | 5953 | 0 | 6016 | 953 | 0 |
| 8 | 6A | 2077 | 0 | 2097 | 86 | 0 |
| 8 | 6B | 2077 | 0 | 2098 | 87 | 0 |
| 8 | 6C | 2077 | 0 | 2099 | 93 | 0 |
| 9 | 7A | 383 | 0 | 390 | 151 | 0 |
| 9 | 7B | 383 | 0 | 392 | 155 | 0 |
| 9 | 7C | 383 | 0 | 390 | 131 | 0 |
| 9 | 7D | 383 | 0 | 392 | 155 | 0 |
| 9 | 7E | 383 | 0 | 391 | 105 | 0 |
| 9 | 7F | 383 | 0 | 392 | 109 | 0 |
| 10 | 8A | 189 | 0 | 41 | 8 | 0 |
| 10 | 8B | 189 | 0 | 41 | 7 | 0 |
| 10 | 8C | 189 | 0 | 40 | 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | 8D | 189 | 0 | 41 | 18 | 0 |
| 10 | 8E | 189 | 0 | 41 | 16 | 0 |
| 10 | 8F | 189 | 0 | 40 | 10 | 0 |
| 10 | 8G | 189 | 0 | 41 | 9 | 0 |
| 10 | 8H | 189 | 0 | 41 | 9 | 0 |
| 10 | 8I | 189 | 0 | 40 | 6 | 0 |
| 10 | 8J | 189 | 0 | 41 | 14 | 0 |
| 10 | 8K | 189 | 0 | 41 | 14 | 0 |
| 10 | 8L | 189 | 0 | 40 | 11 | 0 |
| 10 | 8M | 189 | 0 | 41 | 10 | 0 |
| 10 | 8N | 189 | 0 | 41 | 10 | 0 |
| 10 | 8O | 189 | 0 | 40 | 7 | 0 |
| 10 | 8P | 189 | 0 | 41 | 10 | 0 |
| 10 | 8Q | 189 | 0 | 41 | 6 | 0 |
| 10 | 8R | 189 | 0 | 40 | 5 | 0 |
| 10 | 8S | 189 | 0 | 41 | 20 | 0 |
| 10 | 8T | 189 | 0 | 40 | 23 | 0 |
| 10 | 8U | 189 | 0 | 39 | 33 | 0 |
| 10 | 8V | 189 | 0 | 41 | 45 | 0 |
| 10 | 8W | 189 | 0 | 41 | 34 | 0 |
| 10 | 8X | 189 | 0 | 40 | 19 | 0 |
| 10 | 8Y | 189 | 0 | 40 | 25 | 0 |
| 10 | 8Z | 189 | 0 | 40 | 31 | 0 |
| 10 | 9A | 189 | 0 | 38 | 26 | 0 |
| 11 | AA | 32 | 0 | 12 | 0 | 0 |
| 11 | AC | 32 | 0 | 12 | 0 | 0 |
| 11 | AE | 32 | 0 | 12 | 0 | 0 |
| 11 | BA | 32 | 0 | 12 | 0 | 0 |
| 11 | BC | 32 | 0 | 12 | 0 | 0 |
| 11 | BE | 32 | 0 | 12 | 0 | 0 |
| 11 | CA | 32 | 0 | 12 | 0 | 0 |
| 11 | CC | 32 | 0 | 12 | 0 | 0 |
| 11 | CE | 32 | 0 | 12 | 0 | 0 |
| 11 | DA | 32 | 0 | 12 | 0 | 0 |
| 11 | DC | 32 | 0 | 12 | 0 | 0 |
| 11 | DE | 32 | 0 | 12 | 0 | 0 |
| 11 | EA | 32 | 0 | 12 | 0 | 0 |
| 11 | EC | 32 | 0 | 12 | 0 | 0 |
| 11 | EE | 32 | 0 | 12 | 0 | 0 |
| 11 | FA | 32 | 0 | 12 | 0 | 0 |
| 11 | FC | 32 | 0 | 12 | 0 | 0 |
| 11 | FE | 32 | 0 | 12 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | GA | 32 | 0 | 12 | 0 | 0 |
| 11 | GC | 32 | 0 | 12 | 0 | 0 |
| 11 | GE | 32 | 0 | 12 | 0 | 0 |
| 11 | HA | 32 | 0 | 12 | 0 | 0 |
| 11 | HC | 32 | 0 | 12 | 0 | 0 |
| 11 | HE | 32 | 0 | 12 | 0 | 0 |
| 11 | IA | 32 | 0 | 12 | 0 | 0 |
| 11 | IC | 32 | 0 | 12 | 0 | 0 |
| 11 | IE | 32 | 0 | 12 | 0 | 0 |
| 11 | JA | 32 | 0 | 12 | 0 | 0 |
| 11 | JC | 32 | 0 | 12 | 0 | 0 |
| 11 | JE | 32 | 0 | 12 | 0 | 0 |
| 11 | KA | 32 | 0 | 12 | 0 | 0 |
| 11 | KC | 32 | 0 | 12 | 0 | 0 |
| 11 | KE | 32 | 0 | 12 | 0 | 0 |
| 11 | LA | 32 | 0 | 12 | 0 | 0 |
| 11 | LC | 32 | 0 | 12 | 0 | 0 |
| 11 | LE | 32 | 0 | 12 | 0 | 0 |
| 11 | MA | 32 | 0 | 12 | 1 | 0 |
| 11 | MC | 32 | 0 | 12 | 1 | 0 |
| 11 | ME | 32 | 0 | 12 | 0 | 0 |
| 12 | AA | 1 | 0 | 0 | 0 | 0 |
| 12 | AC | 1 | 0 | 0 | 0 | 0 |
| 12 | AE | 1 | 0 | 0 | 0 | 0 |
| 12 | BA | 1 | 0 | 0 | 0 | 0 |
| 12 | BC | 1 | 0 | 0 | 0 | 0 |
| 12 | BE | 1 | 0 | 0 | 0 | 0 |
| 12 | CA | 1 | 0 | 0 | 0 | 0 |
| 12 | CC | 1 | 0 | 0 | 0 | 0 |
| 12 | CE | 1 | 0 | 0 | 0 | 0 |
| 12 | DA | 1 | 0 | 0 | 0 | 0 |
| 12 | DC | 1 | 0 | 0 | 0 | 0 |
| 12 | DE | 1 | 0 | 0 | 0 | 0 |
| 12 | EA | 1 | 0 | 0 | 0 | 0 |
| 12 | ED | 1 | 0 | 0 | 0 | 0 |
| 12 | EE | 1 | 0 | 0 | 0 | 0 |
| 12 | FB | 1 | 0 | 0 | 0 | 0 |
| 12 | FD | 1 | 0 | 0 | 0 | 0 |
| 12 | FE | 1 | 0 | 0 | 0 | 0 |
| 12 | GA | 1 | 0 | 0 | 0 | 0 |
| 12 | GC | 1 | 0 | 0 | 0 | 0 |
| 12 | GE | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 12 | HA | 1 | 0 | 0 | 0 | 0 |
| 12 | HC | 1 | 0 | 0 | 0 | 0 |
| 12 | HE | 1 | 0 | 0 | 0 | 0 |
| 12 | IA | 1 | 0 | 0 | 0 | 0 |
| 12 | IC | 1 | 0 | 0 | 0 | 0 |
| 12 | IE | 1 | 0 | 0 | 0 | 0 |
| 12 | JA | 1 | 0 | 0 | 0 | 0 |
| 12 | JC | 1 | 0 | 0 | 0 | 0 |
| 12 | JE | 1 | 0 | 0 | 0 | 0 |
| 12 | KA | 1 | 0 | 0 | 0 | 0 |
| 12 | KC | 1 | 0 | 0 | 0 | 0 |
| 12 | KE | 1 | 0 | 0 | 0 | 0 |
| 12 | LA | 1 | 0 | 0 | 0 | 0 |
| 12 | LC | 1 | 0 | 0 | 0 | 0 |
| 12 | LE | 1 | 0 | 0 | 0 | 0 |
| 12 | MB | 1 | 0 | 0 | 0 | 0 |
| 12 | MD | 1 | 0 | 0 | 0 | 0 |
| 12 | MF | 1 | 0 | 0 | 0 | 0 |
| 13 | AB | 28 | 0 | 12 | 2 | 0 |
| 13 | AD | 28 | 0 | 12 | 2 | 0 |
| 13 | AF | 28 | 0 | 12 | 1 | 0 |
| 13 | BB | 28 | 0 | 12 | 3 | 0 |
| 13 | BD | 28 | 0 | 12 | 3 | 0 |
| 13 | BF | 28 | 0 | 12 | 2 | 0 |
| 13 | CB | 28 | 0 | 12 | 3 | 0 |
| 13 | CD | 28 | 0 | 12 | 3 | 0 |
| 13 | CF | 28 | 0 | 12 | 2 | 0 |
| 13 | DB | 28 | 0 | 12 | 3 | 0 |
| 13 | DD | 28 | 0 | 12 | 3 | 0 |
| 13 | DF | 28 | 0 | 12 | 2 | 0 |
| 13 | EB | 28 | 0 | 12 | 4 | 0 |
| 13 | ED | 28 | 0 | 12 | 4 | 0 |
| 13 | EF | 28 | 0 | 12 | 2 | 0 |
| 13 | FB | 28 | 0 | 12 | 4 | 0 |
| 13 | FD | 28 | 0 | 12 | 4 | 0 |
| 13 | FF | 28 | 0 | 12 | 2 | 0 |
| 13 | GB | 28 | 0 | 12 | 3 | 0 |
| 13 | GD | 28 | 0 | 12 | 3 | 0 |
| 13 | GF | 28 | 0 | 12 | 2 | 0 |
| 13 | HB | 28 | 0 | 12 | 3 | 0 |
| 13 | HD | 28 | 0 | 12 | 3 | 0 |
| 13 | HF | 28 | 0 | 12 | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 13 | IB | 28 | 0 | 12 | 3 | 0 |
| 13 | ID | 28 | 0 | 12 | 3 | 0 |
| 13 | IF | 28 | 0 | 12 | 2 | 0 |
| 13 | JB | 28 | 0 | 12 | 3 | 0 |
| 13 | JD | 28 | 0 | 12 | 3 | 0 |
| 13 | JF | 28 | 0 | 12 | 2 | 0 |
| 13 | KB | 28 | 0 | 12 | 3 | 0 |
| 13 | KD | 28 | 0 | 12 | 3 | 0 |
| 13 | KF | 28 | 0 | 12 | 2 | 0 |
| 13 | LB | 28 | 0 | 12 | 2 | 0 |
| 13 | LD | 28 | 0 | 12 | 2 | 0 |
| 13 | LF | 28 | 0 | 12 | 2 | 0 |
| 13 | MB | 28 | 0 | 12 | 2 | 0 |
| 13 | MD | 28 | 0 | 12 | 2 | 0 |
| 13 | MF | 28 | 0 | 12 | 2 | 0 |
| All | All | 318666 | 0 | 306569 | 15548 | 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 25.

All (15548) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:DD:212:PHE:CZ | 1:DE:326:LYS:HD3 | 1.22 | 1.73 |
| 2:KB:217:LEU:HD22 | 6:4A:263:CYS:SG | 1.30 | 1.72 |
| 2:DB:212:PHE:CZ | 1:DC:326:LYS:HD3 | 1.24 | 1.68 |
| 2:ED:125:GLU:CA | 7:5A:903:PHE:CE2 | 1.76 | 1.67 |
| 2:ED:212:PHE:CZ | 1:EE:326:LYS:HD3 | 1.27 | 1.67 |
| 2:CB:86:ARG:HA | 2:DB:281:TYR:CE1 | 1.23 | 1.66 |
| 2:LB:212:PHE:CZ | 1:LC:326:LYS:HD3 | 1.31 | 1.65 |
| 1:FE:282:TYR:CE2 | 10:8O:18:UNK:CB | 1.80 | 1.65 |
| 2:BD:212:PHE:CZ | 1:BE:326:LYS:HD3 | 1.29 | 1.65 |
| 9:7A:7:LEU:HD22 | 9:7B:27:GLY:CA | 1.27 | 1.65 |
| 2:EB:212:PHE:CZ | 1:EC:326:LYS:HD3 | 1.28 | 1.64 |
| 2:CB:212:PHE:CZ | 1:CC:326:LYS:HD3 | 1.23 | 1.63 |
| 2:CD:212:PHE:CZ | 1:CE:326:LYS:HD3 | 1.27 | 1.63 |
| 2:FB:55:THR:CG2 | 2:GB:284:LEU:H | 1.07 | 1.63 |
| 9:7C:7:LEU:HD22 | 9:7D:27:GLY:CA | 1.27 | 1.62 |
| 7:5B:1548:VAL:CG1 | 7:5B:1566:GLU:HA | 1.15 | 1.62 |
| 2:CD:86:ARG:HA | 2:DD:281:TYR:CE1 | 1.22 | 1.62 |
| 2:ED:125:GLU:HA | 7:5A:903:PHE:CE2 | 1.20 | 1.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:89:PRO:CG | 1:GA:280:LYS:HD2 | 1.20 | 1.62 |
| 7:5A:1548:VAL:CG1 | 7:5A:1566:GLU:HA | 1.15 | 1.62 |
| 1:FA:89:PRO:CD | 1:GA:280:LYS:HD2 | 1.24 | 1.61 |
| 7:5C:1548:VAL:CG1 | 7:5C:1566:GLU:HA | 1.15 | 1.61 |
| 2:FB:54:ALA:CA | 2:GB:283:ALA:HB2 | 1.26 | 1.61 |
| 2:CF:86:ARG:HA | 2:DF:281:TYR:CE1 | 1.23 | 1.60 |
| 2:LF:55:THR:HG23 | 2:MF:283:ALA:CA | 1.16 | 1.60 |
| 2:EB:125:GLU:HA | 7:5C:903:PHE:CE2 | 1.15 | 1.60 |
| 9:7C:11:TYR:CD1 | 9:7D:26:LEU:HD23 | 1.36 | 1.60 |
| 2:KB:77:ARG:HG2 | 2:LB:281:TYR:CZ | 1.34 | 1.59 |
| 7:5C:1487:ASN:CB | 7:5C:1568:LYS:HE2 | 1.23 | 1.59 |
| 2:KD:221:THR:HG21 | 6:4B:261:SER:C | 1.23 | 1.59 |
| 1:EA:396:ASP:CB | 7:5C:817:LEU:HD21 | 1.13 | 1.59 |
| 1:FC:177:VAL:HG23 | 7:5A:915:PHE:CE2 | 1.11 | 1.59 |
| 7:5A:1487:ASN:CB | 7:5A:1568:LYS:HE2 | 1.23 | 1.59 |
| 2:BB:212:PHE:CZ | 1:BC:326:LYS:HD3 | 1.30 | 1.59 |
| 7:5B:1487:ASN:CB | 7:5B:1568:LYS:HE2 | 1.23 | 1.59 |
| 2:AF:227:HIS:CE1 | 6:4A:135:LEU:HD11 | 1.31 | 1.58 |
| 1:KC:79:ARG:HB3 | 1:LC:280:LYS:CE | 1.26 | 1.58 |
| 9:7A:11:TYR:CD1 | 9:7B:26:LEU:HD23 | 1.36 | 1.58 |
| 2:AD:358:PRO:C | 6:4C:151:ARG:HH21 | 1.10 | 1.58 |
| 2:CB:86:ARG:HA | 2:DB:281:TYR:CZ | 1.38 | 1.58 |
| 1:DC:402:ARG:CZ | 7:5A:777:ALA:HB3 | 1.33 | 1.58 |
| 2:LB:379:LYS:CB | 4:2C:166:ILE:HD12 | 1.33 | 1.58 |
| 2:EB:125:GLU:CA | 7:5C:903:PHE:CE2 | 1.77 | 1.58 |
| 1:FE:177:VAL:HG23 | 7:5B:915:PHE:CE2 | 1.09 | 1.58 |
| 1:EA:396:ASP:HB3 | 7:5C:817:LEU:CD2 | 1.13 | 1.57 |
| 2:LB:55:THR:CG2 | 2:MB:283:ALA:HA | 1.29 | 1.57 |
| 9:7C:7:LEU:CD2 | 9:7D:27:GLY:CA | 1.82 | 1.57 |
| 2:LD:231:ALA:HB2 | 6:4B:226:ILE:CD1 | 1.33 | 1.57 |
| 10:8Y:38:UNK:C | 10:8Z:1:UNK:H2 | 0.93 | 1.57 |
| 2:GB:212:PHE:CZ | 1:GC:326:LYS:HD3 | 1.38 | 1.57 |
| 2:LD:55:THR:CG2 | 2:MD:283:ALA:HA | 1.30 | 1.57 |
| 7:5A:1284:PHE:CZ | 9:7A:12:GLU:HB3 | 1.33 | 1.56 |
| 2:LB:379:LYS:CB | 4:2C:166:ILE:CD1 | 1.77 | 1.56 |
| 2:HB:212:PHE:CZ | 1:HC:326:LYS:HD3 | 1.38 | 1.56 |
| 10:8M:38:UNK:C | 10:8N:1:UNK:H2 | 0.93 | 1.56 |
| 10:8J:38:UNK:C | 10:8K:1:UNK:H2 | 0.93 | 1.56 |
| 2:KB:215:LEU:CD1 | 6:4A:267:ILE:HG22 | 1.36 | 1.56 |
| 9:7A:15:VAL:CG1 | 9:7B:35:ILE:CD1 | 1.79 | 1.55 |
| 10:8A:38:UNK:C | 10:8B:1:UNK:H2 | 0.93 | 1.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:177:VAL:CG2 | 7:5C:915:PHE:HE2 | 1.14 | 1.55 |
| 1:FA:177:VAL:HG23 | 7:5C:915:PHE:CE2 | 1.04 | 1.55 |
| 10:8S:38:UNK:C | 10:8T:1:UNK:H2 | 0.93 | 1.55 |
| 1:FA:282:TYR:CE2 | 10:8M:18:UNK:CB | 1.87 | 1.55 |
| 9:7A:7:LEU:CD2 | 9:7B:27:GLY:CA | 1.82 | 1.55 |
| 10:8P:38:UNK:C | 10:8Q:1:UNK:H2 | 0.93 | 1.55 |
| 2:CD:86:ARG:HA | 2:DD:281:TYR:CZ | 1.40 | 1.54 |
| 2:FD:212:PHE:CZ | 1:FE:326:LYS:HD3 | 1.40 | 1.54 |
| 2:KB:87:PRO:CG | 2:LB:282:ARG:HG3 | 1.19 | 1.54 |
| 2:LB:55:THR:HG23 | 2:MB:283:ALA:CA | 1.10 | 1.54 |
| 2:LB:231:ALA:HB2 | 6:4A:226:ILE:CD1 | 1.29 | 1.54 |
| 10:8V:38:UNK:C | 10:8W:1:UNK:H2 | 0.93 | 1.54 |
| 2:HD:212:PHE:CZ | 1:HE:326:LYS:HD3 | 1.41 | 1.54 |
| 2:KB:212:PHE:CZ | 1:KC:326:LYS:HD3 | 1.38 | 1.54 |
| 2:LB:306:ARG:CZ | 4:2C:151:VAL:HG23 | 1.34 | 1.54 |
| 2:LB:379:LYS:CA | 4:2C:166:ILE:CD1 | 1.85 | 1.54 |
| 4:2B:16:GLN:CA | 4:2B:19:MET:HB2 | 1.36 | 1.54 |
| 2:AB:212:PHE:CZ | 1:AC:326:LYS:HD3 | 1.38 | 1.54 |
| 2:IB:212:PHE:CZ | 1:IC:326:LYS:HD3 | 1.38 | 1.54 |
| 2:KB:55:THR:HG21 | 2:LB:363:MET:CE | 1.35 | 1.54 |
| 10:8D:38:UNK:C | 10:8E:1:UNK:H2 | 0.93 | 1.54 |
| 2:GD:212:PHE:CZ | 1:GE:326:LYS:HD3 | 1.41 | 1.54 |
| 1:GE:409:VAL:HG11 | 5:3A:383:GLU:CD | 1.30 | 1.53 |
| 2:ID:212:PHE:CZ | 1:IE:326:LYS:HD3 | 1.41 | 1.53 |
| 2:KD:212:PHE:CZ | 1:KE:326:LYS:HD3 | 1.41 | 1.53 |
| 4:2A:16:GLN:CA | 4:2A:19:MET:HB2 | 1.36 | 1.53 |
| 7:5A:1284:PHE:CZ | 9:7A:12:GLU:CB | 1.89 | 1.53 |
| 2:CB:86:ARG:CA | 2:DB:281:TYR:CE1 | 1.88 | 1.53 |
| 1:DA:402:ARG:CZ | 7:5C:777:ALA:HB3 | 1.34 | 1.53 |
| 1:FE:177:VAL:CG2 | 7:5B:915:PHE:HE2 | 1.20 | 1.53 |
| 1:KC:79:ARG:CG | 1:LC:280:LYS:NZ | 1.68 | 1.53 |
| 4:2C:16:GLN:CA | 4:2C:19:MET:HB2 | 1.36 | 1.53 |
| 2:KB:54:ALA:CB | 2:LB:285:THR:CG2 | 1.79 | 1.53 |
| 1:LC:60:LYS:CB | 6:4A:101:ARG:NH1 | 1.67 | 1.53 |
| 10:8G:38:UNK:C | 10:8H:1:UNK:H2 | 0.93 | 1.53 |
| 2:GB:55:THR:CG2 | 2:HB:283:ALA:HA | 1.07 | 1.53 |
| 1:IC:278:ALA:HB2 | 10:8W:21:UNK:CB | 1.36 | 1.53 |
| 2:AD:227:HIS:CE1 | 6:4C:135:LEU:HD11 | 1.41 | 1.53 |
| 2:JB:212:PHE:CZ | 1:JC:326:LYS:HD3 | 1.38 | 1.53 |
| 2:LD:55:THR:HG23 | 2:MD:283:ALA:CA | 1.09 | 1.53 |
| 2:KD:77:ARG:HG2 | 2:LD:281:TYR:CZ | 1.39 | 1.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CF:86:ARG:CA | 2:DF:281:TYR:CE1 | 1.88 | 1.52 |
| 1:IC:58:ALA:CB | 10:8Z:13:UNK:HA | 1.35 | 1.52 |
| 2:JD:212:PHE:CZ | 1:JE:326:LYS:HD3 | 1.41 | 1.52 |
| 1:FA:60:LYS:HD3 | 1:GA:283:HIS:CA | 1.39 | 1.52 |
| 1:IC:58:ALA:CB | 10:8Z:13:UNK:CA | 1.85 | 1.52 |
| 2:LD:212:PHE:CZ | 1:LE:326:LYS:HD3 | 1.41 | 1.52 |
| 9:7C:15:VAL:CG1 | 9:7D:35:ILE:CD1 | 1.79 | 1.52 |
| 1:FA:60:LYS:CD | 1:GA:283:HIS:HA | 1.40 | 1.52 |
| 2:KD:87:PRO:CG | 2:LD:282:ARG:HG3 | 1.38 | 1.52 |
| 2:LF:55:THR:CG2 | 2:MF:283:ALA:HA | 1.35 | 1.52 |
| 2:CD:86:ARG:CA | 2:DD:281:TYR:CE1 | 1.88 | 1.51 |
| 1:JC:370:LYS:HE3 | 10:8Z:17:UNK:CB | 1.10 | 1.51 |
| 2:KB:273:LEU:HA | 6:4A:268:LEU:CD2 | 1.33 | 1.51 |
| 7:5B:1491:LEU:HD13 | 7:5B:1495:PHE:CD1 | 1.44 | 1.51 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:CD1 | 1.32 | 1.51 |
| 2:EB:125:GLU:HA | 7:5C:903:PHE:CZ | 1.45 | 1.51 |
| 1:FA:89:PRO:HG3 | 1:GA:280:LYS:CD | 1.40 | 1.51 |
| 2:FB:54:ALA:C | 2:GB:283:ALA:HB2 | 1.24 | 1.51 |
| 1:FC:177:VAL:CG2 | 7:5A:915:PHE:HE2 | 1.23 | 1.51 |
| 2:LF:231:ALA:HB2 | 6:4D:226:ILE:CD1 | 1.41 | 1.51 |
| 1:EA:430:LYS:CE | 7:5C:834:ASN:HD22 | 1.19 | 1.51 |
| 2:GB:55:THR:HG23 | 2:HB:283:ALA:CB | 1.41 | 1.51 |
| 2:KD:273:LEU:HA | 6:4B:268:LEU:CD2 | 1.40 | 1.51 |
| 7:5A:1491:LEU:HD13 | 7:5A:1495:PHE:CD1 | 1.44 | 1.51 |
| 2:JF:86:ARG:NH2 | 2:KF:280:GLN:CB | 1.68 | 1.51 |
| 1:CC:370:LYS:NZ | 10:8E:17:UNK:CB | 1.69 | 1.50 |
| 1:FC:282:TYR:CE2 | 10:8N:18:UNK:CB | 1.94 | 1.50 |
| 1:JC:370:LYS:CE | 10:8Z:17:UNK:CB | 1.87 | 1.50 |
| 7:5C:1491:LEU:HD13 | 7:5C:1495:PHE:CD1 | 1.44 | 1.50 |
| 2:CF:86:ARG:HA | 2:DF:281:TYR:CZ | 1.42 | 1.50 |
| 1:CA:370:LYS:NZ | 10:8D:17:UNK:CB | 1.74 | 1.50 |
| 2:FB:98:GLY:HA2 | 1:FC:254:GLU:CG | 1.38 | 1.50 |
| 2:KF:77:ARG:HG2 | 2:LF:281:TYR:CZ | 1.47 | 1.49 |
| 2:KF:221:THR:HG21 | 6:4D:261:SER:C | 1.27 | 1.49 |
| 9:7A:15:VAL:HA | 9:7B:35:ILE:CD1 | 1.42 | 1.49 |
| 9:7C:15:VAL:HA | 9:7D:35:ILE:CD1 | 1.42 | 1.49 |
| 1:JE:370:LYS:HE3 | 10:9A:17:UNK:CB | 1.37 | 1.49 |
| 4:2B:16:GLN:HA | 4:2B:19:MET:CB | 1.37 | 1.49 |
| 4:2C:16:GLN:HA | 4:2C:19:MET:CB | 1.37 | 1.49 |
| 2:AD:212:PHE:CZ | 1:AE:326:LYS:HD3 | 1.41 | 1.49 |
| 2:JB:55:THR:CG2 | 2:KB:362:LYS:NZ | 1.74 | 1.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2A:16:GLN:HA | 4:2A:19:MET:CB | 1.37 | 1.49 |
| 7:5C:1491:LEU:CD1 | 7:5C:1495:PHE:CD1 | 1.96 | 1.49 |
| 7:5A:1490:LYS:HD2 | 7:5A:1494:LEU:CB | 1.43 | 1.48 |
| 7:5A:1491:LEU:CD1 | 7:5A:1495:PHE:CD1 | 1.96 | 1.48 |
| 7:5B:1490:LYS:HD2 | 7:5B:1494:LEU:CB | 1.43 | 1.48 |
| 7:5C:1490:LYS:HD2 | 7:5C:1494:LEU:CB | 1.43 | 1.48 |
| 2:ED:177:ASP:CG | 1:EE:353:VAL:CG1 | 1.84 | 1.48 |
| 2:HF:261:PRO:HB2 | 5:3A:337:ARG:NH2 | 1.18 | 1.48 |
| 1:CC:370:LYS:CE | 10:8E:17:UNK:CB | 1.91 | 1.48 |
| 2:MD:212:PHE:CZ | 1:ME:326:LYS:HD3 | 1.49 | 1.48 |
| 5:3B:229:PHE:CE2 | 5:3B:331:GLN:HB3 | 1.45 | 1.48 |
| 5:3C:229:PHE:CE2 | 5:3C:331:GLN:HB3 | 1.45 | 1.48 |
| 7:5B:1491:LEU:CD1 | 7:5B:1495:PHE:CD1 | 1.96 | 1.48 |
| 1:FA:422:ARG:HH21 | 7:5C:1170:THR:C | 1.15 | 1.48 |
| 5:3A:229:PHE:CE2 | 5:3A:331:GLN:HB3 | 1.45 | 1.48 |
| 1:JC:89:PRO:CB | 1:KC:280:LYS:HG2 | 1.17 | 1.48 |
| 2:KD:86:ARG:HH12 | 2:LD:283:ALA:CB | 1.24 | 1.47 |
| 2:EB:177:ASP:CG | 1:EC:353:VAL:CG1 | 1.86 | 1.47 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:CD1 | 1.32 | 1.47 |
| 1:JC:88:HIS:CE1 | 1:KC:280:LYS:O | 1.66 | 1.47 |
| 2:LD:306:ARG:NH2 | 4:2A:151:VAL:HG23 | 1.23 | 1.47 |
| 1:LE:60:LYS:HD2 | 6:4B:101:ARG:NH2 | 1.28 | 1.47 |
| 2:ED:125:GLU:HA | 7:5A:903:PHE:CZ | 1.49 | 1.46 |
| 2:LB:224:ASP:N | 6:4A:219:ASN:ND2 | 1.63 | 1.46 |
| 2:LF:77:ARG:NH1 | 6:4D:204:ARG:NH2 | 1.63 | 1.46 |
| 2:DD:212:PHE:HZ | 1:DE:326:LYS:CD | 1.28 | 1.46 |
| 1:FE:422:ARG:HH21 | 7:5B:1170:THR:C | 1.16 | 1.46 |
| 1:JE:279:GLU:CD | 10:9A:22:UNK:HA | 1.36 | 1.46 |
| 2:KD:221:THR:CG2 | 6:4B:261:SER:C | 1.86 | 1.46 |
| 7:5C:1552:LYS:NZ | 7:5C:1563:SER:CB | 1.77 | 1.46 |
| 2:FD:177:ASP:CG | 1:FE:353:VAL:CG1 | 1.85 | 1.45 |
| 1:FE:402:ARG:HH22 | 7:5B:1262:GLU:CD | 1.21 | 1.45 |
| 2:LD:306:ARG:CZ | 4:2A:151:VAL:HG23 | 1.45 | 1.45 |
| 1:LC:176:GLN:NE2 | 4:2A:42:PHE:CG | 1.81 | 1.45 |
| 2:KD:54:ALA:HB1 | 2:LD:285:THR:CG2 | 1.42 | 1.45 |
| 7:5A:1552:LYS:NZ | 7:5A:1563:SER:CB | 1.77 | 1.45 |
| 2:BD:177:ASP:CG | 1:BE:353:VAL:CG1 | 1.90 | 1.45 |
| 1:CE:282:TYR:CE2 | 10:8F:18:UNK:CB | 1.96 | 1.45 |
| 2:DB:177:ASP:CG | 1:DC:353:VAL:CG1 | 1.89 | 1.45 |
| 1:FC:422:ARG:HH21 | 7:5A:1170:THR:C | 1.17 | 1.45 |
| 2:ID:86:ARG:HA | 2:JD:281:TYR:CE1 | 1.51 | 1.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LD:224:ASP:N | 6:4B:219:ASN:ND2 | 1.65 | 1.45 |
| 2:MF:221:THR:CG2 | 6:4D:189:ARG:HH22 | 1.28 | 1.45 |
| 1:FE:101:ASN:ND2 | 2:FF:252:LYS:HD2 | 1.12 | 1.44 |
| 2:EF:125:GLU:HG2 | 7:5B:903:PHE:CE2 | 1.52 | 1.44 |
| 7:5A:1530:ILE:CD1 | 7:5A:1571:MET:HE1 | 1.48 | 1.44 |
| 7:5B:1530:ILE:CD1 | 7:5B:1571:MET:HE1 | 1.48 | 1.44 |
| 1:EE:370:LYS:NZ | 10:8L:17:UNK:CB | 1.80 | 1.44 |
| 2:FF:428:ALA:HB1 | 7:5B:1080:PHE:CE1 | 1.51 | 1.44 |
| 1:IA:282:TYR:HE2 | 10:8V:19:UNK:N | 1.15 | 1.44 |
| 1:IC:101:ASN:ND2 | 2:ID:252:LYS:CD | 1.80 | 1.44 |
| 7:5B:1552:LYS:NZ | 7:5B:1563:SER:CB | 1.77 | 1.44 |
| 7:5C:1530:ILE:CD1 | 7:5C:1571:MET:HE1 | 1.48 | 1.44 |
| 2:CB:212:PHE:HZ | 1:CC:326:LYS:CD | 1.28 | 1.44 |
| 2:EF:125:GLU:CA | 7:5B:903:PHE:CE2 | 1.76 | 1.44 |
| 2:FB:212:PHE:CZ | 1:FC:326:LYS:HD3 | 1.51 | 1.44 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:CG | 1.81 | 1.44 |
| 2:JF:86:ARG:CZ | 2:KF:280:GLN:CB | 1.96 | 1.44 |
| 7:5B:1284:PHE:CZ | 9:7C:12:GLU:CB | 1.99 | 1.44 |
| 9:7A:30:ARG:NH1 | 9:7B:3:GLN:HA | 1.32 | 1.44 |
| 2:AF:358:PRO:C | 6:4A:151:ARG:HH21 | 1.23 | 1.44 |
| 2:DD:177:ASP:CG | 1:DE:353:VAL:CG1 | 1.88 | 1.44 |
| 1:FA:402:ARG:HH22 | 7:5C:1262:GLU:CD | 1.26 | 1.44 |
| 2:FB:177:ASP:CG | 1:FC:353:VAL:CG1 | 1.88 | 1.44 |
| 1:JA:89:PRO:CG | 1:KA:280:LYS:HG2 | 1.45 | 1.44 |
| 2:LD:77:ARG:NH1 | 6:4B:204:ARG:NH2 | 1.64 | 1.44 |
| 7:5B:1487:ASN:HB3 | 7:5B:1568:LYS:CE | 1.43 | 1.44 |
| 2:DB:212:PHE:HZ | 1:DC:326:LYS:CD | 1.29 | 1.43 |
| 1:DE:402:ARG:CZ | 7:5B:777:ALA:HB3 | 1.45 | 1.43 |
| 2:KD:125:GLU:HG3 | 2:LD:336:LYS:CE | 1.48 | 1.43 |
| 2:JD:86:ARG:NH2 | 2:KD:280:GLN:HB2 | 1.21 | 1.43 |
| 1:LE:176:GLN:NE2 | 4:2B:42:PHE:CG | 1.80 | 1.43 |
| 2:MB:212:PHE:CZ | 1:MC:326:LYS:HD3 | 1.53 | 1.43 |
| 2:MD:221:THR:HG21 | 6:4B:189:ARG:NH2 | 1.25 | 1.43 |
| 7:5A:1487:ASN:HB3 | 7:5A:1568:LYS:CE | 1.43 | 1.43 |
| 1:EC:423:GLU:OE2 | 7:5A:830:VAL:CG1 | 1.65 | 1.43 |
| 2:JB:87:PRO:CG | 2:KB:277:GLY:O | 1.66 | 1.43 |
| 7:5B:1284:PHE:HZ | 9:7C:12:GLU:CB | 1.29 | 1.43 |
| 7:5C:1284:PHE:HZ | 9:7E:12:GLU:CB | 1.30 | 1.43 |
| 9:7C:30:ARG:NH1 | 9:7D:3:GLN:HA | 1.32 | 1.43 |
| 2:BD:212:PHE:HZ | 1:BE:326:LYS:CD | 1.32 | 1.43 |
| 1:GE:409:VAL:CG1 | 5:3A:383:GLU:OE2 | 1.67 | 1.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JA:89:PRO:HB2 | 1:KA:280:LYS:CG | 1.44 | 1.43 |
| 7:5C:1284:PHE:CZ | 9:7E:12:GLU:CB | 1.99 | 1.43 |
| 10:8J:38:UNK:C | 10:8K:1:UNK:N | 1.77 | 1.43 |
| 2:LB:306:ARG:NE | 4:2C:149:ILE:HG22 | 1.34 | 1.43 |
| 1:LC:89:PRO:HD3 | 1:MC:280:LYS:NZ | 1.17 | 1.43 |
| 7:5C:1487:ASN:HB3 | 7:5C:1568:LYS:CE | 1.43 | 1.43 |
| 1:AC:101:ASN:ND2 | 2:AD:252:LYS:CD | 1.80 | 1.42 |
| 2:CD:212:PHE:HZ | 1:CE:326:LYS:CD | 1.31 | 1.42 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:NE | 1.79 | 1.42 |
| 1:GC:409:VAL:HG11 | 5:3C:383:GLU:CD | 1.43 | 1.42 |
| 2:HD:261:PRO:HB2 | 5:3C:337:ARG:NH2 | 1.10 | 1.42 |
| 1:JA:89:PRO:CG | 1:KA:279:GLU:O | 1.67 | 1.42 |
| 1:JC:101:ASN:ND2 | 2:JD:252:LYS:CD | 1.80 | 1.42 |
| 2:KB:54:ALA:HB1 | 2:LB:285:THR:CG2 | 1.39 | 1.42 |
| 2:KD:217:LEU:HD22 | 6:4B:263:CYS:SG | 1.57 | 1.42 |
| 2:LB:212:PHE:HZ | 1:LC:326:LYS:CD | 1.27 | 1.42 |
| 1:MA:372:MET:CE | 6:4C:96:VAL:O | 1.65 | 1.42 |
| 1:FC:101:ASN:ND2 | 2:FD:252:LYS:HD2 | 1.11 | 1.42 |
| 1:GC:101:ASN:ND2 | 2:GD:252:LYS:CD | 1.80 | 1.42 |
| 2:IF:86:ARG:HA | 2:JF:281:TYR:CE1 | 1.52 | 1.42 |
| 7:5C:1491:LEU:CD1 | 7:5C:1495:PHE:HD1 | 1.30 | 1.42 |
| 10:8A:38:UNK:C | 10:8B:1:UNK:N | 1.77 | 1.42 |
| 1:DC:402:ARG:NE | 7:5A:777:ALA:CB | 1.80 | 1.42 |
| 1:FE:419:SER:CB | 7:5B:1256:ARG:NE | 1.76 | 1.42 |
| 1:JE:91:GLN:N | 1:KE:280:LYS:HZ2 | 1.11 | 1.42 |
| 2:KF:273:LEU:HA | 6:4D:268:LEU:CD2 | 1.46 | 1.42 |
| 1:LA:176:GLN:NE2 | 4:2C:42:PHE:CG | 1.84 | 1.42 |
| 7:5A:1491:LEU:CD1 | 7:5A:1495:PHE:HD1 | 1.30 | 1.42 |
| 10:8D:38:UNK:C | 10:8E:1:UNK:N | 1.77 | 1.42 |
| 1:GA:89:PRO:HD3 | 1:HA:280:LYS:NZ | 1.14 | 1.42 |
| 1:HC:101:ASN:ND2 | 2:HD:252:LYS:CD | 1.80 | 1.42 |
| 2:LB:231:ALA:CB | 6:4A:226:ILE:HD13 | 1.48 | 1.42 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:NZ | 1.83 | 1.42 |
| 7:5B:1491:LEU:CD1 | 7:5B:1495:PHE:HD1 | 1.30 | 1.42 |
| 1:CA:370:LYS:CE | 10:8D:17:UNK:CB | 1.98 | 1.42 |
| 1:DA:402:ARG:NE | 7:5C:777:ALA:CB | 1.84 | 1.42 |
| 2:JB:86:ARG:NH2 | 2:KB:280:GLN:HB2 | 1.33 | 1.42 |
| 2:KD:125:GLU:CG | 2:LD:336:LYS:NZ | 1.80 | 1.42 |
| 2:KF:54:ALA:HB1 | 2:LF:285:THR:CG2 | 1.49 | 1.42 |
| 2:ED:212:PHE:HZ | 1:EE:326:LYS:CD | 1.32 | 1.41 |
| 2:FB:55:THR:CG2 | 2:GB:284:LEU:N | 1.82 | 1.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FC:402:ARG:HH22 | 7:5A:1262:GLU:CD | 1.25 | 1.41 |
| 1:LA:222:PRO:CD | 2:LB:324:LYS:HD3 | 1.49 | 1.41 |
| 10:8Y:38:UNK:C | 10:8Z:1:UNK:N | 1.77 | 1.41 |
| 2:FB:54:ALA:HA | 2:GB:283:ALA:CB | 1.50 | 1.41 |
| 2:LF:416:ASN:O | 4:2B:168:LEU:CD1 | 1.66 | 1.41 |
| 10:8M:38:UNK:C | 10:8N:1:UNK:N | 1.77 | 1.41 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:NE | 1.82 | 1.41 |
| 2:FD:98:GLY:HA2 | 1:FE:254:GLU:CG | 1.48 | 1.41 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:CE | 1.49 | 1.41 |
| 1:IC:278:ALA:CB | 10:8W:21:UNK:CB | 1.97 | 1.41 |
| 2:MF:221:THR:HG21 | 6:4D:189:ARG:NH2 | 1.15 | 1.41 |
| 7:5A:1548:VAL:HA | 7:5A:1569:GLU:CD | 1.46 | 1.41 |
| 2:KB:87:PRO:CG | 2:LB:282:ARG:CG | 1.96 | 1.41 |
| 2:LF:306:ARG:NH2 | 4:2B:151:VAL:HG23 | 1.19 | 1.41 |
| 7:5B:1548:VAL:HA | 7:5B:1569:GLU:CD | 1.46 | 1.41 |
| 7:5C:1548:VAL:HA | 7:5C:1569:GLU:CD | 1.46 | 1.41 |
| 10:8V:38:UNK:C | 10:8W:1:UNK:N | 1.77 | 1.40 |
| 2:BB:212:PHE:HZ | 1:BC:326:LYS:CD | 1.32 | 1.40 |
| 2:EB:212:PHE:HZ | 1:EC:326:LYS:CD | 1.32 | 1.40 |
| 2:FF:55:THR:HG23 | 2:GF:283:ALA:CA | 1.49 | 1.40 |
| 1:JC:279:GLU:CD | 10:8Z:22:UNK:HA | 1.46 | 1.40 |
| 2:JF:86:ARG:NH2 | 2:KF:280:GLN:HB2 | 1.07 | 1.40 |
| 1:LA:60:LYS:HD2 | 6:4C:101:ARG:NH2 | 1.31 | 1.40 |
| 2:AB:177:ASP:CG | 1:AC:353:VAL:CG1 | 1.95 | 1.40 |
| 2:HB:177:ASP:CG | 1:HC:353:VAL:CG1 | 1.95 | 1.40 |
| 1:KC:101:ASN:ND2 | 2:KD:252:LYS:CD | 1.80 | 1.40 |
| 2:BB:177:ASP:CG | 1:BC:353:VAL:CG1 | 1.94 | 1.40 |
| 2:ED:125:GLU:O | 7:5A:903:PHE:CZ | 1.72 | 1.40 |
| 2:GB:177:ASP:CG | 1:GC:353:VAL:CG1 | 1.95 | 1.40 |
| 2:KB:177:ASP:CG | 1:KC:353:VAL:CG1 | 1.95 | 1.40 |
| 1:ME:372:MET:CE | 6:4B:96:VAL:O | 1.66 | 1.40 |
| 2:CB:177:ASP:CG | 1:CC:353:VAL:CG1 | 1.93 | 1.39 |
| 2:HD:177:ASP:CG | 1:HE:353:VAL:CG1 | 1.96 | 1.39 |
| 2:IB:177:ASP:CG | 1:IC:353:VAL:CG1 | 1.95 | 1.39 |
| 2:AD:177:ASP:CG | 1:AE:353:VAL:CG1 | 1.96 | 1.39 |
| 2:CD:177:ASP:CG | 1:CE:353:VAL:CG1 | 1.93 | 1.39 |
| 1:JE:89:PRO:HB2 | 1:KE:280:LYS:CG | 1.46 | 1.39 |
| 2:KD:177:ASP:CG | 1:KE:353:VAL:CG1 | 1.96 | 1.39 |
| 2:LB:306:ARG:HE | 4:2C:149:ILE:CG2 | 1.32 | 1.39 |
| 7:5B:1490:LYS:CD | 7:5B:1494:LEU:HB3 | 1.50 | 1.39 |
| 10:8S:38:UNK:C | 10:8T:1:UNK:N | 1.77 | 1.39 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:GD:177:ASP:CG | 1:GE:353:VAL:CG1 | 1.96 | 1.39 |
| 1:IA:101:ASN:ND2 | 2:IB:252:LYS:CD | 1.84 | 1.39 |
| 2:KD:54:ALA:CB | 2:LD:285:THR:CG2 | 1.99 | 1.39 |
| 2:LB:77:ARG:NH1 | 6:4A:204:ARG:NH2 | 1.70 | 1.39 |
| 1:MA:101:ASN:ND2 | 2:MB:252:LYS:CD | 1.82 | 1.39 |
| 7:5C:1544:ILE:HA | 7:5C:1573:ARG:CD | 1.53 | 1.39 |
| 2:ID:177:ASP:CG | 1:IE:353:VAL:CG1 | 1.96 | 1.39 |
| 1:LC:222:PRO:CD | 2:LD:324:LYS:HD3 | 1.51 | 1.39 |
| 2:LD:55:THR:N | 2:MD:283:ALA:HB2 | 1.38 | 1.39 |
| 7:5A:1544:ILE:HA | 7:5A:1573:ARG:CD | 1.53 | 1.39 |
| 7:5C:1267:CYS:SG | 9:7E:8:ARG:NE | 1.95 | 1.39 |
| 10:8G:38:UNK:C | 10:8H:1:UNK:N | 1.77 | 1.39 |
| 1:EC:101:ASN:ND2 | 2:ED:252:LYS:CD | 1.85 | 1.39 |
| 1:FA:101:ASN:ND2 | 2:FB:252:LYS:HD2 | 1.12 | 1.39 |
| 2:FB:55:THR:N | 2:GB:283:ALA:CB | 1.84 | 1.39 |
| 1:IC:402:ARG:HH22 | 7:5A:1418:GLN:N | 1.16 | 1.39 |
| 1:JA:101:ASN:ND2 | 2:JB:252:LYS:CD | 1.84 | 1.39 |
| 2:LB:379:LYS:CG | 4:2C:166:ILE:HD12 | 1.53 | 1.39 |
| 6:4A:244:GLU:CG | 6:4A:284:LEU:HD11 | 1.53 | 1.39 |
| 6:4C:244:GLU:CG | 6:4C:284:LEU:HD11 | 1.53 | 1.39 |
| 7:5A:1490:LYS:CD | 7:5A:1494:LEU:HB3 | 1.50 | 1.39 |
| 7:5B:1544:ILE:HA | 7:5B:1573:ARG:CD | 1.53 | 1.39 |
| 1:EE:101:ASN:ND2 | 2:EF:252:LYS:HD2 | 1.12 | 1.38 |
| 1:GA:101:ASN:ND2 | 2:GB:252:LYS:CD | 1.85 | 1.38 |
| 1:JE:89:PRO:CB | 1:KE:280:LYS:HG2 | 1.13 | 1.38 |
| 1:KA:85:GLN:CA | 1:LA:283:HIS:HA | 1.50 | 1.38 |
| 6:4B:244:GLU:CG | 6:4B:284:LEU:HD11 | 1.53 | 1.38 |
| 7:5C:1490:LYS:CD | 7:5C:1494:LEU:HB3 | 1.50 | 1.38 |
| 9:7E:14:SER:OG | 9:7F:34:PRO:CG | 1.67 | 1.38 |
| 1:DC:101:ASN:ND2 | 2:DD:252:LYS:HD2 | 1.09 | 1.38 |
| 2:ED:125:GLU:HG2 | 7:5A:903:PHE:CE2 | 1.56 | 1.38 |
| 1:JE:87:PHE:O | 1:KE:283:HIS:CE1 | 1.72 | 1.38 |
| 2:LD:231:ALA:CB | 6:4B:226:ILE:HD13 | 1.52 | 1.38 |
| 2:LF:416:ASN:C | 4:2B:168:LEU:HD13 | 1.48 | 1.38 |
| 6:4D:244:GLU:CG | 6:4D:284:LEU:HD11 | 1.53 | 1.38 |
| 9:7C:15:VAL:CA | 9:7D:35:ILE:HD11 | 1.51 | 1.38 |
| 1:EC:370:LYS:NZ | 10:8K:17:UNK:CB | 1.83 | 1.38 |
| 2:FB:55:THR:H | 2:GB:283:ALA:CA | 1.37 | 1.38 |
| 1:IE:101:ASN:ND2 | 2:IF:252:LYS:CD | 1.86 | 1.38 |
| 2:LB:306:ARG:NH2 | 4:2C:151:VAL:HG23 | 1.36 | 1.38 |
| 1:AA:101:ASN:ND2 | 2:AB:252:LYS:CD | 1.85 | 1.38 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:DE:101:ASN:ND2 | 2:DF:252:LYS:HD2 | 1.07 | 1.38 |
| 2:IB:86:ARG:HA | 2:JB:281:TYR:CE1 | 1.59 | 1.38 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:NZ | 1.12 | 1.38 |
| 9:7C:15:VAL:CA | 9:7D:35:ILE:CD1 | 2.00 | 1.38 |
| 2:JB:177:ASP:CG | 1:JC:353:VAL:CG1 | 1.95 | 1.38 |
| 2:JD:86:ARG:NH2 | 2:KD:280:GLN:CB | 1.84 | 1.38 |
| 10:8P:38:UNK:C | 10:8Q:1:UNK:N | 1.77 | 1.38 |
| 2:LF:224:ASP:N | 6:4D:219:ASN:ND2 | 1.71 | 1.37 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:NZ | 1.87 | 1.37 |
| 2:LD:212:PHE:HZ | 1:LE:326:LYS:CD | 1.38 | 1.37 |
| 7:5C:874:GLN:HB2 | 8:6C:59:LYS:NZ | 1.37 | 1.37 |
| 9:7A:15:VAL:CA | 9:7B:35:ILE:HD11 | 1.51 | 1.37 |
| 9:7A:15:VAL:CA | 9:7B:35:ILE:CD1 | 2.00 | 1.37 |
| 1:AE:101:ASN:ND2 | 2:AF:252:LYS:CD | 1.86 | 1.37 |
| 1:EA:430:LYS:NZ | 7:5C:834:ASN:CG | 1.81 | 1.37 |
| 1:JE:101:ASN:ND2 | 2:JF:252:LYS:CD | 1.86 | 1.37 |
| 2:KB:215:LEU:HD13 | 6:4A:267:ILE:CG2 | 1.54 | 1.37 |
| 2:LB:379:LYS:HB3 | 4:2C:166:ILE:CD1 | 1.42 | 1.37 |
| 1:DA:101:ASN:ND2 | 2:DB:252:LYS:HD2 | 1.06 | 1.37 |
| 2:EF:125:GLU:CG | 7:5B:903:PHE:CE2 | 2.08 | 1.37 |
| 1:FE:60:LYS:HZ3 | 1:GE:283:HIS:CG | 1.40 | 1.37 |
| 2:JD:177:ASP:CG | 1:JE:353:VAL:CG1 | 1.96 | 1.37 |
| 7:5A:1284:PHE:CE1 | 9:7A:12:GLU:OE1 | 1.78 | 1.37 |
| 9:7E:11:TYR:CD1 | 9:7F:26:LEU:HD23 | 1.59 | 1.37 |
| 2:FB:98:GLY:CA | 1:FC:254:GLU:HG2 | 1.53 | 1.37 |
| 1:GE:101:ASN:ND2 | 2:GF:252:LYS:CD | 1.86 | 1.37 |
| 1:HA:101:ASN:ND2 | 2:HB:252:LYS:CD | 1.85 | 1.37 |
| 1:JA:89:PRO:HD3 | 1:KA:283:HIS:CE1 | 1.60 | 1.37 |
| 1:JC:89:PRO:HB2 | 1:KC:280:LYS:CG | 1.44 | 1.37 |
| 2:LB:340:TYR:CG | 4:2C:147:PHE:HB2 | 1.57 | 1.37 |
| 1:DA:282:TYR:CE2 | 10:8G:18:UNK:CB | 2.08 | 1.36 |
| 1:JA:89:PRO:CB | 1:KA:280:LYS:HG2 | 1.21 | 1.36 |
| 6:4A:221:MET:SD | 6:4A:222:PRO:HD3 | 1.65 | 1.36 |
| 6:4B:221:MET:SD | 6:4B:222:PRO:HD3 | 1.65 | 1.36 |
| 6:4C:221:MET:SD | 6:4C:222:PRO:HD3 | 1.65 | 1.36 |
| 6:4D:221:MET:SD | 6:4D:222:PRO:HD3 | 1.65 | 1.36 |
| 1:HE:101:ASN:ND2 | 2:HF:252:LYS:CD | 1.86 | 1.36 |
| 1:KA:101:ASN:ND2 | 2:KB:252:LYS:CD | 1.85 | 1.36 |
| 2:KF:86:ARG:HH12 | 2:LF:283:ALA:CB | 1.35 | 1.36 |
| 1:LA:89:PRO:HD3 | 1:MA:280:LYS:NZ | 1.08 | 1.36 |
| 2:LB:331:LEU:CD2 | 4:2C:42:PHE:CE2 | 2.07 | 1.36 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1548:VAL:CG1 | 7:5C:1566:GLU:CA | 2.03 | 1.36 |
| 1:CA:101:ASN:ND2 | 2:CB:252:LYS:HD2 | 1.08 | 1.36 |
| 2:FB:55:THR:HG23 | 2:GB:284:LEU:N | 1.40 | 1.36 |
| 2:GB:55:THR:N | 2:HB:283:ALA:HB2 | 1.32 | 1.36 |
| 2:HD:261:PRO:CB | 5:3C:337:ARG:HH21 | 1.37 | 1.36 |
| 1:HE:282:TYR:HE2 | 10:8U:19:UNK:N | 1.17 | 1.36 |
| 2:KF:272:PRO:O | 6:4D:268:LEU:CD2 | 1.70 | 1.36 |
| 2:LD:55:THR:HG23 | 2:MD:283:ALA:CB | 1.54 | 1.36 |
| 1:LE:222:PRO:CD | 2:LF:324:LYS:HD3 | 1.52 | 1.36 |
| 1:BE:101:ASN:ND2 | 2:BF:252:LYS:HD2 | 1.03 | 1.36 |
| 2:EB:125:GLU:HG2 | 7:5C:903:PHE:CE2 | 1.60 | 1.36 |
| 1:IA:402:ARG:NH1 | 7:5C:1417:GLN:O | 1.59 | 1.36 |
| 2:AD:359:LYS:N | 6:4C:151:ARG:NH2 | 1.66 | 1.36 |
| 2:GD:55:THR:N | 2:HD:283:ALA:HB2 | 1.04 | 1.36 |
| 1:IE:402:ARG:HH22 | 7:5B:1418:GLN:N | 1.22 | 1.36 |
| 2:KF:221:THR:CG2 | 6:4D:261:SER:C | 1.97 | 1.36 |
| 7:5A:1548:VAL:CG1 | 7:5A:1566:GLU:CA | 2.03 | 1.36 |
| 1:EA:101:ASN:ND2 | 2:EB:252:LYS:CD | 1.86 | 1.35 |
| 2:LB:331:LEU:HD21 | 4:2C:42:PHE:CE1 | 0.84 | 1.35 |
| 1:CA:282:TYR:CE2 | 10:8D:18:UNK:CB | 2.09 | 1.35 |
| 1:DE:400:ALA:O | 7:5B:775:PRO:CB | 1.70 | 1.35 |
| 1:JA:89:PRO:CD | 1:KA:283:HIS:CE1 | 2.09 | 1.35 |
| 7:5B:1548:VAL:CG1 | 7:5B:1566:GLU:CA | 2.03 | 1.35 |
| 1:EA:370:LYS:NZ | 10:8J:17:UNK:CB | 1.89 | 1.35 |
| 1:KA:88:HIS:CA | 1:LA:284:GLU:HB2 | 1.27 | 1.35 |
| 1:MC:101:ASN:ND2 | 2:MD:252:LYS:CD | 1.87 | 1.35 |
| 9:7A:11:TYR:CE1 | 9:7B:26:LEU:HB3 | 1.61 | 1.35 |
| 1:KE:101:ASN:ND2 | 2:KF:252:LYS:CD | 1.86 | 1.35 |
| 1:LE:89:PRO:HD3 | 1:ME:280:LYS:NZ | 1.04 | 1.35 |
| 7:5A:1284:PHE:HZ | 9:7A:12:GLU:CB | 1.30 | 1.35 |
| 1:EC:430:LYS:CE | 7:5A:834:ASN:HD22 | 1.38 | 1.34 |
| 2:KD:125:GLU:OE1 | 2:LD:332:ASN:ND2 | 1.59 | 1.34 |
| 1:ME:101:ASN:ND2 | 2:MF:252:LYS:CD | 1.88 | 1.34 |
| 9:7A:30:ARG:HH12 | 9:7B:3:GLN:CA | 1.40 | 1.34 |
| 9:7C:30:ARG:HH12 | 9:7D:3:GLN:CA | 1.40 | 1.34 |
| 1:AE:342:GLN:HE22 | 3:1A:55:HIS:CG | 1.44 | 1.34 |
| 1:BA:101:ASN:ND2 | 2:BB:252:LYS:HD2 | 1.03 | 1.34 |
| 1:LC:245:ASP:OD1 | 6:4A:216:ARG:NH2 | 1.59 | 1.34 |
| 7:5B:1284:PHE:CZ | 9:7C:12:GLU:HB3 | 1.56 | 1.34 |
| 1:BC:101:ASN:ND2 | 2:BD:252:LYS:HD2 | 1.02 | 1.34 |
| 1:CE:101:ASN:ND2 | 2:CF:252:LYS:HD2 | 1.07 | 1.34 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DA:101:ASN:ND2 | 2:DB:252:LYS:CD | 1.89 | 1.34 |
| 1:EE:423:GLU:OE2 | 7:5B:830:VAL:CG1 | 1.74 | 1.34 |
| 2:GB:55:THR:HG23 | 2:HB:283:ALA:CA | 0.87 | 1.34 |
| 1:JA:128:ASN:HD22 | 1:KA:285:GLN:CD | 1.35 | 1.34 |
| 2:KD:86:ARG:NH1 | 2:LD:283:ALA:CB | 1.89 | 1.34 |
| 2:LB:55:THR:N | 2:MB:283:ALA:HB2 | 1.43 | 1.34 |
| 1:MC:372:MET:CE | 6:4A:96:VAL:O | 1.73 | 1.34 |
| 1:FC:419:SER:HB2 | 7:5A:1256:ARG:NE | 1.30 | 1.34 |
| 1:FE:60:LYS:HZ2 | 1:GE:283:HIS:CD2 | 1.44 | 1.34 |
| 1:IA:58:ALA:CB | 10:8Y:13:UNK:CA | 2.06 | 1.34 |
| 2:IB:212:PHE:HZ | 1:IC:326:LYS:CD | 1.39 | 1.34 |
| 2:JB:212:PHE:HZ | 1:JC:326:LYS:CD | 1.39 | 1.34 |
| 2:KB:273:LEU:CA | 6:4A:268:LEU:CD2 | 1.94 | 1.34 |
| 7:5C:1475:PHE:CE2 | 7:5C:1565:GLU:OE2 | 1.80 | 1.34 |
| 1:EA:370:LYS:CE | 10:8J:17:UNK:CB | 2.06 | 1.34 |
| 2:KB:212:PHE:HZ | 1:KC:326:LYS:CD | 1.39 | 1.34 |
| 1:LA:176:GLN:NE2 | 4:2C:42:PHE:CD2 | 1.95 | 1.34 |
| 9:7C:11:TYR:CE1 | 9:7D:26:LEU:HB3 | 1.61 | 1.34 |
| 1:CC:282:TYR:CE2 | 10:8E:18:UNK:CB | 2.09 | 1.33 |
| 1:FE:60:LYS:NZ | 1:GE:283:HIS:CG | 1.96 | 1.33 |
| 2:JB:55:THR:HG21 | 2:KB:362:LYS:NZ | 1.04 | 1.33 |
| 2:MB:221:THR:HG21 | 6:4A:189:ARG:NH2 | 1.41 | 1.33 |
| 7:5A:1475:PHE:CE2 | 7:5A:1565:GLU:OE2 | 1.80 | 1.33 |
| 7:5A:1544:ILE:CA | 7:5A:1573:ARG:HD2 | 1.59 | 1.33 |
| 7:5B:1544:ILE:CA | 7:5B:1573:ARG:HD2 | 1.58 | 1.33 |
| 7:5C:1544:ILE:CA | 7:5C:1573:ARG:HD2 | 1.59 | 1.33 |
| 9:7A:15:VAL:CG1 | 9:7B:35:ILE:HD13 | 0.86 | 1.33 |
| 1:BA:101:ASN:ND2 | 2:BB:252:LYS:CD | 1.89 | 1.33 |
| 1:BC:101:ASN:ND2 | 2:BD:252:LYS:CD | 1.88 | 1.33 |
| 1:CC:101:ASN:ND2 | 2:CD:252:LYS:CD | 1.89 | 1.33 |
| 1:CC:101:ASN:ND2 | 2:CD:252:LYS:HD2 | 1.05 | 1.33 |
| 2:FD:212:PHE:HZ | 1:FE:326:LYS:CD | 1.40 | 1.33 |
| 2:HB:212:PHE:HZ | 1:HC:326:LYS:CD | 1.39 | 1.33 |
| 1:IA:282:TYR:CE2 | 10:8V:18:UNK:CB | 1.87 | 1.33 |
| 9:7E:7:LEU:HD22 | 9:7F:27:GLY:CA | 1.58 | 1.33 |
| 1:IA:282:TYR:CD1 | 10:8V:15:UNK:HA | 1.63 | 1.33 |
| 2:LF:55:THR:HG23 | 2:MF:283:ALA:CB | 1.57 | 1.33 |
| 2:MD:221:THR:CG2 | 6:4B:189:ARG:HH22 | 1.39 | 1.33 |
| 7:5B:1475:PHE:CE2 | 7:5B:1565:GLU:OE2 | 1.80 | 1.33 |
| 9:7A:11:TYR:CE1 | 9:7B:26:LEU:HD23 | 1.61 | 1.33 |
| 9:7C:11:TYR:CE1 | 9:7D:26:LEU:HD23 | 1.61 | 1.33 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:7C:15:VAL:CG1 | 9:7D:35:ILE:HD13 | 0.86 | 1.33 |
| 2:KB:276:ARG:NH2 | 6:4A:271:GLU:O | 1.61 | 1.33 |
| 2:KF:88:ASP:OD1 | 2:LF:291:GLN:CD | 1.71 | 1.33 |
| 1:BE:101:ASN:ND2 | 2:BF:252:LYS:CD | 1.89 | 1.33 |
| 1:DE:402:ARG:HH22 | 7:5B:782:LEU:CD1 | 1.34 | 1.33 |
| 2:HF:261:PRO:CB | 5:3A:337:ARG:HH21 | 1.42 | 1.33 |
| 1:KC:85:GLN:CA | 1:LC:283:HIS:HA | 1.58 | 1.33 |
| 1:ME:101:ASN:ND2 | 2:MF:252:LYS:HD2 | 1.01 | 1.33 |
| 2:LB:306:ARG:NE | 4:2C:149:ILE:CG2 | 1.87 | 1.32 |
| 2:JF:88:ASP:HB2 | 2:KF:278:SER:OG | 1.15 | 1.32 |
| 1:LC:60:LYS:HB3 | 6:4A:101:ARG:NH1 | 1.23 | 1.32 |
| 2:AB:212:PHE:HZ | 1:AC:326:LYS:CD | 1.39 | 1.32 |
| 2:AD:358:PRO:C | 6:4C:151:ARG:NH2 | 1.83 | 1.32 |
| 1:DE:101:ASN:ND2 | 2:DF:252:LYS:CD | 1.92 | 1.32 |
| 1:MC:101:ASN:ND2 | 2:MD:252:LYS:HD2 | 1.02 | 1.32 |
| 2:CB:177:ASP:CG | 1:CC:353:VAL:HG12 | 1.53 | 1.32 |
| 1:EA:282:TYR:CE2 | 10:8J:18:UNK:CB | 2.13 | 1.32 |
| 2:ED:177:ASP:CG | 1:EE:353:VAL:HG12 | 1.48 | 1.32 |
| 1:GE:101:ASN:ND2 | 2:GF:252:LYS:HD2 | 1.01 | 1.32 |
| 1:KE:101:ASN:ND2 | 2:KF:252:LYS:HD2 | 1.01 | 1.32 |
| 2:AF:359:LYS:N | 6:4A:151:ARG:NH2 | 1.74 | 1.32 |
| 2:FD:55:THR:HG23 | 2:GD:283:ALA:CA | 1.58 | 1.32 |
| 1:IA:402:ARG:CZ | 7:5C:1417:GLN:HG3 | 1.60 | 1.32 |
| 1:HE:278:ALA:CB | 10:8U:18:UNK:O | 1.76 | 1.31 |
| 1:JA:88:HIS:CE1 | 1:KA:280:LYS:O | 1.83 | 1.31 |
| 1:JC:91:GLN:N | 1:KC:280:LYS:HZ2 | 1.22 | 1.31 |
| 1:JE:91:GLN:H | 1:KE:280:LYS:NZ | 1.24 | 1.31 |
| 2:KB:55:THR:CG2 | 2:LB:363:MET:HE1 | 1.57 | 1.31 |
| 4:2B:16:GLN:O | 4:2B:20:LYS:N | 1.63 | 1.31 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:CD | 1.58 | 1.31 |
| 2:GB:212:PHE:HZ | 1:GC:326:LYS:CD | 1.39 | 1.31 |
| 4:2A:16:GLN:O | 4:2A:20:LYS:N | 1.63 | 1.31 |
| 1:AE:101:ASN:ND2 | 2:AF:252:LYS:HD2 | 1.01 | 1.31 |
| 1:CA:101:ASN:ND2 | 2:CB:252:LYS:CD | 1.91 | 1.31 |
| 1:CE:101:ASN:ND2 | 2:CF:252:LYS:CD | 1.90 | 1.31 |
| 1:EA:370:LYS:HE2 | 10:8J:17:UNK:CB | 1.61 | 1.31 |
| 1:IC:58:ALA:HB1 | 10:8Z:13:UNK:CB | 1.58 | 1.31 |
| 2:LF:55:THR:N | 2:MF:283:ALA:HB2 | 1.45 | 1.31 |
| 2:LF:231:ALA:CB | 6:4D:226:ILE:HD13 | 1.60 | 1.31 |
| 4:2C:16:GLN:O | 4:2C:20:LYS:N | 1.63 | 1.31 |
| 1:FA:89:PRO:CD | 1:GA:280:LYS:CD | 2.05 | 1.31 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JC:87:PHE:O | 1:KC:283:HIS:CE1 | 1.83 | 1.31 |
| 7:5A:1246:LEU:CG | 9:7B:12:GLU:OE2 | 1.79 | 1.31 |
| 2:EF:125:GLU:HA | 7:5B:903:PHE:CE2 | 1.26 | 1.31 |
| 2:ID:424:GLN:NE2 | 7:5A:1413:GLN:CD | 1.89 | 1.31 |
| 1:IE:101:ASN:ND2 | 2:IF:252:LYS:HD2 | 1.01 | 1.31 |
| 1:KA:62:VAL:CG2 | 1:LA:285:GLN:HB3 | 1.59 | 1.31 |
| 1:GA:101:ASN:ND2 | 2:GB:252:LYS:HD2 | 1.00 | 1.30 |
| 1:HE:101:ASN:ND2 | 2:HF:252:LYS:HD2 | 1.01 | 1.30 |
| 2:KB:217:LEU:CD2 | 6:4A:263:CYS:SG | 2.20 | 1.30 |
| 2:LB:177:ASP:CG | 1:LC:353:VAL:CG1 | 2.03 | 1.30 |
| 7:5B:1266:TYR:HA | 7:5B:1269:ASP:OD2 | 1.31 | 1.30 |
| 1:DC:101:ASN:ND2 | 2:DD:252:LYS:CD | 1.94 | 1.30 |
| 1:DE:402:ARG:NE | 7:5B:777:ALA:HB3 | 1.42 | 1.30 |
| 1:EA:101:ASN:ND2 | 2:EB:252:LYS:HD2 | 1.01 | 1.30 |
| 1:EC:101:ASN:ND2 | 2:ED:252:LYS:HD2 | 0.99 | 1.30 |
| 1:EC:370:LYS:CE | 10:8K:17:UNK:CB | 2.09 | 1.30 |
| 1:KA:101:ASN:ND2 | 2:KB:252:LYS:HD2 | 1.00 | 1.30 |
| 1:HE:278:ALA:HB3 | 10:8U:22:UNK:N | 1.41 | 1.30 |
| 1:HE:282:TYR:CE2 | 10:8U:19:UNK:N | 2.00 | 1.30 |
| 1:IA:58:ALA:HB3 | 10:8Y:13:UNK:CA | 1.59 | 1.30 |
| 2:JD:212:PHE:HZ | 1:JE:326:LYS:CD | 1.42 | 1.30 |
| 2:LB:177:ASP:O | 1:LC:352:LYS:HD2 | 1.27 | 1.30 |
| 7:5A:1266:TYR:HA | 7:5A:1269:ASP:OD2 | 1.31 | 1.30 |
| 1:FE:419:SER:HB2 | 7:5B:1256:ARG:NE | 1.30 | 1.30 |
| 2:ID:212:PHE:HZ | 1:IE:326:LYS:CD | 1.42 | 1.30 |
| 1:JE:101:ASN:ND2 | 2:JF:252:LYS:HD2 | 1.01 | 1.30 |
| 1:DA:402:ARG:NH2 | 7:5C:777:ALA:HB3 | 1.47 | 1.30 |
| 2:ED:125:GLU:CG | 7:5A:903:PHE:CE2 | 2.14 | 1.30 |
| 2:EF:125:GLU:HG2 | 7:5B:903:PHE:CD2 | 1.66 | 1.30 |
| 1:IA:58:ALA:HB1 | 10:8Y:13:UNK:CB | 1.62 | 1.30 |
| 1:KA:88:HIS:CA | 1:LA:284:GLU:CB | 1.80 | 1.30 |
| 2:KF:87:PRO:CG | 2:LF:282:ARG:HG3 | 1.58 | 1.30 |
| 7:5C:1266:TYR:HA | 7:5C:1269:ASP:OD2 | 1.31 | 1.30 |
| 1:AA:101:ASN:ND2 | 2:AB:252:LYS:HD2 | 1.00 | 1.29 |
| 2:AD:362:LYS:NZ | 6:4C:143:THR:O | 1.60 | 1.29 |
| 1:DA:402:ARG:HH22 | 7:5C:782:LEU:CD1 | 1.43 | 1.29 |
| 2:KD:212:PHE:HZ | 1:KE:326:LYS:CD | 1.42 | 1.29 |
| 7:5B:1245:GLY:C | 9:7D:12:GLU:OE1 | 1.75 | 1.29 |
| 7:5B:1499:LYS:HE3 | 7:5B:1513:ASP:O | 1.29 | 1.29 |
| 2:CD:177:ASP:CG | 1:CE:353:VAL:HG12 | 1.54 | 1.29 |
| 1:IA:101:ASN:ND2 | 2:IB:252:LYS:HD2 | 1.00 | 1.29 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:JD:98:GLY:HA2 | 1:JE:254:GLU:CG | 1.62 | 1.29 |
| 2:MD:177:ASP:CG | 1:ME:353:VAL:CG1 | 2.05 | 1.29 |
| 2:AF:362:LYS:NZ | 6:4A:143:THR:O | 1.63 | 1.29 |
| 2:EB:98:GLY:HA2 | 1:EC:254:GLU:CG | 1.60 | 1.29 |
| 1:HA:101:ASN:ND2 | 2:HB:252:LYS:HD2 | 1.00 | 1.29 |
| 2:ID:98:GLY:HA2 | 1:IE:254:GLU:CG | 1.62 | 1.29 |
| 2:JB:98:GLY:HA2 | 1:JC:254:GLU:CG | 1.62 | 1.29 |
| 1:KA:85:GLN:OE1 | 1:LA:282:TYR:CB | 1.79 | 1.29 |
| 2:KB:127:CYS:H | 4:2C:38:VAL:CG1 | 1.39 | 1.29 |
| 7:5A:839:GLU:HG2 | 8:6A:107:PRO:O | 1.27 | 1.29 |
| 7:5A:1499:LYS:HE3 | 7:5A:1513:ASP:O | 1.29 | 1.29 |
| 2:ED:98:GLY:HA2 | 1:EE:254:GLU:CG | 1.62 | 1.29 |
| 2:HB:98:GLY:HA2 | 1:HC:254:GLU:CG | 1.62 | 1.29 |
| 1:IA:402:ARG:HH22 | 7:5C:1418:GLN:N | 1.26 | 1.29 |
| 2:IB:98:GLY:HA2 | 1:IC:254:GLU:CG | 1.62 | 1.29 |
| 1:JC:89:PRO:CD | 1:KC:283:HIS:CE1 | 2.12 | 1.29 |
| 2:LB:55:THR:HG23 | 2:MB:283:ALA:CB | 1.60 | 1.29 |
| 2:AB:98:GLY:HA2 | 1:AC:254:GLU:CG | 1.62 | 1.29 |
| 2:DD:177:ASP:CG | 1:DE:353:VAL:HG12 | 1.47 | 1.29 |
| 2:FF:428:ALA:CB | 7:5B:1080:PHE:HE1 | 1.44 | 1.29 |
| 2:HD:98:GLY:HA2 | 1:HE:254:GLU:CG | 1.62 | 1.29 |
| 2:HD:212:PHE:HZ | 1:HE:326:LYS:CD | 1.42 | 1.29 |
| 1:IC:58:ALA:HB3 | 10:8Z:13:UNK:CA | 1.50 | 1.29 |
| 1:JC:89:PRO:CG | 1:KC:280:LYS:HG2 | 1.61 | 1.29 |
| 2:LB:306:ARG:NH1 | 4:2C:151:VAL:CG2 | 1.96 | 1.29 |
| 1:MA:101:ASN:ND2 | 2:MB:252:LYS:HD2 | 0.97 | 1.29 |
| 2:AD:212:PHE:HZ | 1:AE:326:LYS:CD | 1.42 | 1.28 |
| 2:EB:125:GLU:O | 7:5C:903:PHE:CZ | 1.84 | 1.28 |
| 2:GB:98:GLY:HA2 | 1:GC:254:GLU:CG | 1.61 | 1.28 |
| 1:IC:402:ARG:HH22 | 7:5A:1417:GLN:C | 1.37 | 1.28 |
| 2:IF:424:GLN:NE2 | 7:5B:1413:GLN:CD | 1.91 | 1.28 |
| 1:JA:101:ASN:ND2 | 2:JB:252:LYS:HD2 | 1.00 | 1.28 |
| 1:ME:282:TYR:CD2 | 6:4B:104:ARG:HD3 | 1.68 | 1.28 |
| 7:5C:1284:PHE:CZ | 9:7E:12:GLU:HB3 | 1.60 | 1.28 |
| 7:5C:1499:LYS:HE3 | 7:5C:1513:ASP:O | 1.29 | 1.28 |
| 1:IA:58:ALA:CB | 10:8Y:13:UNK:HA | 1.62 | 1.28 |
| 2:KD:98:GLY:HA2 | 1:KE:254:GLU:CG | 1.62 | 1.28 |
| 2:KD:118:ASP:OD2 | 4:2A:148:ASN:ND2 | 1.64 | 1.28 |
| 7:5B:1573:ARG:O | 7:5B:1577:LYS:HB2 | 1.19 | 1.28 |
| 2:AD:98:GLY:HA2 | 1:AE:254:GLU:CG | 1.62 | 1.28 |
| 1:DE:402:ARG:NE | 7:5B:777:ALA:CB | 1.95 | 1.28 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:GD:98:GLY:HA2 | 1:GE:254:GLU:CG | 1.62 | 1.28 |
| 1:JE:91:GLN:N | 1:KE:280:LYS:NZ | 1.76 | 1.28 |
| 2:KD:86:ARG:NH1 | 2:LD:283:ALA:HB3 | 1.44 | 1.28 |
| 1:KE:85:GLN:CA | 1:LE:283:HIS:HA | 1.63 | 1.28 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:NZ | 1.97 | 1.28 |
| 2:LF:306:ARG:CZ | 4:2B:151:VAL:HG23 | 1.62 | 1.28 |
| 2:GD:212:PHE:HZ | 1:GE:326:LYS:CD | 1.42 | 1.28 |
| 1:JA:89:PRO:CB | 1:KA:280:LYS:CG | 2.01 | 1.28 |
| 7:5C:773:ARG:O | 7:5C:775:PRO:CD | 1.81 | 1.28 |
| 1:EA:396:ASP:CB | 7:5C:817:LEU:CD2 | 1.79 | 1.28 |
| 1:EE:430:LYS:CE | 7:5B:834:ASN:HD22 | 1.46 | 1.28 |
| 1:JC:91:GLN:N | 1:KC:280:LYS:NZ | 1.82 | 1.28 |
| 2:KB:98:GLY:HA2 | 1:KC:254:GLU:CG | 1.62 | 1.28 |
| 2:KF:86:ARG:CZ | 2:LF:283:ALA:H | 1.25 | 1.28 |
| 7:5A:773:ARG:O | 7:5A:775:PRO:CD | 1.81 | 1.28 |
| 7:5C:1548:VAL:HG11 | 7:5C:1565:GLU:O | 1.25 | 1.28 |
| 2:DB:86:ARG:HA | 2:EB:281:TYR:CE1 | 1.67 | 1.27 |
| 2:FD:54:ALA:CA | 2:GD:283:ALA:HB2 | 1.64 | 1.27 |
| 1:HC:278:ALA:HB1 | 10:8T:18:UNK:O | 1.12 | 1.27 |
| 2:LB:306:ARG:CZ | 4:2C:151:VAL:CG2 | 2.10 | 1.27 |
| 7:5A:1573:ARG:O | 7:5A:1577:LYS:HB2 | 1.19 | 1.27 |
| 7:5B:773:ARG:O | 7:5B:775:PRO:CD | 1.81 | 1.27 |
| 2:LD:306:ARG:HE | 4:2A:149:ILE:CG2 | 1.47 | 1.27 |
| 1:MA:282:TYR:CD2 | 6:4C:104:ARG:HD3 | 1.68 | 1.27 |
| 7:5A:1548:VAL:CA | 7:5A:1569:GLU:OE2 | 1.81 | 1.27 |
| 7:5B:1548:VAL:CA | 7:5B:1569:GLU:OE2 | 1.81 | 1.27 |
| 2:AF:227:HIS:HE1 | 6:4A:135:LEU:CD1 | 1.46 | 1.27 |
| 1:DA:402:ARG:CZ | 7:5C:777:ALA:CB | 2.08 | 1.27 |
| 2:JD:88:ASP:HB2 | 2:KD:278:SER:OG | 1.34 | 1.27 |
| 2:EB:125:GLU:CG | 7:5C:903:PHE:HE2 | 1.46 | 1.27 |
| 2:FB:54:ALA:C | 2:GB:283:ALA:CB | 2.08 | 1.27 |
| 7:5A:1547:SER:C | 7:5A:1569:GLU:OE1 | 1.78 | 1.27 |
| 7:5B:827:GLU:OE1 | 7:5B:849:ARG:NH2 | 1.67 | 1.27 |
| 7:5C:1547:SER:C | 7:5C:1569:GLU:OE1 | 1.78 | 1.27 |
| 7:5C:1548:VAL:CA | 7:5C:1569:GLU:OE2 | 1.81 | 1.27 |
| 1:AC:342:GLN:HE22 | 3:1C:55:HIS:CG | 1.52 | 1.27 |
| 1:GC:101:ASN:ND2 | 2:GD:252:LYS:HD2 | 0.96 | 1.27 |
| 1:GE:56:THR:C | 1:HE:285:GLN:HB3 | 1.58 | 1.27 |
| 1:JE:89:PRO:HG2 | 1:KE:280:LYS:CA | 1.58 | 1.27 |
| 7:5A:1548:VAL:HG11 | 7:5A:1565:GLU:O | 1.25 | 1.27 |
| 7:5B:1547:SER:C | 7:5B:1569:GLU:OE1 | 1.78 | 1.27 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AD:217:LEU:CD2 | 6:4C:132:LYS:HG2 | 1.64 | 1.26 |
| 1:FA:423:GLU:OE2 | 7:5C:1256:ARG:NH2 | 1.67 | 1.26 |
| 1:FC:101:ASN:ND2 | 2:FD:252:LYS:CD | 1.96 | 1.26 |
| 1:FE:422:ARG:HH21 | 7:5B:1170:THR:CA | 1.45 | 1.26 |
| 1:GE:56:THR:O | 1:HE:285:GLN:HB3 | 1.24 | 1.26 |
| 1:IC:434:GLU:OE1 | 5:3C:61:SER:HB3 | 1.26 | 1.26 |
| 7:5A:827:GLU:OE1 | 7:5A:849:ARG:NH2 | 1.67 | 1.26 |
| 7:5C:1573:ARG:O | 7:5C:1577:LYS:HB2 | 1.19 | 1.26 |
| 9:7D:12:GLU:HA | 9:7D:16:THR:OG1 | 1.28 | 1.26 |
| 2:ED:125:GLU:C | 7:5A:903:PHE:CZ | 2.13 | 1.26 |
| 1:FA:101:ASN:ND2 | 2:FB:252:LYS:CD | 1.98 | 1.26 |
| 1:FC:423:GLU:OE2 | 7:5A:1256:ARG:NH2 | 1.65 | 1.26 |
| 2:KB:86:ARG:NH1 | 2:LB:283:ALA:CB | 1.80 | 1.26 |
| 2:KF:86:ARG:NH1 | 2:LF:283:ALA:HB3 | 1.49 | 1.26 |
| 1:LC:60:LYS:HD2 | 6:4A:101:ARG:NH2 | 1.51 | 1.26 |
| 7:5C:1267:CYS:O | 7:5C:1270:ASP:HB2 | 1.31 | 1.26 |
| 1:AC:101:ASN:ND2 | 2:AD:252:LYS:HD2 | 0.96 | 1.26 |
| 1:EE:370:LYS:CE | 10:8L:17:UNK:CB | 2.12 | 1.26 |
| 1:KE:359:PRO:HB3 | 6:4B:299:TYR:CE2 | 1.71 | 1.26 |
| 7:5A:1267:CYS:O | 7:5A:1270:ASP:HB2 | 1.31 | 1.26 |
| 7:5B:1267:CYS:O | 7:5B:1270:ASP:HB2 | 1.31 | 1.26 |
| 7:5C:827:GLU:OE1 | 7:5C:849:ARG:NH2 | 1.67 | 1.26 |
| 1:FC:422:ARG:HH21 | 7:5A:1170:THR:CA | 1.47 | 1.26 |
| 1:HC:101:ASN:ND2 | 2:HD:252:LYS:HD2 | 0.96 | 1.26 |
| 1:JA:128:ASN:ND2 | 1:KA:285:GLN:OE1 | 1.67 | 1.26 |
| 1:JC:91:GLN:H | 1:KC:280:LYS:NZ | 1.30 | 1.26 |
| 2:LD:296:ALA:CB | 4:2A:149:ILE:CG2 | 2.03 | 1.26 |
| 7:5C:1246:LEU:HG | 9:7F:12:GLU:OE2 | 1.18 | 1.26 |
| 2:EB:177:ASP:CG | 1:EC:353:VAL:HG12 | 1.53 | 1.26 |
| 2:FD:98:GLY:CA | 1:FE:254:GLU:HG2 | 1.63 | 1.26 |
| 1:GE:56:THR:O | 1:HE:285:GLN:CB | 1.83 | 1.26 |
| 1:HE:419:SER:OG | 5:3A:238:ILE:HD12 | 1.33 | 1.26 |
| 2:LD:177:ASP:O | 1:LE:352:LYS:HD2 | 1.22 | 1.26 |
| 2:MB:177:ASP:CG | 1:MC:353:VAL:CG1 | 2.06 | 1.26 |
| 1:GC:409:VAL:HG11 | 5:3C:383:GLU:OE2 | 1.36 | 1.25 |
| 1:IA:278:ALA:HB2 | 10:8V:21:UNK:CB | 1.62 | 1.25 |
| 2:JD:86:ARG:CZ | 2:KD:280:GLN:CB | 2.14 | 1.25 |
| 1:KC:101:ASN:ND2 | 2:KD:252:LYS:HD2 | 0.96 | 1.25 |
| 2:LD:306:ARG:CZ | 4:2A:151:VAL:CG2 | 2.14 | 1.25 |
| 7:5B:1548:VAL:HG11 | 7:5B:1565:GLU:O | 1.25 | 1.25 |
| 9:7F:12:GLU:HA | 9:7F:16:THR:OG1 | 1.28 | 1.25 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:FE:402:ARG:NH2 | 7:5B:1262:GLU:CD | 1.95 | 1.25 |
| 2:GD:55:THR:N | 2:HD:283:ALA:CB | 1.97 | 1.25 |
| 1:IC:279:GLU:OE2 | 10:8W:22:UNK:O | 1.55 | 1.25 |
| 2:ID:424:GLN:CD | 7:5A:1413:GLN:NE2 | 1.92 | 1.25 |
| 1:KA:79:ARG:O | 1:LA:280:LYS:HE2 | 1.30 | 1.25 |
| 1:KC:88:HIS:CA | 1:LC:284:GLU:HB2 | 1.58 | 1.25 |
| 2:KD:215:LEU:CD1 | 6:4B:267:ILE:HG22 | 1.67 | 1.25 |
| 2:BD:98:GLY:HA2 | 1:BE:254:GLU:CG | 1.66 | 1.25 |
| 2:ED:125:GLU:CG | 7:5A:903:PHE:HE2 | 1.44 | 1.25 |
| 1:EE:101:ASN:ND2 | 2:EF:252:LYS:CD | 1.97 | 1.25 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:NZ | 1.97 | 1.25 |
| 1:JC:101:ASN:ND2 | 2:JD:252:LYS:HD2 | 0.96 | 1.25 |
| 1:IC:101:ASN:ND2 | 2:ID:252:LYS:HD2 | 0.96 | 1.25 |
| 1:IC:279:GLU:OE2 | 10:8W:22:UNK:C | 1.85 | 1.25 |
| 2:KF:221:THR:CG2 | 6:4D:261:SER:O | 1.82 | 1.25 |
| 2:KB:276:ARG:HH21 | 6:4A:265:TYR:CA | 1.50 | 1.25 |
| 7:5A:1490:LYS:CG | 7:5A:1494:LEU:HD23 | 1.67 | 1.25 |
| 7:5C:1552:LYS:HZ1 | 7:5C:1563:SER:CB | 1.38 | 1.25 |
| 2:DD:85:PHE:O | 2:ED:281:TYR:OH | 1.55 | 1.25 |
| 1:EC:430:LYS:NZ | 7:5A:834:ASN:CG | 1.95 | 1.25 |
| 1:IA:278:ALA:HB3 | 10:8V:22:UNK:N | 1.50 | 1.25 |
| 1:JC:89:PRO:HD3 | 1:KC:283:HIS:CE1 | 1.68 | 1.25 |
| 5:3A:229:PHE:CE2 | 5:3A:331:GLN:CB | 2.18 | 1.25 |
| 5:3C:229:PHE:CE2 | 5:3C:331:GLN:CB | 2.18 | 1.25 |
| 7:5B:1490:LYS:CG | 7:5B:1494:LEU:HD23 | 1.67 | 1.25 |
| 7:5C:1490:LYS:CG | 7:5C:1494:LEU:HD23 | 1.67 | 1.25 |
| 1:FE:101:ASN:ND2 | 2:FF:252:LYS:CD | 1.98 | 1.25 |
| 1:HC:419:SER:OG | 5:3C:238:ILE:HD12 | 1.34 | 1.25 |
| 1:IE:389:SER:CB | 5:3A:307:LYS:HD3 | 1.66 | 1.25 |
| 2:IF:424:GLN:CD | 7:5B:1413:GLN:NE2 | 1.93 | 1.25 |
| 2:KF:125:GLU:CG | 2:LF:336:LYS:NZ | 1.97 | 1.25 |
| 5:3B:229:PHE:CE2 | 5:3B:331:GLN:CB | 2.18 | 1.25 |
| 1:FE:423:GLU:OE2 | 7:5B:1256:ARG:NH2 | 1.69 | 1.24 |
| 1:KA:85:GLN:OE1 | 1:LA:282:TYR:HB2 | 1.13 | 1.24 |
| 1:KA:88:HIS:HA | 1:LA:284:GLU:CB | 1.06 | 1.24 |
| 2:KD:215:LEU:HD22 | 6:4B:267:ILE:O | 1.32 | 1.24 |
| 2:KF:217:LEU:HD22 | 6:4D:263:CYS:SG | 1.76 | 1.24 |
| 5:3A:229:PHE:HE2 | 5:3A:331:GLN:CB | 1.51 | 1.24 |
| 5:3C:229:PHE:HE2 | 5:3C:331:GLN:CB | 1.51 | 1.24 |
| 7:5A:1267:CYS:SG | 9:7A:8:ARG:NE | 2.10 | 1.24 |
| 9:7E:11:TYR:CE1 | 9:7F:26:LEU:HD23 | 1.71 | 1.24 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:86:ARG:CB | 2:DB:281:TYR:CE1 | 2.20 | 1.24 |
| 2:DB:177:ASP:CG | 1:DC:353:VAL:HG12 | 1.51 | 1.24 |
| 2:FB:55:THR:N | 2:GB:283:ALA:HB2 | 1.45 | 1.24 |
| 2:FB:428:ALA:HB1 | 7:5C:1080:PHE:CE1 | 1.47 | 1.24 |
| 1:JC:279:GLU:OE2 | 10:8Z:22:UNK:HA | 1.28 | 1.24 |
| 2:KD:55:THR:HG21 | 2:LD:363:MET:CE | 1.68 | 1.24 |
| 2:KF:125:GLU:CG | 2:LF:336:LYS:HZ1 | 1.50 | 1.24 |
| 1:LC:176:GLN:NE2 | 4:2A:42:PHE:CD2 | 2.05 | 1.24 |
| 1:LE:89:PRO:HG3 | 1:ME:280:LYS:CE | 1.67 | 1.24 |
| 2:MD:212:PHE:HZ | 1:ME:326:LYS:CD | 1.50 | 1.24 |
| 5:3B:229:PHE:HE2 | 5:3B:331:GLN:CB | 1.51 | 1.24 |
| 5:3B:231:THR:C | 5:3B:335:LYS:HB2 | 1.54 | 1.24 |
| 7:5B:1475:PHE:HE2 | 7:5B:1565:GLU:OE2 | 0.96 | 1.24 |
| 2:CB:177:ASP:O | 1:CC:352:LYS:HD2 | 1.35 | 1.24 |
| 1:FC:89:PRO:CD | 1:GC:280:LYS:HZ2 | 1.48 | 1.24 |
| 1:FE:60:LYS:NZ | 1:GE:283:HIS:CD2 | 2.04 | 1.24 |
| 1:JC:279:GLU:OE2 | 10:8Z:22:UNK:CA | 1.86 | 1.24 |
| 1:EC:370:LYS:HE2 | 10:8K:17:UNK:CB | 1.68 | 1.24 |
| 2:EF:125:GLU:CB | 7:5B:903:PHE:CE2 | 2.21 | 1.24 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:CG | 1.99 | 1.24 |
| 9:7E:30:ARG:NH1 | 9:7F:3:GLN:HA | 1.50 | 1.24 |
| 2:EF:125:GLU:CG | 7:5B:903:PHE:HE2 | 1.41 | 1.24 |
| 1:GC:89:PRO:HD3 | 1:HC:280:LYS:NZ | 1.49 | 1.24 |
| 5:3A:231:THR:C | 5:3A:335:LYS:HB2 | 1.54 | 1.24 |
| 7:5A:1475:PHE:HE2 | 7:5A:1565:GLU:OE2 | 0.96 | 1.24 |
| 2:AD:224:ASP:OD1 | 6:4C:132:LYS:N | 1.70 | 1.23 |
| 2:DB:86:ARG:CA | 2:EB:281:TYR:CE1 | 2.20 | 1.23 |
| 2:ED:157:GLU:OE2 | 7:5A:935:LYS:NZ | 1.70 | 1.23 |
| 1:HE:278:ALA:HB1 | 10:8U:18:UNK:O | 1.11 | 1.23 |
| 2:KD:217:LEU:CB | 6:4B:265:TYR:OH | 1.86 | 1.23 |
| 1:LA:101:ASN:ND2 | 2:LB:252:LYS:HD2 | 1.52 | 1.23 |
| 1:LA:245:ASP:OD1 | 6:4C:216:ARG:NH2 | 1.71 | 1.23 |
| 7:5C:1379:LYS:O | 7:5C:1383:GLU:OE1 | 1.54 | 1.23 |
| 7:5C:1475:PHE:HE2 | 7:5C:1565:GLU:OE2 | 0.96 | 1.23 |
| 1:EE:430:LYS:NZ | 7:5B:834:ASN:CG | 1.94 | 1.23 |
| 1:FE:177:VAL:CG2 | 7:5B:915:PHE:CE2 | 2.00 | 1.23 |
| 1:IC:278:ALA:HB1 | 10:8W:18:UNK:O | 1.09 | 1.23 |
| 1:JA:91:GLN:H | 1:KA:280:LYS:NZ | 1.37 | 1.23 |
| 7:5A:1379:LYS:O | 7:5A:1383:GLU:OE1 | 1.54 | 1.23 |
| 7:5A:1552:LYS:HZ1 | 7:5A:1563:SER:CB | 1.39 | 1.23 |
| 2:AF:358:PRO:C | 6:4A:151:ARG:NH2 | 1.95 | 1.23 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:DC:402:ARG:NE | 7:5A:777:ALA:HB3 | 1.39 | 1.23 |
| 1:FA:89:PRO:HG3 | 1:GA:280:LYS:CG | 1.69 | 1.23 |
| 1:KA:85:GLN:CD | 1:LA:282:TYR:HB2 | 1.63 | 1.23 |
| 2:KF:54:ALA:CB | 2:LF:285:THR:CG2 | 2.14 | 1.23 |
| 2:KF:217:LEU:CB | 6:4D:265:TYR:OH | 1.85 | 1.23 |
| 1:LC:101:ASN:ND2 | 2:LD:252:LYS:HD2 | 1.51 | 1.23 |
| 5:3C:231:THR:C | 5:3C:335:LYS:HB2 | 1.54 | 1.23 |
| 7:5C:1491:LEU:CA | 7:5C:1495:PHE:HB3 | 1.69 | 1.23 |
| 9:7B:12:GLU:HA | 9:7B:16:THR:OG1 | 1.28 | 1.23 |
| 2:AF:227:HIS:CE1 | 6:4A:135:LEU:CD1 | 2.19 | 1.23 |
| 2:FB:212:PHE:HZ | 1:FC:326:LYS:CD | 1.50 | 1.23 |
| 2:JB:86:ARG:NH2 | 2:KB:280:GLN:CB | 2.01 | 1.23 |
| 1:JE:89:PRO:CB | 1:KE:280:LYS:CG | 2.04 | 1.23 |
| 2:KB:127:CYS:N | 4:2C:38:VAL:HG12 | 1.42 | 1.23 |
| 2:KD:273:LEU:CA | 6:4B:268:LEU:CD2 | 2.12 | 1.23 |
| 7:5A:1491:LEU:CA | 7:5A:1495:PHE:HB3 | 1.69 | 1.23 |
| 7:5B:1379:LYS:O | 7:5B:1383:GLU:OE1 | 1.54 | 1.23 |
| 7:5B:1491:LEU:CA | 7:5B:1495:PHE:HB3 | 1.69 | 1.23 |
| 7:5B:1548:VAL:CA | 7:5B:1569:GLU:CD | 2.11 | 1.23 |
| 9:7C:11:TYR:HE1 | 9:7D:26:LEU:CB | 1.52 | 1.23 |
| 1:AC:342:GLN:NE2 | 3:1C:55:HIS:CD2 | 2.07 | 1.23 |
| 1:DC:402:ARG:HH22 | 7:5A:782:LEU:CD1 | 1.39 | 1.23 |
| 1:IE:402:ARG:NH2 | 7:5B:1417:GLN:C | 1.94 | 1.23 |
| 2:KD:125:GLU:HG3 | 2:LD:336:LYS:NZ | 0.93 | 1.23 |
| 7:5C:1125:LEU:HD11 | 8:6C:245:GLN:OE1 | 1.05 | 1.23 |
| 9:7A:11:TYR:HE1 | 9:7B:26:LEU:CB | 1.52 | 1.23 |
| 1:EC:282:TYR:CE2 | 10:8K:18:UNK:CB | 2.22 | 1.22 |
| 1:HE:282:TYR:CZ | 10:8U:15:UNK:O | 1.90 | 1.22 |
| 1:AC:342:GLN:HE22 | 3:1C:55:HIS:CD2 | 1.58 | 1.22 |
| 2:BB:98:GLY:HA2 | 1:BC:254:GLU:CG | 1.69 | 1.22 |
| 1:EE:402:ARG:NE | 7:5B:824:ARG:HH22 | 1.32 | 1.22 |
| 1:FA:419:SER:OG | 7:5C:1256:ARG:NE | 1.70 | 1.22 |
| 1:FC:177:VAL:CG2 | 7:5A:915:PHE:CE2 | 2.03 | 1.22 |
| 2:KB:127:CYS:N | 4:2C:38:VAL:CG1 | 1.87 | 1.22 |
| 5:3B:231:THR:O | 5:3B:332:MET:HA | 1.32 | 1.22 |
| 7:5A:1246:LEU:HG | 9:7B:12:GLU:OE2 | 1.10 | 1.22 |
| 7:5A:1548:VAL:CA | 7:5A:1569:GLU:CD | 2.11 | 1.22 |
| 7:5C:1548:VAL:CA | 7:5C:1569:GLU:CD | 2.11 | 1.22 |
| 2:DD:86:ARG:HA | 2:ED:281:TYR:CE1 | 1.72 | 1.22 |
| 1:IA:282:TYR:CE2 | 10:8V:19:UNK:N | 2.05 | 1.22 |
| 2:KB:273:LEU:CA | 6:4A:268:LEU:HD23 | 1.57 | 1.22 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LF:274:THR:O | 6:4D:228:LEU:CD2 | 1.88 | 1.22 |
| 7:5A:1491:LEU:HD22 | 7:5A:1495:PHE:CG | 1.73 | 1.22 |
| 7:5B:1491:LEU:HD22 | 7:5B:1495:PHE:CG | 1.73 | 1.22 |
| 7:5C:1491:LEU:HD22 | 7:5C:1495:PHE:CG | 1.74 | 1.22 |
| 1:CE:60:LYS:NZ | 1:DE:283:HIS:NE2 | 1.86 | 1.22 |
| 2:FB:55:THR:HG23 | 2:GB:283:ALA:CA | 1.68 | 1.22 |
| 1:JE:89:PRO:CG | 1:KE:280:LYS:HG2 | 1.67 | 1.22 |
| 1:KC:79:ARG:CA | 1:LC:280:LYS:NZ | 2.02 | 1.22 |
| 2:LB:331:LEU:CG | 4:2C:42:PHE:CZ | 2.23 | 1.22 |
| 5:3B:231:THR:C | 5:3B:332:MET:HA | 1.63 | 1.22 |
| 5:3C:231:THR:C | 5:3C:332:MET:HA | 1.63 | 1.22 |
| 2:EB:125:GLU:CG | 7:5C:903:PHE:CE2 | 2.20 | 1.21 |
| 1:EE:282:TYR:CE2 | 10:8L:18:UNK:CB | 2.21 | 1.21 |
| 1:FC:402:ARG:NH2 | 7:5A:1262:GLU:CD | 1.97 | 1.21 |
| 2:FD:55:THR:CG2 | 2:GD:284:LEU:H | 1.53 | 1.21 |
| 2:LB:296:ALA:CB | 4:2C:149:ILE:CG2 | 2.12 | 1.21 |
| 5:3A:231:THR:C | 5:3A:332:MET:HA | 1.63 | 1.21 |
| 5:3A:231:THR:O | 5:3A:332:MET:HA | 1.32 | 1.21 |
| 2:ED:125:GLU:CB | 7:5A:903:PHE:CE2 | 2.23 | 1.21 |
| 1:IC:389:SER:CB | 5:3C:307:LYS:HD3 | 1.69 | 1.21 |
| 1:JA:87:PHE:O | 1:KA:283:HIS:CE1 | 1.92 | 1.21 |
| 1:LA:89:PRO:HG3 | 1:MA:280:LYS:CE | 1.70 | 1.21 |
| 1:LE:176:GLN:NE2 | 4:2B:42:PHE:CD2 | 2.09 | 1.21 |
| 7:5B:1487:ASN:CG | 7:5B:1568:LYS:HE2 | 1.65 | 1.21 |
| 7:5B:1552:LYS:HZ1 | 7:5B:1563:SER:CB | 1.40 | 1.21 |
| 7:5C:1246:LEU:CG | 9:7F:12:GLU:OE2 | 1.89 | 1.21 |
| 9:7C:7:LEU:CD2 | 9:7D:27:GLY:HA3 | 1.57 | 1.21 |
| 2:CD:86:ARG:CB | 2:DD:281:TYR:CE1 | 2.22 | 1.21 |
| 1:FA:419:SER:HB2 | 7:5C:1256:ARG:NE | 1.40 | 1.21 |
| 1:FE:422:ARG:NH2 | 7:5B:1170:THR:C | 1.98 | 1.21 |
| 7:5A:1487:ASN:CG | 7:5A:1568:LYS:HE2 | 1.65 | 1.21 |
| 7:5C:1487:ASN:CG | 7:5C:1568:LYS:HE2 | 1.65 | 1.21 |
| 1:JE:370:LYS:CE | 10:9A:17:UNK:CB | 2.17 | 1.21 |
| 2:JF:86:ARG:CZ | 2:KF:280:GLN:HB2 | 1.62 | 1.21 |
| 5:3C:231:THR:O | 5:3C:332:MET:HA | 1.32 | 1.21 |
| 2:GF:58:ARG:NH2 | 2:HF:281:TYR:CZ | 2.08 | 1.21 |
| 1:KA:62:VAL:CG2 | 1:LA:285:GLN:CB | 2.17 | 1.21 |
| 2:KD:87:PRO:CG | 2:LD:282:ARG:CG | 2.19 | 1.21 |
| 1:MC:282:TYR:CD2 | 6:4A:104:ARG:HD3 | 1.76 | 1.21 |
| 2:KB:158:GLU:CA | 4:2C:34:ASN:CB | 2.12 | 1.20 |
| 1:KE:85:GLN:HA | 1:LE:283:HIS:CA | 1.70 | 1.20 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KF:86:ARG:NH1 | 2:LF:283:ALA:CB | 1.99 | 1.20 |
| 1:LA:60:LYS:CD | 6:4C:101:ARG:HH22 | 1.53 | 1.20 |
| 2:KD:221:THR:CG2 | 6:4B:261:SER:O | 1.83 | 1.20 |
| 2:LD:274:THR:O | 6:4B:228:LEU:CD2 | 1.89 | 1.20 |
| 1:LE:60:LYS:CD | 6:4B:101:ARG:HH22 | 1.54 | 1.20 |
| 1:LE:101:ASN:ND2 | 2:LF:252:LYS:HD2 | 1.55 | 1.20 |
| 2:MB:98:GLY:HA2 | 1:MC:254:GLU:CG | 1.69 | 1.20 |
| 1:AE:342:GLN:NE2 | 3:1A:55:HIS:CD2 | 2.08 | 1.20 |
| 2:DB:98:GLY:HA2 | 1:DC:254:GLU:CG | 1.69 | 1.20 |
| 2:ED:125:GLU:HG2 | 7:5A:903:PHE:CD2 | 1.76 | 1.20 |
| 1:FA:422:ARG:NH2 | 7:5C:1170:THR:C | 1.97 | 1.20 |
| 7:5B:829:GLY:O | 8:6B:110:ASN:ND2 | 1.75 | 1.20 |
| 1:FE:419:SER:OG | 7:5B:1256:ARG:NE | 1.72 | 1.20 |
| 1:KC:372:MET:CB | 6:4A:299:TYR:CE1 | 2.18 | 1.20 |
| 2:MD:98:GLY:HA2 | 1:ME:254:GLU:CG | 1.70 | 1.20 |
| 7:5A:1152:GLU:OE1 | 8:6A:66:ARG:NH1 | 1.73 | 1.20 |
| 1:EA:402:ARG:NE | 7:5C:824:ARG:HH22 | 1.38 | 1.20 |
| 2:FF:55:THR:CG2 | 2:GF:283:ALA:HA | 1.72 | 1.20 |
| 1:IA:402:ARG:HH22 | 7:5C:1417:GLN:C | 1.48 | 1.20 |
| 2:IB:424:GLN:NE2 | 7:5C:1413:GLN:CD | 1.97 | 1.20 |
| 1:IE:389:SER:HB2 | 5:3A:307:LYS:CD | 1.71 | 1.20 |
| 1:JA:89:PRO:HG3 | 1:KA:279:GLU:O | 1.04 | 1.20 |
| 2:LD:306:ARG:NE | 4:2A:149:ILE:HG22 | 1.57 | 1.20 |
| 2:LF:296:ALA:CB | 4:2B:149:ILE:CG2 | 2.17 | 1.20 |
| 2:MB:221:THR:CG2 | 6:4A:189:ARG:HH22 | 1.54 | 1.20 |
| 2:MD:177:ASP:O | 1:ME:352:LYS:HD2 | 1.42 | 1.20 |
| 7:5A:874:GLN:HB2 | 8:6A:59:LYS:NZ | 1.55 | 1.20 |
| 2:BB:177:ASP:O | 1:BC:352:LYS:HD2 | 1.36 | 1.19 |
| 2:DD:177:ASP:O | 1:DE:352:LYS:HD2 | 1.37 | 1.19 |
| 2:FD:428:ALA:CB | 7:5A:1080:PHE:HE1 | 1.35 | 1.19 |
| 2:GB:55:THR:CG2 | 2:HB:283:ALA:CA | 1.76 | 1.19 |
| 2:KD:158:GLU:HA | 4:2A:34:ASN:HB2 | 1.20 | 1.19 |
| 2:KD:177:ASP:O | 1:KE:352:LYS:HD2 | 1.43 | 1.19 |
| 7:5B:1548:VAL:HG12 | 7:5B:1566:GLU:CA | 1.64 | 1.19 |
| 2:AD:227:HIS:CE1 | 6:4C:135:LEU:CD1 | 2.26 | 1.19 |
| 2:EB:54:ALA:HA | 2:FB:283:ALA:HB2 | 1.22 | 1.19 |
| 2:FB:55:THR:HG23 | 2:GB:283:ALA:C | 1.65 | 1.19 |
| 1:FC:402:ARG:NH2 | 7:5A:1262:GLU:OE2 | 1.75 | 1.19 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:HZ3 | 1.53 | 1.19 |
| 1:JC:89:PRO:HG2 | 1:KC:280:LYS:CA | 1.65 | 1.19 |
| 9:7E:14:SER:OG | 9:7F:34:PRO:HG2 | 1.40 | 1.19 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CE:282:TYR:CD2 | 10:8F:18:UNK:CB | 2.25 | 1.19 |
| 2:HD:160:PRO:HB3 | 5:3C:330:ARG:HH21 | 1.07 | 1.19 |
| 2:HD:177:ASP:O | 1:HE:352:LYS:HD2 | 1.43 | 1.19 |
| 2:IB:424:GLN:CD | 7:5C:1413:GLN:NE2 | 2.01 | 1.19 |
| 2:KB:215:LEU:HD22 | 6:4A:267:ILE:O | 1.03 | 1.19 |
| 2:KF:77:ARG:O | 2:LF:281:TYR:OH | 1.59 | 1.19 |
| 7:5A:1548:VAL:HG12 | 7:5A:1566:GLU:CA | 1.64 | 1.19 |
| 7:5B:839:GLU:HG2 | 8:6B:107:PRO:O | 1.42 | 1.19 |
| 9:7E:35:ILE:CG2 | 9:7F:42:LEU:O | 1.91 | 1.19 |
| 2:CF:86:ARG:CB | 2:DF:281:TYR:CE1 | 2.24 | 1.19 |
| 2:DD:86:ARG:CA | 2:ED:281:TYR:CE1 | 2.26 | 1.19 |
| 2:EB:157:GLU:OE2 | 7:5C:935:LYS:NZ | 1.73 | 1.19 |
| 1:FA:177:VAL:CG2 | 7:5C:915:PHE:CE2 | 1.97 | 1.19 |
| 2:FD:428:ALA:HB1 | 7:5A:1080:PHE:CE1 | 1.49 | 1.19 |
| 1:GE:60:LYS:HD3 | 1:HE:283:HIS:CB | 1.73 | 1.19 |
| 2:HB:177:ASP:O | 1:HC:352:LYS:HD2 | 1.43 | 1.19 |
| 2:ID:177:ASP:O | 1:IE:352:LYS:HD2 | 1.43 | 1.19 |
| 1:KA:85:GLN:C | 1:LA:283:HIS:HA | 1.67 | 1.19 |
| 1:LA:89:PRO:CG | 1:MA:280:LYS:HD2 | 1.72 | 1.19 |
| 1:MC:372:MET:HE3 | 6:4A:96:VAL:O | 1.02 | 1.19 |
| 7:5C:1548:VAL:HG12 | 7:5C:1566:GLU:CA | 1.64 | 1.19 |
| 2:CD:98:GLY:HA2 | 1:CE:254:GLU:CG | 1.72 | 1.18 |
| 1:FA:56:THR:CA | 1:GA:285:GLN:HB3 | 1.73 | 1.18 |
| 1:FA:89:PRO:CG | 1:GA:280:LYS:CD | 2.00 | 1.18 |
| 1:HA:278:ALA:HB1 | 10:8S:18:UNK:O | 1.07 | 1.18 |
| 1:IA:282:TYR:CD2 | 10:8V:18:UNK:CB | 2.26 | 1.18 |
| 2:KB:177:ASP:O | 1:KC:352:LYS:HD2 | 1.43 | 1.18 |
| 2:LB:179:VAL:HG21 | 1:LC:258:ASN:O | 1.41 | 1.18 |
| 2:LD:55:THR:CG2 | 2:MD:283:ALA:CA | 2.00 | 1.18 |
| 1:MA:279:GLU:OE1 | 6:4C:107:MET:N | 1.76 | 1.18 |
| 7:5A:1243:ASP:CG | 9:7B:8:ARG:HH12 | 1.49 | 1.18 |
| 1:FC:422:ARG:NH2 | 7:5A:1170:THR:C | 1.99 | 1.18 |
| 1:KC:85:GLN:HA | 1:LC:283:HIS:CA | 1.72 | 1.18 |
| 2:KD:276:ARG:NH2 | 6:4B:271:GLU:O | 1.77 | 1.18 |
| 7:5A:841:VAL:HG21 | 8:6A:11:PRO:HA | 1.21 | 1.18 |
| 2:BD:177:ASP:CG | 1:BE:353:VAL:HG12 | 1.55 | 1.18 |
| 1:DC:402:ARG:CZ | 7:5A:777:ALA:CB | 2.14 | 1.18 |
| 2:DD:98:GLY:HA2 | 1:DE:254:GLU:CG | 1.72 | 1.18 |
| 1:FE:402:ARG:NH2 | 7:5B:1262:GLU:OE2 | 1.75 | 1.18 |
| 2:KF:217:LEU:HB3 | 6:4D:265:TYR:OH | 1.02 | 1.18 |
| 2:BD:179:VAL:HG21 | 1:BE:258:ASN:O | 1.44 | 1.18 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:422:ARG:HH21 | 7:5C:1170:THR:CA | 1.55 | 1.18 |
| 2:KB:217:LEU:CB | 6:4A:265:TYR:OH | 1.90 | 1.18 |
| 4:2A:176:ARG:O | 4:2A:180:LYS:N | 1.75 | 1.18 |
| 4:2B:176:ARG:O | 4:2B:180:LYS:N | 1.75 | 1.18 |
| 4:2C:176:ARG:O | 4:2C:180:LYS:N | 1.75 | 1.18 |
| 9:7A:7:LEU:CD2 | 9:7B:27:GLY:HA2 | 1.60 | 1.18 |
| 2:DB:177:ASP:O | 1:DC:352:LYS:HD2 | 1.40 | 1.18 |
| 2:FF:428:ALA:CB | 7:5B:1080:PHE:CE1 | 2.20 | 1.18 |
| 2:JB:87:PRO:HG3 | 2:KB:277:GLY:O | 1.41 | 1.18 |
| 2:KB:276:ARG:HE | 6:4A:265:TYR:HB2 | 1.05 | 1.18 |
| 2:KF:77:ARG:HG2 | 2:LF:281:TYR:OH | 1.44 | 1.18 |
| 2:LF:306:ARG:HE | 4:2B:149:ILE:CG2 | 1.56 | 1.18 |
| 2:CD:177:ASP:O | 1:CE:352:LYS:HD2 | 1.42 | 1.17 |
| 2:EB:125:GLU:CB | 7:5C:903:PHE:CE2 | 2.25 | 1.17 |
| 1:EE:370:LYS:HE2 | 10:8L:17:UNK:CB | 1.73 | 1.17 |
| 1:KA:85:GLN:HA | 1:LA:283:HIS:CA | 1.72 | 1.17 |
| 9:7E:14:SER:OG | 9:7F:34:PRO:HG3 | 1.29 | 1.17 |
| 1:DE:282:TYR:CE2 | 10:8I:18:UNK:CB | 2.26 | 1.17 |
| 1:FA:282:TYR:HE2 | 10:8M:18:UNK:CB | 1.30 | 1.17 |
| 1:FA:402:ARG:NH2 | 7:5C:1262:GLU:CD | 2.02 | 1.17 |
| 1:HA:278:ALA:CB | 10:8S:18:UNK:O | 1.92 | 1.17 |
| 2:IB:177:ASP:O | 1:IC:352:LYS:HD2 | 1.43 | 1.17 |
| 2:KB:87:PRO:HG2 | 2:LB:282:ARG:CG | 1.61 | 1.17 |
| 2:KB:158:GLU:HA | 4:2C:34:ASN:CB | 1.72 | 1.17 |
| 1:KC:88:HIS:HA | 1:LC:284:GLU:CB | 1.37 | 1.17 |
| 2:LB:340:TYR:CD1 | 4:2C:147:PHE:HB2 | 1.78 | 1.17 |
| 7:5A:1105:TYR:CB | 7:5A:1166:LEU:H | 1.56 | 1.17 |
| 7:5B:1105:TYR:CB | 7:5B:1166:LEU:H | 1.56 | 1.17 |
| 7:5C:1105:TYR:CB | 7:5C:1166:LEU:H | 1.56 | 1.17 |
| 1:DC:282:TYR:CE2 | 10:8H:18:UNK:CB | 2.26 | 1.17 |
| 2:KB:54:ALA:HB1 | 2:LB:285:THR:HG23 | 1.27 | 1.17 |
| 1:KC:88:HIS:CA | 1:LC:284:GLU:CB | 2.12 | 1.17 |
| 2:KD:221:THR:HG22 | 6:4B:261:SER:O | 1.38 | 1.17 |
| 2:LB:379:LYS:HA | 4:2C:166:ILE:CD1 | 1.59 | 1.17 |
| 2:LD:276:ARG:HH12 | 6:4B:229:GLU:CA | 1.48 | 1.17 |
| 2:CD:98:GLY:HA2 | 1:CE:254:GLU:HG2 | 1.19 | 1.17 |
| 1:EE:430:LYS:HZ1 | 7:5B:834:ASN:CG | 1.51 | 1.17 |
| 2:EF:157:GLU:OE2 | 7:5B:935:LYS:NZ | 1.75 | 1.17 |
| 2:FB:55:THR:H | 2:GB:283:ALA:HA | 1.01 | 1.17 |
| 2:FB:428:ALA:CB | 7:5C:1080:PHE:CE1 | 2.11 | 1.17 |
| 2:LD:340:TYR:CG | 4:2A:147:PHE:HB2 | 1.78 | 1.17 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:MB:212:PHE:HZ | 1:MC:326:LYS:CD | 1.55 | 1.17 |
| 7:5A:839:GLU:CG | 8:6A:107:PRO:O | 1.92 | 1.17 |
| 7:5C:1284:PHE:CZ | 9:7E:12:GLU:HB2 | 1.70 | 1.17 |
| 2:BB:179:VAL:HG21 | 1:BC:258:ASN:O | 1.45 | 1.17 |
| 1:JC:279:GLU:OE2 | 10:8Z:22:UNK:C | 1.91 | 1.17 |
| 2:KF:54:ALA:CB | 2:LF:285:THR:HG21 | 1.71 | 1.17 |
| 2:KF:273:LEU:CA | 6:4D:268:LEU:CD2 | 2.24 | 1.17 |
| 1:LE:89:PRO:CG | 1:ME:280:LYS:HD2 | 1.75 | 1.17 |
| 7:5B:1544:ILE:HG23 | 7:5B:1569:GLU:O | 1.43 | 1.17 |
| 7:5B:1552:LYS:NZ | 7:5B:1563:SER:HB2 | 0.86 | 1.17 |
| 2:BD:177:ASP:O | 1:BE:352:LYS:HD2 | 1.40 | 1.16 |
| 2:CD:397:TRP:CE3 | 1:CE:257:THR:CG2 | 2.19 | 1.16 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:HE | 1.46 | 1.16 |
| 1:FE:177:VAL:HG23 | 7:5B:915:PHE:CZ | 1.81 | 1.16 |
| 1:IC:389:SER:HB2 | 5:3C:307:LYS:CD | 1.73 | 1.16 |
| 1:JE:279:GLU:OE2 | 10:9A:22:UNK:HA | 1.41 | 1.16 |
| 2:LB:274:THR:O | 6:4A:228:LEU:CD2 | 1.92 | 1.16 |
| 7:5B:1152:GLU:OE1 | 8:6B:66:ARG:NH1 | 1.78 | 1.16 |
| 2:AD:98:GLY:HA2 | 1:AE:254:GLU:HG2 | 1.19 | 1.16 |
| 2:EB:98:GLY:CA | 1:EC:254:GLU:HG2 | 1.75 | 1.16 |
| 2:EB:125:GLU:C | 7:5C:903:PHE:CZ | 2.21 | 1.16 |
| 2:FD:54:ALA:C | 2:GD:283:ALA:HB2 | 1.68 | 1.16 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:HG3 | 1.47 | 1.16 |
| 2:IB:177:ASP:CG | 1:IC:353:VAL:HG12 | 1.66 | 1.16 |
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:CA | 1.72 | 1.16 |
| 2:JD:177:ASP:O | 1:JE:352:LYS:HD2 | 1.43 | 1.16 |
| 2:JD:397:TRP:CG | 1:JE:256:GLN:NE2 | 1.80 | 1.16 |
| 1:KA:359:PRO:HB3 | 6:4C:299:TYR:CE2 | 1.80 | 1.16 |
| 1:KE:85:GLN:OE1 | 1:LE:282:TYR:C | 1.87 | 1.16 |
| 2:LB:340:TYR:CG | 4:2C:147:PHE:CB | 2.27 | 1.16 |
| 1:LC:60:LYS:HB2 | 6:4A:101:ARG:NH1 | 1.57 | 1.16 |
| 2:LD:306:ARG:NE | 4:2A:149:ILE:CG2 | 2.05 | 1.16 |
| 7:5A:1552:LYS:NZ | 7:5A:1563:SER:HB2 | 0.85 | 1.16 |
| 7:5C:773:ARG:O | 7:5C:775:PRO:HD3 | 1.34 | 1.16 |
| 2:AD:284:LEU:HD11 | 6:4C:144:LEU:CD1 | 1.47 | 1.16 |
| 2:CB:179:VAL:HG21 | 1:CC:258:ASN:O | 1.45 | 1.16 |
| 2:KF:272:PRO:O | 6:4D:268:LEU:HD22 | 1.31 | 1.16 |
| 2:LD:179:VAL:HG21 | 1:LE:258:ASN:O | 1.44 | 1.16 |
| 7:5A:1524:PHE:CD1 | 7:5A:1567:PHE:HZ | 1.64 | 1.16 |
| 7:5B:1524:PHE:CD1 | 7:5B:1567:PHE:HZ | 1.64 | 1.16 |
| 7:5C:1552:LYS:NZ | 7:5C:1563:SER:HB2 | 0.85 | 1.16 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:177:ASP:O | 1:AC:352:LYS:HD2 | 1.43 | 1.16 |
| 2:CB:98:GLY:HA2 | 1:CC:254:GLU:HG2 | 1.26 | 1.16 |
| 2:FB:331:LEU:HD22 | 7:5C:915:PHE:CZ | 1.79 | 1.16 |
| 1:HC:278:ALA:CB | 10:8T:18:UNK:O | 1.91 | 1.16 |
| 2:KB:158:GLU:CA | 4:2C:34:ASN:HB2 | 1.70 | 1.16 |
| 2:KF:88:ASP:OD1 | 2:LF:291:GLN:OE1 | 1.64 | 1.16 |
| 2:MB:98:GLY:HA2 | 1:MC:254:GLU:HG2 | 1.16 | 1.16 |
| 7:5A:773:ARG:O | 7:5A:775:PRO:HD3 | 1.34 | 1.16 |
| 7:5C:1524:PHE:CD1 | 7:5C:1567:PHE:HZ | 1.64 | 1.16 |
| 2:AD:177:ASP:O | 1:AE:352:LYS:HD2 | 1.43 | 1.16 |
| 2:DD:179:VAL:HG21 | 1:DE:258:ASN:O | 1.42 | 1.16 |
| 2:JB:397:TRP:CG | 1:JC:256:GLN:NE2 | 1.84 | 1.16 |
| 1:JE:89:PRO:CD | 1:KE:283:HIS:CE1 | 2.22 | 1.16 |
| 2:KB:54:ALA:CB | 2:LB:285:THR:HG22 | 1.68 | 1.16 |
| 1:KC:372:MET:HB3 | 6:4A:299:TYR:CE1 | 1.57 | 1.16 |
| 7:5B:773:ARG:O | 7:5B:775:PRO:HD3 | 1.34 | 1.16 |
| 2:DD:220:PRO:O | 1:DE:324:VAL:CG1 | 1.95 | 1.15 |
| 2:FB:428:ALA:CB | 7:5C:1080:PHE:HE1 | 1.36 | 1.15 |
| 1:FE:422:ARG:NH2 | 7:5B:1170:THR:HA | 1.60 | 1.15 |
| 1:GE:56:THR:OG1 | 1:HE:284:GLU:HA | 1.41 | 1.15 |
| 1:HE:159:VAL:HG21 | 5:3A:209:ARG:CZ | 1.75 | 1.15 |
| 2:KB:217:LEU:HB3 | 6:4A:265:TYR:OH | 0.99 | 1.15 |
| 1:LA:222:PRO:HD2 | 2:LB:324:LYS:HD3 | 1.25 | 1.15 |
| 2:LB:340:TYR:CD1 | 4:2C:147:PHE:CB | 2.29 | 1.15 |
| 2:LF:296:ALA:HB3 | 4:2B:149:ILE:HG23 | 1.19 | 1.15 |
| 2:MD:179:VAL:HG21 | 1:ME:258:ASN:O | 1.46 | 1.15 |
| 6:4C:244:GLU:HG2 | 6:4C:284:LEU:CD1 | 1.75 | 1.15 |
| 7:5A:1544:ILE:HG23 | 7:5A:1569:GLU:O | 1.43 | 1.15 |
| 7:5C:1125:LEU:CD1 | 8:6C:245:GLN:OE1 | 1.94 | 1.15 |
| 9:7A:7:LEU:HD21 | 9:7B:27:GLY:O | 1.46 | 1.15 |
| 9:7C:7:LEU:HD21 | 9:7D:27:GLY:O | 1.46 | 1.15 |
| 1:FE:422:ARG:NH2 | 7:5B:1170:THR:CA | 2.06 | 1.15 |
| 2:GB:177:ASP:O | 1:GC:352:LYS:HD2 | 1.43 | 1.15 |
| 2:HD:261:PRO:CB | 5:3C:337:ARG:NH2 | 2.01 | 1.15 |
| 1:IE:434:GLU:OE1 | 5:3A:61:SER:HB3 | 1.46 | 1.15 |
| 1:JA:128:ASN:ND2 | 1:KA:285:GLN:CD | 2.03 | 1.15 |
| 6:4A:244:GLU:HG2 | 6:4A:284:LEU:CD1 | 1.75 | 1.15 |
| 7:5B:874:GLN:HB2 | 8:6B:59:LYS:NZ | 1.59 | 1.15 |
| 9:7A:11:TYR:CD1 | 9:7B:26:LEU:CD2 | 2.28 | 1.15 |
| 9:7C:11:TYR:CD1 | 9:7D:26:LEU:CD2 | 2.28 | 1.15 |
| 1:FC:422:ARG:NH2 | 7:5A:1170:THR:CA | 2.09 | 1.15 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FE:60:LYS:HD3 | 1:GE:283:HIS:HA | 1.28 | 1.15 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:C | 2.04 | 1.15 |
| 2:ID:177:ASP:CG | 1:IE:353:VAL:HG12 | 1.66 | 1.15 |
| 1:JC:279:GLU:OE2 | 10:8Z:22:UNK:O | 1.64 | 1.15 |
| 2:KB:215:LEU:CD1 | 6:4A:267:ILE:CG2 | 2.16 | 1.15 |
| 2:LD:177:ASP:CG | 1:LE:353:VAL:CG1 | 2.19 | 1.15 |
| 1:ME:279:GLU:O | 6:4B:107:MET:CG | 1.88 | 1.15 |
| 1:ME:279:GLU:OE1 | 6:4B:107:MET:N | 1.80 | 1.15 |
| 6:4B:244:GLU:HG2 | 6:4B:284:LEU:CD1 | 1.76 | 1.15 |
| 2:AD:224:ASP:OD1 | 6:4C:131:VAL:C | 1.89 | 1.15 |
| 2:AD:227:HIS:HE1 | 6:4C:135:LEU:CD1 | 1.57 | 1.15 |
| 2:CB:98:GLY:HA2 | 1:CC:254:GLU:CG | 1.76 | 1.15 |
| 2:EF:55:THR:HG23 | 2:FF:283:ALA:CA | 1.74 | 1.15 |
| 2:FB:54:ALA:CA | 2:GB:283:ALA:CB | 2.07 | 1.15 |
| 2:GD:177:ASP:O | 1:GE:352:LYS:HD2 | 1.43 | 1.15 |
| 1:HC:159:VAL:HG21 | 5:3C:209:ARG:CZ | 1.76 | 1.15 |
| 2:ID:397:TRP:CG | 1:IE:256:GLN:NE2 | 1.80 | 1.15 |
| 1:IE:402:ARG:HH22 | 7:5B:1417:GLN:C | 1.46 | 1.15 |
| 2:LF:276:ARG:NH1 | 6:4D:229:GLU:HA | 1.60 | 1.15 |
| 6:4D:244:GLU:HG2 | 6:4D:284:LEU:CD1 | 1.76 | 1.15 |
| 2:AB:98:GLY:CA | 1:AC:254:GLU:HG2 | 1.77 | 1.15 |
| 2:AD:98:GLY:CA | 1:AE:254:GLU:HG2 | 1.77 | 1.15 |
| 1:CC:370:LYS:HE2 | 10:8E:17:UNK:CB | 1.67 | 1.15 |
| 2:DD:397:TRP:CE3 | 1:DE:257:THR:CG2 | 2.24 | 1.15 |
| 1:FC:419:SER:OG | 7:5A:1256:ARG:NE | 1.79 | 1.15 |
| 2:GD:98:GLY:HA2 | 1:GE:254:GLU:HG2 | 1.19 | 1.15 |
| 2:GD:98:GLY:CA | 1:GE:254:GLU:HG2 | 1.77 | 1.15 |
| 2:LB:276:ARG:HH12 | 6:4A:229:GLU:CA | 1.53 | 1.15 |
| 2:LD:276:ARG:NH1 | 6:4B:229:GLU:HA | 1.61 | 1.15 |
| 2:MB:177:ASP:CG | 1:MC:353:VAL:HG12 | 1.70 | 1.15 |
| 1:ME:372:MET:HE3 | 6:4B:96:VAL:O | 0.97 | 1.15 |
| 2:DB:179:VAL:HG21 | 1:DC:258:ASN:O | 1.46 | 1.14 |
| 1:EC:402:ARG:NE | 7:5A:824:ARG:HH22 | 1.43 | 1.14 |
| 1:FC:177:VAL:HG23 | 7:5A:915:PHE:CZ | 1.82 | 1.14 |
| 2:GB:98:GLY:CA | 1:GC:254:GLU:HG2 | 1.77 | 1.14 |
| 2:IB:397:TRP:CG | 1:IC:256:GLN:NE2 | 1.84 | 1.14 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:C | 1.89 | 1.14 |
| 2:JB:177:ASP:O | 1:JC:352:LYS:HD2 | 1.43 | 1.14 |
| 2:KF:221:THR:HG22 | 6:4D:261:SER:O | 1.47 | 1.14 |
| 1:LA:89:PRO:HG3 | 1:MA:280:LYS:CD | 1.76 | 1.14 |
| 1:MA:372:MET:HE3 | 6:4C:96:VAL:C | 1.72 | 1.14 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5C:1544:ILE:HG23 | 7:5C:1569:GLU:O | 1.43 | 1.14 |
| 9:7E:7:LEU:CD2 | 9:7F:27:GLY:CA | 2.24 | 1.14 |
| 2:AD:356:ILE:HD12 | 6:4C:152:PHE:CE1 | 1.82 | 1.14 |
| 1:CC:60:LYS:NZ | 1:DC:283:HIS:NE2 | 1.94 | 1.14 |
| 2:DB:86:ARG:HA | 2:EB:281:TYR:CZ | 1.82 | 1.14 |
| 2:DB:98:GLY:HA2 | 1:DC:254:GLU:HG2 | 1.19 | 1.14 |
| 2:DF:86:ARG:HA | 2:EF:281:TYR:CE1 | 1.82 | 1.14 |
| 1:FA:402:ARG:NH2 | 7:5C:1262:GLU:OE2 | 1.79 | 1.14 |
| 2:IB:424:GLN:CD | 7:5C:1413:GLN:HE21 | 1.51 | 1.14 |
| 2:KB:177:ASP:CG | 1:KC:353:VAL:HG12 | 1.66 | 1.14 |
| 1:KC:359:PRO:HB3 | 6:4A:299:TYR:CE2 | 1.82 | 1.14 |
| 2:KD:217:LEU:HB3 | 6:4B:265:TYR:OH | 0.98 | 1.14 |
| 2:KD:273:LEU:CA | 6:4B:268:LEU:HD23 | 1.76 | 1.14 |
| 1:LC:89:PRO:CG | 1:MC:280:LYS:HD2 | 1.78 | 1.14 |
| 7:5A:839:GLU:OE2 | 8:6A:11:PRO:CG | 1.94 | 1.14 |
| 9:7C:15:VAL:CB | 9:7D:35:ILE:CD1 | 2.24 | 1.14 |
| 2:CB:397:TRP:CE3 | 1:CC:257:THR:CG2 | 2.18 | 1.14 |
| 2:CB:397:TRP:CE3 | 1:CC:257:THR:HG22 | 1.81 | 1.14 |
| 2:HD:98:GLY:CA | 1:HE:254:GLU:HG2 | 1.77 | 1.14 |
| 1:IA:402:ARG:HH21 | 7:5C:1417:GLN:CG | 1.50 | 1.14 |
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:HA | 1.22 | 1.14 |
| 2:JB:177:ASP:CG | 1:JC:353:VAL:HG12 | 1.66 | 1.14 |
| 2:KB:86:ARG:HG2 | 2:LB:288:GLU:OE2 | 1.48 | 1.14 |
| 2:KB:98:GLY:HA2 | 1:KC:254:GLU:HG2 | 1.18 | 1.14 |
| 2:MB:177:ASP:O | 1:MC:352:LYS:HD2 | 1.46 | 1.14 |
| 5:3B:231:THR:O | 5:3B:332:MET:CA | 1.95 | 1.14 |
| 1:DC:400:ALA:O | 7:5A:775:PRO:CB | 1.96 | 1.14 |
| 2:ED:177:ASP:OD2 | 1:EE:353:VAL:CG1 | 1.94 | 1.14 |
| 2:ED:177:ASP:O | 1:EE:352:LYS:HD2 | 1.44 | 1.14 |
| 2:ED:179:VAL:HG21 | 1:EE:258:ASN:O | 1.43 | 1.14 |
| 2:FD:428:ALA:CB | 7:5A:1080:PHE:CE1 | 2.12 | 1.14 |
| 1:FE:419:SER:CB | 7:5B:1256:ARG:HE | 1.46 | 1.14 |
| 1:IC:58:ALA:CB | 10:8Z:13:UNK:N | 2.10 | 1.14 |
| 2:JB:87:PRO:HG2 | 2:KB:277:GLY:O | 1.33 | 1.14 |
| 1:JE:89:PRO:HD3 | 1:KE:283:HIS:CE1 | 1.82 | 1.14 |
| 1:LA:60:LYS:HZ3 | 1:MA:283:HIS:CG | 1.65 | 1.14 |
| 1:LE:245:ASP:OD1 | 6:4B:216:ARG:NH2 | 1.79 | 1.14 |
| 2:EB:125:GLU:CA | 7:5C:903:PHE:CZ | 2.11 | 1.14 |
| 2:ED:220:PRO:O | 1:EE:324:VAL:CG1 | 1.96 | 1.14 |
| 2:HB:98:GLY:CA | 1:HC:254:GLU:HG2 | 1.77 | 1.14 |
| 2:ID:98:GLY:CA | 1:IE:254:GLU:HG2 | 1.77 | 1.14 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:JD:98:GLY:CA | 1:JE:254:GLU:HG2 | 1.77 | 1.14 |
| 2:KB:215:LEU:CD2 | 6:4A:267:ILE:O | 1.96 | 1.14 |
| 2:LF:276:ARG:HH12 | 6:4D:229:GLU:CA | 1.44 | 1.14 |
| 5:3A:231:THR:O | 5:3A:332:MET:CA | 1.95 | 1.14 |
| 9:7A:15:VAL:CB | 9:7B:35:ILE:CD1 | 2.24 | 1.14 |
| 2:ED:125:GLU:CA | 7:5A:903:PHE:CZ | 2.10 | 1.13 |
| 2:ID:86:ARG:CA | 2:JD:281:TYR:CE1 | 2.30 | 1.13 |
| 2:KB:77:ARG:CG | 2:LB:281:TYR:CZ | 2.29 | 1.13 |
| 2:KD:179:VAL:HG21 | 1:KE:258:ASN:O | 1.48 | 1.13 |
| 5:3C:231:THR:O | 5:3C:332:MET:CA | 1.95 | 1.13 |
| 2:BB:177:ASP:CG | 1:BC:353:VAL:HG12 | 1.60 | 1.13 |
| 2:BD:86:ARG:HA | 2:CD:281:TYR:CE1 | 1.84 | 1.13 |
| 2:CF:86:ARG:NH1 | 2:DF:281:TYR:HA | 1.63 | 1.13 |
| 1:EA:430:LYS:HZ2 | 7:5C:834:ASN:CG | 1.47 | 1.13 |
| 2:ED:98:GLY:CA | 1:EE:254:GLU:HG2 | 1.77 | 1.13 |
| 1:FC:422:ARG:NH2 | 7:5A:1170:THR:HA | 1.62 | 1.13 |
| 2:GB:55:THR:OG1 | 2:HB:282:ARG:O | 1.65 | 1.13 |
| 2:GD:179:VAL:HG21 | 1:GE:258:ASN:O | 1.48 | 1.13 |
| 2:HB:177:ASP:CG | 1:HC:353:VAL:HG12 | 1.66 | 1.13 |
| 2:ID:179:VAL:HG21 | 1:IE:258:ASN:O | 1.48 | 1.13 |
| 2:JB:98:GLY:CA | 1:JC:254:GLU:HG2 | 1.77 | 1.13 |
| 2:AB:98:GLY:HA2 | 1:AC:254:GLU:HG2 | 1.18 | 1.13 |
| 2:AD:177:ASP:CG | 1:AE:353:VAL:HG12 | 1.66 | 1.13 |
| 2:AD:223:GLY:CA | 6:4C:131:VAL:HB | 1.77 | 1.13 |
| 2:AF:224:ASP:OD1 | 6:4A:132:LYS:N | 1.80 | 1.13 |
| 2:CB:87:PRO:HD2 | 2:DB:281:TYR:CE2 | 1.84 | 1.13 |
| 2:EB:177:ASP:O | 1:EC:352:LYS:HD2 | 1.48 | 1.13 |
| 2:HD:177:ASP:CG | 1:HE:353:VAL:HG12 | 1.66 | 1.13 |
| 2:IB:98:GLY:CA | 1:IC:254:GLU:HG2 | 1.77 | 1.13 |
| 2:JF:86:ARG:CZ | 2:KF:280:GLN:HB3 | 1.70 | 1.13 |
| 2:KB:98:GLY:CA | 1:KC:254:GLU:HG2 | 1.77 | 1.13 |
| 2:KD:177:ASP:CG | 1:KE:353:VAL:HG12 | 1.66 | 1.13 |
| 2:LD:306:ARG:NH1 | 4:2A:151:VAL:CG2 | 2.12 | 1.13 |
| 2:LF:55:THR:CG2 | 2:MF:283:ALA:CA | 2.06 | 1.13 |
| 1:FA:177:VAL:HG23 | 7:5C:915:PHE:CZ | 1.84 | 1.13 |
| 2:FD:55:THR:N | 2:GD:283:ALA:HB2 | 1.62 | 1.13 |
| 2:FD:331:LEU:HD22 | 7:5A:915:PHE:CZ | 1.84 | 1.13 |
| 2:IF:86:ARG:CA | 2:JF:281:TYR:CE1 | 2.31 | 1.13 |
| 1:JA:91:GLN:N | 1:KA:280:LYS:NZ | 1.93 | 1.13 |
| 2:JD:177:ASP:CG | 1:JE:353:VAL:HG12 | 1.66 | 1.13 |
| 2:LB:177:ASP:OD2 | 1:LC:248:LEU:CD2 | 1.97 | 1.13 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MB:179:VAL:HG21 | 1:MC:258:ASN:O | 1.48 | 1.13 |
| 7:5A:1091:LYS:O | 7:5A:1095:GLU:CG | 1.96 | 1.13 |
| 7:5B:1091:LYS:O | 7:5B:1095:GLU:CG | 1.96 | 1.13 |
| 7:5C:1091:LYS:O | 7:5C:1095:GLU:CG | 1.96 | 1.13 |
| 2:AB:177:ASP:CG | 1:AC:353:VAL:HG12 | 1.66 | 1.12 |
| 2:DD:177:ASP:OD2 | 1:DE:353:VAL:HG13 | 1.49 | 1.12 |
| 2:EB:220:PRO:O | 1:EC:324:VAL:CG1 | 1.98 | 1.12 |
| 2:GD:177:ASP:CG | 1:GE:353:VAL:HG12 | 1.66 | 1.12 |
| 1:KC:85:GLN:OE1 | 1:LC:282:TYR:HB2 | 1.45 | 1.13 |
| 2:KD:87:PRO:HG2 | 2:LD:282:ARG:CG | 1.77 | 1.13 |
| 1:LC:89:PRO:HG3 | 1:MC:280:LYS:CE | 1.78 | 1.12 |
| 1:MA:279:GLU:O | 6:4C:107:MET:CG | 1.90 | 1.13 |
| 2:JF:88:ASP:CB | 2:KF:278:SER:OG | 1.95 | 1.12 |
| 2:LF:306:ARG:CZ | 4:2B:151:VAL:CG2 | 2.27 | 1.12 |
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:N | 1.82 | 1.12 |
| 6:4C:264:GLY:O | 6:4C:273:ARG:HB2 | 1.43 | 1.12 |
| 7:5B:1284:PHE:CZ | 9:7C:12:GLU:HB2 | 1.74 | 1.13 |
| 9:7C:7:LEU:HD21 | 9:7D:27:GLY:C | 1.72 | 1.13 |
| 1:ME:372:MET:HE3 | 6:4B:96:VAL:C | 1.73 | 1.12 |
| 2:AB:397:TRP:CG | 1:AC:256:GLN:NE2 | 1.84 | 1.12 |
| 1:FC:60:LYS:HD3 | 1:GC:283:HIS:CA | 1.78 | 1.12 |
| 1:HC:415:GLU:CG | 5:3C:235:LEU:HB2 | 1.79 | 1.12 |
| 1:LE:89:PRO:HG3 | 1:ME:280:LYS:CD | 1.78 | 1.12 |
| 6:4A:264:GLY:O | 6:4A:273:ARG:HB2 | 1.43 | 1.12 |
| 7:5B:1499:LYS:CE | 7:5B:1513:ASP:O | 1.96 | 1.12 |
| 2:AD:397:TRP:CG | 1:AE:256:GLN:NE2 | 1.80 | 1.12 |
| 1:AE:342:GLN:HE22 | 3:1A:55:HIS:CD2 | 1.66 | 1.12 |
| 2:CD:87:PRO:HD2 | 2:DD:281:TYR:CE2 | 1.85 | 1.12 |
| 1:DE:400:ALA:O | 7:5B:775:PRO:HB2 | 1.34 | 1.12 |
| 2:GB:177:ASP:CG | 1:GC:353:VAL:HG12 | 1.66 | 1.12 |
| 2:KD:54:ALA:CB | 2:LD:285:THR:HG21 | 1.67 | 1.12 |
| 2:KD:98:GLY:CA | 1:KE:254:GLU:HG2 | 1.77 | 1.12 |
| 2:LB:77:ARG:NH1 | 6:4A:204:ARG:HH21 | 1.33 | 1.12 |
| 2:LB:177:ASP:CG | 1:LC:353:VAL:HG12 | 1.71 | 1.12 |
| 2:LB:296:ALA:CB | 4:2C:149:ILE:HG23 | 1.55 | 1.12 |
| 2:MD:98:GLY:HA2 | 1:ME:254:GLU:HG2 | 1.21 | 1.12 |
| 7:5A:1499:LYS:CE | 7:5A:1513:ASP:O | 1.96 | 1.12 |
| 2:AD:217:LEU:HD22 | 6:4C:132:LYS:HG2 | 1.30 | 1.12 |
| 2:AD:223:GLY:HA3 | 6:4C:131:VAL:HB | 1.31 | 1.12 |
| 2:DB:220:PRO:O | 1:DC:324:VAL:CG1 | 1.98 | 1.12 |
| 1:DC:402:ARG:NH2 | 7:5A:777:ALA:HB3 | 1.64 | 1.12 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:FD:177:ASP:CG | 1:FE:353:VAL:HG12 | 1.60 | 1.12 |
| 1:HE:415:GLU:CG | 5:3A:235:LEU:HB2 | 1.78 | 1.12 |
| 1:IA:402:ARG:NE | 7:5C:1417:GLN:HG3 | 1.65 | 1.12 |
| 1:JC:89:PRO:CB | 1:KC:280:LYS:CG | 2.04 | 1.12 |
| 2:KD:98:GLY:HA2 | 1:KE:254:GLU:HG2 | 1.19 | 1.12 |
| 2:MD:106:TYR:CE1 | 3:1B:32:ARG:NH1 | 2.18 | 1.12 |
| 7:5C:1499:LYS:CE | 7:5C:1513:ASP:O | 1.96 | 1.12 |
| 2:AF:40:SER:OG | 6:4A:152:PHE:CE2 | 2.00 | 1.12 |
| 2:DD:85:PHE:C | 2:ED:281:TYR:OH | 1.92 | 1.12 |
| 2:EB:397:TRP:CG | 1:EC:256:GLN:NE2 | 1.96 | 1.12 |
| 2:HD:98:GLY:HA2 | 1:HE:254:GLU:HG2 | 1.19 | 1.12 |
| 2:KF:77:ARG:CG | 2:LF:281:TYR:CZ | 2.33 | 1.12 |
| 2:KF:215:LEU:HD22 | 6:4D:267:ILE:O | 1.49 | 1.12 |
| 1:LC:60:LYS:HZ3 | 1:MC:283:HIS:CG | 1.66 | 1.12 |
| 2:LD:306:ARG:HE | 4:2A:149:ILE:HG22 | 0.95 | 1.12 |
| 1:ME:76:ASP:OD1 | 2:MF:46:ARG:NH2 | 1.81 | 1.12 |
| 6:4B:264:GLY:O | 6:4B:273:ARG:HB2 | 1.43 | 1.12 |
| 6:4D:264:GLY:O | 6:4D:273:ARG:HB2 | 1.43 | 1.12 |
| 2:AD:179:VAL:HG21 | 1:AE:258:ASN:O | 1.48 | 1.11 |
| 2:DD:98:GLY:HA2 | 1:DE:254:GLU:HG2 | 1.22 | 1.11 |
| 2:FB:177:ASP:OD1 | 1:FC:353:VAL:HG11 | 1.50 | 1.11 |
| 1:IA:58:ALA:CB | 10:8Y:13:UNK:CB | 2.26 | 1.11 |
| 2:JD:86:ARG:CZ | 2:KD:280:GLN:HB2 | 1.77 | 1.11 |
| 2:KD:77:ARG:CG | 2:LD:281:TYR:CZ | 2.31 | 1.11 |
| 2:MD:106:TYR:CZ | 3:1B:32:ARG:NH1 | 2.18 | 1.11 |
| 7:5A:1284:PHE:CZ | 9:7A:12:GLU:HB2 | 1.72 | 1.11 |
| 2:BF:86:ARG:HA | 2:CF:281:TYR:CE1 | 1.85 | 1.11 |
| 2:DD:177:ASP:OD2 | 1:DE:353:VAL:CG1 | 1.95 | 1.11 |
| 2:GB:98:GLY:HA2 | 1:GC:254:GLU:HG2 | 1.18 | 1.11 |
| 2:HD:179:VAL:HG21 | 1:HE:258:ASN:O | 1.48 | 1.11 |
| 2:IB:179:VAL:HG21 | 1:IC:258:ASN:O | 1.50 | 1.11 |
| 1:IC:402:ARG:CZ | 7:5A:1417:GLN:HG3 | 1.80 | 1.11 |
| 1:KA:62:VAL:HG22 | 1:LA:285:GLN:HB3 | 1.16 | 1.11 |
| 2:KB:77:ARG:HG2 | 2:LB:281:TYR:CE1 | 1.85 | 1.11 |
| 2:KB:179:VAL:HG21 | 1:KC:258:ASN:O | 1.51 | 1.11 |
| 2:KF:55:THR:HG21 | 2:LF:363:MET:HE1 | 1.12 | 1.11 |
| 2:LF:416:ASN:O | 4:2B:168:LEU:HD11 | 1.50 | 1.11 |
| 7:5B:1491:LEU:CD2 | 7:5B:1495:PHE:CD1 | 2.32 | 1.11 |
| 7:5B:1530:ILE:HD13 | 7:5B:1571:MET:CE | 1.78 | 1.11 |
| 7:5C:1530:ILE:HD13 | 7:5C:1571:MET:CE | 1.78 | 1.11 |
| 9:7A:11:TYR:CE1 | 9:7B:26:LEU:CD2 | 2.34 | 1.11 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AD:223:GLY:C | 6:4C:131:VAL:HB | 1.74 | 1.11 |
| 2:BB:397:TRP:CG | 1:BC:256:GLN:HE22 | 1.41 | 1.11 |
| 1:CA:370:LYS:HE2 | 10:8D:17:UNK:CB | 1.72 | 1.11 |
| 2:EB:177:ASP:OD2 | 1:EC:353:VAL:CG1 | 1.98 | 1.11 |
| 1:EC:398:MET:SD | 2:ED:345:ILE:HG13 | 1.91 | 1.11 |
| 2:FB:177:ASP:CG | 1:FC:353:VAL:HG12 | 1.69 | 1.11 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:HG2 | 1.55 | 1.11 |
| 2:LB:55:THR:CG2 | 2:MB:283:ALA:CA | 2.02 | 1.11 |
| 7:5A:1530:ILE:HD13 | 7:5A:1571:MET:CE | 1.78 | 1.11 |
| 7:5B:1491:LEU:HA | 7:5B:1495:PHE:HB3 | 1.23 | 1.11 |
| 9:7C:15:VAL:HA | 9:7D:35:ILE:HD12 | 1.32 | 1.11 |
| 2:CD:179:VAL:HG21 | 1:CE:258:ASN:O | 1.49 | 1.11 |
| 2:EB:55:THR:HG23 | 2:FB:283:ALA:HA | 1.14 | 1.11 |
| 2:FD:54:ALA:HA | 2:GD:283:ALA:HB2 | 1.23 | 1.11 |
| 2:FD:98:GLY:HA2 | 1:FE:254:GLU:HG3 | 1.33 | 1.11 |
| 2:GB:86:ARG:NH2 | 2:HB:281:TYR:CD2 | 1.86 | 1.11 |
| 2:GB:179:VAL:HG21 | 1:GC:258:ASN:O | 1.51 | 1.11 |
| 1:HE:278:ALA:CB | 10:8U:22:UNK:N | 2.11 | 1.11 |
| 2:JD:98:GLY:HA2 | 1:JE:254:GLU:HG2 | 1.19 | 1.11 |
| 2:KD:215:LEU:HD13 | 6:4B:267:ILE:CG2 | 1.81 | 1.11 |
| 7:5A:1491:LEU:CD2 | 7:5A:1495:PHE:CD1 | 2.32 | 1.11 |
| 9:7A:7:LEU:HD21 | 9:7B:27:GLY:C | 1.72 | 1.11 |
| 9:7E:12:GLU:O | 9:7E:16:THR:OG1 | 1.69 | 1.11 |
| 2:AF:217:LEU:CD2 | 6:4A:132:LYS:HG2 | 1.81 | 1.11 |
| 1:FA:398:MET:SD | 2:FB:345:ILE:HG13 | 1.91 | 1.11 |
| 1:HC:415:GLU:HG2 | 5:3C:235:LEU:CB | 1.81 | 1.11 |
| 1:HE:415:GLU:HG2 | 5:3A:235:LEU:CB | 1.81 | 1.11 |
| 2:KB:83:GLN:NE2 | 2:LB:281:TYR:CE2 | 2.03 | 1.11 |
| 2:KB:273:LEU:CA | 6:4A:268:LEU:HD21 | 1.73 | 1.11 |
| 2:LD:177:ASP:OD2 | 1:LE:248:LEU:HD21 | 1.47 | 1.11 |
| 1:LE:222:PRO:CG | 2:LF:324:LYS:HD3 | 1.80 | 1.11 |
| 2:DB:177:ASP:OD2 | 1:DC:353:VAL:HG13 | 1.51 | 1.10 |
| 1:IA:279:GLU:OE2 | 10:8V:22:UNK:C | 1.99 | 1.10 |
| 1:IE:278:ALA:HB1 | 10:8X:18:UNK:O | 1.50 | 1.10 |
| 2:JF:86:ARG:NH1 | 2:KF:280:GLN:HB3 | 1.64 | 1.10 |
| 1:MA:372:MET:HE3 | 6:4C:96:VAL:O | 0.93 | 1.10 |
| 7:5A:1491:LEU:HA | 7:5A:1495:PHE:HB3 | 1.23 | 1.10 |
| 7:5B:839:GLU:OE2 | 8:6B:11:PRO:CG | 1.99 | 1.10 |
| 7:5C:829:GLY:O | 8:6C:110:ASN:ND2 | 1.84 | 1.10 |
| 7:5C:1491:LEU:CD2 | 7:5C:1495:PHE:CD1 | 2.32 | 1.10 |
| 2:AD:362:LYS:HG2 | 6:4C:146:ILE:HB | 1.25 | 1.10 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:FD:55:THR:HG21 | 2:GD:284:LEU:H | 1.07 | 1.10 |
| 2:HD:397:TRP:CG | 1:HE:256:GLN:NE2 | 1.80 | 1.10 |
| 1:IC:402:ARG:NH2 | 7:5A:1418:GLN:N | 1.98 | 1.10 |
| 2:JD:179:VAL:HG21 | 1:JE:258:ASN:O | 1.48 | 1.10 |
| 1:KC:79:ARG:O | 1:LC:280:LYS:HE2 | 1.45 | 1.10 |
| 9:7C:12:GLU:O | 9:7C:16:THR:OG1 | 1.69 | 1.10 |
| 1:EC:430:LYS:HZ2 | 7:5A:834:ASN:CG | 1.57 | 1.10 |
| 2:ED:125:GLU:O | 7:5A:903:PHE:HZ | 1.05 | 1.10 |
| 1:FA:422:ARG:NH2 | 7:5C:1170:THR:CA | 2.13 | 1.10 |
| 2:FD:177:ASP:OD1 | 1:FE:353:VAL:HG11 | 1.51 | 1.10 |
| 2:HB:397:TRP:CG | 1:HC:256:GLN:NE2 | 1.84 | 1.10 |
| 1:IC:58:ALA:HB2 | 10:8Z:13:UNK:N | 1.66 | 1.10 |
| 2:KD:276:ARG:HH21 | 6:4B:265:TYR:CA | 1.63 | 1.10 |
| 2:LB:331:LEU:CG | 4:2C:42:PHE:HZ | 1.62 | 1.10 |
| 1:LC:89:PRO:HG3 | 1:MC:280:LYS:CD | 1.82 | 1.10 |
| 2:LD:296:ALA:CB | 4:2A:149:ILE:HG23 | 1.55 | 1.10 |
| 9:7C:11:TYR:CE1 | 9:7D:26:LEU:CD2 | 2.34 | 1.10 |
| 1:EC:423:GLU:OE2 | 7:5A:830:VAL:HG12 | 0.94 | 1.10 |
| 1:EC:423:GLU:CD | 7:5A:830:VAL:HG12 | 1.76 | 1.10 |
| 1:EE:423:GLU:OE2 | 7:5B:830:VAL:HG12 | 0.94 | 1.10 |
| 1:FE:402:ARG:CZ | 7:5B:1262:GLU:OE2 | 1.99 | 1.10 |
| 1:HE:415:GLU:HG2 | 5:3A:235:LEU:HB2 | 1.28 | 1.10 |
| 1:IC:402:ARG:HH21 | 7:5A:1417:GLN:CG | 1.62 | 1.10 |
| 2:KF:158:GLU:O | 4:2B:34:ASN:O | 1.69 | 1.10 |
| 9:7C:14:SER:C | 9:7D:35:ILE:HD11 | 1.77 | 1.10 |
| 9:7E:7:LEU:HD22 | 9:7F:27:GLY:HA3 | 1.12 | 1.10 |
| 2:BD:98:GLY:HA2 | 1:BE:254:GLU:HG2 | 1.19 | 1.10 |
| 2:DB:177:ASP:OD2 | 1:DC:353:VAL:CG1 | 1.98 | 1.10 |
| 2:DF:85:PHE:O | 2:EF:281:TYR:OH | 1.67 | 1.10 |
| 2:EB:125:GLU:O | 7:5C:903:PHE:HZ | 1.17 | 1.10 |
| 2:ED:55:THR:HG23 | 2:FD:283:ALA:HA | 1.17 | 1.10 |
| 1:IC:282:TYR:CE2 | 10:8W:15:UNK:O | 2.03 | 1.10 |
| 2:ID:98:GLY:HA2 | 1:IE:254:GLU:HG2 | 1.19 | 1.10 |
| 1:MA:76:ASP:OD1 | 2:MB:46:ARG:NH2 | 1.82 | 1.10 |
| 4:2B:172:ASP:HB2 | 4:2B:173:PRO:HD2 | 1.14 | 1.10 |
| 6:4D:221:MET:SD | 6:4D:222:PRO:CD | 2.38 | 1.10 |
| 7:5C:1491:LEU:HA | 7:5C:1495:PHE:HB3 | 1.23 | 1.10 |
| 9:7D:12:GLU:CA | 9:7D:16:THR:OG1 | 2.00 | 1.10 |
| 1:AE:283:HIS:O | 2:MB:54:ALA:CB | 1.98 | 1.09 |
| 2:BB:98:GLY:HA2 | 1:BC:254:GLU:HG2 | 1.24 | 1.09 |
| 2:GB:55:THR:CG2 | 2:HB:283:ALA:CB | 2.17 | 1.09 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HC:278:ALA:HB3 | 10:8T:22:UNK:N | 1.67 | 1.09 |
| 2:IB:98:GLY:HA2 | 1:IC:254:GLU:HG2 | 1.19 | 1.09 |
| 1:JC:89:PRO:HG2 | 1:KC:280:LYS:HA | 1.12 | 1.09 |
| 1:JE:279:GLU:OE2 | 10:9A:22:UNK:CA | 1.99 | 1.09 |
| 2:LB:276:ARG:NH1 | 6:4A:229:GLU:HA | 1.64 | 1.09 |
| 6:4B:221:MET:SD | 6:4B:222:PRO:CD | 2.38 | 1.09 |
| 7:5B:1484:TYR:CA | 7:5B:1487:ASN:HB2 | 1.82 | 1.09 |
| 9:7A:14:SER:C | 9:7B:35:ILE:HD11 | 1.77 | 1.09 |
| 2:AB:179:VAL:HG21 | 1:AC:258:ASN:O | 1.51 | 1.09 |
| 2:BD:397:TRP:CG | 1:BE:256:GLN:HE22 | 1.45 | 1.09 |
| 1:EA:282:TYR:HE2 | 10:8J:18:UNK:CB | 1.55 | 1.09 |
| 2:ED:125:GLU:C | 7:5A:903:PHE:CE2 | 2.29 | 1.09 |
| 1:FC:60:LYS:CD | 1:GC:283:HIS:HA | 1.82 | 1.09 |
| 4:2C:172:ASP:HB2 | 4:2C:173:PRO:HD2 | 1.15 | 1.09 |
| 6:4C:221:MET:SD | 6:4C:222:PRO:CD | 2.38 | 1.09 |
| 7:5A:1484:TYR:CA | 7:5A:1487:ASN:HB2 | 1.82 | 1.09 |
| 7:5C:1484:TYR:CA | 7:5C:1487:ASN:HB2 | 1.82 | 1.09 |
| 9:7F:12:GLU:CA | 9:7F:16:THR:OG1 | 2.00 | 1.09 |
| 2:AF:356:ILE:HD12 | 6:4A:152:PHE:CE1 | 1.86 | 1.09 |
| 2:BD:98:GLY:CA | 1:BE:254:GLU:HG2 | 1.82 | 1.09 |
| 1:CA:60:LYS:NZ | 1:DA:283:HIS:NE2 | 2.01 | 1.09 |
| 2:EB:125:GLU:HG2 | 7:5C:903:PHE:CD2 | 1.88 | 1.09 |
| 2:ED:177:ASP:OD2 | 1:EE:353:VAL:HG13 | 1.48 | 1.09 |
| 2:GB:412:GLU:OE2 | 7:5C:1323:MET:CE | 1.99 | 1.09 |
| 2:HB:179:VAL:HG21 | 1:HC:258:ASN:O | 1.51 | 1.09 |
| 2:KB:54:ALA:HB1 | 2:LB:285:THR:HG22 | 1.18 | 1.09 |
| 2:KB:54:ALA:HB2 | 2:LB:285:THR:HG21 | 1.10 | 1.09 |
| 4:2A:172:ASP:HB2 | 4:2A:173:PRO:HD2 | 1.14 | 1.09 |
| 6:4A:221:MET:SD | 6:4A:222:PRO:CD | 2.38 | 1.09 |
| 7:5B:1552:LYS:HZ3 | 7:5B:1563:SER:CB | 1.53 | 1.09 |
| 9:7A:12:GLU:O | 9:7A:16:THR:OG1 | 1.69 | 1.09 |
| 9:7B:12:GLU:CA | 9:7B:16:THR:OG1 | 2.00 | 1.09 |
| 9:7C:7:LEU:CD2 | 9:7D:27:GLY:HA2 | 1.60 | 1.09 |
| 1:CC:282:TYR:CD2 | 10:8E:18:UNK:CB | 2.35 | 1.09 |
| 2:DD:86:ARG:HA | 2:ED:281:TYR:CZ | 1.87 | 1.09 |
| 2:FB:98:GLY:HA2 | 1:FC:254:GLU:HG3 | 1.28 | 1.09 |
| 2:GF:405:GLU:OE2 | 7:5B:1337:ASP:OD2 | 1.70 | 1.09 |
| 1:IC:389:SER:HB2 | 5:3C:307:LYS:HD3 | 1.10 | 1.09 |
| 2:KD:77:ARG:HG2 | 2:LD:281:TYR:CE1 | 1.86 | 1.09 |
| 2:KF:125:GLU:OE1 | 2:LF:332:ASN:ND2 | 1.86 | 1.09 |
| 2:LF:416:ASN:C | 4:2B:168:LEU:CD1 | 2.19 | 1.09 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:4D:244:GLU:HG2 | 6:4D:284:LEU:HD11 | 1.19 | 1.09 |
| 9:7C:15:VAL:CB | 9:7D:35:ILE:HD13 | 1.83 | 1.09 |
| 1:DC:414:GLU:OE2 | 7:5A:789:LYS:HE3 | 1.52 | 1.09 |
| 2:FD:179:VAL:HG21 | 1:FE:258:ASN:O | 1.48 | 1.09 |
| 1:HE:420:GLU:OE1 | 5:3A:215:TYR:CZ | 2.06 | 1.09 |
| 2:KB:276:ARG:NH2 | 6:4A:265:TYR:HA | 1.67 | 1.09 |
| 2:KB:276:ARG:HH21 | 6:4A:265:TYR:HA | 0.92 | 1.09 |
| 1:LC:407:TRP:CH2 | 2:LD:254:ALA:O | 2.05 | 1.09 |
| 7:5B:1490:LYS:C | 7:5B:1495:PHE:CB | 2.26 | 1.09 |
| 9:7A:7:LEU:CD2 | 9:7B:27:GLY:HA3 | 1.57 | 1.09 |
| 1:AE:285:GLN:HA | 2:MB:55:THR:CG2 | 1.81 | 1.08 |
| 2:FB:98:GLY:C | 1:FC:254:GLU:HG2 | 1.78 | 1.08 |
| 1:HE:159:VAL:HG22 | 5:3A:209:ARG:NH2 | 1.67 | 1.08 |
| 2:KB:273:LEU:CG | 6:4A:268:LEU:HD21 | 1.80 | 1.08 |
| 1:KE:372:MET:HB3 | 6:4B:299:TYR:CE1 | 1.83 | 1.08 |
| 2:LB:98:GLY:HA2 | 1:LC:254:GLU:HG2 | 1.35 | 1.08 |
| 2:LB:177:ASP:OD1 | 1:LC:353:VAL:CG1 | 1.99 | 1.08 |
| 1:LC:222:PRO:HD2 | 2:LD:324:LYS:HD3 | 1.31 | 1.08 |
| 7:5C:1284:PHE:CE2 | 9:7E:12:GLU:HB3 | 1.88 | 1.08 |
| 2:HB:98:GLY:HA2 | 1:HC:254:GLU:HG2 | 1.19 | 1.08 |
| 2:JB:98:GLY:HA2 | 1:JC:254:GLU:HG2 | 1.19 | 1.08 |
| 2:JB:179:VAL:HG21 | 1:JC:258:ASN:O | 1.50 | 1.08 |
| 2:KF:87:PRO:HG3 | 2:LF:282:ARG:HG3 | 1.12 | 1.08 |
| 1:LA:221:ARG:NH1 | 2:LB:323:THR:C | 2.11 | 1.08 |
| 2:MD:397:TRP:CG | 1:ME:256:GLN:NE2 | 1.90 | 1.08 |
| 6:4B:244:GLU:HG2 | 6:4B:284:LEU:HD11 | 1.18 | 1.08 |
| 7:5A:1490:LYS:C | 7:5A:1495:PHE:CB | 2.26 | 1.08 |
| 7:5B:826:LEU:HD23 | 7:5B:840:GLY:HA2 | 1.24 | 1.08 |
| 9:7A:15:VAL:HA | 9:7B:35:ILE:HD12 | 1.31 | 1.08 |
| 2:FD:54:ALA:HA | 2:GD:283:ALA:CB | 1.84 | 1.08 |
| 2:LD:397:TRP:CE3 | 1:LE:257:THR:HG22 | 1.87 | 1.08 |
| 7:5A:1533:GLU:HB3 | 7:5A:1581:ILE:HG21 | 1.34 | 1.08 |
| 7:5B:1533:GLU:HB3 | 7:5B:1581:ILE:HG21 | 1.34 | 1.08 |
| 2:DF:54:ALA:HA | 2:EF:283:ALA:HB2 | 1.36 | 1.08 |
| 2:ED:157:GLU:CD | 7:5A:935:LYS:NZ | 2.11 | 1.08 |
| 1:FA:422:ARG:NH2 | 7:5C:1170:THR:HA | 1.68 | 1.08 |
| 2:KF:276:ARG:NH2 | 6:4D:271:GLU:O | 1.87 | 1.08 |
| 2:LB:177:ASP:OD2 | 1:LC:248:LEU:HD21 | 1.51 | 1.08 |
| 1:MC:76:ASP:OD1 | 2:MD:46:ARG:NH2 | 1.84 | 1.08 |
| 6:4C:244:GLU:HG2 | 6:4C:284:LEU:HD11 | 1.18 | 1.08 |
| 7:5A:826:LEU:HD23 | 7:5A:840:GLY:HA2 | 1.24 | 1.08 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5C:826:LEU:HD23 | 7:5C:840:GLY:HA2 | 1.24 | 1.08 |
| 7:5C:1490:LYS:C | 7:5C:1495:PHE:CB | 2.26 | 1.08 |
| 2:BB:86:ARG:HA | 2:CB:281:TYR:CE1 | 1.89 | 1.08 |
| 2:CF:87:PRO:HD2 | 2:DF:281:TYR:CE2 | 1.89 | 1.08 |
| 1:GE:402:ARG:HD2 | 5:3A:381:ASN:ND2 | 1.68 | 1.08 |
| 1:HE:278:ALA:HB3 | 10:8U:22:UNK:CA | 1.83 | 1.08 |
| 2:HF:261:PRO:CB | 5:3A:337:ARG:NH2 | 2.06 | 1.08 |
| 2:LD:397:TRP:CE3 | 1:LE:257:THR:CG2 | 2.26 | 1.08 |
| 1:MA:283:HIS:CD2 | 6:4C:101:ARG:HH22 | 1.72 | 1.08 |
| 6:4A:244:GLU:HG2 | 6:4A:284:LEU:HD11 | 1.18 | 1.08 |
| 7:5B:1544:ILE:HD12 | 7:5B:1574:ILE:CG1 | 1.81 | 1.08 |
| 7:5C:1533:GLU:HB3 | 7:5C:1581:ILE:HG21 | 1.34 | 1.08 |
| 2:AF:361:LEU:HD22 | 6:4A:144:LEU:CD1 | 1.83 | 1.07 |
| 2:BD:177:ASP:OD2 | 1:BE:353:VAL:HG13 | 1.54 | 1.07 |
| 2:CB:220:PRO:O | 1:CC:324:VAL:CG1 | 2.01 | 1.07 |
| 2:EB:179:VAL:HG21 | 1:EC:258:ASN:O | 1.50 | 1.07 |
| 1:EE:398:MET:SD | 2:EF:345:ILE:HG13 | 1.94 | 1.07 |
| 2:GB:55:THR:HG21 | 2:HB:283:ALA:HA | 1.33 | 1.07 |
| 2:LB:379:LYS:HG2 | 4:2C:166:ILE:HD12 | 1.30 | 1.07 |
| 2:LB:397:TRP:CE3 | 1:LC:257:THR:HG22 | 1.88 | 1.07 |
| 2:LF:296:ALA:HB2 | 4:2B:149:ILE:CG2 | 1.70 | 1.07 |
| 7:5C:1547:SER:O | 7:5C:1569:GLU:OE1 | 1.70 | 1.07 |
| 2:DB:397:TRP:CE3 | 1:DC:257:THR:HG22 | 1.85 | 1.07 |
| 2:EB:177:ASP:OD2 | 1:EC:353:VAL:HG13 | 1.51 | 1.07 |
| 1:FA:419:SER:OG | 7:5C:1256:ARG:CZ | 2.01 | 1.07 |
| 2:KF:215:LEU:HD13 | 6:4D:267:ILE:HG22 | 1.13 | 1.07 |
| 2:LB:306:ARG:NH1 | 4:2C:151:VAL:HG23 | 1.56 | 1.07 |
| 2:LD:340:TYR:CD1 | 4:2A:147:PHE:HB2 | 1.90 | 1.07 |
| 7:5A:1284:PHE:CE2 | 9:7A:12:GLU:HB3 | 1.88 | 1.07 |
| 7:5A:1481:GLN:O | 7:5A:1485:LYS:N | 1.86 | 1.07 |
| 7:5A:1544:ILE:HD12 | 7:5A:1574:ILE:CG1 | 1.81 | 1.07 |
| 7:5A:1547:SER:O | 7:5A:1569:GLU:OE1 | 1.70 | 1.07 |
| 7:5B:1284:PHE:CE2 | 9:7C:12:GLU:HB3 | 1.90 | 1.07 |
| 7:5B:1481:GLN:O | 7:5B:1485:LYS:N | 1.86 | 1.07 |
| 7:5C:1481:GLN:O | 7:5C:1485:LYS:N | 1.86 | 1.07 |
| 7:5C:1490:LYS:HG3 | 7:5C:1494:LEU:HD23 | 1.22 | 1.07 |
| 7:5C:1565:GLU:HB2 | 7:5C:1568:LYS:HB2 | 1.11 | 1.07 |
| 9:7A:14:SER:O | 9:7B:35:ILE:HD11 | 1.52 | 1.07 |
| 9:7E:11:TYR:OH | 9:7F:23:LEU:O | 1.72 | 1.07 |
| 1:DC:400:ALA:O | 7:5A:775:PRO:HB2 | 1.51 | 1.07 |
| 2:DD:397:TRP:CE3 | 1:DE:257:THR:HG22 | 1.88 | 1.07 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:ED:54:ALA:HA | 2:FD:283:ALA:HB2 | 1.31 | 1.07 |
| 2:ED:98:GLY:HA2 | 1:EE:254:GLU:HG2 | 1.14 | 1.07 |
| 1:HC:282:TYR:CE2 | 10:8T:19:UNK:N | 2.22 | 1.07 |
| 1:JE:279:GLU:CD | 10:9A:22:UNK:CA | 2.25 | 1.07 |
| 2:LD:177:ASP:CG | 1:LE:353:VAL:HG12 | 1.79 | 1.07 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:HZ3 | 1.47 | 1.07 |
| 7:5A:1565:GLU:HB2 | 7:5A:1568:LYS:HB2 | 1.11 | 1.07 |
| 7:5B:1547:SER:O | 7:5B:1569:GLU:OE1 | 1.70 | 1.07 |
| 7:5B:1565:GLU:HB2 | 7:5B:1568:LYS:HB2 | 1.11 | 1.07 |
| 7:5C:829:GLY:HA2 | 8:6C:109:ILE:HG21 | 1.29 | 1.07 |
| 7:5C:1544:ILE:HD12 | 7:5C:1574:ILE:CG1 | 1.81 | 1.07 |
| 7:5C:1548:VAL:CG1 | 7:5C:1565:GLU:O | 2.02 | 1.07 |
| 9:7E:11:TYR:CE1 | 9:7F:26:LEU:HB3 | 1.89 | 1.07 |
| 2:CD:397:TRP:CE3 | 1:CE:257:THR:HG22 | 1.83 | 1.07 |
| 1:EA:396:ASP:HB2 | 7:5C:817:LEU:CD2 | 1.78 | 1.07 |
| 1:GE:56:THR:HG1 | 1:HE:284:GLU:HA | 1.04 | 1.07 |
| 1:GE:409:VAL:HG11 | 5:3A:383:GLU:OE2 | 0.90 | 1.07 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:HG3 | 1.65 | 1.07 |
| 1:LE:101:ASN:HD21 | 2:LF:252:LYS:HD2 | 0.91 | 1.07 |
| 1:MC:279:GLU:O | 6:4A:107:MET:CG | 1.97 | 1.07 |
| 7:5A:1490:LYS:HG3 | 7:5A:1494:LEU:HD23 | 1.22 | 1.07 |
| 7:5A:1548:VAL:CG1 | 7:5A:1565:GLU:O | 2.02 | 1.07 |
| 9:7E:30:ARG:HH12 | 9:7F:3:GLN:HA | 0.92 | 1.07 |
| 2:CD:86:ARG:NH1 | 2:DD:281:TYR:HA | 1.69 | 1.07 |
| 2:CD:177:ASP:OD2 | 1:CE:353:VAL:CG1 | 2.01 | 1.07 |
| 2:DB:98:GLY:CA | 1:DC:254:GLU:HG2 | 1.84 | 1.07 |
| 2:ED:177:ASP:OD1 | 1:EE:353:VAL:CG1 | 2.02 | 1.07 |
| 2:FB:397:TRP:CG | 1:FC:256:GLN:NE2 | 1.95 | 1.07 |
| 1:GA:89:PRO:HG3 | 1:HA:280:LYS:CE | 1.85 | 1.07 |
| 1:HC:159:VAL:HG22 | 5:3C:209:ARG:NH2 | 1.68 | 1.07 |
| 2:KD:273:LEU:CA | 6:4B:268:LEU:HD21 | 1.81 | 1.07 |
| 2:KF:158:GLU:CA | 4:2B:34:ASN:HB2 | 1.81 | 1.07 |
| 2:LF:306:ARG:NH2 | 4:2B:151:VAL:CG2 | 2.16 | 1.07 |
| 7:5C:1355:GLN:HA | 7:5C:1358:LYS:HG3 | 1.37 | 1.07 |
| 2:AF:359:LYS:CA | 6:4A:151:ARG:NH2 | 2.17 | 1.06 |
| 2:EF:55:THR:HG23 | 2:FF:283:ALA:HA | 1.08 | 1.06 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:HE | 1.51 | 1.06 |
| 1:IE:402:ARG:NH2 | 7:5B:1418:GLN:N | 2.00 | 1.06 |
| 2:LB:306:ARG:CZ | 4:2C:149:ILE:HG22 | 1.85 | 1.06 |
| 2:LB:397:TRP:CE3 | 1:LC:257:THR:CG2 | 2.21 | 1.06 |
| 2:LD:306:ARG:NH2 | 4:2A:151:VAL:CG2 | 2.16 | 1.06 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:MD:177:ASP:CG | 1:ME:353:VAL:HG12 | 1.71 | 1.06 |
| 7:5A:1355:GLN:HA | 7:5A:1358:LYS:HG3 | 1.37 | 1.06 |
| 7:5B:1245:GLY:CA | 9:7D:12:GLU:OE1 | 2.03 | 1.06 |
| 7:5B:1490:LYS:HG3 | 7:5B:1494:LEU:HD23 | 1.22 | 1.06 |
| 7:5B:1548:VAL:CG1 | 7:5B:1565:GLU:O | 2.02 | 1.06 |
| 2:AF:40:SER:CB | 6:4A:152:PHE:CD2 | 2.37 | 1.06 |
| 2:BD:177:ASP:OD2 | 1:BE:353:VAL:CG1 | 2.03 | 1.06 |
| 2:EB:98:GLY:HA2 | 1:EC:254:GLU:HG2 | 1.11 | 1.06 |
| 1:FA:222:PRO:CG | 2:FB:324:LYS:HD3 | 1.83 | 1.06 |
| 1:IE:402:ARG:HH22 | 7:5B:1418:GLN:CA | 1.66 | 1.06 |
| 2:JB:88:ASP:HB2 | 2:KB:278:SER:OG | 1.54 | 1.06 |
| 1:JE:279:GLU:OE2 | 10:9A:22:UNK:C | 2.04 | 1.06 |
| 2:KF:215:LEU:CD1 | 6:4D:267:ILE:HG22 | 1.86 | 1.06 |
| 2:LB:379:LYS:HA | 4:2C:166:ILE:HD13 | 1.11 | 1.06 |
| 1:LE:407:TRP:CH2 | 2:LF:254:ALA:O | 2.07 | 1.06 |
| 2:LF:276:ARG:HH12 | 6:4D:229:GLU:HA | 0.91 | 1.06 |
| 1:MA:372:MET:HE2 | 6:4C:96:VAL:N | 1.70 | 1.06 |
| 2:MB:98:GLY:CA | 1:MC:254:GLU:HG2 | 1.83 | 1.06 |
| 2:MD:98:GLY:CA | 1:ME:254:GLU:HG2 | 1.85 | 1.06 |
| 4:2C:12:LEU:CD2 | 4:2C:20:LYS:HB2 | 1.85 | 1.06 |
| 7:5C:874:GLN:CB | 8:6C:59:LYS:NZ | 2.18 | 1.06 |
| 7:5C:1545:TYR:CA | 7:5C:1570:ALA:HB2 | 1.84 | 1.06 |
| 9:7A:30:ARG:HH11 | 9:7B:3:GLN:HG2 | 1.17 | 1.06 |
| 1:CA:282:TYR:CD2 | 10:8D:18:UNK:CB | 2.39 | 1.06 |
| 2:CD:220:PRO:O | 1:CE:324:VAL:CG1 | 2.03 | 1.06 |
| 1:DE:402:ARG:CZ | 7:5B:777:ALA:CB | 2.32 | 1.06 |
| 1:GE:370:LYS:CE | 10:8R:18:UNK:N | 2.19 | 1.06 |
| 2:ID:424:GLN:CD | 7:5A:1413:GLN:HE21 | 1.52 | 1.06 |
| 1:KA:88:HIS:HA | 1:LA:284:GLU:CA | 1.83 | 1.06 |
| 2:KD:54:ALA:HB1 | 2:LD:285:THR:HG22 | 1.32 | 1.06 |
| 2:KD:54:ALA:HB1 | 2:LD:285:THR:HG23 | 1.35 | 1.06 |
| 1:LC:222:PRO:CG | 2:LD:324:LYS:HD3 | 1.84 | 1.06 |
| 2:LD:177:ASP:OD2 | 1:LE:248:LEU:CD2 | 2.03 | 1.06 |
| 4:2A:12:LEU:CD2 | 4:2A:20:LYS:HB2 | 1.85 | 1.06 |
| 7:5B:1243:ASP:CG | 9:7D:8:ARG:HH12 | 1.63 | 1.06 |
| 7:5B:1355:GLN:HA | 7:5B:1358:LYS:HG3 | 1.37 | 1.06 |
| 7:5B:1515:GLU:HG2 | 7:5B:1563:SER:HA | 1.25 | 1.06 |
| 9:7A:42:LEU:CD1 | 9:7B:39:GLY:HA2 | 1.84 | 1.06 |
| 2:AD:361:LEU:HD22 | 6:4C:144:LEU:CD1 | 1.85 | 1.06 |
| 2:FF:55:THR:N | 2:GF:283:ALA:HB2 | 1.70 | 1.06 |
| 1:JE:89:PRO:CG | 1:KE:280:LYS:HA | 1.85 | 1.06 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MB:397:TRP:CG | 1:MC:256:GLN:NE2 | 1.96 | 1.06 |
| 1:ME:372:MET:HE2 | 6:4B:96:VAL:N | 1.70 | 1.06 |
| 7:5A:1545:TYR:CA | 7:5A:1570:ALA:HB2 | 1.84 | 1.06 |
| 7:5C:1484:TYR:HA | 7:5C:1487:ASN:CB | 1.86 | 1.06 |
| 7:5C:1515:GLU:HG2 | 7:5C:1563:SER:HA | 1.25 | 1.06 |
| 9:7C:42:LEU:CD1 | 9:7D:39:GLY:HA2 | 1.84 | 1.06 |
| 2:BB:98:GLY:CA | 1:BC:254:GLU:HG2 | 1.85 | 1.06 |
| 2:BB:177:ASP:OD1 | 1:BC:353:VAL:CG1 | 2.03 | 1.06 |
| 2:CB:397:TRP:CG | 1:CC:256:GLN:NE2 | 1.96 | 1.06 |
| 2:CD:98:GLY:CA | 1:CE:254:GLU:HG2 | 1.86 | 1.06 |
| 2:DB:397:TRP:CE3 | 1:DC:257:THR:CG2 | 2.20 | 1.06 |
| 2:EB:157:GLU:CD | 7:5C:935:LYS:NZ | 2.14 | 1.06 |
| 2:FB:54:ALA:HA | 2:GB:283:ALA:HB3 | 1.30 | 1.06 |
| 1:FC:402:ARG:HD3 | 7:5A:1259:TYR:CD2 | 1.90 | 1.06 |
| 2:FD:55:THR:CG2 | 2:GD:283:ALA:HA | 1.85 | 1.06 |
| 1:GC:409:VAL:CG1 | 5:3C:383:GLU:OE2 | 2.03 | 1.06 |
| 1:IC:278:ALA:CB | 10:8W:18:UNK:O | 2.02 | 1.06 |
| 4:2B:12:LEU:CD2 | 4:2B:20:LYS:HB2 | 1.85 | 1.06 |
| 7:5A:1484:TYR:HA | 7:5A:1487:ASN:HB2 | 1.09 | 1.06 |
| 7:5A:1484:TYR:HA | 7:5A:1487:ASN:CB | 1.86 | 1.06 |
| 7:5A:1515:GLU:HG2 | 7:5A:1563:SER:HA | 1.25 | 1.06 |
| 7:5B:1484:TYR:HA | 7:5B:1487:ASN:CB | 1.86 | 1.06 |
| 7:5B:1545:TYR:CA | 7:5B:1570:ALA:HB2 | 1.84 | 1.06 |
| 7:5C:1484:TYR:HA | 7:5C:1487:ASN:HB2 | 1.09 | 1.06 |
| 2:EF:125:GLU:HA | 7:5B:903:PHE:CD2 | 1.90 | 1.05 |
| 2:FB:177:ASP:CG | 1:FC:353:VAL:HG11 | 1.78 | 1.05 |
| 2:FD:177:ASP:O | 1:FE:352:LYS:HD2 | 1.53 | 1.05 |
| 1:FE:419:SER:OG | 7:5B:1256:ARG:CZ | 2.03 | 1.05 |
| 1:IA:282:TYR:CE2 | 10:8V:18:UNK:C | 2.26 | 1.05 |
| 1:MC:372:MET:HE3 | 6:4A:96:VAL:C | 1.80 | 1.05 |
| 7:5A:1105:TYR:CD1 | 7:5A:1165:PRO:HA | 1.92 | 1.05 |
| 7:5B:1105:TYR:CD1 | 7:5B:1165:PRO:HA | 1.91 | 1.05 |
| 7:5B:1475:PHE:CE2 | 7:5B:1565:GLU:CD | 2.34 | 1.05 |
| 7:5C:1105:TYR:CD1 | 7:5C:1165:PRO:HA | 1.92 | 1.05 |
| 9:7C:14:SER:O | 9:7D:35:ILE:HD11 | 1.52 | 1.05 |
| 9:7C:15:VAL:HG13 | 9:7D:35:ILE:HD13 | 1.07 | 1.05 |
| 2:AB:55:THR:HG23 | 2:BB:283:ALA:CB | 1.86 | 1.05 |
| 2:AF:223:GLY:HA3 | 6:4A:131:VAL:HB | 1.38 | 1.05 |
| 2:DF:86:ARG:CA | 2:EF:281:TYR:CE1 | 2.40 | 1.05 |
| 2:EB:177:ASP:OD1 | 1:EC:353:VAL:CG1 | 2.04 | 1.05 |
| 1:EE:423:GLU:CD | 7:5B:830:VAL:HG12 | 1.80 | 1.05 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:HG2 | 1.34 | 1.05 |
| 1:KC:85:GLN:OE1 | 1:LC:282:TYR:CB | 2.03 | 1.05 |
| 2:KD:158:GLU:CA | 4:2A:34:ASN:HB2 | 1.74 | 1.05 |
| 1:MC:283:HIS:CD2 | 6:4A:101:ARG:HH22 | 1.74 | 1.05 |
| 7:5A:1475:PHE:CE2 | 7:5A:1565:GLU:CD | 2.34 | 1.05 |
| 7:5B:1484:TYR:HA | 7:5B:1487:ASN:HB2 | 1.09 | 1.05 |
| 2:CB:177:ASP:OD2 | 1:CC:353:VAL:CG1 | 2.02 | 1.05 |
| 1:FC:402:ARG:CZ | 7:5A:1262:GLU:OE2 | 2.03 | 1.05 |
| 1:FC:423:GLU:OE2 | 7:5A:1256:ARG:CZ | 2.04 | 1.05 |
| 1:GE:402:ARG:CZ | 5:3A:381:ASN:HD22 | 1.55 | 1.05 |
| 2:IB:86:ARG:CA | 2:JB:281:TYR:CE1 | 2.39 | 1.05 |
| 2:KB:86:ARG:NH1 | 2:LB:283:ALA:HB3 | 1.44 | 1.05 |
| 1:KE:88:HIS:CA | 1:LE:284:GLU:HB2 | 1.84 | 1.05 |
| 2:LB:379:LYS:HB3 | 4:2C:166:ILE:HD11 | 1.05 | 1.05 |
| 7:5B:841:VAL:HG21 | 8:6B:11:PRO:HA | 1.38 | 1.05 |
| 7:5B:1284:PHE:HZ | 9:7C:12:GLU:HB2 | 0.91 | 1.05 |
| 7:5C:1475:PHE:CE2 | 7:5C:1565:GLU:CD | 2.34 | 1.05 |
| 9:7A:15:VAL:HG13 | 9:7B:35:ILE:HD13 | 1.07 | 1.05 |
| 1:EA:396:ASP:CB | 7:5C:817:LEU:HD23 | 1.81 | 1.05 |
| 2:FB:331:LEU:CD2 | 7:5C:915:PHE:CZ | 2.40 | 1.05 |
| 2:FF:331:LEU:HD22 | 7:5B:915:PHE:CZ | 1.92 | 1.05 |
| 2:GD:86:ARG:NH2 | 2:HD:281:TYR:CD2 | 2.09 | 1.05 |
| 1:JA:89:PRO:HB2 | 1:KA:280:LYS:HG3 | 1.37 | 1.05 |
| 2:KD:77:ARG:HG2 | 2:LD:281:TYR:OH | 1.55 | 1.05 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:HZ3 | 1.51 | 1.05 |
| 1:LA:407:TRP:CH2 | 2:LB:254:ALA:O | 2.09 | 1.05 |
| 7:5B:1105:TYR:CG | 7:5B:1165:PRO:HA | 1.92 | 1.05 |
| 7:5C:1545:TYR:HA | 7:5C:1570:ALA:HB2 | 1.39 | 1.05 |
| 2:BB:397:TRP:CG | 1:BC:256:GLN:NE2 | 1.89 | 1.05 |
| 2:BD:177:ASP:OD1 | 1:BE:353:VAL:CG1 | 2.03 | 1.05 |
| 2:ED:125:GLU:HA | 7:5A:903:PHE:CD2 | 1.92 | 1.05 |
| 2:KD:55:THR:CG2 | 2:LD:363:MET:HE1 | 1.87 | 1.05 |
| 2:KF:77:ARG:HG2 | 2:LF:281:TYR:CE1 | 1.89 | 1.05 |
| 2:LB:98:GLY:HA2 | 1:LC:254:GLU:CG | 1.87 | 1.05 |
| 7:5A:1105:TYR:CG | 7:5A:1165:PRO:HA | 1.92 | 1.05 |
| 7:5A:1271:ILE:HA | 9:7A:20:LEU:HD21 | 1.37 | 1.05 |
| 7:5A:1545:TYR:HA | 7:5A:1570:ALA:HB2 | 1.39 | 1.05 |
| 7:5B:1545:TYR:HA | 7:5B:1570:ALA:HB2 | 1.39 | 1.05 |
| 2:AD:359:LYS:CA | 6:4C:151:ARG:NH2 | 2.19 | 1.04 |
| 2:AD:362:LYS:HG3 | 6:4C:144:LEU:O | 1.57 | 1.04 |
| 2:CD:397:TRP:CG | 1:CE:256:GLN:NE2 | 2.00 | 1.04 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:DB:177:ASP:OD1 | 1:DC:353:VAL:CG1 | 2.03 | 1.04 |
| 2:LB:296:ALA:HB3 | 4:2C:149:ILE:HG23 | 1.08 | 1.04 |
| 1:LC:101:ASN:HD21 | 2:LD:252:LYS:HD2 | 0.87 | 1.04 |
| 2:LF:306:ARG:HE | 4:2B:149:ILE:HG22 | 1.18 | 1.04 |
| 1:MA:283:HIS:CD2 | 6:4C:101:ARG:NH2 | 2.25 | 1.04 |
| 7:5C:1549:THR:CA | 7:5C:1566:GLU:HG2 | 1.84 | 1.04 |
| 1:DE:402:ARG:NH2 | 7:5B:782:LEU:CD1 | 1.95 | 1.04 |
| 1:HC:415:GLU:CG | 5:3C:235:LEU:CB | 2.34 | 1.04 |
| 1:LA:101:ASN:HD21 | 2:LB:252:LYS:HD2 | 0.88 | 1.04 |
| 2:MB:106:TYR:CZ | 3:1A:32:ARG:NH1 | 2.25 | 1.04 |
| 1:MC:279:GLU:HG3 | 6:4A:110:LYS:CE | 1.87 | 1.04 |
| 7:5C:1105:TYR:CG | 7:5C:1165:PRO:HA | 1.92 | 1.04 |
| 7:5C:1544:ILE:HD13 | 7:5C:1570:ALA:O | 1.55 | 1.04 |
| 1:FA:56:THR:OG1 | 1:GA:284:GLU:C | 2.00 | 1.04 |
| 1:FE:207:GLU:OE1 | 7:5B:915:PHE:HB2 | 1.57 | 1.04 |
| 2:GB:397:TRP:CG | 1:GC:256:GLN:NE2 | 1.84 | 1.04 |
| 1:JA:279:GLU:CD | 10:8Y:22:UNK:HA | 1.59 | 1.04 |
| 2:KB:82:GLY:O | 2:LB:281:TYR:CE1 | 2.09 | 1.04 |
| 2:KF:86:ARG:CZ | 2:LF:283:ALA:N | 1.93 | 1.04 |
| 1:LA:222:PRO:CG | 2:LB:324:LYS:HD3 | 1.87 | 1.04 |
| 7:5A:1487:ASN:CB | 7:5A:1568:LYS:CE | 2.15 | 1.04 |
| 7:5A:1544:ILE:HD13 | 7:5A:1570:ALA:O | 1.55 | 1.04 |
| 7:5B:1482:SER:HA | 7:5B:1485:LYS:HB2 | 1.35 | 1.04 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:CE | 2.05 | 1.04 |
| 7:5C:1487:ASN:CB | 7:5C:1568:LYS:CE | 2.15 | 1.04 |
| 9:7C:30:ARG:HH11 | 9:7D:3:GLN:HG2 | 1.17 | 1.04 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:CG | 1.87 | 1.04 |
| 2:AD:227:HIS:ND1 | 6:4C:135:LEU:HD11 | 1.72 | 1.04 |
| 2:DD:178:THR:HG23 | 1:DE:258:ASN:HD21 | 1.22 | 1.04 |
| 1:DE:402:ARG:NH2 | 7:5B:782:LEU:HD11 | 1.05 | 1.04 |
| 2:FD:55:THR:HG23 | 2:GD:283:ALA:HA | 1.08 | 1.04 |
| 2:FD:177:ASP:OD1 | 1:FE:353:VAL:CG1 | 2.03 | 1.04 |
| 2:GD:397:TRP:CG | 1:GE:256:GLN:NE2 | 1.80 | 1.04 |
| 2:ID:86:ARG:HA | 2:JD:281:TYR:CZ | 1.92 | 1.04 |
| 2:KD:276:ARG:HE | 6:4B:265:TYR:HB2 | 1.23 | 1.04 |
| 2:KF:273:LEU:CA | 6:4D:268:LEU:HD21 | 1.87 | 1.04 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:CE | 2.05 | 1.04 |
| 1:DA:60:LYS:HD3 | 1:EA:283:HIS:HD2 | 1.23 | 1.04 |
| 1:FA:207:GLU:OE1 | 7:5C:915:PHE:HB2 | 1.58 | 1.04 |
| 2:FD:55:THR:N | 2:GD:283:ALA:CB | 2.21 | 1.04 |
| 2:IB:424:GLN:HE22 | 7:5C:1413:GLN:CD | 1.56 | 1.04 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LB:340:TYR:CB | 4:2C:147:PHE:HB2 | 1.88 | 1.04 |
| 7:5A:1549:THR:CA | 7:5A:1566:GLU:HG2 | 1.84 | 1.04 |
| 7:5B:1487:ASN:CB | 7:5B:1568:LYS:CE | 2.15 | 1.04 |
| 7:5B:1549:THR:CA | 7:5B:1566:GLU:HG2 | 1.84 | 1.04 |
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:CE | 2.05 | 1.04 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:CG | 1.87 | 1.04 |
| 9:7E:11:TYR:HE1 | 9:7F:26:LEU:HB3 | 1.16 | 1.04 |
| 2:CB:86:ARG:NH1 | 2:DB:281:TYR:HA | 1.70 | 1.03 |
| 1:DA:402:ARG:NE | 7:5C:777:ALA:HB3 | 1.53 | 1.03 |
| 1:EA:398:MET:SD | 2:EB:345:ILE:HG13 | 1.98 | 1.03 |
| 1:FA:402:ARG:CZ | 7:5C:1262:GLU:OE2 | 2.06 | 1.03 |
| 2:FD:177:ASP:OD2 | 1:FE:353:VAL:HG13 | 1.56 | 1.03 |
| 2:FD:177:ASP:OD2 | 1:FE:353:VAL:CG1 | 2.05 | 1.03 |
| 1:HC:415:GLU:HG2 | 5:3C:235:LEU:HB2 | 1.32 | 1.03 |
| 1:IA:278:ALA:CB | 10:8V:21:UNK:CB | 2.36 | 1.03 |
| 1:KE:88:HIS:HA | 1:LE:284:GLU:HB2 | 1.11 | 1.03 |
| 7:5B:1544:ILE:HD13 | 7:5B:1570:ALA:O | 1.55 | 1.03 |
| 7:5C:1573:ARG:O | 7:5C:1577:LYS:CB | 2.05 | 1.03 |
| 9:7A:15:VAL:CB | 9:7B:35:ILE:HD13 | 1.83 | 1.03 |
| 2:DD:98:GLY:CA | 1:DE:254:GLU:HG2 | 1.87 | 1.03 |
| 2:DD:177:ASP:OD1 | 1:DE:353:VAL:CG1 | 2.02 | 1.03 |
| 1:HE:419:SER:OG | 5:3A:238:ILE:CD1 | 2.04 | 1.03 |
| 1:IC:429:GLU:OE1 | 5:3C:307:LYS:NZ | 1.90 | 1.03 |
| 1:JE:89:PRO:HG2 | 1:KE:280:LYS:HA | 1.09 | 1.03 |
| 1:KA:85:GLN:CD | 1:LA:282:TYR:CB | 2.27 | 1.03 |
| 1:KA:87:PHE:O | 1:LA:283:HIS:O | 1.75 | 1.03 |
| 2:KB:273:LEU:HA | 6:4A:268:LEU:CG | 1.88 | 1.03 |
| 7:5A:1482:SER:HA | 7:5A:1485:LYS:HB2 | 1.36 | 1.03 |
| 7:5B:1573:ARG:O | 7:5B:1577:LYS:CB | 2.05 | 1.03 |
| 7:5C:1243:ASP:CG | 9:7F:8:ARG:HH12 | 1.66 | 1.03 |
| 7:5C:1491:LEU:HD11 | 7:5C:1495:PHE:CE1 | 1.93 | 1.03 |
| 9:7E:38:LEU:HD23 | 9:7F:42:LEU:HD13 | 1.35 | 1.03 |
| 2:AB:177:ASP:OD1 | 1:AC:353:VAL:CG1 | 2.06 | 1.03 |
| 2:AD:40:SER:OG | 6:4C:152:PHE:CE2 | 2.08 | 1.03 |
| 2:BD:397:TRP:CG | 1:BE:256:GLN:NE2 | 1.92 | 1.03 |
| 2:EB:125:GLU:C | 7:5C:903:PHE:CE2 | 2.37 | 1.03 |
| 1:FA:71:GLU:OE1 | 2:FB:247:ASN:ND2 | 1.92 | 1.03 |
| 2:GD:54:ALA:C | 2:HD:283:ALA:HB2 | 1.82 | 1.03 |
| 1:IE:402:ARG:NH2 | 7:5B:1417:GLN:CG | 2.21 | 1.03 |
| 2:JB:86:ARG:CZ | 2:KB:280:GLN:CB | 2.36 | 1.03 |
| 7:5A:1491:LEU:HD11 | 7:5A:1495:PHE:CE1 | 1.93 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1573:ARG:O | 7:5A:1577:LYS:CB | 2.05 | 1.03 |
| 7:5B:1548:VAL:HA | 7:5B:1569:GLU:OE2 | 0.87 | 1.03 |
| 9:7E:35:ILE:HG21 | 9:7F:42:LEU:O | 1.52 | 1.03 |
| 2:CB:177:ASP:OD1 | 1:CC:353:VAL:CG1 | 2.04 | 1.03 |
| 2:EF:157:GLU:CD | 7:5B:935:LYS:NZ | 2.16 | 1.03 |
| 2:FB:55:THR:HG23 | 2:GB:283:ALA:HA | 1.38 | 1.03 |
| 1:FE:423:GLU:OE2 | 7:5B:1256:ARG:CZ | 2.07 | 1.03 |
| 2:LD:276:ARG:HH12 | 6:4B:229:GLU:HA | 0.87 | 1.03 |
| 7:5A:1548:VAL:HA | 7:5A:1569:GLU:OE2 | 0.87 | 1.03 |
| 7:5B:1491:LEU:N | 7:5B:1495:PHE:HB3 | 1.72 | 1.03 |
| 7:5B:1491:LEU:HD11 | 7:5B:1495:PHE:CE1 | 1.93 | 1.03 |
| 7:5B:1544:ILE:HD12 | 7:5B:1574:ILE:HG13 | 1.04 | 1.03 |
| 7:5C:1544:ILE:HD12 | 7:5C:1574:ILE:HG13 | 1.05 | 1.03 |
| 7:5C:1548:VAL:HG11 | 7:5C:1566:GLU:HA | 1.33 | 1.03 |
| 2:AD:177:ASP:OD1 | 1:AE:353:VAL:CG1 | 2.07 | 1.03 |
| 2:AF:362:LYS:HG2 | 6:4A:146:ILE:HB | 1.37 | 1.03 |
| 2:BB:177:ASP:OD2 | 1:BC:353:VAL:HG13 | 1.59 | 1.03 |
| 2:CD:177:ASP:OD2 | 1:CE:353:VAL:HG13 | 1.56 | 1.03 |
| 1:DA:402:ARG:NH2 | 7:5C:782:LEU:HD11 | 1.34 | 1.03 |
| 2:FD:98:GLY:C | 1:FE:254:GLU:HG2 | 1.83 | 1.03 |
| 1:HE:159:VAL:HG21 | 5:3A:209:ARG:NE | 1.73 | 1.03 |
| 1:HE:415:GLU:CG | 5:3A:235:LEU:CB | 2.36 | 1.03 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:HG2 | 1.72 | 1.03 |
| 2:KD:397:TRP:CG | 1:KE:256:GLN:NE2 | 1.80 | 1.03 |
| 2:LB:276:ARG:HH12 | 6:4A:229:GLU:HA | 0.88 | 1.03 |
| 2:MB:106:TYR:CE1 | 3:1A:32:ARG:NH1 | 2.27 | 1.03 |
| 7:5A:1491:LEU:N | 7:5A:1495:PHE:HB3 | 1.72 | 1.03 |
| 7:5C:1482:SER:HA | 7:5C:1485:LYS:HB2 | 1.35 | 1.03 |
| 7:5C:1548:VAL:HA | 7:5C:1569:GLU:OE2 | 0.87 | 1.03 |
| 2:AF:217:LEU:HD22 | 6:4A:132:LYS:HG2 | 1.37 | 1.02 |
| 2:AF:362:LYS:HG3 | 6:4A:144:LEU:O | 1.58 | 1.02 |
| 2:GB:177:ASP:OD1 | 1:GC:353:VAL:HG11 | 1.60 | 1.02 |
| 1:GC:409:VAL:HG11 | 5:3C:383:GLU:OE1 | 1.57 | 1.02 |
| 1:HC:410:GLY:O | 5:3C:329:ARG:NH2 | 1.92 | 1.02 |
| 1:HE:282:TYR:CE2 | 10:8U:18:UNK:C | 2.33 | 1.02 |
| 2:IB:177:ASP:OD1 | 1:IC:353:VAL:CG1 | 2.06 | 1.02 |
| 2:KB:177:ASP:OD1 | 1:KC:353:VAL:CG1 | 2.06 | 1.02 |
| 1:LE:221:ARG:NH1 | 2:LF:323:THR:C | 2.15 | 1.02 |
| 1:ME:283:HIS:CD2 | 6:4B:101:ARG:HH22 | 1.77 | 1.02 |
| 7:5A:1544:ILE:HD12 | 7:5A:1574:ILE:HG13 | 1.04 | 1.02 |
| 2:BD:220:PRO:O | 1:BE:324:VAL:CG1 | 2.07 | 1.02 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:EA:430:LYS:HZ1 | 7:5C:834:ASN:CG | 1.51 | 1.02 |
| 2:EB:55:THR:HG23 | 2:FB:283:ALA:CA | 1.89 | 1.02 |
| 2:ED:55:THR:HG23 | 2:FD:283:ALA:CA | 1.88 | 1.02 |
| 2:HD:98:GLY:HA2 | 1:HE:254:GLU:HG3 | 1.41 | 1.02 |
| 2:IB:177:ASP:OD1 | 1:IC:353:VAL:HG11 | 1.60 | 1.02 |
| 2:KD:98:GLY:HA2 | 1:KE:254:GLU:HG3 | 1.41 | 1.02 |
| 2:KD:177:ASP:OD1 | 1:KE:353:VAL:CG1 | 2.07 | 1.02 |
| 2:LB:397:TRP:CG | 1:LC:256:GLN:NE2 | 1.98 | 1.02 |
| 2:LF:224:ASP:H | 6:4D:219:ASN:ND2 | 1.44 | 1.02 |
| 2:LF:296:ALA:CB | 4:2B:149:ILE:HG23 | 1.78 | 1.02 |
| 1:MA:282:TYR:HD2 | 6:4C:104:ARG:HD3 | 1.06 | 1.02 |
| 7:5C:1491:LEU:N | 7:5C:1495:PHE:HB3 | 1.72 | 1.02 |
| 9:7E:7:LEU:HD21 | 9:7F:27:GLY:O | 1.57 | 1.02 |
| 2:AB:177:ASP:OD1 | 1:AC:353:VAL:HG11 | 1.60 | 1.02 |
| 1:DE:414:GLU:OE2 | 7:5B:789:LYS:HE3 | 1.57 | 1.02 |
| 2:EF:54:ALA:HA | 2:FF:283:ALA:HB2 | 1.39 | 1.02 |
| 2:FB:179:VAL:HG21 | 1:FC:258:ASN:O | 1.58 | 1.02 |
| 1:FC:222:PRO:CG | 2:FD:324:LYS:HD3 | 1.88 | 1.02 |
| 1:FC:398:MET:SD | 2:FD:345:ILE:HG13 | 1.99 | 1.02 |
| 2:HB:98:GLY:HA2 | 1:HC:254:GLU:HG3 | 1.42 | 1.02 |
| 1:HC:419:SER:OG | 5:3C:238:ILE:CD1 | 2.07 | 1.02 |
| 2:KB:177:ASP:OD1 | 1:KC:353:VAL:HG11 | 1.59 | 1.02 |
| 2:KD:54:ALA:HB2 | 2:LD:285:THR:HG21 | 1.29 | 1.02 |
| 1:MA:11:GLN:OE1 | 2:MB:245:GLN:O | 1.76 | 1.02 |
| 7:5A:1489:PHE:HA | 7:5A:1492:SER:HB2 | 1.42 | 1.02 |
| 1:DA:402:ARG:NE | 7:5C:777:ALA:HB2 | 1.74 | 1.02 |
| 2:EB:220:PRO:HD2 | 1:EC:326:LYS:HE2 | 1.41 | 1.02 |
| 1:EC:370:LYS:HZ3 | 10:8K:17:UNK:CB | 1.56 | 1.02 |
| 1:FA:211:ASP:OD1 | 7:5C:913:ASN:O | 1.78 | 1.02 |
| 1:FC:419:SER:OG | 7:5A:1256:ARG:CZ | 2.06 | 1.02 |
| 2:ID:177:ASP:OD1 | 1:IE:353:VAL:CG1 | 2.07 | 1.02 |
| 2:JD:86:ARG:CZ | 2:KD:280:GLN:HB3 | 1.87 | 1.02 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:HZ2 | 1.68 | 1.02 |
| 2:LB:306:ARG:NH1 | 4:2C:151:VAL:HG21 | 1.72 | 1.02 |
| 1:LC:60:LYS:HD2 | 6:4A:101:ARG:HH22 | 0.88 | 1.02 |
| 7:5A:1491:LEU:HD22 | 7:5A:1495:PHE:CD1 | 1.92 | 1.02 |
| 7:5A:1548:VAL:HG11 | 7:5A:1566:GLU:HA | 1.33 | 1.02 |
| 7:5B:1487:ASN:CG | 7:5B:1568:LYS:HG2 | 1.84 | 1.02 |
| 7:5B:1489:PHE:HA | 7:5B:1492:SER:HB2 | 1.42 | 1.02 |
| 7:5B:1491:LEU:HD22 | 7:5B:1495:PHE:CD1 | 1.92 | 1.02 |
| 7:5C:1489:PHE:HA | 7:5C:1492:SER:HB2 | 1.42 | 1.02 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5C:1491:LEU:HD22 | 7:5C:1495:PHE:CD1 | 1.92 | 1.02 |
| 2:CB:177:ASP:OD2 | 1:CC:353:VAL:HG13 | 1.55 | 1.02 |
| 1:EE:282:TYR:HE2 | 10:8L:18:UNK:CB | 1.68 | 1.02 |
| 1:FA:56:THR:HA | 1:GA:285:GLN:HB3 | 1.06 | 1.02 |
| 1:FC:207:GLU:OE1 | 7:5A:915:PHE:HB2 | 1.59 | 1.02 |
| 1:FE:402:ARG:HD3 | 7:5B:1259:TYR:CD2 | 1.94 | 1.02 |
| 2:KF:158:GLU:HA | 4:2B:34:ASN:HB2 | 1.39 | 1.02 |
| 1:LC:221:ARG:NH1 | 2:LD:323:THR:C | 2.14 | 1.02 |
| 7:5A:1487:ASN:CG | 7:5A:1568:LYS:HG2 | 1.84 | 1.02 |
| 2:CB:178:THR:HG23 | 1:CC:258:ASN:HD21 | 1.25 | 1.01 |
| 2:GB:177:ASP:OD1 | 1:GC:353:VAL:CG1 | 2.06 | 1.01 |
| 1:IA:282:TYR:HE2 | 10:8V:18:UNK:C | 1.65 | 1.01 |
| 1:IA:402:ARG:HH21 | 7:5C:1417:GLN:HG2 | 1.14 | 1.01 |
| 1:IC:402:ARG:NE | 7:5A:1417:GLN:HG3 | 1.73 | 1.01 |
| 2:ID:98:GLY:HA2 | 1:IE:254:GLU:HG3 | 1.41 | 1.01 |
| 2:KD:276:ARG:HH21 | 6:4B:265:TYR:HA | 1.20 | 1.01 |
| 2:LB:379:LYS:CB | 4:2C:166:ILE:HD11 | 1.58 | 1.01 |
| 1:MC:11:GLN:OE1 | 2:MD:245:GLN:O | 1.76 | 1.01 |
| 7:5A:826:LEU:CD2 | 7:5A:840:GLY:HA2 | 1.89 | 1.01 |
| 7:5B:826:LEU:CD2 | 7:5B:840:GLY:HA2 | 1.89 | 1.01 |
| 7:5B:1152:GLU:OE1 | 8:6B:66:ARG:CZ | 2.08 | 1.01 |
| 7:5C:826:LEU:CD2 | 7:5C:840:GLY:HA2 | 1.89 | 1.01 |
| 7:5C:1091:LYS:O | 7:5C:1095:GLU:HG3 | 1.57 | 1.01 |
| 7:5C:1487:ASN:CG | 7:5C:1568:LYS:HG2 | 1.84 | 1.01 |
| 9:7A:35:ILE:CG2 | 9:7B:42:LEU:O | 2.08 | 1.01 |
| 2:AD:356:ILE:HD12 | 6:4C:152:PHE:CD1 | 1.95 | 1.01 |
| 1:EA:62:VAL:HG21 | 1:FA:283:HIS:O | 1.60 | 1.01 |
| 2:GD:177:ASP:OD1 | 1:GE:353:VAL:CG1 | 2.07 | 1.01 |
| 2:HB:177:ASP:OD1 | 1:HC:353:VAL:CG1 | 2.06 | 1.01 |
| 1:IC:279:GLU:OE2 | 10:8W:22:UNK:CA | 2.08 | 1.01 |
| 2:KD:125:GLU:CG | 2:LD:336:LYS:HZ1 | 1.54 | 1.01 |
| 2:LB:83:GLN:O | 2:MB:281:TYR:OH | 1.78 | 1.01 |
| 2:LB:379:LYS:C | 4:2C:166:ILE:HD11 | 1.85 | 1.01 |
| 7:5A:1091:LYS:O | 7:5A:1095:GLU:HG3 | 1.57 | 1.01 |
| 9:7C:35:ILE:CG2 | 9:7D:42:LEU:O | 2.08 | 1.01 |
| 1:DC:402:ARG:NH2 | 7:5A:782:LEU:HD11 | 1.21 | 1.01 |
| 2:EB:177:ASP:OD1 | 1:EC:353:VAL:HG11 | 1.57 | 1.01 |
| 2:ED:177:ASP:OD1 | 1:EE:353:VAL:HG11 | 1.59 | 1.01 |
| 2:JB:177:ASP:OD1 | 1:JC:353:VAL:HG11 | 1.59 | 1.01 |
| 2:KB:98:GLY:HA2 | 1:KC:254:GLU:HG3 | 1.42 | 1.01 |
| 7:5B:1091:LYS:O | 7:5B:1095:GLU:HG3 | 1.57 | 1.01 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5C:827:GLU:CD | 7:5C:849:ARG:HH21 | 1.69 | 1.01 |
| 9:7A:15:VAL:N | 9:7B:35:ILE:HD11 | 1.76 | 1.01 |
| 1:AE:283:HIS:O | 2:MB:54:ALA:HB1 | 1.60 | 1.01 |
| 1:CE:60:LYS:NZ | 1:DE:283:HIS:CD2 | 2.28 | 1.01 |
| 1:DA:414:GLU:OE2 | 7:5C:789:LYS:HE3 | 1.58 | 1.01 |
| 2:FB:391:ARG:HG3 | 1:FC:346:TRP:CD1 | 1.95 | 1.01 |
| 2:GD:177:ASP:OD1 | 1:GE:353:VAL:HG11 | 1.61 | 1.01 |
| 2:HF:362:LYS:NZ | 10:8U:36:UNK:O | 1.93 | 1.01 |
| 2:ID:177:ASP:OD1 | 1:IE:353:VAL:HG11 | 1.61 | 1.01 |
| 2:JB:177:ASP:OD1 | 1:JC:353:VAL:CG1 | 2.06 | 1.01 |
| 1:JC:279:GLU:CD | 10:8Z:22:UNK:CA | 2.28 | 1.01 |
| 2:JD:177:ASP:OD1 | 1:JE:353:VAL:CG1 | 2.07 | 1.01 |
| 1:KC:85:GLN:OE1 | 1:LC:282:TYR:C | 2.03 | 1.01 |
| 2:KD:177:ASP:OD1 | 1:KE:353:VAL:HG11 | 1.61 | 1.01 |
| 2:KD:217:LEU:CD2 | 6:4B:263:CYS:SG | 2.48 | 1.01 |
| 1:KE:88:HIS:HA | 1:LE:284:GLU:CB | 1.67 | 1.01 |
| 2:KF:87:PRO:CG | 2:LF:282:ARG:CG | 2.39 | 1.01 |
| 1:LE:222:PRO:HD2 | 2:LF:324:LYS:HD3 | 1.37 | 1.01 |
| 1:ME:279:GLU:HG3 | 6:4B:110:LYS:CE | 1.91 | 1.01 |
| 7:5A:827:GLU:CD | 7:5A:849:ARG:HH21 | 1.69 | 1.01 |
| 7:5A:1246:LEU:CB | 9:7B:12:GLU:OE2 | 2.07 | 1.01 |
| 7:5B:827:GLU:CD | 7:5B:849:ARG:HH21 | 1.69 | 1.01 |
| 7:5B:839:GLU:OE2 | 8:6B:11:PRO:HG3 | 1.57 | 1.01 |
| 7:5B:1548:VAL:HG11 | 7:5B:1566:GLU:HA | 1.33 | 1.01 |
| 7:5C:829:GLY:HA2 | 8:6C:109:ILE:CG2 | 1.90 | 1.01 |
| 7:5C:1246:LEU:N | 9:7F:12:GLU:OE2 | 1.91 | 1.01 |
| 2:AD:55:THR:HG23 | 2:BD:283:ALA:CB | 1.89 | 1.01 |
| 2:AD:177:ASP:OD1 | 1:AE:353:VAL:HG11 | 1.61 | 1.01 |
| 2:FD:98:GLY:HA2 | 1:FE:254:GLU:HG2 | 1.06 | 1.01 |
| 1:GE:60:LYS:HD3 | 1:HE:283:HIS:HB3 | 1.41 | 1.01 |
| 1:GE:409:VAL:CG1 | 5:3A:383:GLU:CD | 2.26 | 1.01 |
| 1:KE:85:GLN:HE22 | 1:LE:282:TYR:HB3 | 1.26 | 1.01 |
| 1:LE:60:LYS:HZ3 | 1:ME:283:HIS:CG | 1.77 | 1.01 |
| 2:LF:340:TYR:CD1 | 4:2B:147:PHE:HB2 | 1.94 | 1.01 |
| 1:ME:282:TYR:HD2 | 6:4B:104:ARG:HD3 | 1.06 | 1.01 |
| 7:5A:1552:LYS:HZ3 | 7:5A:1563:SER:CB | 1.54 | 1.01 |
| 7:5B:1355:GLN:O | 7:5B:1358:LYS:HG2 | 1.60 | 1.01 |
| 1:GE:56:THR:OG1 | 1:HE:284:GLU:CA | 2.09 | 1.00 |
| 1:JA:279:GLU:CD | 10:8Y:22:UNK:CA | 2.23 | 1.00 |
| 2:KF:273:LEU:HA | 6:4D:268:LEU:HD23 | 1.02 | 1.00 |
| 2:LD:306:ARG:HH22 | 4:2A:151:VAL:HG23 | 1.21 | 1.00 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5A:839:GLU:OE2 | 8:6A:11:PRO:HG2 | 1.56 | 1.00 |
| 7:5B:842:LEU:HD22 | 7:5B:842:LEU:H | 1.25 | 1.00 |
| 7:5B:1490:LYS:CD | 7:5B:1494:LEU:CB | 2.22 | 1.00 |
| 9:7C:15:VAL:N | 9:7D:35:ILE:HD11 | 1.76 | 1.00 |
| 2:AB:98:GLY:HA2 | 1:AC:254:GLU:HG3 | 1.42 | 1.00 |
| 2:AF:227:HIS:ND1 | 6:4A:135:LEU:HD11 | 1.76 | 1.00 |
| 2:BB:177:ASP:OD2 | 1:BC:353:VAL:CG1 | 2.10 | 1.00 |
| 1:DE:400:ALA:O | 7:5B:775:PRO:HB3 | 1.61 | 1.00 |
| 2:ED:220:PRO:HD2 | 1:EE:326:LYS:HE2 | 1.43 | 1.00 |
| 2:FF:83:GLN:O | 2:GF:281:TYR:OH | 1.76 | 1.00 |
| 2:HD:177:ASP:OD1 | 1:HE:353:VAL:CG1 | 2.06 | 1.00 |
| 1:IA:402:ARG:NH1 | 7:5C:1417:GLN:C | 2.17 | 1.00 |
| 2:KB:397:TRP:CG | 1:KC:256:GLN:NE2 | 1.84 | 1.00 |
| 1:KE:79:ARG:O | 1:LE:280:LYS:HE2 | 1.61 | 1.00 |
| 2:KF:276:ARG:HH21 | 6:4D:265:TYR:CA | 1.73 | 1.00 |
| 1:LA:89:PRO:CG | 1:MA:280:LYS:CD | 2.37 | 1.00 |
| 2:LB:306:ARG:CZ | 4:2C:149:ILE:CG2 | 2.36 | 1.00 |
| 2:MD:397:TRP:CG | 1:ME:256:GLN:HE22 | 1.44 | 1.00 |
| 1:ME:282:TYR:HD2 | 6:4B:104:ARG:CD | 1.74 | 1.00 |
| 7:5A:1355:GLN:O | 7:5A:1358:LYS:HG2 | 1.60 | 1.00 |
| 7:5A:1490:LYS:CD | 7:5A:1494:LEU:CB | 2.22 | 1.00 |
| 7:5C:1355:GLN:O | 7:5C:1358:LYS:HG2 | 1.60 | 1.00 |
| 7:5C:1549:THR:HA | 7:5C:1566:GLU:HG2 | 1.43 | 1.00 |
| 2:BD:178:THR:HG23 | 1:BE:258:ASN:HD21 | 1.23 | 1.00 |
| 1:CA:370:LYS:HZ3 | 10:8D:17:UNK:CB | 1.52 | 1.00 |
| 2:CD:177:ASP:OD1 | 1:CE:353:VAL:CG1 | 2.07 | 1.00 |
| 2:FB:55:THR:N | 2:GB:283:ALA:HA | 1.76 | 1.00 |
| 2:FD:397:TRP:CG | 1:FE:256:GLN:NE2 | 1.91 | 1.00 |
| 5:3C:231:THR:O | 5:3C:332:MET:C | 2.05 | 1.00 |
| 7:5A:842:LEU:HD22 | 7:5A:842:LEU:H | 1.26 | 1.00 |
| 7:5A:1549:THR:HA | 7:5A:1566:GLU:HG2 | 1.43 | 1.00 |
| 7:5B:1549:THR:HA | 7:5B:1566:GLU:HG2 | 1.43 | 1.00 |
| 7:5C:1284:PHE:HZ | 9:7E:12:GLU:HB2 | 0.86 | 1.00 |
| 7:5C:1490:LYS:CD | 7:5C:1494:LEU:CB | 2.22 | 1.00 |
| 2:AF:40:SER:OG | 6:4A:152:PHE:HE2 | 1.36 | 1.00 |
| 2:CB:98:GLY:CA | 1:CC:254:GLU:HG2 | 1.92 | 1.00 |
| 1:FC:89:PRO:CD | 1:GC:280:LYS:NZ | 2.01 | 1.00 |
| 2:HD:178:THR:HG23 | 1:HE:258:ASN:HD21 | 1.26 | 1.00 |
| 1:KA:85:GLN:HA | 1:LA:283:HIS:HA | 1.03 | 1.00 |
| 2:LF:306:ARG:NE | 4:2B:149:ILE:CG2 | 2.25 | 1.00 |
| 5:3A:231:THR:O | 5:3A:332:MET:C | 2.05 | 1.00 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:841:VAL:O | 8:6A:9:LEU:O | 1.80 | 1.00 |
| 2:IB:98:GLY:HA2 | 1:IC:254:GLU:HG3 | 1.42 | 1.00 |
| 2:JD:177:ASP:OD1 | 1:JE:353:VAL:HG11 | 1.61 | 1.00 |
| 2:JD:178:THR:HG23 | 1:JE:258:ASN:HD21 | 1.26 | 1.00 |
| 2:KF:55:THR:HG21 | 2:LF:363:MET:CE | 1.92 | 1.00 |
| 6:4D:244:GLU:C | 6:4D:247:LYS:HG2 | 1.86 | 1.00 |
| 2:AD:98:GLY:HA2 | 1:AE:254:GLU:HG3 | 1.41 | 1.00 |
| 2:BD:177:ASP:OD1 | 1:BE:353:VAL:HG11 | 1.60 | 1.00 |
| 1:FE:422:ARG:NE | 7:5B:1170:THR:HB | 1.76 | 1.00 |
| 1:LA:221:ARG:NH1 | 2:LB:324:LYS:N | 2.10 | 1.00 |
| 7:5A:1381:ILE:HD12 | 7:5A:1381:ILE:H | 1.26 | 1.00 |
| 2:EB:125:GLU:HA | 7:5C:903:PHE:CD2 | 1.96 | 1.00 |
| 1:HC:101:ASN:HD21 | 2:HD:252:LYS:CD | 1.58 | 1.00 |
| 1:IC:402:ARG:HH21 | 7:5A:1417:GLN:HG2 | 1.23 | 1.00 |
| 2:LB:224:ASP:N | 6:4A:219:ASN:CG | 2.19 | 1.00 |
| 1:LE:89:PRO:CG | 1:ME:280:LYS:CD | 2.38 | 1.00 |
| 5:3B:231:THR:O | 5:3B:332:MET:C | 2.05 | 1.00 |
| 7:5B:1381:ILE:HD12 | 7:5B:1381:ILE:H | 1.26 | 1.00 |
| 7:5C:1381:ILE:H | 7:5C:1381:ILE:HD12 | 1.26 | 1.00 |
| 2:AB:55:THR:HG23 | 2:BB:283:ALA:HA | 1.44 | 0.99 |
| 2:DB:178:THR:HG23 | 1:DC:258:ASN:HD21 | 1.25 | 0.99 |
| 1:EA:430:LYS:CE | 7:5C:834:ASN:ND2 | 1.91 | 0.99 |
| 2:EB:177:ASP:CG | 1:EC:353:VAL:HG11 | 1.86 | 0.99 |
| 2:HB:177:ASP:OD1 | 1:HC:353:VAL:HG11 | 1.59 | 0.99 |
| 2:LB:331:LEU:CG | 4:2C:42:PHE:CE1 | 2.45 | 0.99 |
| 2:LF:296:ALA:HB2 | 4:2B:149:ILE:HG21 | 1.40 | 0.99 |
| 6:4B:244:GLU:C | 6:4B:247:LYS:HG2 | 1.86 | 0.99 |
| 7:5A:1284:PHE:HZ | 9:7A:12:GLU:HB2 | 1.10 | 0.99 |
| 7:5C:842:LEU:HD22 | 7:5C:842:LEU:H | 1.26 | 0.99 |
| 1:BA:398:MET:SD | 2:BB:345:ILE:HG13 | 2.02 | 0.99 |
| 2:DB:397:TRP:CG | 1:DC:256:GLN:NE2 | 1.98 | 0.99 |
| 1:IA:279:GLU:OE2 | 10:8V:22:UNK:O | 1.80 | 0.99 |
| 1:KC:62:VAL:CG2 | 1:LC:285:GLN:HB3 | 1.91 | 0.99 |
| 1:LC:60:LYS:CD | 6:4A:101:ARG:HH22 | 1.74 | 0.99 |
| 2:LD:55:THR:CG2 | 2:MD:283:ALA:CB | 2.36 | 0.99 |
| 9:7C:7:LEU:HD23 | 9:7D:27:GLY:HA2 | 1.43 | 0.99 |
| 2:KF:273:LEU:CA | 6:4D:268:LEU:HD23 | 1.88 | 0.99 |
| 1:MC:372:MET:HE2 | 6:4A:96:VAL:N | 1.76 | 0.99 |
| 1:GE:409:VAL:HG21 | 5:3A:383:GLU:OE1 | 1.60 | 0.99 |
| 2:LD:83:GLN:O | 2:MD:281:TYR:OH | 1.79 | 0.99 |
| 1:LE:178:SER:OG | 2:LF:347:ASN:HB3 | 1.61 | 0.99 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LF:231:ALA:HB2 | 6:4D:226:ILE:HD11 | 1.43 | 0.99 |
| 6:4A:244:GLU:C | 6:4A:247:LYS:HG2 | 1.86 | 0.99 |
| 2:AB:55:THR:CG2 | 2:BB:283:ALA:HA | 1.92 | 0.99 |
| 2:FD:55:THR:CG2 | 2:GD:284:LEU:N | 2.24 | 0.99 |
| 1:GC:60:LYS:HZ2 | 1:HC:283:HIS:CG | 1.78 | 0.99 |
| 2:LB:231:ALA:HB2 | 6:4A:226:ILE:HD11 | 1.42 | 0.99 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:HZ2 | 1.60 | 0.99 |
| 7:5C:1475:PHE:HE2 | 7:5C:1565:GLU:CD | 1.70 | 0.99 |
| 9:7A:7:LEU:HD23 | 9:7B:27:GLY:HA2 | 1.43 | 0.99 |
| 1:DA:400:ALA:O | 7:5C:775:PRO:CB | 2.09 | 0.99 |
| 1:EE:393:HIS:CE1 | 7:5B:814:LYS:HG3 | 1.95 | 0.99 |
| 2:FD:331:LEU:CD2 | 7:5A:915:PHE:CZ | 2.45 | 0.99 |
| 2:GB:55:THR:CB | 2:HB:283:ALA:HA | 1.92 | 0.99 |
| 2:IB:397:TRP:CG | 1:IC:256:GLN:HE22 | 1.38 | 0.99 |
| 2:KB:82:GLY:O | 2:LB:281:TYR:HE1 | 1.42 | 0.99 |
| 1:KC:79:ARG:CB | 1:LC:280:LYS:NZ | 0.84 | 0.99 |
| 1:KC:87:PHE:O | 1:LC:283:HIS:O | 1.80 | 0.99 |
| 2:LB:306:ARG:NE | 4:2C:149:ILE:HG21 | 1.77 | 0.99 |
| 7:5A:839:GLU:OE2 | 8:6A:11:PRO:HG3 | 1.61 | 0.99 |
| 1:AA:398:MET:SD | 2:AB:345:ILE:HG13 | 2.03 | 0.99 |
| 1:AC:398:MET:SD | 2:AD:345:ILE:HG13 | 2.03 | 0.99 |
| 2:GB:98:GLY:HA2 | 1:GC:254:GLU:HG3 | 1.42 | 0.99 |
| 2:JB:177:ASP:OD2 | 1:JC:353:VAL:HG13 | 1.63 | 0.99 |
| 2:KB:276:ARG:NE | 6:4A:265:TYR:HB2 | 1.78 | 0.99 |
| 1:MC:398:MET:SD | 2:MD:345:ILE:HG13 | 2.02 | 0.99 |
| 6:4C:244:GLU:C | 6:4C:247:LYS:HG2 | 1.86 | 0.99 |
| 7:5A:1475:PHE:HE2 | 7:5A:1565:GLU:CD | 1.70 | 0.99 |
| 7:5C:1355:GLN:O | 7:5C:1358:LYS:CG | 2.10 | 0.99 |
| 2:AF:223:GLY:CA | 6:4A:131:VAL:HB | 1.92 | 0.99 |
| 1:GC:398:MET:SD | 2:GD:345:ILE:HG13 | 2.03 | 0.99 |
| 2:GF:86:ARG:NH2 | 2:HF:281:TYR:CG | 2.07 | 0.99 |
| 7:5A:1533:GLU:HG2 | 7:5A:1604:ALA:HB1 | 1.45 | 0.99 |
| 7:5B:1533:GLU:HG2 | 7:5B:1604:ALA:HB1 | 1.45 | 0.99 |
| 7:5C:1552:LYS:HZ3 | 7:5C:1563:SER:CB | 1.56 | 0.99 |
| 2:AD:40:SER:CB | 6:4C:152:PHE:CD2 | 2.45 | 0.99 |
| 2:GB:86:ARG:NH2 | 2:HB:281:TYR:CE2 | 2.17 | 0.99 |
| 2:GB:177:ASP:OD2 | 1:GC:353:VAL:HG13 | 1.63 | 0.99 |
| 2:HB:178:THR:HG23 | 1:HC:258:ASN:HD21 | 1.28 | 0.99 |
| 2:KF:86:ARG:HH12 | 2:LF:283:ALA:HB2 | 1.26 | 0.99 |
| 2:KF:86:ARG:NH1 | 2:LF:283:ALA:N | 2.10 | 0.99 |
| 1:ME:11:GLN:OE1 | 2:MF:245:GLN:O | 1.79 | 0.99 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1475:PHE:HE2 | 7:5B:1565:GLU:CD | 1.70 | 0.99 |
| 7:5B:1574:ILE:O | 7:5B:1577:LYS:O | 1.80 | 0.99 |
| 2:AB:177:ASP:OD2 | 1:AC:353:VAL:HG13 | 1.63 | 0.99 |
| 1:AE:283:HIS:HB3 | 2:MB:86:ARG:NH1 | 1.77 | 0.99 |
| 2:ED:178:THR:HG23 | 1:EE:258:ASN:HD21 | 1.23 | 0.99 |
| 2:EF:55:THR:CG2 | 2:FF:283:ALA:HA | 1.93 | 0.99 |
| 2:GB:55:THR:N | 2:HB:283:ALA:CB | 2.25 | 0.99 |
| 1:GC:56:THR:O | 1:HC:285:GLN:HB3 | 1.63 | 0.99 |
| 1:HA:398:MET:SD | 2:HB:345:ILE:HG13 | 2.03 | 0.99 |
| 1:JA:398:MET:SD | 2:JB:345:ILE:HG13 | 2.03 | 0.99 |
| 1:KA:398:MET:SD | 2:KB:345:ILE:HG13 | 2.03 | 0.99 |
| 1:MC:282:TYR:HD2 | 6:4A:104:ARG:HD3 | 1.14 | 0.99 |
| 7:5A:1487:ASN:CG | 7:5A:1568:LYS:CE | 2.35 | 0.99 |
| 7:5B:1487:ASN:CG | 7:5B:1568:LYS:CE | 2.35 | 0.99 |
| 7:5C:1533:GLU:HG2 | 7:5C:1604:ALA:HB1 | 1.45 | 0.99 |
| 1:AE:285:GLN:CA | 2:MB:55:THR:HG23 | 1.92 | 0.98 |
| 1:FE:222:PRO:CG | 2:FF:324:LYS:HD3 | 1.91 | 0.98 |
| 2:JB:178:THR:HG23 | 1:JC:258:ASN:HD21 | 1.27 | 0.98 |
| 2:KF:54:ALA:HB1 | 2:LF:285:THR:HG23 | 1.44 | 0.98 |
| 2:LB:77:ARG:HH12 | 6:4A:204:ARG:NH2 | 1.59 | 0.98 |
| 6:4A:244:GLU:CG | 6:4A:284:LEU:CD1 | 2.35 | 0.98 |
| 7:5A:1355:GLN:O | 7:5A:1358:LYS:CG | 2.10 | 0.98 |
| 7:5B:1126:PRO:HD2 | 8:6B:246:TYR:OH | 1.62 | 0.98 |
| 7:5B:1355:GLN:O | 7:5B:1358:LYS:CG | 2.10 | 0.98 |
| 7:5C:1487:ASN:CG | 7:5C:1568:LYS:CE | 2.35 | 0.98 |
| 1:AC:101:ASN:HD21 | 2:AD:252:LYS:CD | 1.58 | 0.98 |
| 1:DC:398:MET:SD | 2:DD:345:ILE:HG13 | 2.03 | 0.98 |
| 1:GA:398:MET:SD | 2:GB:345:ILE:HG13 | 2.03 | 0.98 |
| 2:HD:177:ASP:OD1 | 1:HE:353:VAL:HG11 | 1.61 | 0.98 |
| 1:JA:89:PRO:CG | 1:KA:280:LYS:CG | 2.34 | 0.98 |
| 2:JB:98:GLY:HA2 | 1:JC:254:GLU:HG3 | 1.42 | 0.98 |
| 2:JD:98:GLY:HA2 | 1:JE:254:GLU:HG3 | 1.41 | 0.98 |
| 2:KD:125:GLU:CD | 2:LD:332:ASN:ND2 | 2.20 | 0.98 |
| 1:LE:222:PRO:CG | 2:LF:324:LYS:CD | 2.41 | 0.98 |
| 6:4C:244:GLU:CG | 6:4C:284:LEU:CD1 | 2.35 | 0.98 |
| 7:5A:1574:ILE:O | 7:5A:1577:LYS:O | 1.80 | 0.98 |
| 2:GD:177:ASP:OD2 | 1:GE:353:VAL:HG13 | 1.64 | 0.98 |
| 2:GD:397:TRP:CG | 1:GE:256:GLN:HE22 | 1.35 | 0.98 |
| 1:HC:398:MET:SD | 2:HD:345:ILE:HG13 | 2.03 | 0.98 |
| 2:IF:86:ARG:HA | 2:JF:281:TYR:CZ | 1.97 | 0.98 |
| 1:JC:398:MET:SD | 2:JD:345:ILE:HG13 | 2.03 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:JD:177:ASP:OD2 | 1:JE:353:VAL:HG13 | 1.64 | 0.98 |
| 2:KB:87:PRO:CD | 2:LB:282:ARG:HG3 | 1.94 | 0.98 |
| 2:LB:178:THR:HG23 | 1:LC:258:ASN:HD21 | 1.24 | 0.98 |
| 2:LD:177:ASP:OD1 | 1:LE:353:VAL:CG1 | 2.11 | 0.98 |
| 9:7A:11:TYR:HE1 | 9:7B:26:LEU:HB3 | 0.93 | 0.98 |
| 2:DD:177:ASP:OD1 | 1:DE:353:VAL:HG11 | 1.63 | 0.98 |
| 1:FE:211:ASP:OD1 | 7:5B:913:ASN:O | 1.81 | 0.98 |
| 2:KD:273:LEU:CG | 6:4B:268:LEU:HD21 | 1.88 | 0.98 |
| 1:LA:407:TRP:CE3 | 2:LB:255:VAL:HG13 | 1.97 | 0.98 |
| 2:LB:177:ASP:OD1 | 1:LC:353:VAL:HG11 | 1.61 | 0.98 |
| 2:LB:296:ALA:HB2 | 4:2C:149:ILE:CG2 | 1.58 | 0.98 |
| 1:LE:60:LYS:HD2 | 6:4B:101:ARG:CZ | 1.81 | 0.98 |
| 5:3C:231:THR:O | 5:3C:335:LYS:HB2 | 1.63 | 0.98 |
| 2:AD:178:THR:HG23 | 1:AE:258:ASN:HD21 | 1.26 | 0.98 |
| 2:BB:178:THR:HG23 | 1:BC:258:ASN:HD21 | 1.23 | 0.98 |
| 1:DC:402:ARG:NE | 7:5A:777:ALA:HB2 | 1.76 | 0.98 |
| 2:FD:178:THR:HG23 | 1:FE:258:ASN:HD21 | 1.25 | 0.98 |
| 2:GB:397:TRP:CG | 1:GC:256:GLN:HE22 | 1.38 | 0.98 |
| 1:IC:398:MET:SD | 2:ID:345:ILE:HG13 | 2.03 | 0.98 |
| 2:JB:86:ARG:CZ | 2:KB:280:GLN:HB2 | 1.93 | 0.98 |
| 1:JC:89:PRO:CG | 1:KC:280:LYS:HA | 1.92 | 0.98 |
| 1:JE:279:GLU:OE2 | 10:9A:22:UNK:O | 1.81 | 0.98 |
| 1:KC:398:MET:SD | 2:KD:345:ILE:HG13 | 2.03 | 0.98 |
| 2:KF:87:PRO:HG2 | 2:LF:282:ARG:CG | 1.93 | 0.98 |
| 1:LC:101:ASN:ND2 | 2:LD:252:LYS:CD | 2.26 | 0.98 |
| 1:LC:101:ASN:HD21 | 2:LD:252:LYS:CD | 1.76 | 0.98 |
| 2:LF:83:GLN:O | 2:MF:281:TYR:OH | 1.80 | 0.98 |
| 6:4B:244:GLU:CG | 6:4B:284:LEU:CD1 | 2.35 | 0.98 |
| 2:AD:177:ASP:OD2 | 1:AE:353:VAL:HG13 | 1.64 | 0.98 |
| 2:DD:54:ALA:HA | 2:ED:283:ALA:HB2 | 1.46 | 0.98 |
| 1:EE:370:LYS:HZ1 | 10:8L:17:UNK:CB | 1.72 | 0.98 |
| 1:HE:159:VAL:CG2 | 5:3A:209:ARG:CZ | 2.41 | 0.98 |
| 2:KF:88:ASP:OD1 | 2:LF:291:GLN:NE2 | 1.96 | 0.98 |
| 1:MA:398:MET:SD | 2:MB:345:ILE:HG13 | 2.03 | 0.98 |
| 1:MC:283:HIS:CD2 | 6:4A:101:ARG:NH2 | 2.31 | 0.98 |
| 7:5C:1574:ILE:O | 7:5C:1577:LYS:O | 1.80 | 0.98 |
| 1:AE:398:MET:SD | 2:AF:345:ILE:HG13 | 2.04 | 0.98 |
| 1:EA:396:ASP:HB2 | 7:5C:817:LEU:HD21 | 1.36 | 0.98 |
| 1:FC:211:ASP:OD1 | 7:5A:913:ASN:O | 1.81 | 0.98 |
| 2:FF:428:ALA:CA | 7:5B:1080:PHE:CE1 | 2.39 | 0.98 |
| 1:GC:402:ARG:CD | 5:3C:381:ASN:ND2 | 2.27 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:GD:98:GLY:HA2 | 1:GE:254:GLU:HG3 | 1.41 | 0.98 |
| 2:IB:177:ASP:OD2 | 1:IC:353:VAL:HG13 | 1.63 | 0.98 |
| 2:JB:86:ARG:NE | 2:KB:281:TYR:CD2 | 2.32 | 0.98 |
| 2:KB:86:ARG:HH11 | 2:LB:283:ALA:HB3 | 1.20 | 0.98 |
| 2:KD:86:ARG:HG2 | 2:LD:288:GLU:OE2 | 1.62 | 0.98 |
| 2:LD:340:TYR:CD1 | 4:2A:147:PHE:CB | 2.46 | 0.98 |
| 7:5B:1548:VAL:CB | 7:5B:1566:GLU:HA | 1.93 | 0.98 |
| 2:HB:177:ASP:OD2 | 1:HC:353:VAL:HG13 | 1.63 | 0.98 |
| 2:IB:177:ASP:OD2 | 1:IC:248:LEU:CD2 | 2.12 | 0.98 |
| 1:JE:398:MET:SD | 2:JF:345:ILE:HG13 | 2.04 | 0.98 |
| 2:KB:177:ASP:OD2 | 1:KC:248:LEU:CD2 | 2.12 | 0.98 |
| 2:KB:397:TRP:CG | 1:KC:256:GLN:HE22 | 1.38 | 0.98 |
| 2:KD:397:TRP:CG | 1:KE:256:GLN:HE22 | 1.34 | 0.98 |
| 2:KF:125:GLU:CG | 2:LF:336:LYS:CE | 2.39 | 0.98 |
| 1:MA:282:TYR:HD2 | 6:4C:104:ARG:CD | 1.76 | 0.98 |
| 5:3A:231:THR:O | 5:3A:335:LYS:HB2 | 1.63 | 0.98 |
| 7:5A:1548:VAL:CB | 7:5A:1566:GLU:HA | 1.93 | 0.98 |
| 7:5C:1152:GLU:OE2 | 8:6C:66:ARG:NH2 | 1.96 | 0.98 |
| 2:AF:224:ASP:OD1 | 6:4A:131:VAL:C | 2.07 | 0.98 |
| 2:DB:177:ASP:OD1 | 1:DC:353:VAL:HG11 | 1.62 | 0.98 |
| 2:FF:55:THR:HG21 | 2:GF:284:LEU:H | 1.27 | 0.98 |
| 2:GB:177:ASP:OD2 | 1:GC:248:LEU:CD2 | 2.12 | 0.98 |
| 1:HC:159:VAL:CG2 | 5:3C:209:ARG:CZ | 2.41 | 0.98 |
| 1:HE:398:MET:SD | 2:HF:345:ILE:HG13 | 2.04 | 0.98 |
| 1:IC:434:GLU:OE1 | 5:3C:61:SER:CB | 2.12 | 0.98 |
| 1:KA:85:GLN:NE2 | 1:LA:282:TYR:CB | 2.25 | 0.98 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:HZ1 | 1.75 | 0.98 |
| 1:ME:283:HIS:CD2 | 6:4B:101:ARG:NH2 | 2.31 | 0.98 |
| 6:4D:244:GLU:CG | 6:4D:284:LEU:CD1 | 2.35 | 0.98 |
| 2:ED:177:ASP:CG | 1:EE:353:VAL:HG11 | 1.87 | 0.98 |
| 1:GC:89:PRO:HD3 | 1:HC:280:LYS:HZ2 | 0.83 | 0.98 |
| 1:GE:398:MET:SD | 2:GF:345:ILE:HG13 | 2.04 | 0.98 |
| 2:HB:177:ASP:OD2 | 1:HC:248:LEU:CD2 | 2.12 | 0.98 |
| 2:HD:177:ASP:OD2 | 1:HE:353:VAL:HG13 | 1.64 | 0.98 |
| 2:JB:177:ASP:OD2 | 1:JC:248:LEU:CD2 | 2.12 | 0.98 |
| 2:LD:231:ALA:HB2 | 6:4B:226:ILE:HD11 | 1.41 | 0.98 |
| 7:5C:1548:VAL:CB | 7:5C:1566:GLU:HA | 1.93 | 0.98 |
| 2:FD:177:ASP:CG | 1:FE:353:VAL:HG11 | 1.81 | 0.97 |
| 1:KE:398:MET:SD | 2:KF:345:ILE:HG13 | 2.04 | 0.97 |
| 1:LC:176:GLN:NE2 | 4:2A:42:PHE:CB | 2.26 | 0.97 |
| 1:EE:370:LYS:HZ3 | 10:8L:17:UNK:CB | 1.58 | 0.97 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FA:11:GLN:OE1 | 2:FB:245:GLN:O | 1.82 | 0.97 |
| 2:GD:178:THR:HG23 | 1:GE:258:ASN:HD21 | 1.26 | 0.97 |
| 2:JF:86:ARG:NH2 | 2:KF:280:GLN:HB3 | 1.66 | 0.97 |
| 6:4A:139:ASP:OD2 | 6:4A:140:PRO:HD2 | 1.64 | 0.97 |
| 7:5B:1105:TYR:HB3 | 7:5B:1166:LEU:H | 1.24 | 0.97 |
| 9:7C:42:LEU:HD12 | 9:7D:39:GLY:HA2 | 1.45 | 0.97 |
| 2:CB:86:ARG:CA | 2:DB:281:TYR:CZ | 2.30 | 0.97 |
| 2:DF:85:PHE:C | 2:EF:281:TYR:OH | 2.07 | 0.97 |
| 1:IA:398:MET:SD | 2:IB:345:ILE:HG13 | 2.03 | 0.97 |
| 2:IB:86:ARG:HA | 2:JB:281:TYR:CZ | 1.99 | 0.97 |
| 1:LC:178:SER:OG | 2:LD:347:ASN:HB3 | 1.63 | 0.97 |
| 5:3B:231:THR:O | 5:3B:335:LYS:HB2 | 1.63 | 0.97 |
| 6:4B:139:ASP:OD2 | 6:4B:140:PRO:HD2 | 1.64 | 0.97 |
| 6:4D:151:ARG:HH11 | 6:4D:151:ARG:HG2 | 1.28 | 0.97 |
| 7:5A:1524:PHE:CD1 | 7:5A:1567:PHE:CZ | 2.52 | 0.97 |
| 7:5B:1524:PHE:CD1 | 7:5B:1567:PHE:CZ | 2.52 | 0.97 |
| 2:AB:55:THR:HG23 | 2:BB:283:ALA:CA | 1.95 | 0.97 |
| 2:AB:177:ASP:OD2 | 1:AC:248:LEU:CD2 | 2.12 | 0.97 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:HD2 | 1.24 | 0.97 |
| 2:FB:55:THR:HG21 | 2:GB:284:LEU:H | 0.83 | 0.97 |
| 2:FB:177:ASP:O | 1:FC:352:LYS:HD2 | 1.65 | 0.97 |
| 1:FC:89:PRO:N | 1:GC:280:LYS:NZ | 2.12 | 0.97 |
| 2:KB:177:ASP:OD2 | 1:KC:353:VAL:HG13 | 1.63 | 0.97 |
| 2:KD:86:ARG:HH12 | 2:LD:283:ALA:HB2 | 1.27 | 0.97 |
| 6:4C:139:ASP:OD2 | 6:4C:140:PRO:HD2 | 1.64 | 0.97 |
| 6:4D:139:ASP:OD2 | 6:4D:140:PRO:HD2 | 1.64 | 0.97 |
| 7:5C:1524:PHE:CD1 | 7:5C:1567:PHE:CZ | 2.52 | 0.97 |
| 9:7C:7:LEU:HD21 | 9:7D:27:GLY:CA | 1.89 | 0.97 |
| 1:DE:398:MET:SD | 2:DF:345:ILE:HG13 | 2.05 | 0.97 |
| 1:HC:420:GLU:OE1 | 5:3C:215:TYR:CZ | 2.17 | 0.97 |
| 1:IA:402:ARG:NH2 | 7:5C:1418:GLN:N | 2.11 | 0.97 |
| 1:IE:398:MET:SD | 2:IF:345:ILE:HG13 | 2.04 | 0.97 |
| 2:IF:85:PHE:O | 2:JF:281:TYR:OH | 1.81 | 0.97 |
| 1:KE:372:MET:CB | 6:4B:299:TYR:CE1 | 2.45 | 0.97 |
| 2:KF:273:LEU:CG | 6:4D:268:LEU:HD21 | 1.94 | 0.97 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:HZ2 | 1.63 | 0.97 |
| 2:MD:106:TYR:OH | 3:1B:32:ARG:NH1 | 1.94 | 0.97 |
| 7:5B:1544:ILE:CD1 | 7:5B:1574:ILE:HG13 | 1.92 | 0.97 |
| 7:5C:1548:VAL:HG11 | 7:5C:1566:GLU:CA | 1.81 | 0.97 |
| 1:AE:342:GLN:NE2 | 3:1A:55:HIS:CG | 2.26 | 0.97 |
| 2:ID:177:ASP:OD2 | 1:IE:353:VAL:HG13 | 1.64 | 0.97 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:2B:12:LEU:HD23 | 4:2B:20:LYS:HB2 | 1.43 | 0.97 |
| 7:5A:1544:ILE:CD1 | 7:5A:1574:ILE:HG13 | 1.93 | 0.97 |
| 7:5C:1091:LYS:O | 7:5C:1095:GLU:HG2 | 1.65 | 0.97 |
| 1:FC:422:ARG:NE | 7:5A:1170:THR:HB | 1.78 | 0.97 |
| 2:ID:177:ASP:OD2 | 1:IE:248:LEU:CD2 | 2.13 | 0.97 |
| 1:IE:429:GLU:OE1 | 5:3A:307:LYS:NZ | 1.97 | 0.97 |
| 6:4B:151:ARG:HH11 | 6:4B:151:ARG:HG2 | 1.28 | 0.97 |
| 7:5A:1091:LYS:O | 7:5A:1095:GLU:HG2 | 1.65 | 0.97 |
| 7:5A:1105:TYR:HB3 | 7:5A:1166:LEU:H | 1.24 | 0.97 |
| 2:AF:55:THR:HG23 | 2:BF:283:ALA:CB | 1.94 | 0.97 |
| 2:BB:177:ASP:OD1 | 1:BC:353:VAL:HG11 | 1.61 | 0.97 |
| 1:DA:400:ALA:O | 7:5C:775:PRO:HB2 | 1.62 | 0.97 |
| 1:EE:430:LYS:CE | 7:5B:834:ASN:ND2 | 2.12 | 0.97 |
| 1:FA:423:GLU:OE2 | 7:5C:1256:ARG:CZ | 2.12 | 0.97 |
| 1:JC:101:ASN:HD21 | 2:JD:252:LYS:CD | 1.58 | 0.97 |
| 1:KE:359:PRO:CB | 6:4B:299:TYR:CE2 | 2.48 | 0.97 |
| 7:5C:1544:ILE:CD1 | 7:5C:1574:ILE:HG13 | 1.93 | 0.97 |
| 2:AB:178:THR:HG23 | 1:AC:258:ASN:HD21 | 1.27 | 0.97 |
| 2:EB:98:GLY:HA2 | 1:EC:254:GLU:HG3 | 1.47 | 0.97 |
| 2:ED:98:GLY:HA2 | 1:EE:254:GLU:HG3 | 1.47 | 0.97 |
| 2:GD:55:THR:H | 2:HD:283:ALA:CB | 1.68 | 0.97 |
| 2:GD:177:ASP:OD2 | 1:GE:248:LEU:CD2 | 2.13 | 0.97 |
| 2:JD:177:ASP:OD2 | 1:JE:248:LEU:CD2 | 2.13 | 0.97 |
| 2:KD:177:ASP:OD2 | 1:KE:248:LEU:CD2 | 2.13 | 0.97 |
| 7:5B:1091:LYS:O | 7:5B:1095:GLU:HG2 | 1.65 | 0.97 |
| 9:7E:11:TYR:HD1 | 9:7F:26:LEU:HD23 | 1.22 | 0.97 |
| 2:AD:177:ASP:OD2 | 1:AE:248:LEU:CD2 | 2.13 | 0.97 |
| 1:FE:402:ARG:NH1 | 7:5B:1262:GLU:OE2 | 1.98 | 0.97 |
| 1:HA:101:ASN:HD21 | 2:HB:252:LYS:CD | 1.62 | 0.97 |
| 2:JD:86:ARG:NH1 | 2:KD:280:GLN:HB3 | 1.79 | 0.97 |
| 2:KD:177:ASP:OD2 | 1:KE:353:VAL:HG13 | 1.64 | 0.97 |
| 2:KF:118:ASP:OD2 | 4:2B:148:ASN:ND2 | 1.96 | 0.97 |
| 2:LD:224:ASP:N | 6:4B:219:ASN:CG | 2.21 | 0.97 |
| 5:3A:231:THR:O | 5:3A:332:MET:O | 1.82 | 0.97 |
| 7:5A:1548:VAL:HG11 | 7:5A:1566:GLU:CA | 1.81 | 0.97 |
| 1:BC:398:MET:SD | 2:BD:345:ILE:HG13 | 2.05 | 0.96 |
| 2:CD:177:ASP:OD1 | 1:CE:353:VAL:HG11 | 1.65 | 0.96 |
| 2:DD:397:TRP:CG | 1:DE:256:GLN:NE2 | 1.99 | 0.96 |
| 2:FB:177:ASP:OD1 | 1:FC:353:VAL:CG1 | 2.09 | 0.96 |
| 1:LE:407:TRP:CE3 | 2:LF:255:VAL:HG13 | 1.99 | 0.96 |
| 2:MD:111:GLU:HG2 | 3:1B:62:SER:CA | 1.95 | 0.96 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2A:172:ASP:HB2 | 4:2A:173:PRO:CD | 1.95 | 0.96 |
| 5:3B:231:THR:O | 5:3B:332:MET:O | 1.82 | 0.96 |
| 6:4A:151:ARG:HH11 | 6:4A:151:ARG:HG2 | 1.28 | 0.96 |
| 7:5C:1105:TYR:HB3 | 7:5C:1166:LEU:H | 1.24 | 0.96 |
| 7:5C:1548:VAL:N | 7:5C:1569:GLU:CD | 2.22 | 0.96 |
| 1:DA:62:VAL:HG21 | 1:EA:283:HIS:O | 1.64 | 0.96 |
| 1:DE:62:VAL:HG21 | 1:EE:283:HIS:O | 1.65 | 0.96 |
| 2:HD:177:ASP:OD2 | 1:HE:248:LEU:CD2 | 2.13 | 0.96 |
| 1:IC:282:TYR:CD2 | 10:8W:15:UNK:O | 2.17 | 0.96 |
| 2:JD:397:TRP:CG | 1:JE:256:GLN:HE22 | 1.35 | 0.96 |
| 1:KC:101:ASN:HD21 | 2:KD:252:LYS:CD | 1.58 | 0.96 |
| 1:LA:101:ASN:HD21 | 2:LB:252:LYS:CD | 1.78 | 0.96 |
| 5:3C:231:THR:O | 5:3C:332:MET:O | 1.82 | 0.96 |
| 6:4C:289:LYS:HA | 6:4C:289:LYS:HE3 | 1.44 | 0.96 |
| 1:DC:62:VAL:HG21 | 1:EC:283:HIS:O | 1.66 | 0.96 |
| 2:FB:55:THR:H | 2:GB:283:ALA:CB | 1.58 | 0.96 |
| 1:GC:402:ARG:HD2 | 5:3C:381:ASN:ND2 | 1.80 | 0.96 |
| 2:ID:85:PHE:O | 2:JD:281:TYR:OH | 1.82 | 0.96 |
| 1:LA:101:ASN:ND2 | 2:LB:252:LYS:CD | 2.27 | 0.96 |
| 2:MB:397:TRP:CG | 1:MC:256:GLN:HE22 | 1.50 | 0.96 |
| 2:MD:111:GLU:HG2 | 3:1B:62:SER:HA | 1.43 | 0.96 |
| 1:ME:279:GLU:CB | 6:4B:110:LYS:HE3 | 1.96 | 0.96 |
| 4:2B:172:ASP:HB2 | 4:2B:173:PRO:CD | 1.95 | 0.96 |
| 7:5B:1548:VAL:N | 7:5B:1569:GLU:CD | 2.22 | 0.96 |
| 7:5C:1544:ILE:C | 7:5C:1570:ALA:HA | 1.75 | 0.96 |
| 9:7E:7:LEU:CD2 | 9:7F:27:GLY:HA2 | 1.94 | 0.96 |
| 2:BB:220:PRO:O | 1:BC:324:VAL:CG1 | 2.14 | 0.96 |
| 2:CD:178:THR:HG23 | 1:CE:258:ASN:HD21 | 1.29 | 0.96 |
| 1:FC:56:THR:HA | 1:GC:285:GLN:HB3 | 1.44 | 0.96 |
| 1:FC:89:PRO:CA | 1:GC:280:LYS:HZ1 | 1.76 | 0.96 |
| 2:JB:397:TRP:CG | 1:JC:256:GLN:HE22 | 1.38 | 0.96 |
| 2:JD:86:ARG:NH2 | 2:KD:280:GLN:HB3 | 1.79 | 0.96 |
| 2:LD:55:THR:N | 2:MD:283:ALA:CB | 2.27 | 0.96 |
| 1:LE:89:PRO:CG | 1:ME:280:LYS:CE | 2.42 | 0.96 |
| 2:MB:106:TYR:OH | 3:1A:32:ARG:NH1 | 1.97 | 0.96 |
| 4:2A:12:LEU:HD23 | 4:2A:20:LYS:HB2 | 1.43 | 0.96 |
| 4:2C:172:ASP:HB2 | 4:2C:173:PRO:CD | 1.95 | 0.96 |
| 7:5A:1548:VAL:N | 7:5A:1569:GLU:CD | 2.22 | 0.96 |
| 1:AE:285:GLN:HA | 2:MB:55:THR:HG23 | 0.96 | 0.96 |
| 1:AE:308:ARG:O | 3:1A:56:ASN:OD1 | 1.82 | 0.96 |
| 2:EB:220:PRO:O | 1:EC:324:VAL:HG11 | 1.63 | 0.96 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:FB:177:ASP:OD2 | 1:FC:353:VAL:CG1 | 2.12 | 0.96 |
| 2:KD:86:ARG:HH12 | 2:LD:283:ALA:CA | 1.71 | 0.96 |
| 7:5B:1125:LEU:HD11 | 8:6B:245:GLN:OE1 | 1.66 | 0.96 |
| 7:5B:1548:VAL:HG11 | 7:5B:1566:GLU:CA | 1.81 | 0.96 |
| 2:AF:40:SER:CB | 6:4A:152:PHE:HD2 | 1.74 | 0.96 |
| 2:LF:274:THR:O | 6:4D:228:LEU:HD23 | 1.64 | 0.96 |
| 7:5B:839:GLU:CG | 8:6B:107:PRO:O | 2.12 | 0.96 |
| 7:5B:1265:ALA:O | 7:5B:1269:ASP:OD1 | 1.82 | 0.96 |
| 7:5C:1355:GLN:HA | 7:5C:1358:LYS:CG | 1.92 | 0.96 |
| 9:7A:42:LEU:HD12 | 9:7B:39:GLY:HA2 | 1.45 | 0.96 |
| 2:KF:54:ALA:HB2 | 2:LF:285:THR:HG21 | 1.46 | 0.96 |
| 4:2C:12:LEU:HD23 | 4:2C:20:LYS:HB2 | 1.43 | 0.96 |
| 6:4C:151:ARG:HH11 | 6:4C:151:ARG:HG2 | 1.28 | 0.96 |
| 2:AD:40:SER:CB | 6:4C:152:PHE:HD2 | 1.79 | 0.96 |
| 2:ED:220:PRO:O | 1:EE:324:VAL:HG11 | 1.64 | 0.96 |
| 2:GB:178:THR:HG23 | 1:GC:258:ASN:HD21 | 1.28 | 0.96 |
| 1:GE:56:THR:O | 1:HE:285:GLN:CA | 2.14 | 0.96 |
| 2:HD:98:GLY:C | 1:HE:254:GLU:HG2 | 1.90 | 0.96 |
| 2:LD:306:ARG:NH1 | 4:2A:151:VAL:HG21 | 1.79 | 0.96 |
| 6:4A:289:LYS:HA | 6:4A:289:LYS:HE3 | 1.44 | 0.96 |
| 7:5A:1355:GLN:HA | 7:5A:1358:LYS:CG | 1.91 | 0.96 |
| 2:HB:177:ASP:OD2 | 1:HC:353:VAL:CG1 | 2.14 | 0.96 |
| 2:HD:177:ASP:OD2 | 1:HE:353:VAL:CG1 | 2.14 | 0.96 |
| 1:JA:87:PHE:O | 1:KA:283:HIS:HE1 | 1.48 | 0.96 |
| 7:5A:1246:LEU:N | 9:7B:12:GLU:OE2 | 1.94 | 0.96 |
| 7:5A:1265:ALA:O | 7:5A:1269:ASP:OD1 | 1.82 | 0.96 |
| 7:5C:1152:GLU:OE1 | 8:6C:66:ARG:CZ | 2.14 | 0.96 |
| 9:7A:7:LEU:HD21 | 9:7B:27:GLY:CA | 1.89 | 0.96 |
| 9:7C:11:TYR:HE1 | 9:7D:26:LEU:HB3 | 0.93 | 0.96 |
| 2:CB:220:PRO:HD2 | 1:CC:326:LYS:HG2 | 1.46 | 0.96 |
| 2:ED:397:TRP:CG | 1:EE:256:GLN:NE2 | 1.95 | 0.96 |
| 2:FB:98:GLY:HA2 | 1:FC:254:GLU:HG2 | 0.97 | 0.96 |
| 2:FB:177:ASP:OD2 | 1:FC:353:VAL:HG13 | 1.63 | 0.96 |
| 1:JC:370:LYS:HE2 | 10:8Z:17:UNK:CB | 1.94 | 0.96 |
| 2:KF:54:ALA:HB1 | 2:LF:285:THR:HG22 | 1.46 | 0.96 |
| 1:LE:101:ASN:HD21 | 2:LF:252:LYS:CD | 1.79 | 0.96 |
| 1:CC:60:LYS:NZ | 1:DC:283:HIS:CD2 | 2.33 | 0.95 |
| 2:ED:125:GLU:O | 7:5A:903:PHE:CE2 | 2.19 | 0.95 |
| 2:FF:55:THR:HG23 | 2:GF:283:ALA:HA | 0.96 | 0.95 |
| 2:LD:274:THR:O | 6:4B:228:LEU:HD23 | 1.66 | 0.95 |
| 2:MB:111:GLU:HG2 | 3:1A:62:SER:CA | 1.95 | 0.95 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MD:110:ALA:O | 3:1B:61:HIS:CB | 2.13 | 0.95 |
| 6:4D:252:VAL:HG13 | 6:4D:292:VAL:HG23 | 1.45 | 0.95 |
| 7:5C:1265:ALA:O | 7:5C:1269:ASP:OD1 | 1.82 | 0.95 |
| 1:CC:398:MET:SD | 2:CD:345:ILE:HG13 | 2.06 | 0.95 |
| 1:GA:60:LYS:HZ3 | 1:HA:283:HIS:CG | 1.84 | 0.95 |
| 2:GB:177:ASP:OD2 | 1:GC:353:VAL:CG1 | 2.14 | 0.95 |
| 2:GD:177:ASP:OD2 | 1:GE:353:VAL:CG1 | 2.14 | 0.95 |
| 1:JA:282:TYR:OH | 10:8Y:17:UNK:CB | 2.14 | 0.95 |
| 2:JB:177:ASP:OD2 | 1:JC:353:VAL:CG1 | 2.14 | 0.95 |
| 2:JD:88:ASP:CB | 2:KD:278:SER:OG | 2.13 | 0.95 |
| 2:JD:177:ASP:OD2 | 1:JE:353:VAL:CG1 | 2.14 | 0.95 |
| 1:JE:124:LYS:HD2 | 1:KE:284:GLU:OE1 | 1.66 | 0.95 |
| 1:LA:60:LYS:HD2 | 6:4C:101:ARG:CZ | 1.84 | 0.95 |
| 1:LC:407:TRP:CE3 | 2:LD:255:VAL:HG13 | 1.99 | 0.95 |
| 1:LE:101:ASN:ND2 | 2:LF:252:LYS:CD | 2.29 | 0.95 |
| 6:4B:289:LYS:HA | 6:4B:289:LYS:HE3 | 1.44 | 0.95 |
| 7:5A:1544:ILE:C | 7:5A:1570:ALA:HA | 1.76 | 0.95 |
| 1:AA:101:ASN:HD21 | 2:AB:252:LYS:CD | 1.62 | 0.95 |
| 2:DD:220:PRO:HD2 | 1:DE:326:LYS:HG2 | 1.46 | 0.95 |
| 1:EE:396:ASP:OD1 | 7:5B:821:LEU:HD11 | 1.65 | 0.95 |
| 1:GE:402:ARG:CD | 5:3A:381:ASN:ND2 | 2.30 | 0.95 |
| 1:IA:282:TYR:CE1 | 10:8V:18:UNK:CB | 2.33 | 0.95 |
| 1:LC:222:PRO:CG | 2:LD:324:LYS:CD | 2.43 | 0.95 |
| 6:4B:252:VAL:HG13 | 6:4B:292:VAL:HG23 | 1.45 | 0.95 |
| 7:5A:1246:LEU:CA | 9:7B:12:GLU:OE2 | 2.14 | 0.95 |
| 7:5B:1355:GLN:HA | 7:5B:1358:LYS:CG | 1.92 | 0.95 |
| 2:CB:87:PRO:CD | 2:DB:281:TYR:CE2 | 2.50 | 0.95 |
| 1:DA:402:ARG:HH22 | 7:5C:782:LEU:HD11 | 0.78 | 0.95 |
| 1:HA:282:TYR:CE2 | 10:8S:19:UNK:N | 2.34 | 0.95 |
| 1:IA:402:ARG:CZ | 7:5C:1417:GLN:C | 2.38 | 0.95 |
| 6:4C:252:VAL:HG13 | 6:4C:292:VAL:HG23 | 1.45 | 0.95 |
| 7:5A:841:VAL:CG2 | 8:6A:11:PRO:HA | 1.95 | 0.95 |
| 7:5B:874:GLN:HB2 | 8:6B:59:LYS:HZ3 | 1.25 | 0.95 |
| 1:CA:398:MET:SD | 2:CB:345:ILE:HG13 | 2.06 | 0.95 |
| 2:GD:98:GLY:C | 1:GE:254:GLU:HG2 | 1.90 | 0.95 |
| 2:ID:178:THR:HG23 | 1:IE:258:ASN:HD21 | 1.26 | 0.95 |
| 2:JD:98:GLY:C | 1:JE:254:GLU:HG2 | 1.90 | 0.95 |
| 1:KC:79:ARG:HB2 | 1:LC:280:LYS:HZ1 | 0.81 | 0.95 |
| 2:KD:125:GLU:CG | 2:LD:336:LYS:CE | 2.33 | 0.95 |
| 1:LA:222:PRO:CG | 2:LB:324:LYS:CD | 2.44 | 0.95 |
| 1:LE:176:GLN:O | 2:LF:347:ASN:ND2 | 2.00 | 0.95 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:4A:252:VAL:HG13 | 6:4A:292:VAL:HG23 | 1.45 | 0.95 |
| 6:4D:252:VAL:HG13 | 6:4D:292:VAL:CG2 | 1.96 | 0.95 |
| 2:AD:217:LEU:HD22 | 6:4C:132:LYS:CG | 1.95 | 0.95 |
| 2:CB:177:ASP:OD1 | 1:CC:353:VAL:HG11 | 1.66 | 0.95 |
| 2:CD:87:PRO:CD | 2:DD:281:TYR:CE2 | 2.50 | 0.95 |
| 1:GC:409:VAL:CG1 | 5:3C:383:GLU:CD | 2.39 | 0.95 |
| 1:IE:389:SER:HB2 | 5:3A:307:LYS:HD3 | 0.97 | 0.95 |
| 1:LA:178:SER:OG | 2:LB:347:ASN:HB3 | 1.66 | 0.95 |
| 2:LD:98:GLY:HA2 | 1:LE:254:GLU:HG2 | 1.48 | 0.95 |
| 2:LD:340:TYR:CG | 4:2A:147:PHE:CB | 2.50 | 0.95 |
| 1:MA:279:GLU:OE2 | 6:4C:106:ALA:HB3 | 1.66 | 0.95 |
| 1:MC:71:GLU:OE1 | 2:MD:247:ASN:ND2 | 1.98 | 0.95 |
| 2:MF:221:THR:HG21 | 6:4D:189:ARG:CZ | 1.95 | 0.95 |
| 7:5C:874:GLN:HB2 | 8:6C:59:LYS:HZ1 | 0.85 | 0.95 |
| 2:BD:98:GLY:HA2 | 1:BE:254:GLU:HG3 | 1.48 | 0.95 |
| 2:EB:178:THR:HG23 | 1:EC:258:ASN:HD21 | 1.29 | 0.95 |
| 2:IB:177:ASP:OD2 | 1:IC:353:VAL:CG1 | 2.14 | 0.95 |
| 2:ID:98:GLY:C | 1:IE:254:GLU:HG2 | 1.90 | 0.95 |
| 1:JA:89:PRO:HG2 | 1:KA:279:GLU:O | 1.65 | 0.95 |
| 1:KC:85:GLN:CD | 1:LC:282:TYR:HB2 | 1.91 | 0.95 |
| 2:KD:87:PRO:HG3 | 2:LD:282:ARG:HG3 | 0.97 | 0.95 |
| 2:LB:379:LYS:CA | 4:2C:166:ILE:HD11 | 1.75 | 0.95 |
| 2:LD:296:ALA:HB3 | 4:2A:149:ILE:HG23 | 0.99 | 0.95 |
| 2:LD:379:LYS:HZ1 | 4:2A:166:ILE:H | 0.99 | 0.95 |
| 2:MB:111:GLU:HG2 | 3:1A:62:SER:HA | 1.46 | 0.95 |
| 6:4B:252:VAL:HG13 | 6:4B:292:VAL:CG2 | 1.96 | 0.95 |
| 6:4D:289:LYS:HA | 6:4D:289:LYS:HE3 | 1.44 | 0.95 |
| 1:FC:60:LYS:CD | 1:GC:283:HIS:CD2 | 2.42 | 0.95 |
| 1:FE:282:TYR:HE2 | 10:8O:18:UNK:CB | 1.36 | 0.95 |
| 2:HB:98:GLY:C | 1:HC:254:GLU:HG2 | 1.91 | 0.95 |
| 1:HC:159:VAL:CG2 | 5:3C:209:ARG:NH2 | 2.29 | 0.95 |
| 1:HE:101:ASN:HD21 | 2:HF:252:LYS:CD | 1.64 | 0.95 |
| 1:HE:282:TYR:CE2 | 10:8U:15:UNK:O | 2.18 | 0.95 |
| 2:ID:177:ASP:OD2 | 1:IE:353:VAL:CG1 | 2.14 | 0.95 |
| 1:KA:85:GLN:HE22 | 1:LA:282:TYR:CB | 1.79 | 0.95 |
| 2:KD:178:THR:HG23 | 1:KE:258:ASN:HD21 | 1.26 | 0.95 |
| 2:KD:273:LEU:HA | 6:4B:268:LEU:HD23 | 0.96 | 0.95 |
| 2:LB:331:LEU:HD22 | 4:2C:42:PHE:CE2 | 1.87 | 0.95 |
| 2:LF:379:LYS:HZ1 | 4:2B:166:ILE:H | 1.11 | 0.95 |
| 6:4C:252:VAL:HG13 | 6:4C:292:VAL:CG2 | 1.96 | 0.95 |
| 7:5A:1490:LYS:HG3 | 7:5A:1494:LEU:CD2 | 1.96 | 0.95 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1490:LYS:HG3 | 7:5B:1494:LEU:CD2 | 1.96 | 0.95 |
| 7:5B:1544:ILE:C | 7:5B:1570:ALA:HA | 1.76 | 0.95 |
| 7:5C:1490:LYS:HG3 | 7:5C:1494:LEU:CD2 | 1.96 | 0.95 |
| 2:AD:98:GLY:C | 1:AE:254:GLU:HG2 | 1.90 | 0.95 |
| 2:BB:177:ASP:OD2 | 1:BC:248:LEU:CD2 | 2.15 | 0.95 |
| 1:FA:402:ARG:HD3 | 7:5C:1259:TYR:CD2 | 2.02 | 0.95 |
| 2:IB:178:THR:HG23 | 1:IC:258:ASN:HD21 | 1.27 | 0.95 |
| 2:KD:98:GLY:C | 1:KE:254:GLU:HG2 | 1.90 | 0.95 |
| 1:LE:222:PRO:HG2 | 2:LF:324:LYS:HB2 | 1.49 | 0.95 |
| 2:LF:379:LYS:NZ | 4:2B:166:ILE:H | 1.63 | 0.95 |
| 2:CF:86:ARG:CA | 2:DF:281:TYR:HE1 | 1.65 | 0.95 |
| 1:EE:402:ARG:NE | 7:5B:824:ARG:NH2 | 2.14 | 0.95 |
| 1:FA:402:ARG:NH1 | 7:5C:1262:GLU:OE2 | 2.00 | 0.95 |
| 2:JB:55:THR:HG22 | 2:KB:362:LYS:NZ | 1.81 | 0.95 |
| 2:KB:124:ALA:O | 4:2C:38:VAL:HG13 | 1.65 | 0.95 |
| 2:LB:223:GLY:C | 6:4A:219:ASN:ND2 | 2.24 | 0.95 |
| 2:MD:177:ASP:OD1 | 1:ME:353:VAL:CG1 | 2.13 | 0.95 |
| 6:4A:252:VAL:HG13 | 6:4A:292:VAL:CG2 | 1.96 | 0.95 |
| 7:5A:1152:GLU:OE1 | 8:6A:66:ARG:CZ | 2.14 | 0.95 |
| 7:5C:1490:LYS:HD2 | 7:5C:1494:LEU:HB2 | 1.45 | 0.95 |
| 1:DA:282:TYR:HE2 | 10:8G:18:UNK:CB | 1.65 | 0.94 |
| 1:FE:419:SER:CB | 7:5B:1256:ARG:CD | 2.45 | 0.94 |
| 2:GB:98:GLY:C | 1:GC:254:GLU:HG2 | 1.91 | 0.94 |
| 2:ID:424:GLN:HE22 | 7:5A:1413:GLN:CD | 1.57 | 0.94 |
| 1:KA:88:HIS:CA | 1:LA:284:GLU:HB3 | 1.69 | 0.94 |
| 1:MA:101:ASN:CG | 2:MB:252:LYS:HD2 | 1.90 | 0.94 |
| 7:5B:1355:GLN:C | 7:5B:1358:LYS:CG | 2.40 | 0.94 |
| 2:HF:160:PRO:HB3 | 5:3A:330:ARG:HH21 | 1.31 | 0.94 |
| 2:KB:54:ALA:HB2 | 2:LB:285:THR:CG2 | 1.69 | 0.94 |
| 2:KB:177:ASP:OD2 | 1:KC:353:VAL:CG1 | 2.14 | 0.94 |
| 2:KD:177:ASP:OD2 | 1:KE:353:VAL:CG1 | 2.14 | 0.94 |
| 7:5A:1246:LEU:HG | 9:7B:12:GLU:CD | 1.91 | 0.94 |
| 7:5B:773:ARG:O | 7:5B:775:PRO:HD2 | 1.62 | 0.94 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:HD21 | 1.49 | 0.94 |
| 2:BB:98:GLY:HA2 | 1:BC:254:GLU:HG3 | 1.48 | 0.94 |
| 1:DE:414:GLU:OE2 | 7:5B:789:LYS:CE | 2.16 | 0.94 |
| 2:HD:160:PRO:HB3 | 5:3C:330:ARG:NH2 | 1.80 | 0.94 |
| 2:HD:397:TRP:CG | 1:HE:256:GLN:HE22 | 1.34 | 0.94 |
| 2:JB:55:THR:CG2 | 2:KB:362:LYS:HZ1 | 1.54 | 0.94 |
| 1:LC:84:ARG:NH1 | 6:4A:108:LYS:HE2 | 1.78 | 0.94 |
| 1:LE:84:ARG:NH2 | 6:4B:108:LYS:O | 1.88 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MB:110:ALA:O | 3:1A:61:HIS:CB | 2.15 | 0.94 |
| 7:5A:773:ARG:O | 7:5A:775:PRO:HD2 | 1.62 | 0.94 |
| 7:5A:1530:ILE:HD13 | 7:5A:1571:MET:HE1 | 0.95 | 0.94 |
| 7:5B:1530:ILE:HD13 | 7:5B:1571:MET:HE1 | 0.95 | 0.94 |
| 2:KF:215:LEU:HD13 | 6:4D:267:ILE:CG2 | 1.98 | 0.94 |
| 2:MB:178:THR:HG23 | 1:MC:258:ASN:HD21 | 1.32 | 0.94 |
| 7:5A:1355:GLN:C | 7:5A:1358:LYS:CG | 2.40 | 0.94 |
| 7:5C:1126:PRO:HD2 | 8:6C:246:TYR:OH | 1.67 | 0.94 |
| 7:5C:1490:LYS:CD | 7:5C:1494:LEU:HD23 | 1.97 | 0.94 |
| 2:AB:98:GLY:C | 1:AC:254:GLU:HG2 | 1.91 | 0.94 |
| 1:HE:159:VAL:CG2 | 5:3A:209:ARG:NH2 | 2.29 | 0.94 |
| 2:JB:98:GLY:C | 1:JC:254:GLU:HG2 | 1.91 | 0.94 |
| 2:KF:221:THR:HG21 | 6:4D:261:SER:CA | 1.88 | 0.94 |
| 2:LB:55:THR:OG1 | 2:MB:282:ARG:O | 1.85 | 0.94 |
| 1:LC:221:ARG:NH1 | 2:LD:324:LYS:N | 2.16 | 0.94 |
| 7:5A:1490:LYS:HD2 | 7:5A:1494:LEU:HB2 | 1.45 | 0.94 |
| 7:5C:773:ARG:O | 7:5C:775:PRO:HD2 | 1.62 | 0.94 |
| 7:5C:1355:GLN:CA | 7:5C:1358:LYS:CG | 2.46 | 0.94 |
| 7:5C:1530:ILE:HD13 | 7:5C:1571:MET:HE1 | 0.95 | 0.94 |
| 2:BF:86:ARG:HA | 2:CF:281:TYR:CZ | 2.01 | 0.94 |
| 1:CE:398:MET:SD | 2:CF:345:ILE:HG13 | 2.07 | 0.94 |
| 1:JC:89:PRO:HB2 | 1:KC:280:LYS:HG3 | 1.46 | 0.94 |
| 1:KC:62:VAL:HG22 | 1:LC:285:GLN:HB3 | 1.50 | 0.94 |
| 1:LC:176:GLN:O | 2:LD:347:ASN:ND2 | 2.01 | 0.94 |
| 1:MA:283:HIS:NE2 | 6:4C:101:ARG:NH2 | 2.16 | 0.94 |
| 2:MD:178:THR:HG23 | 1:ME:258:ASN:HD21 | 1.29 | 0.94 |
| 7:5A:1490:LYS:CD | 7:5A:1494:LEU:HD23 | 1.97 | 0.94 |
| 7:5C:1355:GLN:C | 7:5C:1358:LYS:CG | 2.40 | 0.94 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:CD2 | 1.98 | 0.94 |
| 1:CC:282:TYR:HE2 | 10:8E:18:UNK:CB | 1.78 | 0.94 |
| 2:EB:54:ALA:CA | 2:FB:283:ALA:HB2 | 1.97 | 0.94 |
| 2:IB:98:GLY:C | 1:IC:254:GLU:HG2 | 1.91 | 0.94 |
| 1:IE:402:ARG:NH2 | 7:5B:1417:GLN:HG3 | 1.82 | 0.94 |
| 2:KB:87:PRO:HG3 | 2:LB:282:ARG:CG | 1.76 | 0.94 |
| 2:KB:158:GLU:HA | 4:2C:34:ASN:HB2 | 0.94 | 0.94 |
| 7:5A:1355:GLN:CA | 7:5A:1358:LYS:CG | 2.46 | 0.94 |
| 7:5C:874:GLN:CB | 8:6C:59:LYS:HZ1 | 1.76 | 0.94 |
| 9:7C:11:TYR:HD1 | 9:7D:26:LEU:CD2 | 1.75 | 0.94 |
| 1:CE:60:LYS:HZ2 | 1:DE:283:HIS:CD2 | 1.86 | 0.94 |
| 1:DA:398:MET:SD | 2:DB:345:ILE:HG13 | 2.08 | 0.94 |
| 2:DB:54:ALA:HA | 2:EB:283:ALA:HB2 | 1.50 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:GC:60:LYS:HD3 | 1:HC:283:HIS:CB | 1.98 | 0.94 |
| 2:HB:397:TRP:CG | 1:HC:256:GLN:HE22 | 1.38 | 0.94 |
| 1:HE:410:GLY:O | 5:3A:329:ARG:NH2 | 1.99 | 0.94 |
| 2:HF:261:PRO:HB2 | 5:3A:337:ARG:HH22 | 1.30 | 0.94 |
| 1:IC:58:ALA:HB1 | 10:8Z:13:UNK:CA | 1.73 | 0.94 |
| 2:KB:178:THR:HG23 | 1:KC:258:ASN:HD21 | 1.27 | 0.94 |
| 2:KB:273:LEU:CB | 6:4A:268:LEU:HD21 | 1.98 | 0.94 |
| 1:LA:89:PRO:CG | 1:MA:280:LYS:CE | 2.45 | 0.94 |
| 2:LD:177:ASP:O | 1:LE:352:LYS:CD | 2.13 | 0.94 |
| 2:LF:413:SER:HB2 | 4:2B:171:VAL:HG21 | 1.46 | 0.94 |
| 7:5A:841:VAL:HG12 | 8:6A:9:LEU:HD23 | 1.48 | 0.94 |
| 7:5A:1243:ASP:CB | 9:7B:8:ARG:HH12 | 1.79 | 0.94 |
| 7:5B:1490:LYS:HD2 | 7:5B:1494:LEU:HB2 | 1.45 | 0.94 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:HD21 | 1.49 | 0.94 |
| 9:7E:11:TYR:HE1 | 9:7F:26:LEU:CB | 1.80 | 0.94 |
| 9:7E:30:ARG:HH12 | 9:7F:3:GLN:CA | 1.80 | 0.94 |
| 1:AE:101:ASN:HD21 | 2:AF:252:LYS:CD | 1.64 | 0.94 |
| 1:FC:71:GLU:OE1 | 2:FD:247:ASN:ND2 | 2.01 | 0.94 |
| 1:FE:398:MET:SD | 2:FF:345:ILE:HG13 | 2.08 | 0.94 |
| 1:GA:89:PRO:HD3 | 1:HA:280:LYS:HZ2 | 1.31 | 0.94 |
| 1:HA:282:TYR:CE2 | 10:8S:15:UNK:O | 2.20 | 0.94 |
| 1:JA:88:HIS:HE1 | 1:KA:280:LYS:O | 1.49 | 0.94 |
| 1:JE:87:PHE:O | 1:KE:283:HIS:HE1 | 1.35 | 0.94 |
| 7:5A:1284:PHE:CD1 | 9:7A:12:GLU:OE1 | 2.20 | 0.94 |
| 7:5B:1355:GLN:CA | 7:5B:1358:LYS:CG | 2.46 | 0.94 |
| 7:5B:1490:LYS:CD | 7:5B:1494:LEU:HD23 | 1.97 | 0.94 |
| 7:5C:1548:VAL:HG11 | 7:5C:1565:GLU:C | 1.92 | 0.94 |
| 2:FB:177:ASP:OD2 | 1:FC:248:LEU:CD2 | 2.15 | 0.94 |
| 1:FC:282:TYR:HE2 | 10:8N:18:UNK:CB | 1.47 | 0.94 |
| 2:FD:220:PRO:O | 1:FE:324:VAL:CG1 | 2.15 | 0.94 |
| 2:LD:296:ALA:HB2 | 4:2A:149:ILE:HG21 | 1.47 | 0.94 |
| 2:LF:296:ALA:CB | 4:2B:149:ILE:HG21 | 1.94 | 0.94 |
| 9:7E:42:LEU:HD12 | 9:7F:39:GLY:HA2 | 1.48 | 0.94 |
| 2:BD:86:ARG:HA | 2:CD:281:TYR:CZ | 2.02 | 0.93 |
| 1:EC:282:TYR:HE2 | 10:8K:18:UNK:CB | 1.68 | 0.93 |
| 1:FA:422:ARG:NE | 7:5C:1170:THR:HB | 1.83 | 0.93 |
| 1:IA:278:ALA:HB3 | 10:8V:21:UNK:C | 1.98 | 0.93 |
| 2:KB:54:ALA:CB | 2:LB:285:THR:HG21 | 1.64 | 0.93 |
| 2:KD:215:LEU:HD13 | 6:4B:267:ILE:HG22 | 0.95 | 0.93 |
| 7:5B:1089:PHE:CD1 | 7:5B:1101:LEU:CD2 | 2.51 | 0.93 |
| 9:7C:18:VAL:HG21 | 9:7D:35:ILE:HG21 | 1.49 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:EC:430:LYS:HZ1 | 7:5A:834:ASN:CG | 1.64 | 0.93 |
| 2:KB:98:GLY:C | 1:KC:254:GLU:HG2 | 1.91 | 0.93 |
| 2:LB:340:TYR:CD1 | 4:2C:147:PHE:CA | 2.44 | 0.93 |
| 7:5A:1089:PHE:CD1 | 7:5A:1101:LEU:CD2 | 2.51 | 0.93 |
| 7:5A:1548:VAL:HG11 | 7:5A:1565:GLU:C | 1.92 | 0.93 |
| 7:5C:1552:LYS:CE | 7:5C:1563:SER:HB2 | 1.98 | 0.93 |
| 9:7E:7:LEU:HD23 | 9:7F:30:ARG:HE | 1.31 | 0.93 |
| 1:IA:279:GLU:CD | 10:8V:22:UNK:CB | 2.41 | 0.93 |
| 1:IE:402:ARG:CZ | 7:5B:1417:GLN:HG3 | 1.99 | 0.93 |
| 2:JD:86:ARG:CZ | 2:KD:280:GLN:C | 2.41 | 0.93 |
| 1:LE:89:PRO:HG3 | 1:ME:280:LYS:HE3 | 1.47 | 0.93 |
| 7:5A:1552:LYS:CE | 7:5A:1563:SER:HB2 | 1.98 | 0.93 |
| 7:5C:1089:PHE:CD1 | 7:5C:1101:LEU:CD2 | 2.51 | 0.93 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:CD2 | 1.97 | 0.93 |
| 2:CD:86:ARG:CA | 2:DD:281:TYR:CZ | 2.33 | 0.93 |
| 1:CE:282:TYR:HE2 | 10:8F:18:UNK:CB | 1.67 | 0.93 |
| 1:FC:89:PRO:HD3 | 1:GC:280:LYS:NZ | 1.53 | 0.93 |
| 2:GB:55:THR:H | 2:HB:283:ALA:HB2 | 1.17 | 0.93 |
| 1:GC:89:PRO:CD | 1:HC:280:LYS:HZ2 | 1.78 | 0.93 |
| 1:JA:101:ASN:HD21 | 2:JB:252:LYS:CD | 1.62 | 0.93 |
| 2:LB:55:THR:H | 2:MB:283:ALA:HB2 | 1.20 | 0.93 |
| 2:LF:55:THR:H | 2:MF:283:ALA:HB2 | 1.17 | 0.93 |
| 2:MD:177:ASP:OD2 | 1:ME:248:LEU:CD2 | 2.16 | 0.93 |
| 7:5B:1548:VAL:HG11 | 7:5B:1565:GLU:C | 1.92 | 0.93 |
| 2:AD:359:LYS:N | 6:4C:151:ARG:HH22 | 1.42 | 0.93 |
| 2:KB:54:ALA:CA | 2:LB:285:THR:HG22 | 1.98 | 0.93 |
| 7:5B:841:VAL:HG12 | 8:6B:9:LEU:HD23 | 1.51 | 0.93 |
| 7:5B:1245:GLY:HA3 | 9:7D:12:GLU:OE1 | 1.66 | 0.93 |
| 2:AB:177:ASP:OD2 | 1:AC:353:VAL:CG1 | 2.14 | 0.93 |
| 2:GB:412:GLU:OE2 | 7:5C:1323:MET:HE1 | 1.68 | 0.93 |
| 1:GC:56:THR:OG1 | 1:HC:284:GLU:HA | 1.66 | 0.93 |
| 1:KA:101:ASN:HD21 | 2:KB:252:LYS:CD | 1.61 | 0.93 |
| 2:MD:221:THR:HG21 | 6:4B:189:ARG:CZ | 1.99 | 0.93 |
| 7:5B:1355:GLN:C | 7:5B:1358:LYS:HG2 | 1.94 | 0.93 |
| 7:5B:1552:LYS:CE | 7:5B:1563:SER:HB2 | 1.98 | 0.93 |
| 1:BA:101:ASN:HD21 | 2:BB:252:LYS:CD | 1.66 | 0.93 |
| 1:DA:101:ASN:HD21 | 2:DB:252:LYS:CD | 1.61 | 0.93 |
| 1:IC:278:ALA:HB3 | 10:8W:21:UNK:C | 1.98 | 0.93 |
| 1:IC:402:ARG:HH22 | 7:5A:1418:GLN:CA | 1.81 | 0.93 |
| 7:5A:1355:GLN:C | 7:5A:1358:LYS:HG2 | 1.94 | 0.93 |
| 2:AD:177:ASP:OD2 | 1:AE:353:VAL:CG1 | 2.14 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:JF:86:ARG:CZ | 2:KF:280:GLN:C | 2.31 | 0.93 |
| 1:LA:222:PRO:CD | 2:LB:324:LYS:CD | 2.43 | 0.93 |
| 1:MA:71:GLU:OE1 | 2:MB:247:ASN:ND2 | 2.01 | 0.93 |
| 7:5B:1490:LYS:HD2 | 7:5B:1494:LEU:CD2 | 1.99 | 0.93 |
| 7:5C:1355:GLN:C | 7:5C:1358:LYS:HG2 | 1.94 | 0.93 |
| 1:EA:370:LYS:HZ3 | 10:8J:17:UNK:CB | 1.64 | 0.93 |
| 1:IC:278:ALA:HB3 | 10:8W:21:UNK:CB | 1.94 | 0.93 |
| 2:LB:55:THR:CG2 | 2:MB:283:ALA:CB | 2.42 | 0.93 |
| 2:LD:55:THR:OG1 | 2:MD:282:ARG:O | 1.85 | 0.93 |
| 2:LD:178:THR:HG23 | 1:LE:258:ASN:HD21 | 1.31 | 0.93 |
| 2:MD:111:GLU:HG2 | 3:1B:62:SER:CB | 1.99 | 0.93 |
| 7:5A:1490:LYS:HD2 | 7:5A:1494:LEU:CD2 | 1.99 | 0.93 |
| 7:5B:1530:ILE:CD1 | 7:5B:1571:MET:CE | 2.42 | 0.93 |
| 7:5C:1490:LYS:HD2 | 7:5C:1494:LEU:CD2 | 1.99 | 0.93 |
| 2:AF:359:LYS:N | 6:4A:151:ARG:HH21 | 1.52 | 0.93 |
| 2:LF:224:ASP:H | 6:4D:219:ASN:HD21 | 0.93 | 0.93 |
| 1:ME:279:GLU:CG | 6:4B:110:LYS:HE3 | 1.99 | 0.93 |
| 7:5C:1548:VAL:HG13 | 7:5C:1565:GLU:OE1 | 1.68 | 0.93 |
| 9:7A:18:VAL:HG21 | 9:7B:35:ILE:HG21 | 1.49 | 0.93 |
| 1:CA:370:LYS:HZ1 | 10:8D:17:UNK:CB | 1.76 | 0.92 |
| 2:FB:98:GLY:CA | 1:FC:254:GLU:CG | 2.26 | 0.92 |
| 2:JD:86:ARG:HH22 | 2:KD:280:GLN:CB | 1.82 | 0.92 |
| 2:KF:86:ARG:NH1 | 2:LF:283:ALA:H | 1.65 | 0.92 |
| 1:MC:279:GLU:CG | 6:4A:110:LYS:HE3 | 1.98 | 0.92 |
| 1:MC:282:TYR:HD2 | 6:4A:104:ARG:CD | 1.82 | 0.92 |
| 2:MD:177:ASP:OD2 | 1:ME:248:LEU:HD21 | 1.68 | 0.92 |
| 2:EF:157:GLU:CD | 7:5B:935:LYS:HZ2 | 1.74 | 0.92 |
| 2:FD:177:ASP:OD2 | 1:FE:248:LEU:CD2 | 2.18 | 0.92 |
| 2:FF:55:THR:HG23 | 2:GF:283:ALA:CB | 1.98 | 0.92 |
| 7:5A:1521:PHE:CE2 | 7:5A:1571:MET:HG2 | 2.03 | 0.92 |
| 7:5A:1530:ILE:CD1 | 7:5A:1571:MET:CE | 2.42 | 0.92 |
| 7:5B:1246:LEU:N | 9:7D:12:GLU:CD | 2.27 | 0.92 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:CG | 2.18 | 0.92 |
| 7:5B:1491:LEU:CD1 | 7:5B:1495:PHE:CE1 | 2.52 | 0.92 |
| 7:5B:1491:LEU:HD11 | 7:5B:1495:PHE:CD1 | 1.97 | 0.92 |
| 7:5C:1521:PHE:CE2 | 7:5C:1571:MET:HG2 | 2.03 | 0.92 |
| 9:7A:7:LEU:CD2 | 9:7B:27:GLY:C | 2.36 | 0.92 |
| 1:BE:398:MET:SD | 2:BF:345:ILE:HG13 | 2.09 | 0.92 |
| 1:GE:60:LYS:HD3 | 1:HE:283:HIS:CA | 1.97 | 0.92 |
| 1:HC:282:TYR:CZ | 10:8T:15:UNK:O | 2.21 | 0.92 |
| 1:JE:101:ASN:HD21 | 2:JF:252:LYS:CD | 1.64 | 0.92 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:KC:79:ARG:CB | 1:LC:280:LYS:HZ1 | 0.73 | 0.92 |
| 2:KF:227:HIS:HB3 | 6:4D:267:ILE:HD11 | 1.48 | 0.92 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:CG | 2.17 | 0.92 |
| 7:5A:1491:LEU:CD1 | 7:5A:1495:PHE:CE1 | 2.52 | 0.92 |
| 7:5A:1549:THR:N | 7:5A:1566:GLU:HG2 | 1.84 | 0.92 |
| 7:5B:1521:PHE:CE2 | 7:5B:1571:MET:HG2 | 2.03 | 0.92 |
| 7:5B:1549:THR:N | 7:5B:1566:GLU:HG2 | 1.84 | 0.92 |
| 7:5C:1491:LEU:HD11 | 7:5C:1495:PHE:CD1 | 1.97 | 0.92 |
| 2:AD:276:ARG:NH1 | 6:4C:137:ASN:O | 2.01 | 0.92 |
| 2:DB:220:PRO:HD2 | 1:DC:326:LYS:HE2 | 1.50 | 0.92 |
| 2:GD:412:GLU:OE2 | 7:5A:1323:MET:CE | 2.17 | 0.92 |
| 2:HD:261:PRO:HB2 | 5:3C:337:ARG:HH22 | 1.31 | 0.92 |
| 1:JE:89:PRO:HB2 | 1:KE:280:LYS:HG3 | 1.48 | 0.92 |
| 2:KD:118:ASP:CG | 4:2A:148:ASN:HD21 | 1.77 | 0.92 |
| 2:LB:274:THR:O | 6:4A:228:LEU:HD23 | 1.70 | 0.92 |
| 7:5A:1491:LEU:HD11 | 7:5A:1495:PHE:CD1 | 1.97 | 0.92 |
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:CG | 2.17 | 0.92 |
| 7:5C:1491:LEU:CD1 | 7:5C:1495:PHE:CE1 | 2.52 | 0.92 |
| 7:5C:1530:ILE:CD1 | 7:5C:1571:MET:CE | 2.42 | 0.92 |
| 7:5C:1549:THR:N | 7:5C:1566:GLU:HG2 | 1.84 | 0.92 |
| 2:EB:125:GLU:CB | 7:5C:903:PHE:HE2 | 1.75 | 0.92 |
| 1:KE:101:ASN:HD21 | 2:KF:252:LYS:CD | 1.64 | 0.92 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CE2 | 2.36 | 0.92 |
| 7:5A:1548:VAL:HG13 | 7:5A:1565:GLU:OE1 | 1.68 | 0.92 |
| 7:5B:1545:TYR:N | 7:5B:1570:ALA:HB2 | 1.84 | 0.92 |
| 7:5C:1246:LEU:CB | 9:7F:12:GLU:OE2 | 2.16 | 0.92 |
| 2:DB:220:PRO:O | 1:DC:324:VAL:HG11 | 1.69 | 0.92 |
| 1:FC:422:ARG:HE | 7:5A:1170:THR:HB | 1.29 | 0.92 |
| 2:KB:87:PRO:HG2 | 2:LB:282:ARG:CD | 1.99 | 0.92 |
| 2:LB:379:LYS:HZ1 | 4:2C:166:ILE:H | 1.10 | 0.92 |
| 7:5A:1077:ASN:OD1 | 7:5A:1083:THR:HG21 | 1.69 | 0.92 |
| 7:5C:1077:ASN:OD1 | 7:5C:1083:THR:HG21 | 1.70 | 0.92 |
| 2:AD:359:LYS:N | 6:4C:151:ARG:HH21 | 1.47 | 0.92 |
| 2:CB:86:ARG:CA | 2:DB:281:TYR:HE1 | 1.64 | 0.92 |
| 2:DD:220:PRO:O | 1:DE:324:VAL:HG11 | 1.68 | 0.92 |
| 2:DF:86:ARG:HA | 2:EF:281:TYR:CZ | 2.04 | 0.92 |
| 1:FC:89:PRO:N | 1:GC:280:LYS:HZ2 | 1.68 | 0.92 |
| 1:IC:101:ASN:HD21 | 2:ID:252:LYS:CD | 1.58 | 0.92 |
| 2:KB:83:GLN:HE22 | 2:LB:281:TYR:HE2 | 0.95 | 0.92 |
| 2:LF:306:ARG:HH22 | 4:2B:151:VAL:HG23 | 1.25 | 0.92 |
| 1:MC:283:HIS:NE2 | 6:4A:101:ARG:NH2 | 2.18 | 0.92 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1545:TYR:N | 7:5A:1570:ALA:HB2 | 1.84 | 0.92 |
| 7:5B:839:GLU:OE2 | 8:6B:11:PRO:HG2 | 1.69 | 0.92 |
| 9:7A:42:LEU:CD1 | 9:7B:39:GLY:CA | 2.47 | 0.92 |
| 2:IF:86:ARG:NH1 | 2:JF:281:TYR:HA | 1.81 | 0.92 |
| 1:KA:85:GLN:NE2 | 1:LA:282:TYR:HB3 | 1.84 | 0.92 |
| 2:KF:87:PRO:HG2 | 2:LF:282:ARG:HG3 | 1.48 | 0.92 |
| 1:LC:222:PRO:CD | 2:LD:324:LYS:CD | 2.46 | 0.92 |
| 5:3B:231:THR:C | 5:3B:335:LYS:CB | 2.43 | 0.92 |
| 7:5B:1077:ASN:OD1 | 7:5B:1083:THR:HG21 | 1.70 | 0.92 |
| 9:7E:36:GLN:HA | 9:7F:43:LEU:CD2 | 2.00 | 0.92 |
| 1:FC:402:ARG:CD | 7:5A:1259:TYR:HD2 | 1.83 | 0.92 |
| 1:FE:60:LYS:HZ2 | 1:GE:283:HIS:CE1 | 1.88 | 0.92 |
| 1:FE:60:LYS:NZ | 1:GE:283:HIS:ND1 | 2.18 | 0.92 |
| 1:KC:101:ASN:CG | 2:KD:252:LYS:HD2 | 1.95 | 0.92 |
| 1:KE:88:HIS:CA | 1:LE:284:GLU:CB | 2.42 | 0.92 |
| 1:LE:222:PRO:CD | 2:LF:324:LYS:CD | 2.47 | 0.92 |
| 1:AE:342:GLN:NE2 | 3:1A:55:HIS:NE2 | 2.18 | 0.92 |
| 1:CC:101:ASN:HD21 | 2:CD:252:LYS:CD | 1.63 | 0.92 |
| 2:CF:87:PRO:CD | 2:DF:281:TYR:CE2 | 2.53 | 0.92 |
| 1:KC:85:GLN:HE22 | 1:LC:282:TYR:CB | 1.82 | 0.92 |
| 2:LB:310:TYR:HE2 | 4:2C:147:PHE:CZ | 1.88 | 0.92 |
| 2:LD:55:THR:H | 2:MD:283:ALA:HB2 | 1.13 | 0.92 |
| 2:LD:223:GLY:C | 6:4B:219:ASN:ND2 | 2.27 | 0.92 |
| 2:LF:416:ASN:CA | 4:2B:168:LEU:CD1 | 2.47 | 0.92 |
| 2:MB:111:GLU:HG2 | 3:1A:62:SER:CB | 2.00 | 0.92 |
| 7:5B:1243:ASP:CG | 9:7D:8:ARG:NH1 | 2.27 | 0.92 |
| 7:5B:1548:VAL:HG13 | 7:5B:1565:GLU:OE1 | 1.68 | 0.92 |
| 1:FE:71:GLU:OE1 | 2:FF:247:ASN:ND2 | 2.03 | 0.91 |
| 1:JC:88:HIS:NE2 | 1:KC:280:LYS:O | 2.03 | 0.91 |
| 2:LD:306:ARG:CZ | 4:2A:149:ILE:CG2 | 2.48 | 0.91 |
| 2:LF:340:TYR:CG | 4:2B:147:PHE:HB2 | 2.03 | 0.91 |
| 7:5A:1243:ASP:HB3 | 9:7B:8:ARG:NH1 | 1.85 | 0.91 |
| 7:5C:1545:TYR:N | 7:5C:1570:ALA:HB2 | 1.84 | 0.91 |
| 1:LE:76:ASP:OD1 | 2:LF:46:ARG:NH2 | 2.03 | 0.91 |
| 5:3A:231:THR:C | 5:3A:335:LYS:CB | 2.43 | 0.91 |
| 7:5A:1482:SER:O | 7:5A:1486:THR:OG1 | 1.88 | 0.91 |
| 7:5B:1482:SER:O | 7:5B:1486:THR:OG1 | 1.88 | 0.91 |
| 7:5C:1482:SER:O | 7:5C:1486:THR:OG1 | 1.88 | 0.91 |
| 1:AE:342:GLN:NE2 | 3:1A:55:HIS:CE1 | 2.39 | 0.91 |
| 2:DD:220:PRO:HD2 | 1:DE:326:LYS:HE2 | 1.50 | 0.91 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:CD | 2.48 | 0.91 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KC:85:GLN:C | 1:LC:283:HIS:HA | 1.94 | 0.91 |
| 1:ME:71:GLU:OE1 | 2:MF:247:ASN:ND2 | 2.02 | 0.91 |
| 6:4C:285:ARG:HB3 | 6:4C:285:ARG:NH1 | 1.85 | 0.91 |
| 1:CA:282:TYR:HE2 | 10:8D:18:UNK:CB | 1.75 | 0.91 |
| 1:DC:402:ARG:NH2 | 7:5A:782:LEU:CD1 | 2.03 | 0.91 |
| 1:FE:419:SER:OG | 7:5B:1256:ARG:CD | 2.18 | 0.91 |
| 1:HC:282:TYR:HE2 | 10:8T:19:UNK:N | 1.35 | 0.91 |
| 1:IC:101:ASN:CG | 2:ID:252:LYS:HD2 | 1.95 | 0.91 |
| 2:JF:86:ARG:NH1 | 2:KF:280:GLN:C | 2.29 | 0.91 |
| 2:KB:127:CYS:N | 4:2C:38:VAL:CB | 2.25 | 0.91 |
| 2:MD:110:ALA:O | 3:1B:61:HIS:HB3 | 1.70 | 0.91 |
| 7:5B:1423:LYS:HA | 7:5B:1423:LYS:NZ | 1.85 | 0.91 |
| 7:5B:1547:SER:C | 7:5B:1569:GLU:CD | 2.37 | 0.91 |
| 2:EF:125:GLU:CG | 7:5B:903:PHE:CD2 | 2.43 | 0.91 |
| 1:KE:85:GLN:HE22 | 1:LE:282:TYR:CB | 1.82 | 0.91 |
| 6:4A:285:ARG:NH1 | 6:4A:285:ARG:HB3 | 1.85 | 0.91 |
| 9:7A:38:LEU:HD23 | 9:7B:42:LEU:HD13 | 1.50 | 0.91 |
| 9:7E:18:VAL:CG1 | 9:7E:42:LEU:CD2 | 2.49 | 0.91 |
| 2:AF:223:GLY:C | 6:4A:131:VAL:HB | 1.94 | 0.91 |
| 2:DB:220:PRO:HD2 | 1:DC:326:LYS:HG2 | 1.52 | 0.91 |
| 1:EE:426:ALA:HB3 | 7:5B:833:PHE:HB2 | 1.52 | 0.91 |
| 2:GD:55:THR:CA | 2:HD:283:ALA:HB2 | 1.99 | 0.91 |
| 1:HC:101:ASN:CG | 2:HD:252:LYS:HD2 | 1.95 | 0.91 |
| 2:KB:77:ARG:CG | 2:LB:281:TYR:CE1 | 2.53 | 0.91 |
| 2:KB:127:CYS:H | 4:2C:38:VAL:HG12 | 0.75 | 0.91 |
| 1:KC:79:ARG:CD | 1:LC:280:LYS:NZ | 2.34 | 0.91 |
| 7:5C:1423:LYS:HA | 7:5C:1423:LYS:NZ | 1.85 | 0.91 |
| 9:7C:18:VAL:CG1 | 9:7C:42:LEU:CD2 | 2.49 | 0.91 |
| 2:BD:177:ASP:CG | 1:BE:353:VAL:HG11 | 1.94 | 0.91 |
| 1:CC:60:LYS:HZ2 | 1:DC:283:HIS:CD2 | 1.88 | 0.91 |
| 1:FA:60:LYS:CD | 1:GA:283:HIS:CD2 | 2.48 | 0.91 |
| 2:FB:212:PHE:HZ | 1:FC:326:LYS:HD3 | 0.74 | 0.91 |
| 1:HA:278:ALA:HB3 | 10:8S:22:UNK:N | 1.84 | 0.91 |
| 2:LF:294:PHE:HD2 | 4:2B:147:PHE:CZ | 1.87 | 0.91 |
| 6:4B:285:ARG:NH1 | 6:4B:285:ARG:HB3 | 1.85 | 0.91 |
| 7:5A:1547:SER:C | 7:5A:1569:GLU:CD | 2.37 | 0.91 |
| 7:5C:1246:LEU:CA | 9:7F:12:GLU:OE2 | 2.19 | 0.91 |
| 2:FF:428:ALA:HB1 | 7:5B:1080:PHE:HE1 | 0.87 | 0.91 |
| 1:GC:101:ASN:HD21 | 2:GD:252:LYS:CD | 1.58 | 0.91 |
| 1:IE:402:ARG:HH21 | 7:5B:1417:GLN:CG | 1.84 | 0.91 |
| 1:JA:87:PHE:C | 1:KA:283:HIS:CE1 | 2.41 | 0.91 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KC:88:HIS:HA | 1:LC:284:GLU:CA | 2.01 | 0.91 |
| 2:LB:379:LYS:C | 4:2C:166:ILE:CD1 | 2.42 | 0.91 |
| 1:MA:101:ASN:HD22 | 2:MB:252:LYS:HG3 | 1.35 | 0.91 |
| 2:MB:177:ASP:OD2 | 1:MC:353:VAL:CG1 | 2.17 | 0.91 |
| 1:MC:101:ASN:CG | 2:MD:252:LYS:HD2 | 1.94 | 0.91 |
| 5:3C:231:THR:C | 5:3C:335:LYS:CB | 2.43 | 0.91 |
| 7:5A:1423:LYS:NZ | 7:5A:1423:LYS:HA | 1.85 | 0.91 |
| 9:7A:30:ARG:NH1 | 9:7B:3:GLN:CA | 2.14 | 0.91 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:NZ | 1.84 | 0.91 |
| 1:GA:89:PRO:CG | 1:HA:280:LYS:HD2 | 2.00 | 0.91 |
| 2:KB:177:ASP:OD2 | 1:KC:248:LEU:HD21 | 1.71 | 0.91 |
| 2:KB:217:LEU:HB3 | 6:4A:265:TYR:HH | 1.23 | 0.91 |
| 2:KD:177:ASP:OD2 | 1:KE:248:LEU:HD21 | 1.71 | 0.91 |
| 2:KF:217:LEU:HB3 | 6:4D:265:TYR:HH | 1.10 | 0.91 |
| 2:LB:55:THR:N | 2:MB:283:ALA:CB | 2.31 | 0.91 |
| 2:LD:55:THR:HG21 | 2:MD:284:LEU:H | 1.36 | 0.91 |
| 9:7C:38:LEU:HD23 | 9:7D:42:LEU:HD13 | 1.50 | 0.91 |
| 2:AB:177:ASP:OD2 | 1:AC:248:LEU:HD21 | 1.70 | 0.91 |
| 2:AD:356:ILE:HD12 | 6:4C:152:PHE:HE1 | 1.35 | 0.91 |
| 1:EC:101:ASN:CG | 2:ED:252:LYS:HD2 | 1.95 | 0.91 |
| 2:GB:177:ASP:CG | 1:GC:353:VAL:HG11 | 1.95 | 0.91 |
| 1:IA:76:ASP:OD1 | 2:IB:46:ARG:NH2 | 2.04 | 0.91 |
| 1:JA:128:ASN:HD22 | 1:KA:285:GLN:NE2 | 1.68 | 0.91 |
| 1:JC:101:ASN:CG | 2:JD:252:LYS:HD2 | 1.95 | 0.91 |
| 1:KA:76:ASP:OD1 | 2:KB:46:ARG:NH2 | 2.04 | 0.91 |
| 2:LF:340:TYR:CD1 | 4:2B:147:PHE:CB | 2.54 | 0.91 |
| 1:ME:398:MET:SD | 2:MF:345:ILE:HG13 | 2.10 | 0.91 |
| 9:7C:42:LEU:CD1 | 9:7D:39:GLY:CA | 2.47 | 0.91 |
| 9:7E:11:TYR:CE1 | 9:7F:26:LEU:CD2 | 2.53 | 0.91 |
| 1:CE:101:ASN:HD21 | 2:CF:252:LYS:CD | 1.65 | 0.90 |
| 1:JA:76:ASP:OD1 | 2:JB:46:ARG:NH2 | 2.04 | 0.90 |
| 2:KD:55:THR:HG21 | 2:LD:363:MET:HE1 | 0.92 | 0.90 |
| 1:KE:85:GLN:N | 1:LE:283:HIS:CD2 | 2.23 | 0.90 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:HD2 | 1.99 | 0.90 |
| 2:LB:306:ARG:NH2 | 4:2C:151:VAL:CG2 | 2.27 | 0.90 |
| 2:LD:306:ARG:CZ | 4:2A:149:ILE:HG22 | 2.00 | 0.90 |
| 2:LF:379:LYS:HZ1 | 4:2B:166:ILE:N | 1.69 | 0.90 |
| 7:5C:1547:SER:C | 7:5C:1569:GLU:CD | 2.37 | 0.90 |
| 1:FE:422:ARG:HE | 7:5B:1170:THR:HB | 1.28 | 0.90 |
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:CG | 2.00 | 0.90 |
| 1:LC:89:PRO:CG | 1:MC:280:LYS:CD | 2.45 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4C:244:GLU:HG3 | 6:4C:284:LEU:HD11 | 1.54 | 0.90 |
| 6:4D:285:ARG:HB3 | 6:4D:285:ARG:NH1 | 1.85 | 0.90 |
| 2:CB:397:TRP:CG | 1:CC:256:GLN:HE22 | 1.43 | 0.90 |
| 2:FB:178:THR:HG23 | 1:FC:258:ASN:HD21 | 1.34 | 0.90 |
| 2:LB:98:GLY:CA | 1:LC:254:GLU:HG2 | 2.01 | 0.90 |
| 1:MC:279:GLU:HG3 | 6:4A:110:LYS:HE2 | 1.51 | 0.90 |
| 6:4A:244:GLU:HG3 | 6:4A:284:LEU:HD11 | 1.54 | 0.90 |
| 9:7A:18:VAL:CG1 | 9:7A:42:LEU:CD2 | 2.49 | 0.90 |
| 2:AD:177:ASP:OD2 | 1:AE:248:LEU:HD21 | 1.71 | 0.90 |
| 2:KF:77:ARG:CG | 2:LF:281:TYR:CE1 | 2.52 | 0.90 |
| 6:4B:244:GLU:HG3 | 6:4B:284:LEU:HD11 | 1.54 | 0.90 |
| 7:5B:1530:ILE:HD11 | 7:5B:1571:MET:HE1 | 1.52 | 0.90 |
| 1:AC:101:ASN:CG | 2:AD:252:LYS:HD2 | 1.95 | 0.90 |
| 2:AF:356:ILE:HD12 | 6:4A:152:PHE:CD1 | 2.06 | 0.90 |
| 2:CD:220:PRO:HD2 | 1:CE:326:LYS:HG2 | 1.52 | 0.90 |
| 2:DB:98:GLY:HA2 | 1:DC:254:GLU:HG3 | 1.53 | 0.90 |
| 1:FE:60:LYS:CD | 1:GE:283:HIS:CD2 | 2.53 | 0.90 |
| 1:GC:101:ASN:CG | 2:GD:252:LYS:HD2 | 1.95 | 0.90 |
| 2:LF:296:ALA:HB3 | 4:2B:149:ILE:CG2 | 1.89 | 0.90 |
| 7:5A:1530:ILE:HD11 | 7:5A:1571:MET:HE1 | 1.52 | 0.90 |
| 7:5C:1105:TYR:CB | 7:5C:1166:LEU:N | 2.34 | 0.90 |
| 2:AD:177:ASP:CG | 1:AE:353:VAL:HG11 | 1.96 | 0.90 |
| 1:GE:402:ARG:CZ | 5:3A:381:ASN:ND2 | 2.24 | 0.90 |
| 2:HB:177:ASP:CG | 1:HC:353:VAL:HG11 | 1.95 | 0.90 |
| 1:HC:101:ASN:HD22 | 2:HD:252:LYS:HG3 | 1.36 | 0.90 |
| 1:JA:89:PRO:CD | 1:KA:283:HIS:ND1 | 2.16 | 0.90 |
| 2:KD:86:ARG:NH1 | 2:LD:283:ALA:CA | 2.19 | 0.90 |
| 1:MA:279:GLU:HG3 | 6:4C:110:LYS:CE | 2.01 | 0.90 |
| 5:3C:229:PHE:CE2 | 5:3C:331:GLN:CG | 2.46 | 0.90 |
| 6:4D:244:GLU:HG3 | 6:4D:284:LEU:HD11 | 1.53 | 0.90 |
| 7:5C:1530:ILE:HD11 | 7:5C:1571:MET:HE1 | 1.52 | 0.90 |
| 2:AD:397:TRP:CG | 1:AE:256:GLN:HE22 | 1.34 | 0.90 |
| 2:CD:177:ASP:CG | 1:CE:353:VAL:HG11 | 1.96 | 0.90 |
| 2:FD:55:THR:H | 2:GD:283:ALA:CA | 1.84 | 0.90 |
| 2:KD:217:LEU:HD22 | 6:4B:263:CYS:HG | 1.14 | 0.90 |
| 2:KF:88:ASP:OD2 | 4:2B:150:GLN:NE2 | 2.05 | 0.90 |
| 2:KF:276:ARG:NH1 | 6:4D:271:GLU:CA | 1.70 | 0.90 |
| 1:LA:176:GLN:NE2 | 4:2C:42:PHE:CB | 2.33 | 0.90 |
| 2:MB:177:ASP:OD2 | 1:MC:353:VAL:HG13 | 1.72 | 0.90 |
| 7:5A:839:GLU:CD | 8:6A:107:PRO:O | 2.14 | 0.90 |
| 7:5A:1105:TYR:CB | 7:5A:1166:LEU:N | 2.34 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1105:TYR:CB | 7:5B:1166:LEU:N | 2.34 | 0.90 |
| 7:5C:1490:LYS:C | 7:5C:1495:PHE:HB3 | 1.94 | 0.90 |
| 7:5C:1544:ILE:CD1 | 7:5C:1570:ALA:O | 2.03 | 0.90 |
| 2:FB:55:THR:N | 2:GB:283:ALA:CA | 2.16 | 0.90 |
| 2:FF:331:LEU:CD2 | 7:5B:915:PHE:CZ | 2.54 | 0.90 |
| 1:GC:56:THR:C | 1:HC:285:GLN:HB3 | 1.97 | 0.90 |
| 1:HA:76:ASP:OD1 | 2:HB:46:ARG:NH2 | 2.04 | 0.90 |
| 1:JC:76:ASP:OD1 | 2:JD:46:ARG:NH2 | 2.05 | 0.90 |
| 2:KD:86:ARG:HH11 | 2:LD:283:ALA:HB3 | 1.29 | 0.90 |
| 1:KE:76:ASP:OD1 | 2:KF:46:ARG:NH2 | 2.05 | 0.90 |
| 1:LE:221:ARG:NH1 | 2:LF:324:LYS:N | 2.20 | 0.90 |
| 7:5B:1490:LYS:CD | 7:5B:1494:LEU:CD2 | 2.49 | 0.90 |
| 7:5C:1515:GLU:CG | 7:5C:1563:SER:HA | 2.01 | 0.90 |
| 8:6B:131:ASP:N | 8:6B:136:LEU:HD12 | 1.87 | 0.90 |
| 9:7C:7:LEU:CD2 | 9:7D:27:GLY:C | 2.36 | 0.90 |
| 2:ED:86:ARG:HA | 2:FD:281:TYR:CE1 | 2.06 | 0.90 |
| 1:GA:89:PRO:HG3 | 1:HA:280:LYS:CD | 2.02 | 0.90 |
| 1:GC:89:PRO:CD | 1:HC:280:LYS:NZ | 2.33 | 0.90 |
| 2:GD:177:ASP:CG | 1:GE:353:VAL:HG11 | 1.96 | 0.90 |
| 2:GD:177:ASP:OD2 | 1:GE:248:LEU:HD21 | 1.71 | 0.90 |
| 1:HC:159:VAL:HG21 | 5:3C:209:ARG:NE | 1.86 | 0.90 |
| 1:IE:76:ASP:OD1 | 2:IF:46:ARG:NH2 | 2.05 | 0.90 |
| 1:KA:85:GLN:OE1 | 1:LA:282:TYR:C | 2.14 | 0.90 |
| 2:KB:127:CYS:CB | 4:2C:38:VAL:HG21 | 1.98 | 0.90 |
| 1:KC:76:ASP:OD1 | 2:KD:46:ARG:NH2 | 2.05 | 0.90 |
| 1:MC:279:GLU:CB | 6:4A:110:LYS:HE3 | 2.02 | 0.90 |
| 7:5A:1243:ASP:CG | 9:7B:8:ARG:NH1 | 2.30 | 0.90 |
| 7:5A:1490:LYS:CD | 7:5A:1494:LEU:CD2 | 2.49 | 0.90 |
| 7:5A:1490:LYS:C | 7:5A:1495:PHE:HB3 | 1.94 | 0.90 |
| 7:5A:1544:ILE:CD1 | 7:5A:1570:ALA:O | 2.03 | 0.90 |
| 7:5B:1544:ILE:CD1 | 7:5B:1570:ALA:O | 2.03 | 0.90 |
| 7:5C:1491:LEU:N | 7:5C:1495:PHE:CB | 2.33 | 0.90 |
| 8:6A:131:ASP:N | 8:6A:136:LEU:HD12 | 1.86 | 0.90 |
| 2:AB:220:PRO:O | 1:AC:324:VAL:CG1 | 2.20 | 0.90 |
| 2:AD:55:THR:HG23 | 2:BD:283:ALA:HA | 1.54 | 0.90 |
| 2:AF:359:LYS:HA | 6:4A:151:ARG:NH2 | 1.85 | 0.90 |
| 2:BB:177:ASP:OD2 | 1:BC:248:LEU:HD21 | 1.71 | 0.90 |
| 1:FC:402:ARG:NH1 | 7:5A:1262:GLU:OE2 | 2.05 | 0.90 |
| 2:GD:58:ARG:NH2 | 2:HD:281:TYR:CZ | 2.40 | 0.90 |
| 1:JE:76:ASP:OD1 | 2:JF:46:ARG:NH2 | 2.05 | 0.90 |
| 2:KF:276:ARG:HE | 6:4D:265:TYR:HB2 | 1.36 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LC:60:LYS:HD2 | 6:4A:101:ARG:CZ | 2.00 | 0.90 |
| 7:5A:1515:GLU:CG | 7:5A:1563:SER:HA | 2.01 | 0.90 |
| 7:5B:1491:LEU:N | 7:5B:1495:PHE:CB | 2.33 | 0.90 |
| 2:ED:54:ALA:CA | 2:FD:283:ALA:HB2 | 2.03 | 0.89 |
| 1:FA:56:THR:OG1 | 1:GA:285:GLN:N | 2.04 | 0.89 |
| 1:FC:76:ASP:OD1 | 2:FD:46:ARG:NH2 | 2.05 | 0.89 |
| 2:IB:177:ASP:OD2 | 1:IC:248:LEU:HD21 | 1.70 | 0.89 |
| 1:JA:89:PRO:HB2 | 1:KA:280:LYS:HG2 | 0.98 | 0.89 |
| 1:LA:89:PRO:HG3 | 1:MA:280:LYS:HE3 | 1.51 | 0.89 |
| 7:5C:839:GLU:CD | 8:6C:107:PRO:O | 2.15 | 0.89 |
| 2:AB:397:TRP:CG | 1:AC:256:GLN:HE22 | 1.38 | 0.89 |
| 1:BC:101:ASN:HD21 | 2:BD:252:LYS:CD | 1.64 | 0.89 |
| 2:CF:86:ARG:CA | 2:DF:281:TYR:CZ | 2.34 | 0.89 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:CE | 2.01 | 0.89 |
| 2:GB:177:ASP:OD2 | 1:GC:248:LEU:HD21 | 1.71 | 0.89 |
| 1:IC:76:ASP:OD1 | 2:ID:46:ARG:NH2 | 2.05 | 0.89 |
| 1:IC:101:ASN:HD22 | 2:ID:252:LYS:CD | 1.85 | 0.89 |
| 2:JB:220:PRO:O | 1:JC:324:VAL:CG1 | 2.20 | 0.89 |
| 1:LA:84:ARG:NH2 | 6:4C:108:LYS:O | 2.01 | 0.89 |
| 2:LF:55:THR:N | 2:MF:283:ALA:CB | 2.34 | 0.89 |
| 1:MA:279:GLU:CB | 6:4C:110:LYS:HE3 | 2.01 | 0.89 |
| 2:MB:177:ASP:OD1 | 1:MC:353:VAL:CG1 | 2.19 | 0.89 |
| 4:2B:33:GLN:NE2 | 4:2B:51:VAL:O | 2.05 | 0.89 |
| 4:2C:162:GLN:HE21 | 4:2C:162:GLN:HA | 1.37 | 0.89 |
| 7:5A:1491:LEU:N | 7:5A:1495:PHE:CB | 2.33 | 0.89 |
| 7:5B:1515:GLU:CG | 7:5B:1563:SER:HA | 2.01 | 0.89 |
| 7:5C:1490:LYS:CD | 7:5C:1494:LEU:CD2 | 2.49 | 0.89 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:HZ2 | 1.79 | 0.89 |
| 2:HD:177:ASP:OD2 | 1:HE:248:LEU:HD21 | 1.71 | 0.89 |
| 1:JC:101:ASN:ND2 | 2:JD:252:LYS:CG | 2.36 | 0.89 |
| 1:KA:88:HIS:CB | 1:LA:284:GLU:HB2 | 2.02 | 0.89 |
| 1:KC:85:GLN:HE22 | 1:LC:282:TYR:HB3 | 1.37 | 0.89 |
| 1:KE:85:GLN:OE1 | 1:LE:282:TYR:CB | 2.20 | 0.89 |
| 1:LE:176:GLN:NE2 | 4:2B:42:PHE:CB | 2.35 | 0.89 |
| 5:3B:229:PHE:CE2 | 5:3B:331:GLN:CG | 2.46 | 0.89 |
| 7:5B:841:VAL:O | 8:6B:9:LEU:O | 1.90 | 0.89 |
| 7:5B:1490:LYS:C | 7:5B:1495:PHE:HB3 | 1.94 | 0.89 |
| 8:6C:131:ASP:N | 8:6C:136:LEU:HD12 | 1.87 | 0.89 |
| 1:AA:76:ASP:OD1 | 2:AB:46:ARG:NH2 | 2.04 | 0.89 |
| 1:EA:396:ASP:HB3 | 7:5C:817:LEU:CG | 2.02 | 0.89 |
| 1:GA:76:ASP:OD1 | 2:GB:46:ARG:NH2 | 2.04 | 0.89 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:HB:177:ASP:OD2 | 1:HC:248:LEU:HD21 | 1.70 | 0.89 |
| 2:HB:220:PRO:O | 1:HC:324:VAL:CG1 | 2.20 | 0.89 |
| 2:ID:177:ASP:OD2 | 1:IE:248:LEU:HD21 | 1.71 | 0.89 |
| 2:KF:272:PRO:C | 6:4D:268:LEU:CD2 | 2.46 | 0.89 |
| 2:LB:397:TRP:CG | 1:LC:256:GLN:HE22 | 1.50 | 0.89 |
| 1:LC:245:ASP:OD1 | 6:4A:216:ARG:CZ | 2.20 | 0.89 |
| 2:MD:177:ASP:OD2 | 1:ME:353:VAL:HG13 | 1.72 | 0.89 |
| 4:2A:33:GLN:NE2 | 4:2A:51:VAL:O | 2.05 | 0.89 |
| 6:4D:244:GLU:HA | 6:4D:247:LYS:HG3 | 1.54 | 0.89 |
| 1:AC:76:ASP:OD1 | 2:AD:46:ARG:NH2 | 2.05 | 0.89 |
| 1:DC:414:GLU:OE2 | 7:5A:789:LYS:CE | 2.20 | 0.89 |
| 1:FE:76:ASP:OD1 | 2:FF:46:ARG:NH2 | 2.05 | 0.89 |
| 1:GC:76:ASP:OD1 | 2:GD:46:ARG:NH2 | 2.05 | 0.89 |
| 1:IA:282:TYR:CG | 10:8V:15:UNK:HA | 2.08 | 0.89 |
| 2:IF:424:GLN:CD | 7:5B:1413:GLN:HE21 | 1.63 | 0.89 |
| 2:LF:55:THR:OG1 | 2:MF:282:ARG:O | 1.90 | 0.89 |
| 4:2A:162:GLN:HE21 | 4:2A:162:GLN:HA | 1.38 | 0.89 |
| 4:2C:33:GLN:NE2 | 4:2C:51:VAL:O | 2.05 | 0.89 |
| 6:4C:244:GLU:HA | 6:4C:247:LYS:HG3 | 1.54 | 0.89 |
| 7:5B:1423:LYS:HA | 7:5B:1423:LYS:CE | 2.03 | 0.89 |
| 7:5C:1491:LEU:CG | 7:5C:1495:PHE:CD1 | 2.55 | 0.89 |
| 1:AE:283:HIS:ND1 | 2:MB:86:ARG:NH2 | 2.20 | 0.89 |
| 1:BE:101:ASN:HD21 | 2:BF:252:LYS:CD | 1.66 | 0.89 |
| 1:CA:101:ASN:HD21 | 2:CB:252:LYS:CD | 1.65 | 0.89 |
| 1:EC:101:ASN:HD22 | 2:ED:252:LYS:HG3 | 1.38 | 0.89 |
| 1:FA:56:THR:O | 1:GA:285:GLN:HA | 1.72 | 0.89 |
| 1:GC:402:ARG:NE | 5:3C:381:ASN:ND2 | 2.06 | 0.89 |
| 2:HD:177:ASP:CG | 1:HE:353:VAL:HG11 | 1.96 | 0.89 |
| 1:JA:88:HIS:ND1 | 1:KA:280:LYS:HD3 | 1.87 | 0.89 |
| 1:JC:101:ASN:HD22 | 2:JD:252:LYS:CD | 1.86 | 0.89 |
| 4:2B:162:GLN:HE21 | 4:2B:162:GLN:HA | 1.38 | 0.89 |
| 5:3A:229:PHE:CE2 | 5:3A:331:GLN:CG | 2.46 | 0.89 |
| 7:5A:1491:LEU:CG | 7:5A:1495:PHE:CD1 | 2.55 | 0.89 |
| 7:5B:1491:LEU:CG | 7:5B:1495:PHE:CD1 | 2.55 | 0.89 |
| 9:7A:18:VAL:CG1 | 9:7A:42:LEU:HD23 | 2.03 | 0.89 |
| 1:AC:101:ASN:HD22 | 2:AD:252:LYS:CD | 1.86 | 0.89 |
| 1:EC:430:LYS:CE | 7:5A:834:ASN:ND2 | 2.10 | 0.89 |
| 1:FC:402:ARG:NH1 | 7:5A:1259:TYR:HA | 1.86 | 0.89 |
| 2:FD:55:THR:HG23 | 2:GD:283:ALA:C | 1.98 | 0.89 |
| 1:FE:60:LYS:NZ | 1:GE:283:HIS:CE1 | 2.38 | 0.89 |
| 1:GC:101:ASN:ND2 | 2:GD:252:LYS:CG | 2.36 | 0.89 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HE:76:ASP:OD1 | 2:HF:46:ARG:NH2 | 2.05 | 0.89 |
| 1:IA:101:ASN:HD21 | 2:IB:252:LYS:CD | 1.61 | 0.89 |
| 1:JC:101:ASN:HD22 | 2:JD:252:LYS:HG3 | 1.36 | 0.89 |
| 2:KD:77:ARG:CG | 2:LD:281:TYR:CE1 | 2.52 | 0.89 |
| 2:LD:179:VAL:CG2 | 1:LE:258:ASN:HA | 2.03 | 0.89 |
| 2:MD:177:ASP:OD2 | 1:ME:353:VAL:CG1 | 2.20 | 0.89 |
| 6:4B:244:GLU:HA | 6:4B:247:LYS:HG3 | 1.54 | 0.89 |
| 7:5A:826:LEU:HD23 | 7:5A:840:GLY:CA | 2.02 | 0.89 |
| 7:5A:1423:LYS:HA | 7:5A:1423:LYS:CE | 2.03 | 0.89 |
| 7:5B:826:LEU:HD23 | 7:5B:840:GLY:CA | 2.02 | 0.89 |
| 7:5C:1503:TYR:HA | 7:5C:1508:ARG:HD2 | 1.52 | 0.89 |
| 2:GB:220:PRO:O | 1:GC:324:VAL:CG1 | 2.20 | 0.89 |
| 1:IA:402:ARG:CZ | 7:5C:1417:GLN:CG | 2.34 | 0.89 |
| 1:IC:279:GLU:CD | 10:8W:22:UNK:CB | 2.45 | 0.89 |
| 1:KC:85:GLN:HA | 1:LC:283:HIS:HA | 0.90 | 0.89 |
| 2:LB:391:ARG:HG3 | 1:LC:346:TRP:CD1 | 2.07 | 0.89 |
| 1:LC:222:PRO:HG2 | 2:LD:324:LYS:HB2 | 1.55 | 0.89 |
| 2:LF:224:ASP:N | 6:4D:219:ASN:CG | 2.30 | 0.89 |
| 6:4A:244:GLU:HA | 6:4A:247:LYS:HG3 | 1.54 | 0.89 |
| 7:5A:1503:TYR:HA | 7:5A:1508:ARG:HD2 | 1.52 | 0.89 |
| 7:5C:826:LEU:HD23 | 7:5C:840:GLY:CA | 2.02 | 0.89 |
| 7:5C:1423:LYS:HA | 7:5C:1423:LYS:CE | 2.03 | 0.89 |
| 2:BD:177:ASP:OD2 | 1:BE:248:LEU:CD2 | 2.21 | 0.89 |
| 2:EB:98:GLY:C | 1:EC:254:GLU:HG2 | 1.97 | 0.89 |
| 1:HE:415:GLU:HG3 | 5:3A:235:LEU:HD22 | 1.54 | 0.89 |
| 1:IC:278:ALA:HB3 | 10:8W:22:UNK:N | 1.88 | 0.89 |
| 1:KC:372:MET:HB3 | 6:4A:299:TYR:HE1 | 1.23 | 0.89 |
| 1:LC:76:ASP:OD1 | 2:LD:46:ARG:NH2 | 2.05 | 0.89 |
| 1:MA:101:ASN:ND2 | 2:MB:252:LYS:CG | 2.36 | 0.89 |
| 7:5B:1503:TYR:HA | 7:5B:1508:ARG:HD2 | 1.53 | 0.89 |
| 7:5C:773:ARG:HD3 | 7:5C:773:ARG:H | 1.38 | 0.89 |
| 2:AF:55:THR:HG23 | 2:BF:283:ALA:HA | 1.55 | 0.89 |
| 2:CD:86:ARG:CA | 2:DD:281:TYR:HE1 | 1.63 | 0.89 |
| 2:DB:177:ASP:CG | 1:DC:353:VAL:HG11 | 1.94 | 0.89 |
| 1:FC:423:GLU:CD | 7:5A:1256:ARG:NH2 | 2.30 | 0.89 |
| 1:GE:89:PRO:HD3 | 1:HE:280:LYS:NZ | 1.88 | 0.89 |
| 1:IC:101:ASN:ND2 | 2:ID:252:LYS:CG | 2.36 | 0.89 |
| 2:ID:397:TRP:CG | 1:IE:256:GLN:HE22 | 1.35 | 0.89 |
| 1:JA:89:PRO:CG | 1:KA:280:LYS:HA | 2.01 | 0.89 |
| 2:KD:87:PRO:HG3 | 2:LD:282:ARG:CG | 1.93 | 0.89 |
| 1:LA:176:GLN:O | 2:LB:347:ASN:ND2 | 2.06 | 0.89 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MB:110:ALA:O | 3:1A:61:HIS:HB3 | 1.72 | 0.89 |
| 1:ME:282:TYR:CE2 | 6:4B:104:ARG:HD3 | 2.08 | 0.89 |
| 7:5A:773:ARG:HD3 | 7:5A:773:ARG:H | 1.38 | 0.89 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:HD12 | 1.54 | 0.89 |
| 1:DC:282:TYR:HE2 | 10:8H:18:UNK:CB | 1.87 | 0.88 |
| 2:FB:55:THR:CG2 | 2:GB:283:ALA:HA | 2.03 | 0.88 |
| 1:FE:222:PRO:CD | 2:FF:324:LYS:HD3 | 2.02 | 0.88 |
| 2:GF:416:ASN:CG | 7:5B:1327:LYS:HZ1 | 1.81 | 0.88 |
| 1:HC:278:ALA:CB | 10:8T:22:UNK:N | 2.37 | 0.88 |
| 2:IB:220:PRO:O | 1:IC:324:VAL:CG1 | 2.20 | 0.88 |
| 1:LA:60:LYS:HD2 | 6:4C:101:ARG:HH22 | 0.74 | 0.88 |
| 1:LA:60:LYS:CD | 6:4C:101:ARG:NH2 | 2.20 | 0.88 |
| 2:LB:177:ASP:OD2 | 1:LC:353:VAL:HG13 | 1.71 | 0.88 |
| 1:LE:60:LYS:CD | 6:4B:101:ARG:NH2 | 2.20 | 0.88 |
| 2:MD:177:ASP:OD1 | 1:ME:353:VAL:HG11 | 1.70 | 0.88 |
| 5:3B:230:ILE:O | 5:3B:332:MET:HG2 | 1.73 | 0.88 |
| 1:AE:76:ASP:OD1 | 2:AF:46:ARG:NH2 | 2.05 | 0.88 |
| 2:CD:397:TRP:CG | 1:CE:256:GLN:HE22 | 1.48 | 0.88 |
| 1:EC:101:ASN:HD22 | 2:ED:252:LYS:HD2 | 1.38 | 0.88 |
| 1:GE:76:ASP:OD1 | 2:GF:46:ARG:NH2 | 2.05 | 0.88 |
| 1:JC:88:HIS:HE1 | 1:KC:280:LYS:O | 1.27 | 0.88 |
| 1:KC:101:ASN:ND2 | 2:KD:252:LYS:CG | 2.36 | 0.88 |
| 1:KE:359:PRO:HB3 | 6:4B:299:TYR:HE2 | 1.27 | 0.88 |
| 2:LD:306:ARG:NE | 4:2A:149:ILE:HG21 | 1.86 | 0.88 |
| 1:LE:401:LYS:NZ | 2:LF:344:TRP:CE2 | 2.40 | 0.88 |
| 5:3A:230:ILE:O | 5:3A:332:MET:HG2 | 1.73 | 0.88 |
| 5:3C:230:ILE:O | 5:3C:332:MET:HG2 | 1.73 | 0.88 |
| 7:5B:773:ARG:HD3 | 7:5B:773:ARG:H | 1.38 | 0.88 |
| 9:7C:18:VAL:CG1 | 9:7C:42:LEU:HD23 | 2.03 | 0.88 |
| 2:BB:86:ARG:HA | 2:CB:281:TYR:CZ | 2.08 | 0.88 |
| 2:FD:106:TYR:O | 7:5A:1298:LYS:NZ | 2.07 | 0.88 |
| 1:GA:370:LYS:HG2 | 10:8P:17:UNK:C | 2.03 | 0.88 |
| 1:HC:76:ASP:OD1 | 2:HD:46:ARG:NH2 | 2.05 | 0.88 |
| 2:KB:273:LEU:HA | 6:4A:268:LEU:HD23 | 0.92 | 0.88 |
| 2:LB:306:ARG:NH2 | 4:2C:149:ILE:CG2 | 2.37 | 0.88 |
| 1:ME:101:ASN:HD22 | 2:MF:252:LYS:HD2 | 1.37 | 0.88 |
| 1:DA:402:ARG:HE | 7:5C:777:ALA:CB | 1.83 | 0.88 |
| 1:DE:282:TYR:HE2 | 10:8I:18:UNK:CB | 1.86 | 0.88 |
| 1:KA:101:ASN:CG | 2:KB:252:LYS:HD2 | 1.98 | 0.88 |
| 1:MA:101:ASN:HD22 | 2:MB:252:LYS:CG | 1.86 | 0.88 |
| 7:5A:1549:THR:CA | 7:5A:1566:GLU:CG | 2.49 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1484:TYR:CD1 | 7:5B:1568:LYS:CD | 2.52 | 0.88 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:HA | 1.54 | 0.88 |
| 2:AF:40:SER:HB3 | 6:4A:152:PHE:HD2 | 1.37 | 0.88 |
| 1:HC:101:ASN:HD22 | 2:HD:252:LYS:CD | 1.86 | 0.88 |
| 1:IE:393:HIS:HB3 | 5:3A:308:PHE:CE2 | 2.08 | 0.88 |
| 2:JB:177:ASP:OD2 | 1:JC:248:LEU:HD21 | 1.70 | 0.88 |
| 2:KB:276:ARG:CZ | 6:4A:271:GLU:O | 2.08 | 0.88 |
| 2:KD:217:LEU:HB3 | 6:4B:265:TYR:HH | 1.05 | 0.88 |
| 2:LB:306:ARG:HE | 4:2C:149:ILE:HG22 | 0.73 | 0.88 |
| 2:MD:98:GLY:HA2 | 1:ME:254:GLU:HG3 | 1.54 | 0.88 |
| 6:4D:198:ASN:O | 6:4D:202:VAL:HG23 | 1.72 | 0.88 |
| 1:CE:76:ASP:OD1 | 2:CF:46:ARG:NH2 | 2.05 | 0.88 |
| 2:EB:212:PHE:CZ | 1:EC:326:LYS:CD | 2.22 | 0.88 |
| 2:ED:98:GLY:C | 1:EE:254:GLU:HG2 | 1.97 | 0.88 |
| 2:GB:55:THR:CG2 | 2:HB:283:ALA:HB1 | 2.02 | 0.88 |
| 1:HC:101:ASN:ND2 | 2:HD:252:LYS:CG | 2.36 | 0.88 |
| 2:IB:177:ASP:CG | 1:IC:353:VAL:HG11 | 1.96 | 0.88 |
| 1:IC:101:ASN:HD22 | 2:ID:252:LYS:HG3 | 1.36 | 0.88 |
| 1:IE:282:TYR:CD2 | 10:8X:15:UNK:O | 2.27 | 0.88 |
| 2:JF:86:ARG:HH21 | 2:KF:280:GLN:HB2 | 1.29 | 0.88 |
| 2:LB:54:ALA:HB1 | 2:MB:281:TYR:O | 1.74 | 0.88 |
| 2:LD:340:TYR:OH | 4:2A:146:PRO:HA | 1.74 | 0.88 |
| 7:5B:1549:THR:HA | 7:5B:1566:GLU:OE1 | 1.71 | 0.88 |
| 2:AD:55:THR:CG2 | 2:BD:283:ALA:HA | 2.03 | 0.88 |
| 2:CD:220:PRO:HD2 | 1:CE:326:LYS:HE2 | 1.53 | 0.88 |
| 1:FA:76:ASP:OD1 | 2:FB:46:ARG:NH2 | 2.07 | 0.88 |
| 2:FD:220:PRO:HD2 | 1:FE:326:LYS:HE2 | 1.54 | 0.88 |
| 2:GF:58:ARG:NH2 | 2:HF:281:TYR:OH | 2.05 | 0.88 |
| 1:HE:410:GLY:HA2 | 5:3A:329:ARG:HH21 | 1.39 | 0.88 |
| 2:KB:83:GLN:HA | 2:LB:281:TYR:CD1 | 2.08 | 0.88 |
| 2:KB:220:PRO:O | 1:KC:324:VAL:CG1 | 2.20 | 0.88 |
| 1:KC:101:ASN:HD22 | 2:KD:252:LYS:CD | 1.86 | 0.88 |
| 2:KD:227:HIS:HB3 | 6:4B:267:ILE:HD11 | 1.56 | 0.88 |
| 2:LD:55:THR:H | 2:MD:283:ALA:CB | 1.87 | 0.88 |
| 2:LF:416:ASN:CA | 4:2B:168:LEU:HD13 | 1.96 | 0.88 |
| 1:ME:279:GLU:HG3 | 6:4B:110:LYS:HE2 | 1.54 | 0.88 |
| 1:AC:101:ASN:ND2 | 2:AD:252:LYS:CG | 2.36 | 0.88 |
| 2:AD:223:GLY:C | 6:4C:131:VAL:CB | 2.43 | 0.88 |
| 1:KC:101:ASN:HD22 | 2:KD:252:LYS:HG3 | 1.36 | 0.88 |
| 2:KD:221:THR:HG21 | 6:4B:262:ASN:N | 1.88 | 0.88 |
| 1:KE:85:GLN:OE1 | 1:LE:282:TYR:HB2 | 1.71 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LC:60:LYS:CD | 6:4A:101:ARG:NH1 | 2.37 | 0.88 |
| 2:LD:413:SER:HB2 | 4:2A:171:VAL:HG21 | 1.54 | 0.88 |
| 9:7E:11:TYR:OH | 9:7F:27:GLY:N | 2.07 | 0.88 |
| 2:AD:55:THR:HG23 | 2:BD:283:ALA:CA | 2.04 | 0.88 |
| 2:BB:98:GLY:C | 1:BC:254:GLU:HG2 | 1.98 | 0.88 |
| 1:HA:101:ASN:HD22 | 2:HB:252:LYS:HG3 | 1.38 | 0.88 |
| 1:IA:101:ASN:CG | 2:IB:252:LYS:HD2 | 1.98 | 0.88 |
| 2:KD:221:THR:HG21 | 6:4B:261:SER:CA | 1.76 | 0.88 |
| 2:LB:55:THR:HG21 | 2:MB:284:LEU:H | 1.38 | 0.88 |
| 6:4B:198:ASN:O | 6:4B:202:VAL:HG23 | 1.73 | 0.88 |
| 9:7E:18:VAL:CG1 | 9:7E:42:LEU:HD23 | 2.03 | 0.88 |
| 2:AD:220:PRO:O | 1:AE:324:VAL:CG1 | 2.22 | 0.88 |
| 2:DD:98:GLY:HA2 | 1:DE:254:GLU:HG3 | 1.54 | 0.88 |
| 2:FB:177:ASP:CB | 1:FC:353:VAL:HG12 | 2.04 | 0.88 |
| 2:ID:86:ARG:NH1 | 2:JD:281:TYR:HA | 1.89 | 0.88 |
| 2:LD:306:ARG:NH2 | 4:2A:149:ILE:CG2 | 2.37 | 0.88 |
| 2:LD:379:LYS:NZ | 4:2A:166:ILE:H | 1.71 | 0.88 |
| 7:5A:874:GLN:HB2 | 8:6A:59:LYS:HZ2 | 1.28 | 0.88 |
| 7:5B:1549:THR:CA | 7:5B:1566:GLU:CG | 2.49 | 0.88 |
| 9:7C:12:GLU:C | 9:7C:16:THR:HG1 | 1.81 | 0.88 |
| 9:7C:30:ARG:NH1 | 9:7D:3:GLN:HG2 | 1.89 | 0.88 |
| 9:7C:30:ARG:NH1 | 9:7D:3:GLN:CA | 2.14 | 0.88 |
| 1:FA:101:ASN:HD21 | 2:FB:252:LYS:HD2 | 1.06 | 0.87 |
| 2:HD:220:PRO:O | 1:HE:324:VAL:CG1 | 2.22 | 0.87 |
| 2:IB:177:ASP:CG | 1:IC:353:VAL:HG13 | 1.99 | 0.87 |
| 2:JD:220:PRO:O | 1:JE:324:VAL:CG1 | 2.22 | 0.87 |
| 1:LA:76:ASP:OD1 | 2:LB:46:ARG:NH2 | 2.06 | 0.87 |
| 7:5A:1484:TYR:CD1 | 7:5A:1568:LYS:CD | 2.52 | 0.87 |
| 1:IE:101:ASN:HD21 | 2:IF:252:LYS:CD | 1.64 | 0.87 |
| 1:IE:402:ARG:NE | 7:5B:1417:GLN:HG3 | 1.89 | 0.87 |
| 2:JB:86:ARG:HE | 2:KB:281:TYR:HD2 | 1.22 | 0.87 |
| 1:KA:85:GLN:OE1 | 1:LA:282:TYR:CA | 2.21 | 0.87 |
| 2:KB:77:ARG:HG2 | 2:LB:281:TYR:OH | 1.71 | 0.87 |
| 7:5A:1549:THR:HA | 7:5A:1566:GLU:OE1 | 1.71 | 0.87 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:HD12 | 1.54 | 0.87 |
| 2:AF:359:LYS:N | 6:4A:151:ARG:HH22 | 1.51 | 0.87 |
| 2:FB:397:TRP:CG | 1:FC:256:GLN:HE22 | 1.59 | 0.87 |
| 1:FC:11:GLN:OE1 | 2:FD:245:GLN:O | 1.92 | 0.87 |
| 1:GA:101:ASN:HD21 | 2:GB:252:LYS:CD | 1.62 | 0.87 |
| 2:ID:177:ASP:CG | 1:IE:353:VAL:HG11 | 1.96 | 0.87 |
| 2:JB:86:ARG:CZ | 2:KB:280:GLN:C | 2.47 | 0.87 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JC:89:PRO:HG2 | 1:KC:280:LYS:HG2 | 1.56 | 0.87 |
| 1:KC:88:HIS:HA | 1:LC:284:GLU:HB2 | 0.88 | 0.87 |
| 2:LD:98:GLY:HA2 | 1:LE:254:GLU:CG | 2.04 | 0.87 |
| 7:5A:1126:PRO:HD2 | 8:6A:246:TYR:OH | 1.75 | 0.87 |
| 7:5B:1545:TYR:N | 7:5B:1570:ALA:CB | 2.37 | 0.87 |
| 9:7E:12:GLU:C | 9:7E:16:THR:HG1 | 1.81 | 0.87 |
| 2:AB:177:ASP:CG | 1:AC:353:VAL:HG13 | 1.99 | 0.87 |
| 2:BD:98:GLY:C | 1:BE:254:GLU:HG2 | 1.98 | 0.87 |
| 2:EB:397:TRP:CG | 1:EC:256:GLN:HE22 | 1.46 | 0.87 |
| 2:ED:220:PRO:HD2 | 1:EE:326:LYS:HG2 | 1.56 | 0.87 |
| 2:GD:220:PRO:O | 1:GE:324:VAL:CG1 | 2.22 | 0.87 |
| 2:LD:296:ALA:CB | 4:2A:149:ILE:HG21 | 1.98 | 0.87 |
| 2:LF:55:THR:CG2 | 2:MF:283:ALA:CB | 2.41 | 0.87 |
| 1:MA:282:TYR:CE2 | 6:4C:104:ARG:HD3 | 2.10 | 0.87 |
| 6:4A:198:ASN:O | 6:4A:202:VAL:HG23 | 1.72 | 0.87 |
| 7:5A:1545:TYR:N | 7:5A:1570:ALA:CB | 2.37 | 0.87 |
| 9:7A:12:GLU:C | 9:7A:16:THR:HG1 | 1.81 | 0.87 |
| 9:7A:30:ARG:NH1 | 9:7B:3:GLN:HG2 | 1.89 | 0.87 |
| 9:7F:12:GLU:HA | 9:7F:16:THR:HG1 | 1.38 | 0.87 |
| 2:AD:40:SER:OG | 6:4C:152:PHE:HE2 | 1.48 | 0.87 |
| 2:FF:54:ALA:HA | 2:GF:283:ALA:HB2 | 1.56 | 0.87 |
| 2:JB:55:THR:CG2 | 2:KB:362:LYS:HZ3 | 1.55 | 0.87 |
| 2:JD:177:ASP:OD2 | 1:JE:248:LEU:HD21 | 1.71 | 0.87 |
| 2:KB:228:LEU:CD2 | 6:4A:267:ILE:HD12 | 2.05 | 0.87 |
| 1:LA:401:LYS:NZ | 2:LB:344:TRP:CE2 | 2.42 | 0.87 |
| 2:LF:306:ARG:NE | 4:2B:149:ILE:HG21 | 1.88 | 0.87 |
| 1:ME:101:ASN:CG | 2:MF:252:LYS:HD2 | 1.97 | 0.87 |
| 1:ME:283:HIS:NE2 | 6:4B:101:ARG:NH2 | 2.23 | 0.87 |
| 5:3B:230:ILE:HG22 | 5:3B:332:MET:SD | 2.15 | 0.87 |
| 7:5B:1404:LYS:O | 7:5B:1404:LYS:NZ | 2.07 | 0.87 |
| 9:7A:11:TYR:HD1 | 9:7B:26:LEU:HD23 | 1.06 | 0.87 |
| 1:FA:56:THR:C | 1:GA:285:GLN:HB3 | 1.98 | 0.87 |
| 1:HA:282:TYR:HE2 | 10:8S:19:UNK:N | 1.44 | 0.87 |
| 2:LF:231:ALA:HB2 | 6:4D:226:ILE:HD13 | 0.88 | 0.87 |
| 6:4C:198:ASN:O | 6:4C:202:VAL:HG23 | 1.73 | 0.87 |
| 7:5C:1545:TYR:N | 7:5C:1570:ALA:CB | 2.37 | 0.87 |
| 7:5C:1549:THR:HA | 7:5C:1566:GLU:OE1 | 1.70 | 0.87 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:HA | 1.54 | 0.87 |
| 1:CA:76:ASP:OD1 | 2:CB:46:ARG:NH2 | 2.07 | 0.87 |
| 2:CB:177:ASP:O | 1:CC:352:LYS:CD | 2.23 | 0.87 |
| 1:DA:402:ARG:NH2 | 7:5C:782:LEU:CD1 | 2.11 | 0.87 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EA:101:ASN:HD22 | 2:EB:252:LYS:HG3 | 1.38 | 0.87 |
| 1:GC:101:ASN:HD22 | 2:GD:252:LYS:HG3 | 1.36 | 0.87 |
| 2:GD:405:GLU:OE2 | 7:5A:1337:ASP:OD2 | 1.92 | 0.87 |
| 1:JC:89:PRO:HB2 | 1:KC:280:LYS:HG2 | 0.87 | 0.87 |
| 1:KE:359:PRO:HG3 | 6:4B:299:TYR:CD2 | 2.09 | 0.87 |
| 1:ME:279:GLU:HG3 | 6:4B:110:LYS:HE3 | 1.56 | 0.87 |
| 9:7A:14:SER:O | 9:7B:35:ILE:CD1 | 2.22 | 0.87 |
| 1:EA:101:ASN:CG | 2:EB:252:LYS:HD2 | 1.98 | 0.87 |
| 1:FA:89:PRO:HG3 | 1:GA:280:LYS:HG3 | 1.56 | 0.87 |
| 1:FA:419:SER:OG | 7:5C:1256:ARG:CD | 2.23 | 0.87 |
| 1:GC:409:VAL:HG21 | 5:3C:383:GLU:OE1 | 1.75 | 0.87 |
| 2:IB:85:PHE:O | 2:JB:281:TYR:OH | 1.92 | 0.87 |
| 1:JA:101:ASN:CG | 2:JB:252:LYS:HD2 | 1.98 | 0.87 |
| 2:KD:276:ARG:NH2 | 6:4B:265:TYR:HA | 1.90 | 0.87 |
| 1:LE:89:PRO:CG | 1:ME:280:LYS:NZ | 2.37 | 0.87 |
| 1:MC:279:GLU:HG3 | 6:4A:110:LYS:HE3 | 1.51 | 0.87 |
| 7:5A:1404:LYS:O | 7:5A:1404:LYS:NZ | 2.07 | 0.87 |
| 7:5C:1484:TYR:CD1 | 7:5C:1568:LYS:CD | 2.52 | 0.87 |
| 9:7C:15:VAL:HA | 9:7D:35:ILE:HD11 | 1.04 | 0.87 |
| 2:FD:55:THR:HG23 | 2:GD:284:LEU:N | 1.89 | 0.87 |
| 1:IC:101:ASN:HD22 | 2:ID:252:LYS:CG | 1.87 | 0.87 |
| 1:JE:89:PRO:HB2 | 1:KE:280:LYS:HG2 | 0.87 | 0.87 |
| 2:KB:177:ASP:CG | 1:KC:353:VAL:HG13 | 1.99 | 0.87 |
| 2:LB:227:HIS:CE1 | 6:4A:226:ILE:HG13 | 2.09 | 0.87 |
| 5:3A:230:ILE:HG22 | 5:3A:332:MET:SD | 2.15 | 0.87 |
| 9:7A:12:GLU:C | 9:7A:16:THR:OG1 | 2.18 | 0.87 |
| 9:7C:11:TYR:HD1 | 9:7D:26:LEU:HD23 | 1.06 | 0.87 |
| 9:7C:14:SER:O | 9:7D:35:ILE:CD1 | 2.22 | 0.87 |
| 1:AC:101:ASN:HD22 | 2:AD:252:LYS:HG3 | 1.36 | 0.86 |
| 1:EC:370:LYS:HZ1 | 10:8K:17:UNK:CB | 1.84 | 0.86 |
| 1:EE:222:PRO:CG | 2:EF:324:LYS:HD3 | 2.04 | 0.86 |
| 1:GE:101:ASN:HD21 | 2:GF:252:LYS:CD | 1.64 | 0.86 |
| 1:JC:101:ASN:HD22 | 2:JD:252:LYS:CG | 1.87 | 0.86 |
| 9:7C:18:VAL:HG12 | 9:7C:42:LEU:CD2 | 2.05 | 0.86 |
| 2:AF:276:ARG:NH1 | 6:4A:137:ASN:O | 2.09 | 0.86 |
| 2:DB:397:TRP:CG | 1:DC:256:GLN:HE22 | 1.47 | 0.86 |
| 1:EC:101:ASN:HD22 | 2:ED:252:LYS:CD | 1.87 | 0.86 |
| 1:JA:101:ASN:ND2 | 2:JB:252:LYS:CG | 2.38 | 0.86 |
| 2:LF:224:ASP:N | 6:4D:219:ASN:HD21 | 1.49 | 0.86 |
| 7:5C:1404:LYS:O | 7:5C:1404:LYS:NZ | 2.07 | 0.86 |
| 9:7C:12:GLU:C | 9:7C:16:THR:OG1 | 2.18 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:397:TRP:HE3 | 1:CC:257:THR:HG22 | 1.37 | 0.86 |
| 1:EE:426:ALA:CB | 7:5B:833:PHE:HB2 | 2.04 | 0.86 |
| 2:EF:54:ALA:CA | 2:FF:283:ALA:HB2 | 2.05 | 0.86 |
| 2:FF:55:THR:CG2 | 2:GF:283:ALA:CA | 2.43 | 0.86 |
| 1:GA:101:ASN:ND2 | 2:GB:252:LYS:CG | 2.38 | 0.86 |
| 1:HC:101:ASN:HD22 | 2:HD:252:LYS:CG | 1.87 | 0.86 |
| 1:IA:101:ASN:HD22 | 2:IB:252:LYS:HG3 | 1.38 | 0.86 |
| 1:IA:282:TYR:CD1 | 10:8V:15:UNK:CA | 2.55 | 0.86 |
| 2:KD:220:PRO:O | 1:KE:324:VAL:CG1 | 2.22 | 0.86 |
| 2:LB:177:ASP:O | 1:LC:352:LYS:CD | 2.20 | 0.86 |
| 2:LB:310:TYR:HE2 | 4:2C:147:PHE:CE2 | 1.92 | 0.86 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:HD2 | 2.03 | 0.86 |
| 1:ME:404:PHE:HE2 | 2:MF:345:ILE:CD1 | 1.87 | 0.86 |
| 9:7E:18:VAL:HG12 | 9:7E:42:LEU:CD2 | 2.05 | 0.86 |
| 1:FE:402:ARG:HD3 | 7:5B:1259:TYR:HD2 | 1.35 | 0.86 |
| 1:HC:282:TYR:CE2 | 10:8T:15:UNK:O | 2.28 | 0.86 |
| 1:HE:415:GLU:HG3 | 5:3A:235:LEU:CD2 | 2.04 | 0.86 |
| 2:ID:177:ASP:CG | 1:IE:353:VAL:HG13 | 2.00 | 0.86 |
| 1:JA:88:HIS:NE2 | 1:KA:280:LYS:O | 2.07 | 0.86 |
| 1:KA:127:ASP:OD2 | 1:LA:334:THR:HG23 | 1.76 | 0.86 |
| 2:KD:124:ALA:O | 4:2A:37:GLY:O | 1.94 | 0.86 |
| 2:LB:18:ALA:HB3 | 6:4A:217:ASN:ND2 | 1.89 | 0.86 |
| 2:LF:379:LYS:HZ1 | 4:2B:166:ILE:CB | 1.86 | 0.86 |
| 9:7A:18:VAL:HG12 | 9:7A:42:LEU:CD2 | 2.05 | 0.86 |
| 1:AA:101:ASN:HD22 | 2:AB:252:LYS:HG3 | 1.38 | 0.86 |
| 1:CA:60:LYS:NZ | 1:DA:283:HIS:CD2 | 2.43 | 0.86 |
| 1:EE:71:GLU:OE1 | 2:EF:247:ASN:ND2 | 2.09 | 0.86 |
| 1:JC:87:PHE:O | 1:KC:283:HIS:HE1 | 1.43 | 0.86 |
| 1:KA:101:ASN:HD22 | 2:KB:252:LYS:HG3 | 1.38 | 0.86 |
| 1:LE:89:PRO:HD3 | 1:ME:280:LYS:CE | 2.05 | 0.86 |
| 1:MC:101:ASN:HD22 | 2:MD:252:LYS:HG3 | 1.39 | 0.86 |
| 1:MC:101:ASN:HD22 | 2:MD:252:LYS:HD2 | 1.39 | 0.86 |
| 2:GB:177:ASP:CG | 1:GC:353:VAL:HG13 | 1.99 | 0.86 |
| 1:HC:101:ASN:HD22 | 2:HD:252:LYS:HD2 | 1.40 | 0.86 |
| 2:IF:424:GLN:HE21 | 7:5B:1413:GLN:CD | 1.60 | 0.86 |
| 2:KB:87:PRO:HG3 | 2:LB:282:ARG:HG3 | 0.86 | 0.86 |
| 1:LC:407:TRP:CZ2 | 2:LD:254:ALA:O | 2.29 | 0.86 |
| 2:LD:54:ALA:C | 2:MD:283:ALA:HB2 | 2.01 | 0.86 |
| 7:5B:1276:GLU:HG2 | 9:7D:7:LEU:HD12 | 1.56 | 0.86 |
| 1:DE:402:ARG:NH2 | 7:5B:777:ALA:HB3 | 1.88 | 0.86 |
| 2:FF:106:TYR:O | 7:5B:1298:LYS:NZ | 2.09 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GC:101:ASN:HD22 | 2:GD:252:LYS:CG | 1.87 | 0.86 |
| 1:IC:393:HIS:CE1 | 5:3C:306:ASP:OD1 | 2.27 | 0.86 |
| 1:JA:101:ASN:HD22 | 2:JB:252:LYS:HG3 | 1.38 | 0.86 |
| 1:LA:89:PRO:HD3 | 1:MA:280:LYS:CE | 2.05 | 0.86 |
| 2:MB:98:GLY:HA2 | 1:MC:254:GLU:HG3 | 1.56 | 0.86 |
| 2:MB:177:ASP:OD2 | 1:MC:248:LEU:HD21 | 1.75 | 0.86 |
| 5:3C:230:ILE:HG22 | 5:3C:332:MET:SD | 2.15 | 0.86 |
| 2:CD:220:PRO:O | 1:CE:324:VAL:HG11 | 1.74 | 0.86 |
| 1:DA:60:LYS:HD3 | 1:EA:283:HIS:CD2 | 2.10 | 0.86 |
| 2:ED:157:GLU:OE1 | 7:5A:935:LYS:HE3 | 1.76 | 0.86 |
| 1:FC:222:PRO:CD | 2:FD:324:LYS:HD3 | 2.05 | 0.86 |
| 1:GA:101:ASN:CG | 2:GB:252:LYS:HD2 | 1.98 | 0.86 |
| 1:HA:101:ASN:CG | 2:HB:252:LYS:HD2 | 1.98 | 0.86 |
| 2:ID:220:PRO:O | 1:IE:324:VAL:CG1 | 2.22 | 0.86 |
| 1:JC:282:TYR:OH | 10:8Z:17:UNK:CB | 2.24 | 0.86 |
| 2:KB:86:ARG:HG2 | 2:LB:288:GLU:CD | 2.00 | 0.86 |
| 2:KD:54:ALA:CB | 2:LD:285:THR:HG22 | 1.95 | 0.86 |
| 2:KD:125:GLU:HG3 | 2:LD:336:LYS:HZ1 | 1.06 | 0.86 |
| 7:5A:1521:PHE:HA | 7:5A:1567:PHE:CE2 | 2.11 | 0.86 |
| 7:5B:1267:CYS:O | 7:5B:1270:ASP:CB | 2.21 | 0.86 |
| 7:5B:1521:PHE:HA | 7:5B:1567:PHE:CE2 | 2.11 | 0.86 |
| 7:5C:1521:PHE:HA | 7:5C:1567:PHE:CE2 | 2.11 | 0.86 |
| 9:7A:42:LEU:HD13 | 9:7B:39:GLY:CA | 2.06 | 0.86 |
| 1:AA:101:ASN:CG | 2:AB:252:LYS:HD2 | 1.98 | 0.86 |
| 2:AD:177:ASP:CG | 1:AE:353:VAL:HG13 | 2.00 | 0.86 |
| 2:AD:362:LYS:HZ1 | 6:4C:143:THR:C | 1.83 | 0.86 |
| 1:CE:101:ASN:HD22 | 2:CF:252:LYS:HG3 | 1.40 | 0.86 |
| 1:FA:56:THR:HA | 1:GA:285:GLN:CB | 2.01 | 0.86 |
| 2:FD:397:TRP:CG | 1:FE:256:GLN:HE22 | 1.51 | 0.86 |
| 1:FE:423:GLU:CD | 7:5B:1256:ARG:NH2 | 2.32 | 0.86 |
| 1:HE:101:ASN:HD22 | 2:HF:252:LYS:HD2 | 1.41 | 0.86 |
| 1:HE:282:TYR:HE2 | 10:8U:18:UNK:C | 1.81 | 0.86 |
| 2:KB:273:LEU:HG | 6:4A:268:LEU:HD21 | 1.56 | 0.86 |
| 1:KC:85:GLN:NE2 | 1:LC:282:TYR:CB | 2.38 | 0.86 |
| 1:KC:101:ASN:HD22 | 2:KD:252:LYS:CG | 1.87 | 0.86 |
| 2:KF:276:ARG:HH21 | 6:4D:265:TYR:HA | 1.38 | 0.86 |
| 2:LB:306:ARG:HH12 | 4:2C:151:VAL:CG2 | 1.88 | 0.86 |
| 7:5A:1243:ASP:CB | 9:7B:8:ARG:NH1 | 2.38 | 0.86 |
| 7:5A:1267:CYS:O | 7:5A:1270:ASP:CB | 2.21 | 0.86 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:HE3 | 1.74 | 0.86 |
| 7:5C:1267:CYS:O | 7:5C:1270:ASP:CB | 2.21 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:DB:86:ARG:N | 2:EB:281:TYR:CE1 | 2.43 | 0.86 |
| 1:DE:101:ASN:HD21 | 2:DF:252:LYS:CD | 1.68 | 0.86 |
| 1:FA:89:PRO:N | 1:GA:280:LYS:HZ2 | 1.73 | 0.86 |
| 1:IA:101:ASN:ND2 | 2:IB:252:LYS:CG | 2.38 | 0.86 |
| 1:KE:87:PHE:O | 1:LE:283:HIS:O | 1.94 | 0.86 |
| 4:2A:15:GLU:O | 4:2A:19:MET:HG2 | 1.76 | 0.86 |
| 4:2C:15:GLU:O | 4:2C:19:MET:HG2 | 1.76 | 0.86 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:HE3 | 1.74 | 0.86 |
| 7:5A:1490:LYS:CG | 7:5A:1494:LEU:CD2 | 2.54 | 0.86 |
| 7:5A:1533:GLU:CG | 7:5A:1604:ALA:HB1 | 2.06 | 0.86 |
| 7:5A:1565:GLU:HB2 | 7:5A:1568:LYS:CB | 2.04 | 0.86 |
| 7:5B:1276:GLU:HG2 | 9:7D:7:LEU:CD1 | 2.05 | 0.86 |
| 7:5B:1565:GLU:HB2 | 7:5B:1568:LYS:CB | 2.04 | 0.86 |
| 7:5C:1490:LYS:HD2 | 7:5C:1494:LEU:CG | 2.06 | 0.86 |
| 7:5C:1490:LYS:CG | 7:5C:1494:LEU:CD2 | 2.54 | 0.86 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:CD1 | 2.05 | 0.86 |
| 9:7C:42:LEU:HD13 | 9:7D:39:GLY:CA | 2.06 | 0.86 |
| 2:CD:98:GLY:HA2 | 1:CE:254:GLU:HG3 | 1.58 | 0.85 |
| 2:DD:220:PRO:O | 1:DE:324:VAL:HG13 | 1.75 | 0.85 |
| 2:EB:125:GLU:O | 7:5C:903:PHE:CE2 | 2.29 | 0.85 |
| 2:ED:125:GLU:CB | 7:5A:903:PHE:HE2 | 1.78 | 0.85 |
| 1:GC:101:ASN:HD22 | 2:GD:252:LYS:CD | 1.85 | 0.85 |
| 1:HA:101:ASN:ND2 | 2:HB:252:LYS:CG | 2.38 | 0.85 |
| 1:JA:89:PRO:HD2 | 1:KA:283:HIS:ND1 | 1.90 | 0.85 |
| 1:KA:101:ASN:ND2 | 2:KB:252:LYS:CG | 2.38 | 0.85 |
| 2:LF:306:ARG:NE | 4:2B:149:ILE:HG22 | 1.88 | 0.85 |
| 7:5A:1490:LYS:HD2 | 7:5A:1494:LEU:CG | 2.06 | 0.85 |
| 7:5B:1490:LYS:CG | 7:5B:1494:LEU:CD2 | 2.54 | 0.85 |
| 7:5B:1533:GLU:CG | 7:5B:1604:ALA:HB1 | 2.06 | 0.85 |
| 7:5C:1533:GLU:CG | 7:5C:1604:ALA:HB1 | 2.06 | 0.85 |
| 7:5C:1565:GLU:HB2 | 7:5C:1568:LYS:CB | 2.04 | 0.85 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:CD1 | 2.05 | 0.85 |
| 9:7E:12:GLU:C | 9:7E:16:THR:OG1 | 2.18 | 0.85 |
| 2:BD:220:PRO:HD2 | 1:BE:326:LYS:HE2 | 1.58 | 0.85 |
| 1:EC:76:ASP:OD1 | 2:ED:46:ARG:NH2 | 2.08 | 0.85 |
| 1:EC:101:ASN:ND2 | 2:ED:252:LYS:CG | 2.39 | 0.85 |
| 2:FD:391:ARG:HG3 | 1:FE:346:TRP:CD1 | 2.11 | 0.85 |
| 2:KD:273:LEU:CB | 6:4B:268:LEU:HD21 | 2.05 | 0.85 |
| 2:LD:296:ALA:HB3 | 4:2A:149:ILE:CG2 | 1.82 | 0.85 |
| 4:2B:15:GLU:O | 4:2B:19:MET:HG2 | 1.76 | 0.85 |
| 7:5A:1378:GLN:HA | 7:5A:1381:ILE:HD13 | 1.58 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:HE3 | 1.74 | 0.85 |
| 7:5C:1549:THR:HA | 7:5C:1566:GLU:CG | 2.01 | 0.85 |
| 1:EA:101:ASN:ND2 | 2:EB:252:LYS:CG | 2.40 | 0.85 |
| 1:FE:402:ARG:CD | 7:5B:1259:TYR:HD2 | 1.88 | 0.85 |
| 2:GD:177:ASP:CG | 1:GE:353:VAL:HG13 | 2.00 | 0.85 |
| 1:IA:58:ALA:CB | 10:8Y:13:UNK:N | 2.39 | 0.85 |
| 2:LB:306:ARG:HH22 | 4:2C:151:VAL:HG23 | 1.38 | 0.85 |
| 2:LB:331:LEU:HD21 | 4:2C:42:PHE:CE2 | 1.91 | 0.85 |
| 6:4C:132:LYS:HE2 | 6:4C:132:LYS:O | 1.75 | 0.85 |
| 6:4C:244:GLU:CA | 6:4C:247:LYS:CG | 2.53 | 0.85 |
| 7:5B:1378:GLN:HA | 7:5B:1381:ILE:HD13 | 1.58 | 0.85 |
| 7:5B:1490:LYS:HD2 | 7:5B:1494:LEU:CG | 2.06 | 0.85 |
| 7:5C:1378:GLN:HA | 7:5C:1381:ILE:HD13 | 1.58 | 0.85 |
| 2:AF:356:ILE:HD12 | 6:4A:152:PHE:HE1 | 1.33 | 0.85 |
| 2:BB:177:ASP:CG | 1:BC:353:VAL:HG11 | 1.99 | 0.85 |
| 2:DD:177:ASP:CG | 1:DE:353:VAL:HG11 | 1.95 | 0.85 |
| 2:KD:130:LEU:HB2 | 4:2A:37:GLY:HA2 | 1.57 | 0.85 |
| 2:LF:227:HIS:CE1 | 6:4D:226:ILE:HG13 | 2.12 | 0.85 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:HD11 | 1.58 | 0.85 |
| 1:CC:101:ASN:HD22 | 2:CD:252:LYS:HG3 | 1.40 | 0.85 |
| 1:EA:101:ASN:HD22 | 2:EB:252:LYS:HD2 | 1.42 | 0.85 |
| 2:FB:55:THR:HG21 | 2:GB:284:LEU:N | 1.66 | 0.85 |
| 2:GB:55:THR:HG21 | 2:HB:284:LEU:H | 1.39 | 0.85 |
| 1:IA:58:ALA:HB2 | 10:8Y:13:UNK:N | 1.91 | 0.85 |
| 1:IE:279:GLU:CD | 10:8X:22:UNK:CB | 2.49 | 0.85 |
| 1:KA:87:PHE:O | 1:LA:283:HIS:C | 2.18 | 0.85 |
| 2:KB:55:THR:HG21 | 2:LB:363:MET:HE3 | 1.55 | 0.85 |
| 6:4A:132:LYS:HE2 | 6:4A:132:LYS:O | 1.75 | 0.85 |
| 7:5A:1425:LYS:O | 7:5A:1425:LYS:NZ | 2.08 | 0.85 |
| 7:5C:1425:LYS:O | 7:5C:1425:LYS:NZ | 2.08 | 0.85 |
| 7:5C:1490:LYS:HD3 | 7:5C:1494:LEU:HB3 | 1.58 | 0.85 |
| 1:KC:101:ASN:HD22 | 2:KD:252:LYS:HD2 | 1.40 | 0.85 |
| 2:KD:215:LEU:CD2 | 6:4B:267:ILE:O | 2.23 | 0.85 |
| 2:KD:221:THR:CG2 | 6:4B:261:SER:CA | 2.33 | 0.85 |
| 1:LA:60:LYS:HE3 | 6:4C:101:ARG:NH1 | 1.92 | 0.85 |
| 2:LB:54:ALA:C | 2:MB:283:ALA:HB2 | 2.01 | 0.85 |
| 2:LD:379:LYS:HZ1 | 4:2A:166:ILE:N | 1.74 | 0.85 |
| 1:MA:222:PRO:CG | 2:MB:324:LYS:HD3 | 2.06 | 0.85 |
| 6:4D:154:LYS:HZ3 | 6:4D:154:LYS:HB2 | 1.41 | 0.85 |
| 7:5A:1267:CYS:SG | 9:7A:8:ARG:HG3 | 2.17 | 0.85 |
| 7:5B:1425:LYS:O | 7:5B:1425:LYS:NZ | 2.08 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:101:ASN:HD22 | 2:AD:252:LYS:CG | 1.87 | 0.85 |
| 2:BD:87:PRO:HD2 | 2:CD:281:TYR:CZ | 2.12 | 0.85 |
| 1:CC:76:ASP:OD1 | 2:CD:46:ARG:NH2 | 2.09 | 0.85 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:CD | 2.55 | 0.85 |
| 2:FB:106:TYR:O | 7:5C:1298:LYS:NZ | 2.09 | 0.85 |
| 2:FD:177:ASP:CB | 1:FE:353:VAL:HG12 | 2.06 | 0.85 |
| 2:FF:55:THR:CG2 | 2:GF:284:LEU:H | 1.89 | 0.85 |
| 1:GA:101:ASN:HD22 | 2:GB:252:LYS:HG3 | 1.38 | 0.85 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:HD2 | 2.06 | 0.85 |
| 2:LD:227:HIS:CE1 | 6:4B:226:ILE:HG13 | 2.11 | 0.85 |
| 2:LF:223:GLY:C | 6:4D:219:ASN:ND2 | 2.35 | 0.85 |
| 1:ME:279:GLU:OE2 | 6:4B:106:ALA:HB3 | 1.77 | 0.85 |
| 7:5C:1126:PRO:CD | 8:6C:246:TYR:OH | 2.24 | 0.85 |
| 7:5C:1484:TYR:CD1 | 7:5C:1568:LYS:HD3 | 2.12 | 0.85 |
| 9:7A:15:VAL:HA | 9:7B:35:ILE:HD11 | 1.04 | 0.85 |
| 2:AF:55:THR:CG2 | 2:BF:283:ALA:HA | 2.06 | 0.85 |
| 1:CA:101:ASN:HD22 | 2:CB:252:LYS:HG3 | 1.41 | 0.85 |
| 2:CB:98:GLY:HA2 | 1:CC:254:GLU:HG3 | 1.58 | 0.85 |
| 2:CB:177:ASP:OD2 | 1:CC:248:LEU:CD2 | 2.25 | 0.85 |
| 1:GE:101:ASN:CG | 2:GF:252:LYS:HD2 | 2.00 | 0.85 |
| 2:HF:261:PRO:CG | 5:3A:337:ARG:HH21 | 1.89 | 0.85 |
| 1:JE:101:ASN:CG | 2:JF:252:LYS:HD2 | 2.00 | 0.85 |
| 1:KA:90:GLU:N | 1:LA:284:GLU:OE1 | 2.08 | 0.85 |
| 2:KF:86:ARG:HG2 | 2:LF:288:GLU:OE2 | 1.77 | 0.85 |
| 2:LF:77:ARG:HH11 | 6:4D:204:ARG:NH2 | 1.70 | 0.85 |
| 2:MB:177:ASP:OD1 | 1:MC:353:VAL:HG11 | 1.75 | 0.85 |
| 7:5A:1484:TYR:CD1 | 7:5A:1568:LYS:HD3 | 2.12 | 0.85 |
| 7:5A:1549:THR:HA | 7:5A:1566:GLU:CG | 2.01 | 0.85 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:HD11 | 1.58 | 0.85 |
| 1:EC:101:ASN:HD22 | 2:ED:252:LYS:CG | 1.88 | 0.85 |
| 1:HA:282:TYR:CZ | 10:8S:15:UNK:O | 2.30 | 0.85 |
| 2:KF:272:PRO:O | 6:4D:268:LEU:HD21 | 1.76 | 0.85 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CZ2 | 2.45 | 0.85 |
| 1:MC:404:PHE:HE2 | 2:MD:345:ILE:CD1 | 1.90 | 0.85 |
| 6:4A:244:GLU:CA | 6:4A:247:LYS:CG | 2.53 | 0.85 |
| 6:4B:132:LYS:HE2 | 6:4B:132:LYS:O | 1.75 | 0.85 |
| 1:AA:101:ASN:ND2 | 2:AB:252:LYS:CG | 2.38 | 0.85 |
| 1:EC:62:VAL:HG21 | 1:FC:283:HIS:O | 1.77 | 0.85 |
| 1:FE:402:ARG:NH1 | 7:5B:1259:TYR:HA | 1.90 | 0.85 |
| 2:GD:55:THR:H | 2:HD:283:ALA:HB2 | 1.03 | 0.85 |
| 2:KD:215:LEU:CD1 | 6:4B:267:ILE:CG2 | 2.46 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KE:101:ASN:HD22 | 2:KF:252:LYS:HD2 | 1.41 | 0.85 |
| 6:4B:244:GLU:CA | 6:4B:247:LYS:CG | 2.54 | 0.85 |
| 6:4D:132:LYS:HE2 | 6:4D:132:LYS:O | 1.75 | 0.85 |
| 7:5B:1355:GLN:CA | 7:5B:1358:LYS:HG3 | 2.05 | 0.85 |
| 7:5B:1484:TYR:CD1 | 7:5B:1568:LYS:HD3 | 2.12 | 0.85 |
| 7:5B:1549:THR:HA | 7:5B:1566:GLU:CG | 2.01 | 0.85 |
| 9:7E:11:TYR:CD1 | 9:7F:26:LEU:CD2 | 2.54 | 0.85 |
| 2:BB:87:PRO:HD2 | 2:CB:281:TYR:CZ | 2.12 | 0.84 |
| 1:FC:402:ARG:HD3 | 7:5A:1259:TYR:HD2 | 1.33 | 0.84 |
| 2:FF:54:ALA:CA | 2:GF:283:ALA:HB2 | 2.06 | 0.84 |
| 2:GB:54:ALA:HB1 | 2:HB:281:TYR:O | 1.77 | 0.84 |
| 1:GE:409:VAL:HG11 | 5:3A:383:GLU:OE1 | 1.77 | 0.84 |
| 1:HE:101:ASN:CG | 2:HF:252:LYS:HD2 | 2.00 | 0.84 |
| 1:IC:101:ASN:HD22 | 2:ID:252:LYS:HD2 | 1.40 | 0.84 |
| 6:4D:244:GLU:CA | 6:4D:247:LYS:CG | 2.54 | 0.84 |
| 7:5A:1355:GLN:CA | 7:5A:1358:LYS:HG3 | 2.05 | 0.84 |
| 2:AF:55:THR:HG23 | 2:BF:283:ALA:CA | 2.07 | 0.84 |
| 2:BB:220:PRO:HD2 | 1:BC:326:LYS:HG2 | 1.58 | 0.84 |
| 2:DD:397:TRP:CG | 1:DE:256:GLN:HE22 | 1.48 | 0.84 |
| 1:EA:396:ASP:CA | 7:5C:817:LEU:HD21 | 2.07 | 0.84 |
| 1:EA:402:ARG:NE | 7:5C:824:ARG:NH2 | 2.23 | 0.84 |
| 1:GC:56:THR:O | 1:HC:285:GLN:CB | 2.24 | 0.84 |
| 2:KB:55:THR:CG2 | 2:LB:363:MET:CE | 2.31 | 0.84 |
| 2:LD:55:THR:CB | 2:MD:283:ALA:HA | 2.06 | 0.84 |
| 2:MB:177:ASP:OD2 | 1:MC:248:LEU:CD2 | 2.24 | 0.84 |
| 1:MC:222:PRO:CG | 2:MD:324:LYS:HD3 | 2.06 | 0.84 |
| 6:4A:154:LYS:HB2 | 6:4A:154:LYS:HZ3 | 1.41 | 0.84 |
| 7:5B:1490:LYS:C | 7:5B:1495:PHE:HB2 | 2.00 | 0.84 |
| 7:5C:1077:ASN:HA | 7:5C:1083:THR:CG2 | 2.07 | 0.84 |
| 1:AC:342:GLN:NE2 | 3:1C:55:HIS:NE2 | 2.24 | 0.84 |
| 1:EC:11:GLN:OE1 | 2:ED:245:GLN:O | 1.96 | 0.84 |
| 1:HA:101:ASN:HD22 | 2:HB:252:LYS:CD | 1.90 | 0.84 |
| 1:KC:85:GLN:CA | 1:LC:283:HIS:HD2 | 1.86 | 0.84 |
| 2:LD:306:ARG:HH21 | 4:2A:149:ILE:CG2 | 1.90 | 0.84 |
| 7:5C:1355:GLN:CA | 7:5C:1358:LYS:HG3 | 2.05 | 0.84 |
| 9:7A:11:TYR:HE1 | 9:7B:26:LEU:CG | 1.89 | 0.84 |
| 9:7C:11:TYR:HE1 | 9:7D:26:LEU:CG | 1.89 | 0.84 |
| 2:AD:280:GLN:NE2 | 6:4C:141:LYS:HB3 | 1.90 | 0.84 |
| 1:AE:101:ASN:HD22 | 2:AF:252:LYS:CD | 1.90 | 0.84 |
| 2:CB:220:PRO:O | 1:CC:324:VAL:HG11 | 1.75 | 0.84 |
| 2:CB:220:PRO:HD2 | 1:CC:326:LYS:HE2 | 1.57 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LC:89:PRO:CG | 1:MC:280:LYS:CE | 2.55 | 0.84 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CD2 | 2.44 | 0.84 |
| 7:5B:1562:LEU:H | 7:5B:1562:LEU:HD12 | 1.40 | 0.84 |
| 9:7C:35:ILE:O | 9:7D:43:LEU:HD23 | 1.77 | 0.84 |
| 1:DC:101:ASN:HD21 | 2:DD:252:LYS:CD | 1.69 | 0.84 |
| 2:EB:157:GLU:CD | 7:5C:935:LYS:HZ2 | 1.80 | 0.84 |
| 1:EC:71:GLU:OE1 | 2:ED:247:ASN:ND2 | 2.11 | 0.84 |
| 2:ED:157:GLU:CD | 7:5A:935:LYS:HZ1 | 1.76 | 0.84 |
| 1:FC:419:SER:OG | 7:5A:1256:ARG:CD | 2.24 | 0.84 |
| 1:IA:101:ASN:HD22 | 2:IB:252:LYS:CD | 1.90 | 0.84 |
| 1:KE:85:GLN:NE2 | 1:LE:282:TYR:HB3 | 1.91 | 0.84 |
| 2:LB:331:LEU:HD23 | 4:2C:42:PHE:CZ | 1.37 | 0.84 |
| 7:5B:832:ASN:OD1 | 7:5B:832:ASN:N | 2.09 | 0.84 |
| 7:5B:1246:LEU:N | 9:7D:12:GLU:OE1 | 2.09 | 0.84 |
| 1:AE:101:ASN:CG | 2:AF:252:LYS:HD2 | 2.00 | 0.84 |
| 1:DA:101:ASN:HD22 | 2:DB:252:LYS:HG3 | 1.42 | 0.84 |
| 2:EF:55:THR:HG21 | 2:FF:284:LEU:H | 1.41 | 0.84 |
| 1:FC:60:LYS:HD3 | 1:GC:283:HIS:HA | 0.90 | 0.84 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:CZ | 2.55 | 0.84 |
| 1:HE:101:ASN:HD22 | 2:HF:252:LYS:HG3 | 1.42 | 0.84 |
| 1:JE:282:TYR:OH | 10:9A:17:UNK:CB | 2.26 | 0.84 |
| 2:KF:130:LEU:HB2 | 4:2B:37:GLY:HA2 | 1.60 | 0.84 |
| 1:LE:222:PRO:HD2 | 2:LF:324:LYS:HB3 | 1.57 | 0.84 |
| 5:3A:229:PHE:HE2 | 5:3A:331:GLN:HB3 | 0.69 | 0.84 |
| 5:3B:229:PHE:HE2 | 5:3B:331:GLN:HB3 | 0.68 | 0.84 |
| 7:5A:832:ASN:OD1 | 7:5A:832:ASN:N | 2.09 | 0.84 |
| 7:5A:1077:ASN:HA | 7:5A:1083:THR:CG2 | 2.07 | 0.84 |
| 7:5C:1490:LYS:C | 7:5C:1495:PHE:HB2 | 2.00 | 0.84 |
| 7:5C:1562:LEU:H | 7:5C:1562:LEU:HD12 | 1.40 | 0.84 |
| 1:IE:101:ASN:HD22 | 2:IF:252:LYS:CD | 1.90 | 0.84 |
| 1:IE:101:ASN:CG | 2:IF:252:LYS:HD2 | 2.00 | 0.84 |
| 1:KC:85:GLN:NE2 | 1:LC:282:TYR:HB3 | 1.92 | 0.84 |
| 1:KE:84:ARG:NE | 1:LE:283:HIS:CE1 | 2.38 | 0.84 |
| 2:LD:340:TYR:CB | 4:2A:147:PHE:HB2 | 2.07 | 0.84 |
| 1:MC:101:ASN:ND2 | 2:MD:252:LYS:CG | 2.41 | 0.84 |
| 2:DD:177:ASP:O | 1:DE:352:LYS:CD | 2.24 | 0.84 |
| 1:JE:101:ASN:HD22 | 2:JF:252:LYS:CD | 1.90 | 0.84 |
| 2:LB:379:LYS:NZ | 4:2C:166:ILE:H | 1.76 | 0.84 |
| 2:LD:55:THR:HG21 | 2:MD:283:ALA:HA | 1.57 | 0.84 |
| 1:LE:401:LYS:NZ | 2:LF:344:TRP:CD2 | 2.45 | 0.84 |
| 2:LF:55:THR:HG21 | 2:MF:284:LEU:H | 1.43 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:3C:229:PHE:HE2 | 5:3C:331:GLN:HB3 | 0.68 | 0.84 |
| 9:7A:35:ILE:O | 9:7B:43:LEU:HD23 | 1.77 | 0.84 |
| 9:7B:12:GLU:HA | 9:7B:16:THR:HG1 | 1.41 | 0.84 |
| 2:AF:361:LEU:HD22 | 6:4A:144:LEU:HD12 | 1.60 | 0.84 |
| 2:BD:220:PRO:O | 1:BE:324:VAL:HG11 | 1.78 | 0.84 |
| 2:ED:212:PHE:CZ | 1:EE:326:LYS:CD | 2.22 | 0.84 |
| 1:HE:369:ALA:HB1 | 10:8U:18:UNK:HA | 1.60 | 0.84 |
| 1:MC:101:ASN:HD22 | 2:MD:252:LYS:CG | 1.90 | 0.84 |
| 7:5A:1562:LEU:H | 7:5A:1562:LEU:HD12 | 1.40 | 0.84 |
| 2:DB:220:PRO:O | 1:DC:324:VAL:HG13 | 1.78 | 0.84 |
| 2:EB:220:PRO:CD | 1:EC:326:LYS:HE2 | 2.07 | 0.84 |
| 2:ED:220:PRO:CD | 1:EE:326:LYS:HE2 | 2.06 | 0.84 |
| 1:FA:402:ARG:HD3 | 7:5C:1259:TYR:HD2 | 1.42 | 0.84 |
| 1:HC:415:GLU:HG3 | 5:3C:235:LEU:CB | 2.06 | 0.84 |
| 1:JA:91:GLN:H | 1:KA:280:LYS:HZ3 | 1.24 | 0.84 |
| 2:JB:86:ARG:HH22 | 2:KB:280:GLN:CB | 1.90 | 0.84 |
| 2:JB:177:ASP:CG | 1:JC:353:VAL:HG11 | 1.95 | 0.84 |
| 2:KD:158:GLU:CA | 4:2A:34:ASN:CB | 2.34 | 0.84 |
| 1:MA:101:ASN:HD22 | 2:MB:252:LYS:CD | 1.86 | 0.84 |
| 6:4A:244:GLU:CA | 6:4A:247:LYS:HG2 | 2.08 | 0.84 |
| 6:4B:244:GLU:CA | 6:4B:247:LYS:HG2 | 2.08 | 0.84 |
| 6:4D:244:GLU:CA | 6:4D:247:LYS:HG2 | 2.08 | 0.84 |
| 7:5A:1490:LYS:C | 7:5A:1495:PHE:HB2 | 2.00 | 0.84 |
| 7:5C:1367:LYS:HB2 | 7:5C:1367:LYS:NZ | 1.93 | 0.84 |
| 2:FD:55:THR:H | 2:GD:283:ALA:CB | 1.84 | 0.83 |
| 1:FE:419:SER:CB | 7:5B:1256:ARG:CZ | 2.55 | 0.83 |
| 2:FF:54:ALA:C | 2:GF:283:ALA:HB2 | 2.03 | 0.83 |
| 1:JA:101:ASN:HD22 | 2:JB:252:LYS:CD | 1.90 | 0.83 |
| 2:KB:217:LEU:HB3 | 6:4A:265:TYR:CZ | 2.13 | 0.83 |
| 2:KF:86:ARG:HH11 | 2:LF:283:ALA:HB3 | 1.41 | 0.83 |
| 2:LB:177:ASP:CG | 1:LC:353:VAL:HG13 | 2.00 | 0.83 |
| 1:MC:282:TYR:CE2 | 6:4A:104:ARG:HD3 | 2.12 | 0.83 |
| 6:4C:244:GLU:CA | 6:4C:247:LYS:HG2 | 2.08 | 0.83 |
| 7:5A:1267:CYS:SG | 9:7A:8:ARG:CG | 2.66 | 0.83 |
| 7:5A:1367:LYS:HB2 | 7:5A:1367:LYS:NZ | 1.93 | 0.83 |
| 7:5B:1077:ASN:HA | 7:5B:1083:THR:CG2 | 2.07 | 0.83 |
| 1:AA:101:ASN:HD22 | 2:AB:252:LYS:CD | 1.90 | 0.83 |
| 2:BD:220:PRO:HD2 | 1:BE:326:LYS:HG2 | 1.57 | 0.83 |
| 2:CD:87:PRO:HD2 | 2:DD:281:TYR:CZ | 2.13 | 0.83 |
| 1:DE:402:ARG:NE | 7:5B:777:ALA:HB2 | 1.92 | 0.83 |
| 2:ED:397:TRP:CG | 1:EE:256:GLN:HE22 | 1.47 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:HC:415:GLU:HG3 | 5:3C:235:LEU:HD22 | 1.60 | 0.83 |
| 2:JF:88:ASP:HB2 | 2:KF:278:SER:CB | 2.08 | 0.83 |
| 2:KB:124:ALA:O | 4:2C:38:VAL:CG1 | 2.26 | 0.83 |
| 1:KE:101:ASN:CG | 2:KF:252:LYS:HD2 | 2.00 | 0.83 |
| 1:LA:222:PRO:HG2 | 2:LB:324:LYS:HB2 | 1.60 | 0.83 |
| 1:LA:407:TRP:CZ2 | 2:LB:254:ALA:O | 2.31 | 0.83 |
| 2:LD:306:ARG:NH1 | 4:2A:151:VAL:HG23 | 1.79 | 0.83 |
| 1:ME:101:ASN:HD22 | 2:MF:252:LYS:CD | 1.89 | 0.83 |
| 7:5B:841:VAL:CG2 | 8:6B:11:PRO:HA | 2.08 | 0.83 |
| 7:5B:1367:LYS:HB2 | 7:5B:1367:LYS:NZ | 1.93 | 0.83 |
| 1:EA:76:ASP:OD1 | 2:EB:46:ARG:NH2 | 2.10 | 0.83 |
| 1:HC:415:GLU:HG3 | 5:3C:235:LEU:CD2 | 2.07 | 0.83 |
| 1:IE:101:ASN:HD22 | 2:IF:252:LYS:HD2 | 1.41 | 0.83 |
| 1:JA:90:GLU:HG2 | 1:KA:280:LYS:HD2 | 1.59 | 0.83 |
| 1:LA:222:PRO:HD2 | 2:LB:324:LYS:CD | 2.06 | 0.83 |
| 9:7B:12:GLU:C | 9:7B:16:THR:OG1 | 2.20 | 0.83 |
| 2:CB:177:ASP:OD1 | 1:CC:353:VAL:HG12 | 1.73 | 0.83 |
| 2:DB:86:ARG:CB | 2:EB:281:TYR:CE1 | 2.60 | 0.83 |
| 1:DC:402:ARG:HE | 7:5A:777:ALA:CB | 1.83 | 0.83 |
| 1:FE:419:SER:HB3 | 7:5B:1256:ARG:HG2 | 1.60 | 0.83 |
| 1:GE:402:ARG:NE | 5:3A:381:ASN:ND2 | 2.26 | 0.83 |
| 2:IF:424:GLN:CD | 7:5B:1413:GLN:HE22 | 1.73 | 0.83 |
| 1:LC:245:ASP:CG | 6:4A:216:ARG:HE | 1.85 | 0.83 |
| 2:EB:177:ASP:OD2 | 1:EC:248:LEU:CD2 | 2.26 | 0.83 |
| 1:FA:56:THR:C | 1:GA:285:GLN:CB | 2.51 | 0.83 |
| 1:FE:11:GLN:OE1 | 2:FF:245:GLN:O | 1.96 | 0.83 |
| 1:HE:101:ASN:HD22 | 2:HF:252:LYS:CD | 1.90 | 0.83 |
| 2:LB:331:LEU:CD2 | 4:2C:42:PHE:CZ | 0.81 | 0.83 |
| 2:LD:77:ARG:HH11 | 6:4B:204:ARG:NH2 | 1.74 | 0.83 |
| 2:LD:306:ARG:NH2 | 4:2A:149:ILE:HG22 | 1.93 | 0.83 |
| 1:LE:11:GLN:NE2 | 2:LF:247:ASN:OD1 | 2.11 | 0.83 |
| 1:MA:279:GLU:CG | 6:4C:110:LYS:HE3 | 2.08 | 0.83 |
| 1:DE:414:GLU:OE2 | 7:5B:789:LYS:NZ | 2.11 | 0.83 |
| 1:IA:278:ALA:CB | 10:8V:22:UNK:N | 2.38 | 0.83 |
| 1:IC:402:ARG:HE | 7:5A:1417:GLN:HG3 | 1.44 | 0.83 |
| 1:IE:101:ASN:HD22 | 2:IF:252:LYS:HG3 | 1.42 | 0.83 |
| 1:KE:101:ASN:HD22 | 2:KF:252:LYS:CD | 1.90 | 0.83 |
| 1:LA:401:LYS:NZ | 2:LB:344:TRP:CD2 | 2.46 | 0.83 |
| 2:LB:413:SER:HB2 | 4:2C:171:VAL:HG21 | 1.57 | 0.83 |
| 7:5C:1246:LEU:HG | 9:7F:12:GLU:CD | 2.03 | 0.83 |
| 9:7C:11:TYR:CZ | 9:7D:26:LEU:HB3 | 2.13 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AD:322:SER:N | 6:4C:156:PHE:CE2 | 2.47 | 0.83 |
| 1:DA:401:LYS:CE | 2:DB:344:TRP:CE3 | 2.47 | 0.83 |
| 2:FF:55:THR:H | 2:GF:283:ALA:HB2 | 1.37 | 0.83 |
| 1:JA:101:ASN:HD22 | 2:JB:252:LYS:CG | 1.91 | 0.83 |
| 2:JD:86:ARG:HH21 | 2:KD:280:GLN:HB2 | 1.43 | 0.83 |
| 2:KB:54:ALA:CA | 2:LB:285:THR:CG2 | 2.53 | 0.83 |
| 1:KC:85:GLN:CD | 1:LC:282:TYR:CB | 2.50 | 0.83 |
| 2:MD:98:GLY:C | 1:ME:254:GLU:HG2 | 2.03 | 0.83 |
| 1:ME:372:MET:CE | 6:4B:96:VAL:C | 2.43 | 0.83 |
| 5:3C:224:ASP:N | 5:3C:335:LYS:HZ3 | 1.75 | 0.83 |
| 2:AD:280:GLN:HA | 6:4C:142:SER:HB3 | 1.59 | 0.83 |
| 2:CD:177:ASP:OD2 | 1:CE:248:LEU:CD2 | 2.27 | 0.83 |
| 1:FA:422:ARG:HE | 7:5C:1170:THR:HB | 1.38 | 0.83 |
| 1:GE:402:ARG:NE | 5:3A:381:ASN:HD22 | 1.77 | 0.83 |
| 1:IA:101:ASN:HD22 | 2:IB:252:LYS:CG | 1.91 | 0.83 |
| 1:IE:282:TYR:CE2 | 10:8X:15:UNK:O | 2.31 | 0.83 |
| 1:KE:101:ASN:HD22 | 2:KF:252:LYS:HG3 | 1.42 | 0.83 |
| 7:5C:839:GLU:HG2 | 8:6C:107:PRO:O | 1.79 | 0.83 |
| 9:7A:11:TYR:CZ | 9:7B:26:LEU:HB3 | 2.13 | 0.83 |
| 2:BD:177:ASP:OD2 | 1:BE:248:LEU:HD21 | 1.78 | 0.83 |
| 2:CB:87:PRO:HD2 | 2:DB:281:TYR:CZ | 2.13 | 0.83 |
| 1:DA:101:ASN:ND2 | 2:DB:252:LYS:CG | 2.42 | 0.83 |
| 1:EA:101:ASN:HD22 | 2:EB:252:LYS:CG | 1.90 | 0.83 |
| 2:JD:177:ASP:CG | 1:JE:353:VAL:HG11 | 1.96 | 0.83 |
| 1:JE:101:ASN:ND2 | 2:JF:252:LYS:CG | 2.42 | 0.83 |
| 2:KD:125:GLU:HG3 | 2:LD:336:LYS:HZ3 | 1.03 | 0.83 |
| 4:2B:16:GLN:HA | 4:2B:19:MET:CG | 2.09 | 0.83 |
| 5:3B:224:ASP:N | 5:3B:335:LYS:HZ3 | 1.75 | 0.83 |
| 7:5B:1480:VAL:HG11 | 7:5B:1572:LEU:HD22 | 1.61 | 0.83 |
| 9:7D:12:GLU:C | 9:7D:16:THR:OG1 | 2.20 | 0.83 |
| 2:AD:359:LYS:HA | 6:4C:151:ARG:NH2 | 1.92 | 0.83 |
| 1:CE:222:PRO:CG | 2:CF:324:LYS:HD3 | 2.08 | 0.83 |
| 1:FA:423:GLU:CD | 7:5C:1256:ARG:NH2 | 2.35 | 0.83 |
| 2:FD:220:PRO:O | 1:FE:324:VAL:HG11 | 1.78 | 0.83 |
| 1:FE:101:ASN:HD21 | 2:FF:252:LYS:CD | 1.77 | 0.83 |
| 1:GE:101:ASN:ND2 | 2:GF:252:LYS:CG | 2.42 | 0.83 |
| 2:LD:220:PRO:HD2 | 1:LE:326:LYS:HG2 | 1.59 | 0.83 |
| 2:LF:379:LYS:HE3 | 4:2B:166:ILE:HG13 | 1.59 | 0.83 |
| 9:7F:12:GLU:C | 9:7F:16:THR:OG1 | 2.21 | 0.83 |
| 1:BC:101:ASN:HD22 | 2:BD:252:LYS:CD | 1.92 | 0.82 |
| 1:FA:89:PRO:CD | 1:GA:280:LYS:NZ | 2.42 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FC:402:ARG:CD | 7:5A:1259:TYR:CD2 | 2.61 | 0.82 |
| 2:GB:55:THR:HG23 | 2:HB:283:ALA:C | 2.01 | 0.82 |
| 2:GB:412:GLU:OE2 | 7:5C:1323:MET:HE2 | 1.79 | 0.82 |
| 2:JB:86:ARG:NH1 | 2:KB:280:GLN:C | 2.37 | 0.82 |
| 1:LA:60:LYS:NZ | 1:MA:283:HIS:ND1 | 2.27 | 0.82 |
| 2:LB:306:ARG:NH2 | 4:2C:149:ILE:HG22 | 1.94 | 0.82 |
| 2:LF:55:THR:H | 2:MF:283:ALA:CB | 1.92 | 0.82 |
| 2:MB:111:GLU:HG2 | 3:1A:62:SER:HB2 | 1.59 | 0.82 |
| 7:5A:1480:VAL:HG11 | 7:5A:1572:LEU:HD22 | 1.61 | 0.82 |
| 1:CC:101:ASN:ND2 | 2:CD:252:LYS:CG | 2.41 | 0.82 |
| 2:DB:98:GLY:C | 1:DC:254:GLU:HG2 | 2.04 | 0.82 |
| 2:FB:220:PRO:O | 1:FC:324:VAL:CG1 | 2.27 | 0.82 |
| 1:HA:101:ASN:HD22 | 2:HB:252:LYS:CG | 1.91 | 0.82 |
| 1:HC:410:GLY:HA2 | 5:3C:329:ARG:HH21 | 1.42 | 0.82 |
| 1:JC:124:LYS:HD2 | 1:KC:284:GLU:OE1 | 1.78 | 0.82 |
| 1:LA:89:PRO:CG | 1:MA:280:LYS:NZ | 2.42 | 0.82 |
| 2:LB:296:ALA:HB2 | 4:2C:149:ILE:HG21 | 1.61 | 0.82 |
| 2:MD:78:ALA:CB | 6:4B:178:HIS:NE2 | 2.42 | 0.82 |
| 4:2A:16:GLN:HA | 4:2A:19:MET:CG | 2.09 | 0.82 |
| 2:DB:177:ASP:OD2 | 1:DC:248:LEU:CD2 | 2.27 | 0.82 |
| 1:IE:431:ASP:OD2 | 5:3A:61:SER:O | 1.96 | 0.82 |
| 1:JE:101:ASN:HD22 | 2:JF:252:LYS:HG3 | 1.42 | 0.82 |
| 2:LB:55:THR:CB | 2:MB:283:ALA:HA | 2.09 | 0.82 |
| 2:LF:55:THR:HG21 | 2:MF:283:ALA:HA | 1.59 | 0.82 |
| 4:2C:16:GLN:HA | 4:2C:19:MET:CG | 2.09 | 0.82 |
| 4:2C:170:LYS:HB3 | 4:2C:172:ASP:HB3 | 1.61 | 0.82 |
| 6:4A:244:GLU:HA | 6:4A:247:LYS:CG | 2.09 | 0.82 |
| 6:4B:244:GLU:HA | 6:4B:247:LYS:CG | 2.10 | 0.82 |
| 6:4C:244:GLU:HA | 6:4C:247:LYS:CG | 2.09 | 0.82 |
| 7:5C:1480:VAL:HG11 | 7:5C:1572:LEU:HD22 | 1.61 | 0.82 |
| 1:BC:101:ASN:HD22 | 2:BD:252:LYS:HG3 | 1.43 | 0.82 |
| 2:EB:55:THR:CG2 | 2:FB:283:ALA:HA | 2.06 | 0.82 |
| 1:EE:76:ASP:OD1 | 2:EF:46:ARG:NH2 | 2.10 | 0.82 |
| 2:EF:86:ARG:HA | 2:FF:281:TYR:CE1 | 2.15 | 0.82 |
| 2:KD:125:GLU:CD | 2:LD:332:ASN:HD22 | 1.86 | 0.82 |
| 1:MA:279:GLU:HG3 | 6:4C:110:LYS:HE3 | 1.61 | 0.82 |
| 1:ME:101:ASN:HD22 | 2:MF:252:LYS:HG3 | 1.43 | 0.82 |
| 4:2A:170:LYS:HB3 | 4:2A:172:ASP:HB3 | 1.61 | 0.82 |
| 6:4D:244:GLU:HA | 6:4D:247:LYS:CG | 2.10 | 0.82 |
| 1:AE:101:ASN:HD22 | 2:AF:252:LYS:HG3 | 1.42 | 0.82 |
| 1:KA:101:ASN:HD22 | 2:KB:252:LYS:CD | 1.90 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LB:231:ALA:CB | 6:4A:226:ILE:CD1 | 2.24 | 0.82 |
| 7:5B:1487:ASN:CG | 7:5B:1568:LYS:CG | 2.52 | 0.82 |
| 7:5C:1549:THR:CA | 7:5C:1566:GLU:CG | 2.49 | 0.82 |
| 1:BA:101:ASN:HD22 | 2:BB:252:LYS:HG3 | 1.43 | 0.82 |
| 2:DD:220:PRO:CD | 1:DE:326:LYS:HE2 | 2.10 | 0.82 |
| 2:ED:220:PRO:O | 1:EE:324:VAL:HG13 | 1.80 | 0.82 |
| 1:IE:101:ASN:ND2 | 2:IF:252:LYS:CG | 2.42 | 0.82 |
| 1:KA:127:ASP:OD2 | 1:LA:334:THR:CG2 | 2.28 | 0.82 |
| 2:LB:55:THR:H | 2:MB:283:ALA:CB | 1.93 | 0.82 |
| 4:2B:170:LYS:HB3 | 4:2B:172:ASP:HB3 | 1.61 | 0.82 |
| 7:5A:1487:ASN:CG | 7:5A:1568:LYS:CG | 2.52 | 0.82 |
| 7:5A:1544:ILE:HA | 7:5A:1573:ARG:HD2 | 0.84 | 0.82 |
| 7:5A:1548:VAL:HG12 | 7:5A:1566:GLU:HA | 0.84 | 0.82 |
| 7:5C:839:GLU:CG | 8:6C:107:PRO:O | 2.28 | 0.82 |
| 7:5C:1267:CYS:SG | 9:7E:8:ARG:HG3 | 2.19 | 0.82 |
| 7:5C:1471:ILE:HD12 | 7:5C:1471:ILE:H | 1.44 | 0.82 |
| 7:5C:1487:ASN:CG | 7:5C:1568:LYS:CG | 2.52 | 0.82 |
| 2:ED:125:GLU:CG | 7:5A:903:PHE:CD2 | 2.53 | 0.82 |
| 1:FA:60:LYS:HD2 | 1:GA:283:HIS:CD2 | 2.14 | 0.82 |
| 1:FA:60:LYS:HD2 | 1:GA:283:HIS:HD2 | 1.41 | 0.82 |
| 1:GA:101:ASN:HD22 | 2:GB:252:LYS:CG | 1.91 | 0.82 |
| 1:JE:90:GLU:HG2 | 1:KE:280:LYS:HB3 | 1.61 | 0.82 |
| 1:KA:79:ARG:O | 1:LA:280:LYS:CE | 2.22 | 0.82 |
| 1:KE:101:ASN:ND2 | 2:KF:252:LYS:CG | 2.42 | 0.82 |
| 1:ME:279:GLU:CB | 6:4B:110:LYS:CE | 2.57 | 0.82 |
| 5:3A:224:ASP:N | 5:3A:335:LYS:HZ3 | 1.76 | 0.82 |
| 6:4B:132:LYS:HA | 6:4B:132:LYS:CE | 2.07 | 0.82 |
| 6:4D:132:LYS:HA | 6:4D:132:LYS:CE | 2.07 | 0.82 |
| 7:5B:1548:VAL:HG12 | 7:5B:1566:GLU:HA | 0.84 | 0.82 |
| 7:5C:1544:ILE:HA | 7:5C:1573:ARG:HD2 | 0.83 | 0.82 |
| 9:7F:18:VAL:CG1 | 9:7F:42:LEU:HD23 | 2.09 | 0.82 |
| 1:AE:283:HIS:HB3 | 2:MB:86:ARG:HH12 | 1.42 | 0.82 |
| 1:CE:101:ASN:ND2 | 2:CF:252:LYS:CG | 2.42 | 0.82 |
| 2:DD:86:ARG:N | 2:ED:281:TYR:CE1 | 2.47 | 0.82 |
| 1:EC:402:ARG:NE | 7:5A:824:ARG:NH2 | 2.27 | 0.82 |
| 1:GA:60:LYS:HD3 | 1:HA:283:HIS:CG | 2.15 | 0.82 |
| 1:GE:101:ASN:HD22 | 2:GF:252:LYS:HG3 | 1.42 | 0.82 |
| 1:HE:101:ASN:ND2 | 2:HF:252:LYS:CG | 2.42 | 0.82 |
| 1:IE:434:GLU:OE1 | 5:3A:61:SER:CB | 2.27 | 0.82 |
| 1:KA:101:ASN:HD22 | 2:KB:252:LYS:CG | 1.91 | 0.82 |
| 2:KB:159:TYR:CE2 | 4:2C:35:VAL:O | 2.32 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KF:86:ARG:NH1 | 2:LF:283:ALA:CA | 2.42 | 0.82 |
| 2:LD:310:TYR:HE2 | 4:2A:147:PHE:CE2 | 1.98 | 0.82 |
| 1:LE:407:TRP:CZ2 | 2:LF:254:ALA:O | 2.33 | 0.82 |
| 6:4C:101:ARG:HH21 | 6:4C:101:ARG:HG3 | 1.43 | 0.82 |
| 7:5A:1471:ILE:H | 7:5A:1471:ILE:HD12 | 1.44 | 0.82 |
| 7:5B:1544:ILE:HA | 7:5B:1573:ARG:HD2 | 0.83 | 0.82 |
| 9:7A:30:ARG:HH11 | 9:7B:3:GLN:CG | 1.92 | 0.82 |
| 9:7C:30:ARG:HH11 | 9:7D:3:GLN:CG | 1.92 | 0.82 |
| 9:7E:42:LEU:HD12 | 9:7F:39:GLY:CA | 2.09 | 0.82 |
| 2:AD:361:LEU:HD22 | 6:4C:144:LEU:HD12 | 1.60 | 0.82 |
| 2:CD:397:TRP:HE3 | 1:CE:257:THR:HG22 | 1.42 | 0.82 |
| 2:EF:157:GLU:OE1 | 7:5B:935:LYS:HE3 | 1.79 | 0.82 |
| 2:FF:55:THR:N | 2:GF:283:ALA:CB | 2.43 | 0.82 |
| 2:KB:177:ASP:CG | 1:KC:353:VAL:HG11 | 1.96 | 0.82 |
| 2:LB:331:LEU:CD2 | 4:2C:42:PHE:CE1 | 1.75 | 0.82 |
| 2:LD:18:ALA:HB3 | 6:4B:217:ASN:ND2 | 1.94 | 0.82 |
| 6:4A:132:LYS:HA | 6:4A:132:LYS:CE | 2.07 | 0.82 |
| 7:5C:1535:ILE:HG12 | 7:5C:1574:ILE:O | 1.80 | 0.82 |
| 7:5C:1548:VAL:HG12 | 7:5C:1566:GLU:HA | 0.84 | 0.82 |
| 9:7C:15:VAL:CG1 | 9:7D:35:ILE:HA | 2.09 | 0.82 |
| 1:AA:101:ASN:HD22 | 2:AB:252:LYS:CG | 1.91 | 0.82 |
| 1:BE:76:ASP:OD1 | 2:BF:46:ARG:NH2 | 2.11 | 0.82 |
| 2:DD:212:PHE:CZ | 1:DE:326:LYS:CD | 2.18 | 0.82 |
| 2:MB:221:THR:HG21 | 6:4A:189:ARG:CZ | 2.10 | 0.82 |
| 2:MD:78:ALA:HB3 | 6:4B:178:HIS:NE2 | 1.94 | 0.82 |
| 6:4C:132:LYS:HA | 6:4C:132:LYS:CE | 2.07 | 0.82 |
| 9:7A:15:VAL:CG1 | 9:7B:35:ILE:HA | 2.09 | 0.82 |
| 9:7B:18:VAL:CG1 | 9:7B:42:LEU:HD23 | 2.09 | 0.82 |
| 9:7C:30:ARG:HH12 | 9:7D:3:GLN:HA | 0.66 | 0.82 |
| 1:BE:101:ASN:HD22 | 2:BF:252:LYS:CD | 1.92 | 0.81 |
| 2:ED:157:GLU:CD | 7:5A:935:LYS:HZ2 | 1.84 | 0.81 |
| 1:FA:89:PRO:CA | 1:GA:280:LYS:HZ2 | 1.93 | 0.81 |
| 1:FA:222:PRO:CD | 2:FB:324:LYS:HD3 | 2.09 | 0.81 |
| 2:GB:54:ALA:C | 2:HB:283:ALA:HB2 | 2.04 | 0.81 |
| 2:KF:124:ALA:O | 4:2B:37:GLY:O | 1.97 | 0.81 |
| 2:LB:310:TYR:CE2 | 4:2C:147:PHE:CE2 | 2.68 | 0.81 |
| 1:LE:224:TYR:HE2 | 2:LF:246:LEU:HD11 | 1.44 | 0.81 |
| 7:5A:1535:ILE:HG12 | 7:5A:1574:ILE:O | 1.80 | 0.81 |
| 7:5B:1471:ILE:HD12 | 7:5B:1471:ILE:H | 1.44 | 0.81 |
| 9:7D:18:VAL:CG1 | 9:7D:42:LEU:HD23 | 2.08 | 0.81 |
| 2:AD:217:LEU:HD23 | 6:4C:132:LYS:HG2 | 1.59 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:EA:101:ASN:HD22 | 2:EB:252:LYS:CD | 1.89 | 0.81 |
| 1:FA:56:THR:O | 1:GA:285:GLN:CB | 2.27 | 0.81 |
| 1:FA:419:SER:HB2 | 7:5C:1256:ARG:HE | 0.67 | 0.81 |
| 2:FB:100:ASN:HB2 | 1:FC:257:THR:HG21 | 1.62 | 0.81 |
| 2:FB:220:PRO:HD2 | 1:FC:326:LYS:HE2 | 1.60 | 0.81 |
| 1:JC:89:PRO:CG | 1:KC:280:LYS:CG | 2.49 | 0.81 |
| 2:JD:86:ARG:NH1 | 2:KD:280:GLN:C | 2.37 | 0.81 |
| 1:LC:11:GLN:NE2 | 2:LD:247:ASN:OD1 | 2.12 | 0.81 |
| 1:MC:279:GLU:OE2 | 6:4A:106:ALA:HB3 | 1.80 | 0.81 |
| 2:MD:111:GLU:HG2 | 3:1B:62:SER:HB2 | 1.61 | 0.81 |
| 9:7A:30:ARG:HH12 | 9:7B:3:GLN:HA | 0.66 | 0.81 |
| 2:AF:217:LEU:HD22 | 6:4A:132:LYS:CG | 2.10 | 0.81 |
| 1:BC:101:ASN:ND2 | 2:BD:252:LYS:CG | 2.43 | 0.81 |
| 2:CB:220:PRO:O | 1:CC:324:VAL:HG13 | 1.78 | 0.81 |
| 1:DC:222:PRO:CG | 2:DD:324:LYS:HD3 | 2.10 | 0.81 |
| 2:DD:98:GLY:C | 1:DE:254:GLU:HG2 | 2.05 | 0.81 |
| 2:EB:220:PRO:O | 1:EC:324:VAL:HG13 | 1.80 | 0.81 |
| 1:FA:101:ASN:HD22 | 2:FB:252:LYS:HG3 | 1.43 | 0.81 |
| 1:FC:101:ASN:HD22 | 2:FD:252:LYS:HG3 | 1.42 | 0.81 |
| 1:GE:56:THR:HG1 | 1:HE:284:GLU:CA | 1.88 | 0.81 |
| 1:IC:282:TYR:CD1 | 10:8W:15:UNK:HA | 2.14 | 0.81 |
| 1:IE:402:ARG:NH2 | 7:5B:1417:GLN:HG2 | 1.93 | 0.81 |
| 1:JA:279:GLU:CD | 10:8Y:22:UNK:CB | 2.53 | 0.81 |
| 1:KA:79:ARG:C | 1:LA:280:LYS:HE2 | 2.05 | 0.81 |
| 2:KD:276:ARG:NH2 | 6:4B:266:ASN:H | 1.78 | 0.81 |
| 1:LA:35:GLN:HE21 | 6:4C:101:ARG:HB2 | 1.44 | 0.81 |
| 2:LB:177:ASP:OD2 | 1:LC:353:VAL:CG1 | 2.27 | 0.81 |
| 2:LB:413:SER:HB2 | 4:2C:171:VAL:CG2 | 2.10 | 0.81 |
| 1:MC:279:GLU:CG | 6:4A:110:LYS:CE | 2.57 | 0.81 |
| 6:4A:101:ARG:HH21 | 6:4A:101:ARG:HG3 | 1.43 | 0.81 |
| 7:5B:1535:ILE:HG12 | 7:5B:1574:ILE:O | 1.80 | 0.81 |
| 1:AE:101:ASN:ND2 | 2:AF:252:LYS:CG | 2.42 | 0.81 |
| 1:BA:76:ASP:OD1 | 2:BB:46:ARG:NH2 | 2.13 | 0.81 |
| 1:EA:396:ASP:HB3 | 7:5C:817:LEU:HD23 | 1.43 | 0.81 |
| 2:EB:125:GLU:C | 7:5C:903:PHE:HZ | 1.74 | 0.81 |
| 2:ED:125:GLU:C | 7:5A:903:PHE:HZ | 1.69 | 0.81 |
| 1:FC:207:GLU:OE1 | 7:5A:915:PHE:CD2 | 2.33 | 0.81 |
| 1:JE:90:GLU:C | 1:KE:280:LYS:HZ2 | 1.77 | 0.81 |
| 1:LC:89:PRO:HG3 | 1:MC:280:LYS:HE3 | 1.60 | 0.81 |
| 2:LD:54:ALA:HB1 | 2:MD:281:TYR:O | 1.81 | 0.81 |
| 1:LE:35:GLN:HE21 | 6:4B:101:ARG:HB2 | 1.44 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LF:54:ALA:HB1 | 2:MF:281:TYR:O | 1.81 | 0.81 |
| 7:5C:1490:LYS:CG | 7:5C:1494:LEU:HB3 | 2.09 | 0.81 |
| 2:CD:86:ARG:NH1 | 2:DD:281:TYR:CA | 2.43 | 0.81 |
| 2:FD:98:GLY:CA | 1:FE:254:GLU:CG | 2.35 | 0.81 |
| 1:FE:282:TYR:CD2 | 10:8O:18:UNK:CB | 2.60 | 0.81 |
| 2:JB:86:ARG:NH2 | 2:KB:280:GLN:HB3 | 1.96 | 0.81 |
| 2:KB:54:ALA:CB | 2:LB:285:THR:HG23 | 1.88 | 0.81 |
| 1:LC:60:LYS:NZ | 1:MC:283:HIS:ND1 | 2.29 | 0.81 |
| 1:BA:222:PRO:CG | 2:BB:324:LYS:HD3 | 2.10 | 0.81 |
| 1:CA:101:ASN:ND2 | 2:CB:252:LYS:CG | 2.43 | 0.81 |
| 2:DB:177:ASP:O | 1:DC:352:LYS:CD | 2.28 | 0.81 |
| 1:EA:71:GLU:OE1 | 2:EB:247:ASN:ND2 | 2.14 | 0.81 |
| 1:EA:222:PRO:CG | 2:EB:324:LYS:HD3 | 2.10 | 0.81 |
| 1:EE:430:LYS:HZ2 | 7:5B:834:ASN:CG | 1.71 | 0.81 |
| 2:FB:332:ASN:ND2 | 7:5C:909:ASN:OD1 | 2.14 | 0.81 |
| 1:FC:101:ASN:HD21 | 2:FD:252:LYS:CD | 1.76 | 0.81 |
| 1:JC:101:ASN:HD22 | 2:JD:252:LYS:HD2 | 1.40 | 0.81 |
| 2:KD:177:ASP:CG | 1:KE:353:VAL:HG11 | 1.96 | 0.81 |
| 6:4B:101:ARG:HH21 | 6:4B:101:ARG:HG3 | 1.44 | 0.81 |
| 7:5A:1490:LYS:CG | 7:5A:1494:LEU:HB3 | 2.09 | 0.81 |
| 2:AD:362:LYS:HG2 | 6:4C:146:ILE:CB | 2.10 | 0.81 |
| 1:BC:101:ASN:CG | 2:BD:252:LYS:HD2 | 2.03 | 0.81 |
| 1:EC:423:GLU:OE2 | 7:5A:830:VAL:HG11 | 1.79 | 0.81 |
| 2:GB:55:THR:H | 2:HB:283:ALA:CB | 1.91 | 0.81 |
| 1:KA:85:GLN:CA | 1:LA:283:HIS:CA | 2.41 | 0.81 |
| 2:KD:125:GLU:CD | 2:LD:336:LYS:HZ3 | 1.89 | 0.81 |
| 2:LD:231:ALA:CB | 6:4B:226:ILE:CD1 | 2.27 | 0.81 |
| 2:LF:306:ARG:HH21 | 4:2B:149:ILE:CG2 | 1.93 | 0.81 |
| 1:MC:101:ASN:HD21 | 2:MD:252:LYS:HD2 | 0.98 | 0.81 |
| 7:5A:1125:LEU:HD11 | 8:6A:245:GLN:OE1 | 1.80 | 0.81 |
| 7:5B:1490:LYS:CG | 7:5B:1494:LEU:HB3 | 2.09 | 0.81 |
| 7:5C:1152:GLU:CD | 8:6C:66:ARG:CZ | 2.54 | 0.81 |
| 2:EB:86:ARG:HA | 2:FB:281:TYR:CE1 | 2.15 | 0.81 |
| 2:JF:86:ARG:HH12 | 2:KF:280:GLN:HB3 | 1.45 | 0.81 |
| 1:KC:85:GLN:CA | 1:LC:283:HIS:CD2 | 2.48 | 0.81 |
| 1:ME:101:ASN:HD22 | 2:MF:252:LYS:CG | 1.93 | 0.81 |
| 7:5A:1276:GLU:HG2 | 9:7B:7:LEU:CD1 | 2.11 | 0.81 |
| 2:AD:322:SER:N | 6:4C:156:PHE:HE2 | 1.77 | 0.81 |
| 1:CA:60:LYS:HZ2 | 1:DA:283:HIS:CD2 | 1.99 | 0.81 |
| 2:FD:106:TYR:O | 7:5A:1298:LYS:CE | 2.29 | 0.81 |
| 2:FF:428:ALA:HA | 7:5B:1080:PHE:CE1 | 2.15 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GA:101:ASN:HD22 | 2:GB:252:LYS:CD | 1.90 | 0.81 |
| 1:HE:420:GLU:OE1 | 5:3A:215:TYR:CE1 | 2.33 | 0.81 |
| 2:JB:55:THR:CG2 | 2:KB:362:LYS:HZ2 | 1.93 | 0.81 |
| 1:JC:90:GLU:C | 1:KC:280:LYS:NZ | 2.27 | 0.81 |
| 2:KD:276:ARG:NE | 6:4B:265:TYR:HB2 | 1.95 | 0.81 |
| 2:LF:413:SER:HB2 | 4:2B:171:VAL:CG2 | 2.10 | 0.81 |
| 1:MC:101:ASN:HD22 | 2:MD:252:LYS:CD | 1.89 | 0.81 |
| 7:5C:1487:ASN:HB3 | 7:5C:1568:LYS:HE2 | 0.81 | 0.81 |
| 9:7E:42:LEU:CD1 | 9:7F:39:GLY:HA2 | 2.10 | 0.81 |
| 1:BA:101:ASN:HD22 | 2:BB:252:LYS:CD | 1.92 | 0.81 |
| 2:CB:179:VAL:CG2 | 1:CC:258:ASN:HA | 2.11 | 0.81 |
| 2:ED:177:ASP:CB | 1:EE:353:VAL:HG12 | 2.11 | 0.81 |
| 1:FC:60:LYS:CD | 1:GC:283:HIS:HD2 | 1.92 | 0.81 |
| 1:FC:89:PRO:HD3 | 1:GC:280:LYS:HZ2 | 1.00 | 0.81 |
| 1:IE:402:ARG:HH21 | 7:5B:1417:GLN:HG2 | 1.46 | 0.81 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:HZ3 | 1.43 | 0.81 |
| 1:ME:101:ASN:ND2 | 2:MF:252:LYS:CG | 2.44 | 0.81 |
| 1:BA:101:ASN:ND2 | 2:BB:252:LYS:CG | 2.44 | 0.80 |
| 2:EB:177:ASP:CB | 1:EC:353:VAL:HG12 | 2.11 | 0.80 |
| 1:HE:278:ALA:HB2 | 10:8U:18:UNK:O | 1.79 | 0.80 |
| 1:JE:101:ASN:HD22 | 2:JF:252:LYS:CG | 1.94 | 0.80 |
| 2:LB:397:TRP:HE3 | 1:LC:257:THR:HG22 | 1.42 | 0.80 |
| 2:LF:54:ALA:C | 2:MF:283:ALA:HB2 | 2.06 | 0.80 |
| 6:4A:164:ARG:HB3 | 6:4A:164:ARG:NH1 | 1.95 | 0.80 |
| 6:4C:164:ARG:HB3 | 6:4C:164:ARG:NH1 | 1.95 | 0.80 |
| 6:4D:101:ARG:HH21 | 6:4D:101:ARG:HG3 | 1.44 | 0.80 |
| 7:5A:1487:ASN:HB3 | 7:5A:1568:LYS:HE2 | 0.81 | 0.80 |
| 7:5B:841:VAL:CG1 | 8:6B:9:LEU:HD23 | 2.10 | 0.80 |
| 7:5B:1487:ASN:HB3 | 7:5B:1568:LYS:HE2 | 0.81 | 0.80 |
| 7:5C:1105:TYR:HB3 | 7:5C:1166:LEU:HB2 | 1.63 | 0.80 |
| 1:DC:222:PRO:CD | 2:DD:324:LYS:HD3 | 2.11 | 0.80 |
| 1:EE:101:ASN:HD22 | 2:EF:252:LYS:HG3 | 1.44 | 0.80 |
| 1:IE:101:ASN:HD22 | 2:IF:252:LYS:CG | 1.94 | 0.80 |
| 2:LD:177:ASP:OD1 | 1:LE:353:VAL:HG11 | 1.80 | 0.80 |
| 2:LF:379:LYS:NZ | 4:2B:166:ILE:HB | 1.96 | 0.80 |
| 6:4A:132:LYS:HE2 | 6:4A:132:LYS:HA | 1.63 | 0.80 |
| 6:4B:132:LYS:HE2 | 6:4B:132:LYS:HA | 1.63 | 0.80 |
| 7:5A:1105:TYR:HB3 | 7:5A:1166:LEU:HB2 | 1.63 | 0.80 |
| 7:5B:1105:TYR:HB3 | 7:5B:1166:LEU:HB2 | 1.63 | 0.80 |
| 9:7A:11:TYR:HD1 | 9:7B:26:LEU:CD2 | 1.75 | 0.80 |
| 1:AC:101:ASN:HD22 | 2:AD:252:LYS:HD2 | 1.40 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:BC:76:ASP:OD1 | 2:BD:46:ARG:NH2 | 2.13 | 0.80 |
| 1:IA:222:PRO:CG | 2:IB:324:LYS:HD3 | 2.12 | 0.80 |
| 1:IA:282:TYR:CG | 10:8V:18:UNK:CB | 2.65 | 0.80 |
| 2:KF:276:ARG:NH2 | 6:4D:266:ASN:H | 1.79 | 0.80 |
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:CA | 2.28 | 0.80 |
| 6:4C:132:LYS:HE2 | 6:4C:132:LYS:HA | 1.63 | 0.80 |
| 6:4D:132:LYS:HE2 | 6:4D:132:LYS:HA | 1.63 | 0.80 |
| 6:4D:164:ARG:HB3 | 6:4D:164:ARG:NH1 | 1.95 | 0.80 |
| 7:5B:1490:LYS:HD3 | 7:5B:1494:LEU:HB3 | 1.58 | 0.80 |
| 1:BA:101:ASN:CG | 2:BB:252:LYS:HD2 | 2.03 | 0.80 |
| 1:CA:222:PRO:CG | 2:CB:324:LYS:HD3 | 2.11 | 0.80 |
| 2:CB:177:ASP:OD2 | 1:CC:248:LEU:HD21 | 1.80 | 0.80 |
| 2:DD:177:ASP:OD2 | 1:DE:248:LEU:CD2 | 2.29 | 0.80 |
| 1:EC:404:PHE:HE2 | 2:ED:345:ILE:CD1 | 1.94 | 0.80 |
| 1:FA:404:PHE:HE2 | 2:FB:345:ILE:CD1 | 1.94 | 0.80 |
| 2:FB:397:TRP:CD2 | 1:FC:256:GLN:O | 2.05 | 0.80 |
| 1:GA:222:PRO:CG | 2:GB:324:LYS:HD3 | 2.12 | 0.80 |
| 1:HE:101:ASN:HD22 | 2:HF:252:LYS:CG | 1.94 | 0.80 |
| 2:MB:220:PRO:HD2 | 1:MC:326:LYS:HG2 | 1.61 | 0.80 |
| 6:4B:164:ARG:HB3 | 6:4B:164:ARG:NH1 | 1.95 | 0.80 |
| 7:5B:773:ARG:HD3 | 7:5B:773:ARG:N | 1.94 | 0.80 |
| 2:DD:177:ASP:OD1 | 1:DE:353:VAL:HG12 | 1.71 | 0.80 |
| 2:EF:55:THR:CG2 | 2:FF:284:LEU:H | 1.95 | 0.80 |
| 1:GE:101:ASN:HD22 | 2:GF:252:LYS:CD | 1.90 | 0.80 |
| 1:HC:415:GLU:HG2 | 5:3C:235:LEU:HB3 | 1.62 | 0.80 |
| 1:KE:85:GLN:NE2 | 1:LE:282:TYR:CB | 2.44 | 0.80 |
| 4:2B:144:ASN:O | 4:2B:145:GLN:HG3 | 1.80 | 0.80 |
| 7:5A:1490:LYS:HD3 | 7:5A:1494:LEU:HB3 | 1.58 | 0.80 |
| 7:5C:1495:PHE:HE2 | 7:5C:1562:LEU:HD22 | 1.46 | 0.80 |
| 2:AF:40:SER:HB2 | 6:4A:152:PHE:CD2 | 2.15 | 0.80 |
| 2:DB:220:PRO:CD | 1:DC:326:LYS:HE2 | 2.12 | 0.80 |
| 2:EB:212:PHE:CE2 | 1:EC:326:LYS:HD3 | 2.10 | 0.80 |
| 1:FC:101:ASN:HD21 | 2:FD:252:LYS:HD2 | 0.97 | 0.80 |
| 1:GC:89:PRO:CG | 1:HC:280:LYS:HD2 | 2.12 | 0.80 |
| 1:HA:222:PRO:CG | 2:HB:324:LYS:HD3 | 2.12 | 0.80 |
| 1:JA:222:PRO:CG | 2:JB:324:LYS:HD3 | 2.12 | 0.80 |
| 2:KB:273:LEU:CB | 6:4A:268:LEU:CD2 | 2.58 | 0.80 |
| 7:5A:773:ARG:HD3 | 7:5A:773:ARG:N | 1.94 | 0.80 |
| 7:5A:1495:PHE:HE2 | 7:5A:1562:LEU:HD22 | 1.46 | 0.80 |
| 7:5B:1544:ILE:HA | 7:5B:1573:ARG:CG | 2.06 | 0.80 |
| 1:AA:222:PRO:CG | 2:AB:324:LYS:HD3 | 2.12 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AD:284:LEU:HD12 | 6:4C:144:LEU:HA | 1.63 | 0.80 |
| 1:BE:101:ASN:HD22 | 2:BF:252:LYS:HG3 | 1.45 | 0.80 |
| 2:EB:220:PRO:HD2 | 1:EC:326:LYS:HG2 | 1.63 | 0.80 |
| 1:FE:207:GLU:OE1 | 7:5B:915:PHE:CD2 | 2.34 | 0.80 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:HZ1 | 0.97 | 0.80 |
| 1:LA:60:LYS:CD | 1:MA:283:HIS:CD2 | 2.65 | 0.80 |
| 2:MB:78:ALA:CB | 6:4A:178:HIS:NE2 | 2.44 | 0.80 |
| 4:2A:144:ASN:O | 4:2A:145:GLN:HG3 | 1.80 | 0.80 |
| 5:3B:230:ILE:O | 5:3B:332:MET:CG | 2.28 | 0.80 |
| 7:5C:1126:PRO:CG | 8:6C:246:TYR:OH | 2.30 | 0.80 |
| 1:BC:222:PRO:CG | 2:BD:324:LYS:HD3 | 2.11 | 0.80 |
| 1:DC:101:ASN:HD22 | 2:DD:252:LYS:HG3 | 1.45 | 0.80 |
| 2:ED:177:ASP:OD2 | 1:EE:248:LEU:CD2 | 2.29 | 0.80 |
| 1:GE:89:PRO:HD3 | 1:HE:280:LYS:HZ3 | 1.44 | 0.80 |
| 1:IC:58:ALA:CB | 10:8Z:13:UNK:CB | 2.37 | 0.80 |
| 1:IE:60:LYS:HZ2 | 1:JE:283:HIS:CD2 | 1.99 | 0.80 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:CE | 2.60 | 0.80 |
| 5:3A:230:ILE:O | 5:3A:332:MET:CG | 2.28 | 0.80 |
| 6:4D:154:LYS:HB2 | 6:4D:154:LYS:NZ | 1.95 | 0.80 |
| 7:5A:1544:ILE:HA | 7:5A:1573:ARG:CG | 2.06 | 0.80 |
| 7:5B:1495:PHE:HE2 | 7:5B:1562:LEU:HD22 | 1.46 | 0.80 |
| 7:5B:1510:ASN:HB3 | 7:5B:1559:PRO:HD2 | 1.64 | 0.80 |
| 1:EA:370:LYS:HZ1 | 10:8J:17:UNK:CB | 1.91 | 0.80 |
| 2:EB:157:GLU:OE1 | 7:5C:935:LYS:HE3 | 1.81 | 0.80 |
| 1:EE:402:ARG:CD | 7:5B:824:ARG:HH22 | 1.95 | 0.80 |
| 2:FB:55:THR:N | 2:GB:283:ALA:HB1 | 1.97 | 0.80 |
| 2:FD:212:PHE:CE2 | 1:FE:326:LYS:HD3 | 2.15 | 0.80 |
| 1:GA:89:PRO:HG3 | 1:HA:280:LYS:HE3 | 1.62 | 0.80 |
| 1:KA:124:LYS:HD3 | 1:LA:290:GLU:HA | 1.64 | 0.80 |
| 2:KB:276:ARG:NH2 | 6:4A:266:ASN:H | 1.79 | 0.80 |
| 1:LC:222:PRO:HD2 | 2:LD:324:LYS:HB3 | 1.61 | 0.80 |
| 2:LF:231:ALA:CB | 6:4D:226:ILE:CD1 | 2.34 | 0.80 |
| 2:MD:110:ALA:O | 3:1B:61:HIS:HB2 | 1.80 | 0.80 |
| 4:2C:144:ASN:O | 4:2C:145:GLN:HG3 | 1.81 | 0.80 |
| 7:5B:1434:LYS:HA | 7:5B:1434:LYS:CE | 2.10 | 0.80 |
| 1:DC:402:ARG:HH22 | 7:5A:782:LEU:HD11 | 0.72 | 0.80 |
| 1:EA:101:ASN:HD21 | 2:EB:252:LYS:CD | 1.66 | 0.80 |
| 2:FB:331:LEU:HD22 | 7:5C:915:PHE:CE2 | 2.16 | 0.80 |
| 1:GE:101:ASN:HD22 | 2:GF:252:LYS:CG | 1.94 | 0.80 |
| 2:KB:276:ARG:NH2 | 6:4A:265:TYR:CA | 2.32 | 0.80 |
| 2:LF:276:ARG:NH1 | 6:4D:229:GLU:CA | 2.30 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5A:841:VAL:HG21 | 8:6A:11:PRO:CA | 2.10 | 0.80 |
| 7:5A:1434:LYS:HA | 7:5A:1434:LYS:CE | 2.10 | 0.80 |
| 7:5A:1510:ASN:HB3 | 7:5A:1559:PRO:HD2 | 1.64 | 0.80 |
| 7:5C:1401:LYS:HD3 | 7:5C:1401:LYS:H | 1.45 | 0.80 |
| 7:5C:1434:LYS:HA | 7:5C:1434:LYS:CE | 2.10 | 0.80 |
| 9:7E:11:TYR:HE1 | 9:7F:26:LEU:HD23 | 1.47 | 0.80 |
| 1:CC:101:ASN:HD22 | 2:CD:252:LYS:CD | 1.95 | 0.79 |
| 1:FA:402:ARG:NH1 | 7:5C:1259:TYR:HA | 1.96 | 0.79 |
| 1:FC:89:PRO:HA | 1:GC:280:LYS:HZ1 | 1.46 | 0.79 |
| 1:HC:410:GLY:C | 5:3C:329:ARG:NH2 | 2.39 | 0.79 |
| 1:IA:279:GLU:OE2 | 10:8V:22:UNK:CB | 2.30 | 0.79 |
| 1:JC:88:HIS:ND1 | 1:KC:280:LYS:HD3 | 1.97 | 0.79 |
| 2:LB:179:VAL:CG2 | 1:LC:258:ASN:HA | 2.12 | 0.79 |
| 1:LC:60:LYS:CG | 6:4A:101:ARG:NH1 | 2.45 | 0.79 |
| 2:LD:55:THR:CG2 | 2:MD:283:ALA:HB1 | 2.12 | 0.79 |
| 1:ME:279:GLU:CG | 6:4B:110:LYS:CE | 2.59 | 0.79 |
| 5:3C:230:ILE:O | 5:3C:332:MET:CG | 2.28 | 0.79 |
| 6:4A:256:ASN:HD21 | 6:4A:260:ARG:NE | 1.79 | 0.79 |
| 6:4B:256:ASN:HD21 | 6:4B:260:ARG:NE | 1.79 | 0.79 |
| 6:4C:256:ASN:HD21 | 6:4C:260:ARG:NE | 1.79 | 0.79 |
| 7:5A:1401:LYS:HD3 | 7:5A:1401:LYS:H | 1.45 | 0.79 |
| 7:5B:1401:LYS:HD3 | 7:5B:1401:LYS:H | 1.45 | 0.79 |
| 7:5C:773:ARG:HD3 | 7:5C:773:ARG:N | 1.94 | 0.79 |
| 7:5C:1544:ILE:HA | 7:5C:1573:ARG:CG | 2.06 | 0.79 |
| 2:AD:357:PRO:HD2 | 6:4C:151:ARG:HD2 | 1.62 | 0.79 |
| 2:CB:86:ARG:NH1 | 2:DB:281:TYR:CA | 2.44 | 0.79 |
| 1:DA:76:ASP:OD1 | 2:DB:46:ARG:NH2 | 2.15 | 0.79 |
| 1:DE:101:ASN:HD22 | 2:DF:252:LYS:HG3 | 1.46 | 0.79 |
| 1:FE:282:TYR:CZ | 10:8O:18:UNK:CB | 2.61 | 0.79 |
| 2:IB:86:ARG:NH1 | 2:JB:281:TYR:HA | 1.97 | 0.79 |
| 1:JE:11:GLN:OE1 | 2:JF:245:GLN:O | 1.99 | 0.79 |
| 1:JE:101:ASN:HD22 | 2:JF:252:LYS:HD2 | 1.41 | 0.79 |
| 1:KC:359:PRO:CB | 6:4A:299:TYR:CE2 | 2.65 | 0.79 |
| 2:KD:177:ASP:CG | 1:KE:353:VAL:HG13 | 2.00 | 0.79 |
| 1:KE:101:ASN:HD22 | 2:KF:252:LYS:CG | 1.94 | 0.79 |
| 2:KF:273:LEU:CB | 6:4D:268:LEU:HD21 | 2.11 | 0.79 |
| 1:LA:222:PRO:HD3 | 2:LB:324:LYS:HD3 | 1.64 | 0.79 |
| 6:4B:154:LYS:HB2 | 6:4B:154:LYS:NZ | 1.95 | 0.79 |
| 6:4D:252:VAL:CG1 | 6:4D:292:VAL:HG23 | 2.12 | 0.79 |
| 6:4D:256:ASN:HD21 | 6:4D:260:ARG:NE | 1.79 | 0.79 |
| 7:5C:1510:ASN:HB3 | 7:5C:1559:PRO:HD2 | 1.64 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BE:101:ASN:CG | 2:BF:252:LYS:HD2 | 2.05 | 0.79 |
| 1:CE:222:PRO:CD | 2:CF:324:LYS:HD3 | 2.10 | 0.79 |
| 2:ED:212:PHE:CE2 | 1:EE:326:LYS:HD3 | 2.13 | 0.79 |
| 1:EE:404:PHE:HE2 | 2:EF:345:ILE:CD1 | 1.95 | 0.79 |
| 2:HD:362:LYS:NZ | 10:8T:36:UNK:O | 2.11 | 0.79 |
| 1:HE:415:GLU:HG3 | 5:3A:235:LEU:CB | 2.09 | 0.79 |
| 1:KE:11:GLN:OE1 | 2:KF:245:GLN:O | 1.99 | 0.79 |
| 2:LB:77:ARG:CZ | 6:4A:204:ARG:HH21 | 1.94 | 0.79 |
| 1:LE:89:PRO:CG | 1:ME:280:LYS:HZ2 | 1.95 | 0.79 |
| 1:LE:222:PRO:HG3 | 2:LF:324:LYS:CD | 2.10 | 0.79 |
| 7:5A:874:GLN:HB2 | 8:6A:59:LYS:HZ3 | 1.42 | 0.79 |
| 7:5B:1549:THR:CA | 7:5B:1566:GLU:OE1 | 2.13 | 0.79 |
| 1:AE:101:ASN:HD22 | 2:AF:252:LYS:CG | 1.94 | 0.79 |
| 2:DD:178:THR:HG23 | 1:DE:258:ASN:ND2 | 1.97 | 0.79 |
| 1:GE:11:GLN:OE1 | 2:GF:245:GLN:O | 1.99 | 0.79 |
| 1:IE:393:HIS:CE1 | 5:3A:306:ASP:OD1 | 2.35 | 0.79 |
| 2:JB:55:THR:HG22 | 2:KB:362:LYS:HZ1 | 1.41 | 0.79 |
| 1:JE:90:GLU:CG | 1:KE:280:LYS:HD2 | 2.12 | 0.79 |
| 2:JF:86:ARG:CZ | 2:KF:280:GLN:CA | 2.61 | 0.79 |
| 1:LA:221:ARG:HH11 | 2:LB:324:LYS:N | 1.81 | 0.79 |
| 2:LD:413:SER:HB2 | 4:2A:171:VAL:CG2 | 2.12 | 0.79 |
| 2:MB:98:GLY:C | 1:MC:254:GLU:HG2 | 2.06 | 0.79 |
| 6:4B:252:VAL:CG1 | 6:4B:292:VAL:HG23 | 2.12 | 0.79 |
| 6:4C:252:VAL:CG1 | 6:4C:292:VAL:HG23 | 2.12 | 0.79 |
| 7:5C:832:ASN:OD1 | 7:5C:832:ASN:N | 2.09 | 0.79 |
| 2:BB:177:ASP:O | 1:BC:352:LYS:CD | 2.26 | 0.79 |
| 2:CB:177:ASP:CG | 1:CC:353:VAL:HG11 | 2.01 | 0.79 |
| 1:EC:393:HIS:CE1 | 7:5A:814:LYS:HG3 | 2.16 | 0.79 |
| 2:FD:212:PHE:CZ | 1:FE:326:LYS:CD | 2.31 | 0.79 |
| 2:LB:331:LEU:HD11 | 4:2C:42:PHE:CE1 | 2.17 | 0.79 |
| 2:LD:212:PHE:HZ | 1:LE:326:LYS:HD3 | 0.62 | 0.79 |
| 1:ME:101:ASN:HD21 | 2:MF:252:LYS:HD2 | 0.96 | 0.79 |
| 1:ME:279:GLU:OE1 | 6:4B:107:MET:CA | 2.31 | 0.79 |
| 6:4A:252:VAL:CG1 | 6:4A:292:VAL:HG23 | 2.12 | 0.79 |
| 7:5B:773:ARG:C | 7:5B:775:PRO:HD3 | 2.07 | 0.79 |
| 7:5B:836:ARG:HH11 | 7:5B:836:ARG:HB3 | 1.44 | 0.79 |
| 1:AC:342:GLN:NE2 | 3:1C:55:HIS:CG | 2.36 | 0.79 |
| 2:CD:220:PRO:O | 1:CE:324:VAL:HG13 | 1.82 | 0.79 |
| 2:EB:55:THR:CG2 | 2:FB:284:LEU:H | 1.95 | 0.79 |
| 1:HE:11:GLN:OE1 | 2:HF:245:GLN:O | 1.99 | 0.79 |
| 1:HE:159:VAL:HG22 | 5:3A:209:ARG:HH21 | 1.46 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:IA:402:ARG:HE | 7:5C:1417:GLN:HG3 | 1.46 | 0.79 |
| 1:IE:11:GLN:OE1 | 2:IF:245:GLN:O | 1.99 | 0.79 |
| 2:JF:86:ARG:NH1 | 2:KF:280:GLN:O | 2.16 | 0.79 |
| 1:KC:62:VAL:CG2 | 1:LC:285:GLN:CB | 2.51 | 0.79 |
| 1:KC:90:GLU:N | 1:LC:284:GLU:OE1 | 2.15 | 0.79 |
| 1:LA:401:LYS:NZ | 2:LB:344:TRP:CZ2 | 2.51 | 0.79 |
| 2:LB:55:THR:HG21 | 2:MB:283:ALA:HA | 1.59 | 0.79 |
| 2:LD:177:ASP:OD2 | 1:LE:353:VAL:HG13 | 1.83 | 0.79 |
| 1:LE:60:LYS:NZ | 1:ME:283:HIS:ND1 | 2.31 | 0.79 |
| 2:MF:78:ALA:HB3 | 6:4D:178:HIS:NE2 | 1.98 | 0.79 |
| 6:4D:252:VAL:CG1 | 6:4D:292:VAL:CG2 | 2.61 | 0.79 |
| 7:5C:1491:LEU:HD21 | 7:5C:1495:PHE:CE1 | 2.17 | 0.79 |
| 2:AD:40:SER:HB3 | 6:4C:152:PHE:HD2 | 1.45 | 0.79 |
| 2:AD:284:LEU:HD11 | 6:4C:144:LEU:HD11 | 1.62 | 0.79 |
| 1:AE:11:GLN:OE1 | 2:AF:245:GLN:O | 1.99 | 0.79 |
| 2:BF:87:PRO:HD2 | 2:CF:281:TYR:CZ | 2.17 | 0.79 |
| 2:DB:397:TRP:HE3 | 1:DC:257:THR:HG22 | 1.42 | 0.79 |
| 1:FA:101:ASN:HD22 | 2:FB:252:LYS:HD2 | 1.46 | 0.79 |
| 1:FA:101:ASN:CG | 2:FB:252:LYS:HD2 | 2.04 | 0.79 |
| 2:GD:83:GLN:O | 2:HD:281:TYR:OH | 2.00 | 0.79 |
| 2:KF:86:ARG:HH12 | 2:LF:283:ALA:CA | 1.96 | 0.79 |
| 6:4A:154:LYS:HB2 | 6:4A:154:LYS:NZ | 1.95 | 0.79 |
| 7:5A:773:ARG:C | 7:5A:775:PRO:HD3 | 2.07 | 0.79 |
| 7:5A:1491:LEU:HD21 | 7:5A:1495:PHE:CE1 | 2.17 | 0.79 |
| 9:7B:18:VAL:HG12 | 9:7B:42:LEU:CD2 | 2.13 | 0.79 |
| 1:AE:101:ASN:HD22 | 2:AF:252:LYS:HD2 | 1.41 | 0.79 |
| 1:BE:101:ASN:ND2 | 2:BF:252:LYS:CG | 2.46 | 0.79 |
| 1:DA:222:PRO:CD | 2:DB:324:LYS:HD3 | 2.12 | 0.79 |
| 1:EE:11:GLN:OE1 | 2:EF:245:GLN:O | 2.01 | 0.79 |
| 1:IA:282:TYR:CD1 | 10:8V:18:UNK:CB | 2.65 | 0.79 |
| 1:IA:282:TYR:HB3 | 10:8V:15:UNK:CB | 2.13 | 0.79 |
| 1:IE:402:ARG:HH22 | 7:5B:1418:GLN:HA | 1.48 | 0.79 |
| 2:JB:86:ARG:CZ | 2:KB:280:GLN:HB3 | 2.11 | 0.79 |
| 1:JC:11:GLN:OE1 | 2:JD:245:GLN:O | 2.00 | 0.79 |
| 2:KD:82:GLY:O | 2:LD:281:TYR:HE1 | 1.64 | 0.79 |
| 2:KD:273:LEU:HA | 6:4B:268:LEU:CG | 2.12 | 0.79 |
| 1:LA:60:LYS:CE | 6:4C:101:ARG:NH1 | 2.45 | 0.79 |
| 1:LE:401:LYS:NZ | 2:LF:344:TRP:CZ2 | 2.51 | 0.79 |
| 2:LF:306:ARG:NH1 | 4:2B:151:VAL:CG2 | 2.46 | 0.79 |
| 5:3B:229:PHE:CD2 | 5:3B:331:GLN:HB3 | 2.16 | 0.79 |
| 6:4B:252:VAL:CG1 | 6:4B:292:VAL:CG2 | 2.61 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5A:836:ARG:HH11 | 7:5A:836:ARG:HB3 | 1.44 | 0.79 |
| 7:5A:1381:ILE:H | 7:5A:1381:ILE:CD1 | 1.96 | 0.79 |
| 7:5A:1549:THR:CA | 7:5A:1566:GLU:OE1 | 2.13 | 0.79 |
| 7:5B:1381:ILE:H | 7:5B:1381:ILE:CD1 | 1.96 | 0.79 |
| 7:5B:1491:LEU:HD21 | 7:5B:1495:PHE:CE1 | 2.17 | 0.79 |
| 9:7C:35:ILE:HG23 | 9:7D:42:LEU:O | 1.83 | 0.79 |
| 2:CF:86:ARG:NH1 | 2:DF:281:TYR:CA | 2.35 | 0.79 |
| 1:DE:400:ALA:C | 7:5B:775:PRO:HB3 | 2.08 | 0.79 |
| 2:GF:416:ASN:CG | 7:5B:1327:LYS:NZ | 2.41 | 0.79 |
| 1:HC:278:ALA:HB3 | 10:8T:22:UNK:CA | 2.13 | 0.79 |
| 1:LE:60:LYS:CD | 1:ME:283:HIS:CD2 | 2.66 | 0.79 |
| 7:5B:1515:GLU:OE1 | 7:5B:1563:SER:CB | 2.31 | 0.79 |
| 7:5C:773:ARG:C | 7:5C:775:PRO:HD3 | 2.07 | 0.79 |
| 7:5C:1267:CYS:SG | 9:7E:8:ARG:CG | 2.71 | 0.79 |
| 7:5C:1381:ILE:H | 7:5C:1381:ILE:CD1 | 1.96 | 0.79 |
| 1:EE:396:ASP:CG | 7:5B:821:LEU:HD11 | 2.07 | 0.79 |
| 1:FC:101:ASN:CG | 2:FD:252:LYS:HD2 | 2.05 | 0.79 |
| 2:GB:86:ARG:NH2 | 2:HB:281:TYR:CZ | 2.35 | 0.79 |
| 1:LA:11:GLN:NE2 | 2:LB:247:ASN:OD1 | 2.15 | 0.79 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:CE | 2.61 | 0.79 |
| 2:LB:77:ARG:HH11 | 6:4A:204:ARG:NH2 | 1.80 | 0.79 |
| 6:4C:154:LYS:NZ | 6:4C:154:LYS:HB2 | 1.95 | 0.79 |
| 6:4C:266:ASN:HB2 | 6:4C:273:ARG:HH11 | 1.47 | 0.79 |
| 7:5C:836:ARG:HH11 | 7:5C:836:ARG:HB3 | 1.44 | 0.79 |
| 2:ED:55:THR:CG2 | 2:FD:283:ALA:HA | 2.06 | 0.78 |
| 2:EF:125:GLU:CB | 7:5B:903:PHE:HE2 | 1.80 | 0.78 |
| 1:FE:177:VAL:HG21 | 7:5B:915:PHE:HE2 | 1.42 | 0.78 |
| 1:KA:222:PRO:CG | 2:KB:324:LYS:HD3 | 2.12 | 0.78 |
| 1:KC:11:GLN:OE1 | 2:KD:245:GLN:O | 2.00 | 0.78 |
| 2:LD:177:ASP:OD1 | 1:LE:353:VAL:HG12 | 1.77 | 0.78 |
| 1:MA:101:ASN:HD21 | 2:MB:252:LYS:CD | 1.67 | 0.78 |
| 1:MA:404:PHE:HE2 | 2:MB:345:ILE:CD1 | 1.96 | 0.78 |
| 1:ME:279:GLU:HB3 | 6:4B:110:LYS:HE3 | 1.63 | 0.78 |
| 6:4A:252:VAL:CG1 | 6:4A:292:VAL:CG2 | 2.61 | 0.78 |
| 6:4A:266:ASN:HB2 | 6:4A:273:ARG:HH11 | 1.47 | 0.78 |
| 6:4B:251:TYR:CE2 | 6:4B:280:VAL:CG1 | 2.66 | 0.78 |
| 6:4D:251:TYR:CE2 | 6:4D:280:VAL:CG1 | 2.66 | 0.78 |
| 7:5B:1489:PHE:O | 7:5B:1493:GLN:N | 2.15 | 0.78 |
| 7:5C:1424:GLN:NE2 | 7:5C:1424:GLN:O | 2.16 | 0.78 |
| 2:AB:55:THR:HG23 | 2:BB:283:ALA:HB2 | 1.63 | 0.78 |
| 1:DA:282:TYR:CD2 | 10:8G:18:UNK:CB | 2.66 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EA:402:ARG:CZ | 7:5C:824:ARG:HH22 | 1.96 | 0.78 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:CZ | 2.59 | 0.78 |
| 2:FD:55:THR:HG21 | 2:GD:284:LEU:N | 1.93 | 0.78 |
| 2:FD:177:ASP:OD2 | 1:FE:248:LEU:HD21 | 1.81 | 0.78 |
| 1:HC:11:GLN:OE1 | 2:HD:245:GLN:O | 2.00 | 0.78 |
| 1:HE:416:GLY:HA2 | 5:3A:238:ILE:HD11 | 1.64 | 0.78 |
| 5:3A:229:PHE:CD2 | 5:3A:331:GLN:HB3 | 2.16 | 0.78 |
| 6:4B:266:ASN:HB2 | 6:4B:273:ARG:HH11 | 1.47 | 0.78 |
| 6:4C:252:VAL:CG1 | 6:4C:292:VAL:CG2 | 2.61 | 0.78 |
| 7:5A:1284:PHE:CE1 | 9:7A:12:GLU:HB2 | 2.18 | 0.78 |
| 7:5A:1424:GLN:O | 7:5A:1424:GLN:NE2 | 2.16 | 0.78 |
| 7:5A:1515:GLU:OE1 | 7:5A:1563:SER:CB | 2.31 | 0.78 |
| 7:5B:1152:GLU:CD | 8:6B:66:ARG:NH1 | 2.42 | 0.78 |
| 7:5C:1549:THR:CA | 7:5C:1566:GLU:OE1 | 2.13 | 0.78 |
| 9:7A:35:ILE:HG23 | 9:7B:42:LEU:O | 1.83 | 0.78 |
| 1:CC:101:ASN:HD22 | 2:CD:252:LYS:CG | 1.95 | 0.78 |
| 1:CC:101:ASN:CG | 2:CD:252:LYS:HD2 | 2.04 | 0.78 |
| 1:GC:56:THR:OG1 | 1:HC:284:GLU:CA | 2.31 | 0.78 |
| 1:IA:282:TYR:CG | 10:8V:15:UNK:CA | 2.67 | 0.78 |
| 2:JB:86:ARG:NH1 | 2:KB:280:GLN:HB3 | 1.98 | 0.78 |
| 1:JC:88:HIS:CE1 | 1:KC:280:LYS:C | 2.61 | 0.78 |
| 1:LA:222:PRO:HD2 | 2:LB:324:LYS:HB3 | 1.64 | 0.78 |
| 2:LB:224:ASP:HA | 6:4A:219:ASN:OD1 | 1.82 | 0.78 |
| 7:5A:1489:PHE:O | 7:5A:1493:GLN:N | 2.15 | 0.78 |
| 7:5B:841:VAL:N | 8:6B:109:ILE:HD11 | 1.98 | 0.78 |
| 7:5C:1524:PHE:HD1 | 7:5C:1567:PHE:HZ | 1.24 | 0.78 |
| 1:AC:11:GLN:OE1 | 2:AD:245:GLN:O | 2.00 | 0.78 |
| 1:BE:222:PRO:CG | 2:BF:324:LYS:HD3 | 2.13 | 0.78 |
| 2:DB:212:PHE:CZ | 1:DC:326:LYS:CD | 2.20 | 0.78 |
| 1:DC:402:ARG:CD | 7:5A:777:ALA:CB | 2.62 | 0.78 |
| 2:DD:179:VAL:CG2 | 1:DE:258:ASN:HA | 2.14 | 0.78 |
| 1:EE:101:ASN:HD21 | 2:EF:252:LYS:HD2 | 0.96 | 0.78 |
| 1:IC:11:GLN:OE1 | 2:ID:245:GLN:O | 2.00 | 0.78 |
| 1:LA:60:LYS:HD3 | 1:MA:283:HIS:CG | 2.18 | 0.78 |
| 6:4A:251:TYR:CE2 | 6:4A:280:VAL:CG1 | 2.66 | 0.78 |
| 6:4D:266:ASN:HB2 | 6:4D:273:ARG:HH11 | 1.48 | 0.78 |
| 7:5B:1424:GLN:O | 7:5B:1424:GLN:NE2 | 2.16 | 0.78 |
| 7:5C:1489:PHE:O | 7:5C:1493:GLN:N | 2.15 | 0.78 |
| 7:5C:1573:ARG:O | 7:5C:1577:LYS:N | 2.17 | 0.78 |
| 9:7D:18:VAL:HG12 | 9:7D:42:LEU:CD2 | 2.13 | 0.78 |
| 2:AF:280:GLN:NE2 | 6:4A:141:LYS:HB3 | 1.99 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:98:GLY:C | 1:CC:254:GLU:HG2 | 2.08 | 0.78 |
| 1:EE:222:PRO:CD | 2:EF:324:LYS:HD3 | 2.12 | 0.78 |
| 1:FC:60:LYS:HD2 | 1:GC:283:HIS:CD2 | 2.19 | 0.78 |
| 1:IC:389:SER:HB3 | 5:3C:307:LYS:HD3 | 1.64 | 0.78 |
| 1:IE:60:LYS:NZ | 1:JE:283:HIS:CD2 | 2.51 | 0.78 |
| 1:JE:222:PRO:CG | 2:JF:324:LYS:HD3 | 2.14 | 0.78 |
| 2:KD:82:GLY:O | 2:LD:281:TYR:CE1 | 2.36 | 0.78 |
| 2:KD:125:GLU:HG2 | 2:LD:336:LYS:HZ1 | 1.47 | 0.78 |
| 2:KF:221:THR:HG21 | 6:4D:262:ASN:N | 1.97 | 0.78 |
| 7:5A:1573:ARG:O | 7:5A:1577:LYS:N | 2.17 | 0.78 |
| 7:5B:1416:LYS:HA | 7:5B:1416:LYS:NZ | 1.98 | 0.78 |
| 7:5C:1515:GLU:OE1 | 7:5C:1563:SER:CB | 2.31 | 0.78 |
| 9:7C:11:TYR:OH | 9:7D:27:GLY:N | 2.16 | 0.78 |
| 2:FB:177:ASP:OD2 | 1:FC:248:LEU:HD21 | 1.81 | 0.78 |
| 2:FD:55:THR:H | 2:GD:283:ALA:HA | 1.46 | 0.78 |
| 2:GB:55:THR:CG2 | 2:HB:283:ALA:C | 2.56 | 0.78 |
| 1:GE:402:ARG:HD2 | 5:3A:381:ASN:CG | 2.09 | 0.78 |
| 1:IE:222:PRO:CG | 2:IF:324:LYS:HD3 | 2.14 | 0.78 |
| 1:KA:11:GLN:OE1 | 2:KB:245:GLN:O | 2.01 | 0.78 |
| 1:KA:85:GLN:NE2 | 1:LA:282:TYR:HB2 | 1.91 | 0.78 |
| 1:LC:224:TYR:HE2 | 2:LD:246:LEU:HD11 | 1.48 | 0.78 |
| 2:MD:220:PRO:HD2 | 1:ME:326:LYS:HG2 | 1.64 | 0.78 |
| 5:3C:229:PHE:CD2 | 5:3C:331:GLN:HB3 | 2.16 | 0.78 |
| 7:5B:1524:PHE:HD1 | 7:5B:1567:PHE:HZ | 1.24 | 0.78 |
| 7:5C:1152:GLU:CD | 8:6C:66:ARG:NH1 | 2.41 | 0.78 |
| 9:7F:18:VAL:HG12 | 9:7F:42:LEU:CD2 | 2.13 | 0.78 |
| 2:BF:86:ARG:HE | 2:BF:87:PRO:HD2 | 1.49 | 0.78 |
| 1:DE:76:ASP:OD1 | 2:DF:46:ARG:NH2 | 2.16 | 0.78 |
| 2:ED:85:PHE:O | 2:FD:281:TYR:OH | 1.98 | 0.78 |
| 1:FC:419:SER:HB3 | 7:5A:1256:ARG:HG2 | 1.65 | 0.78 |
| 1:GC:11:GLN:OE1 | 2:GD:245:GLN:O | 2.00 | 0.78 |
| 1:GE:60:LYS:CD | 1:HE:283:HIS:CG | 2.67 | 0.78 |
| 1:GE:409:VAL:CG2 | 5:3A:383:GLU:OE1 | 2.31 | 0.78 |
| 2:GF:58:ARG:CZ | 2:HF:281:TYR:CZ | 2.67 | 0.78 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:HE2 | 1.62 | 0.78 |
| 2:LB:310:TYR:CE2 | 4:2C:147:PHE:CZ | 2.72 | 0.78 |
| 6:4C:251:TYR:CE2 | 6:4C:280:VAL:CG1 | 2.66 | 0.78 |
| 7:5A:841:VAL:CG1 | 8:6A:9:LEU:HD23 | 2.12 | 0.78 |
| 7:5A:1521:PHE:HE2 | 7:5A:1571:MET:HG2 | 1.48 | 0.78 |
| 7:5A:1524:PHE:HD1 | 7:5A:1567:PHE:HZ | 1.24 | 0.78 |
| 7:5B:1573:ARG:O | 7:5B:1577:LYS:N | 2.17 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:829:GLY:CA | 8:6C:109:ILE:CG2 | 2.62 | 0.78 |
| 7:5C:1521:PHE:HE2 | 7:5C:1571:MET:HG2 | 1.48 | 0.78 |
| 2:AF:280:GLN:HA | 6:4A:142:SER:HB3 | 1.64 | 0.78 |
| 2:CD:177:ASP:OD1 | 1:CE:353:VAL:HG12 | 1.78 | 0.78 |
| 2:DD:86:ARG:CB | 2:ED:281:TYR:CE1 | 2.66 | 0.78 |
| 2:DF:86:ARG:HE | 2:DF:87:PRO:HD2 | 1.49 | 0.78 |
| 1:GC:60:LYS:HD3 | 1:HC:283:HIS:CG | 2.19 | 0.78 |
| 1:GC:89:PRO:HG3 | 1:HC:280:LYS:HD2 | 1.66 | 0.78 |
| 1:IA:11:GLN:OE1 | 2:IB:245:GLN:O | 2.01 | 0.78 |
| 2:IB:220:PRO:HD2 | 1:IC:326:LYS:HE2 | 1.66 | 0.78 |
| 1:JA:11:GLN:OE1 | 2:JB:245:GLN:O | 2.01 | 0.78 |
| 1:KE:222:PRO:CG | 2:KF:324:LYS:HD3 | 2.14 | 0.78 |
| 2:LF:55:THR:HG23 | 2:MF:283:ALA:HA | 0.78 | 0.78 |
| 1:MA:282:TYR:CD2 | 6:4C:104:ARG:CD | 2.56 | 0.78 |
| 7:5B:1521:PHE:HE2 | 7:5B:1571:MET:HG2 | 1.48 | 0.78 |
| 7:5C:1515:GLU:HG2 | 7:5C:1563:SER:CA | 2.12 | 0.78 |
| 9:7C:42:LEU:HD12 | 9:7D:39:GLY:CA | 2.11 | 0.78 |
| 9:7D:18:VAL:CG1 | 9:7D:42:LEU:CD2 | 2.62 | 0.78 |
| 2:AB:86:ARG:HE | 2:AB:87:PRO:HD2 | 1.49 | 0.78 |
| 2:AD:86:ARG:HE | 2:AD:87:PRO:HD2 | 1.49 | 0.78 |
| 2:AF:86:ARG:HE | 2:AF:87:PRO:HD2 | 1.49 | 0.78 |
| 2:BB:179:VAL:CG2 | 1:BC:258:ASN:HA | 2.14 | 0.78 |
| 2:BD:86:ARG:HE | 2:BD:87:PRO:HD2 | 1.49 | 0.78 |
| 2:CB:86:ARG:HE | 2:CB:87:PRO:HD2 | 1.49 | 0.78 |
| 2:CD:86:ARG:HE | 2:CD:87:PRO:HD2 | 1.49 | 0.78 |
| 1:CE:101:ASN:HD22 | 2:CF:252:LYS:CD | 1.97 | 0.78 |
| 2:DB:86:ARG:HE | 2:DB:87:PRO:HD2 | 1.49 | 0.78 |
| 2:DD:86:ARG:HE | 2:DD:87:PRO:HD2 | 1.49 | 0.78 |
| 1:FA:71:GLU:CD | 2:FB:247:ASN:ND2 | 2.42 | 0.78 |
| 1:FA:282:TYR:CZ | 10:8M:18:UNK:CB | 2.66 | 0.78 |
| 1:FA:402:ARG:CD | 7:5C:1259:TYR:HD2 | 1.96 | 0.78 |
| 1:FE:101:ASN:HD21 | 2:FF:252:LYS:HD2 | 0.96 | 0.78 |
| 1:GE:60:LYS:CD | 1:HE:283:HIS:CB | 2.60 | 0.78 |
| 1:HE:222:PRO:CG | 2:HF:324:LYS:HD3 | 2.14 | 0.78 |
| 1:MA:279:GLU:OE2 | 6:4C:106:ALA:CB | 2.32 | 0.78 |
| 7:5A:1416:LYS:HA | 7:5A:1416:LYS:NZ | 1.99 | 0.78 |
| 7:5A:1515:GLU:HG2 | 7:5A:1563:SER:CA | 2.12 | 0.78 |
| 7:5C:927:ILE:HG12 | 7:5C:952:VAL:HG11 | 1.65 | 0.78 |
| 2:BB:86:ARG:HE | 2:BB:87:PRO:HD2 | 1.49 | 0.78 |
| 2:CD:98:GLY:C | 1:CE:254:GLU:HG2 | 2.08 | 0.78 |
| 2:CF:86:ARG:HE | 2:CF:87:PRO:HD2 | 1.49 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DC:76:ASP:OD1 | 2:DD:46:ARG:NH2 | 2.16 | 0.78 |
| 1:DE:101:ASN:ND2 | 2:DF:252:LYS:CG | 2.47 | 0.78 |
| 1:EA:11:GLN:OE1 | 2:EB:245:GLN:O | 2.02 | 0.78 |
| 2:ED:86:ARG:HE | 2:ED:87:PRO:HD2 | 1.49 | 0.78 |
| 1:FC:101:ASN:ND2 | 2:FD:252:LYS:CG | 2.46 | 0.78 |
| 2:FD:86:ARG:HE | 2:FD:87:PRO:HD2 | 1.49 | 0.78 |
| 2:GB:220:PRO:HD2 | 1:GC:326:LYS:HE2 | 1.66 | 0.78 |
| 2:GD:86:ARG:HE | 2:GD:87:PRO:HD2 | 1.49 | 0.78 |
| 2:GF:86:ARG:HE | 2:GF:87:PRO:HD2 | 1.49 | 0.78 |
| 1:HE:282:TYR:CE1 | 10:8U:15:UNK:HA | 2.18 | 0.78 |
| 1:KC:85:GLN:HA | 1:LC:283:HIS:CD2 | 2.17 | 0.78 |
| 7:5B:1515:GLU:HG2 | 7:5B:1563:SER:CA | 2.12 | 0.78 |
| 9:7F:18:VAL:CG1 | 9:7F:42:LEU:CD2 | 2.62 | 0.78 |
| 1:AE:222:PRO:CG | 2:AF:324:LYS:HD3 | 2.14 | 0.77 |
| 2:BD:177:ASP:CG | 1:BE:353:VAL:HG13 | 1.98 | 0.77 |
| 2:EB:86:ARG:HE | 2:EB:87:PRO:HD2 | 1.49 | 0.77 |
| 2:FB:86:ARG:HE | 2:FB:87:PRO:HD2 | 1.49 | 0.77 |
| 2:FF:86:ARG:HE | 2:FF:87:PRO:HD2 | 1.49 | 0.77 |
| 2:GB:86:ARG:HE | 2:GB:87:PRO:HD2 | 1.49 | 0.77 |
| 1:HA:11:GLN:OE1 | 2:HB:245:GLN:O | 2.01 | 0.77 |
| 1:HE:282:TYR:CD1 | 10:8U:15:UNK:HA | 2.19 | 0.77 |
| 2:ID:86:ARG:CA | 2:JD:281:TYR:HE1 | 1.97 | 0.77 |
| 1:JE:279:GLU:OE1 | 10:9A:22:UNK:HA | 1.83 | 0.77 |
| 2:KD:118:ASP:CG | 4:2A:148:ASN:ND2 | 2.36 | 0.77 |
| 1:LC:222:PRO:HD2 | 2:LD:324:LYS:CD | 2.11 | 0.77 |
| 1:LE:60:LYS:HD3 | 1:ME:283:HIS:CG | 2.19 | 0.77 |
| 7:5A:927:ILE:HG12 | 7:5A:952:VAL:HG11 | 1.65 | 0.77 |
| 7:5B:839:GLU:CD | 8:6B:109:ILE:HG13 | 2.09 | 0.77 |
| 7:5B:1430:GLN:HA | 7:5B:1430:GLN:OE1 | 1.84 | 0.77 |
| 9:7B:18:VAL:CG1 | 9:7B:42:LEU:CD2 | 2.62 | 0.77 |
| 1:BC:101:ASN:HD22 | 2:BD:252:LYS:CG | 1.95 | 0.77 |
| 2:CD:177:ASP:OD2 | 1:CE:248:LEU:HD21 | 1.83 | 0.77 |
| 1:CE:101:ASN:HD22 | 2:CF:252:LYS:CG | 1.96 | 0.77 |
| 1:EE:101:ASN:CG | 2:EF:252:LYS:HD2 | 2.07 | 0.77 |
| 2:EF:86:ARG:HE | 2:EF:87:PRO:HD2 | 1.50 | 0.77 |
| 2:FB:55:THR:CB | 2:GB:283:ALA:HA | 2.15 | 0.77 |
| 1:GE:60:LYS:HZ2 | 1:HE:283:HIS:CG | 2.03 | 0.77 |
| 2:HF:86:ARG:HA | 2:IF:281:TYR:CE1 | 2.19 | 0.77 |
| 2:LB:306:ARG:HH21 | 4:2C:149:ILE:CG2 | 1.97 | 0.77 |
| 2:LD:231:ALA:HB2 | 6:4B:226:ILE:HD13 | 0.78 | 0.77 |
| 1:MC:279:GLU:CB | 6:4A:110:LYS:CE | 2.62 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5B:927:ILE:HG12 | 7:5B:952:VAL:HG11 | 1.65 | 0.77 |
| 7:5C:1416:LYS:HA | 7:5C:1416:LYS:NZ | 1.99 | 0.77 |
| 1:CA:101:ASN:HD22 | 2:CB:252:LYS:CD | 1.98 | 0.77 |
| 1:CE:101:ASN:CG | 2:CF:252:LYS:HD2 | 2.05 | 0.77 |
| 1:DA:222:PRO:CG | 2:DB:324:LYS:HD3 | 2.14 | 0.77 |
| 2:DB:177:ASP:OD2 | 1:DC:248:LEU:HD21 | 1.84 | 0.77 |
| 1:EE:402:ARG:CZ | 7:5B:824:ARG:HH22 | 1.96 | 0.77 |
| 1:GA:11:GLN:OE1 | 2:GB:245:GLN:O | 2.01 | 0.77 |
| 1:IC:278:ALA:HB1 | 10:8W:18:UNK:C | 2.09 | 0.77 |
| 1:KA:85:GLN:C | 1:LA:283:HIS:CA | 2.55 | 0.77 |
| 1:LE:60:LYS:HD2 | 6:4B:101:ARG:HH22 | 0.71 | 0.77 |
| 2:LF:416:ASN:O | 4:2B:168:LEU:HD13 | 1.43 | 0.77 |
| 2:MB:177:ASP:CG | 1:MC:353:VAL:HG11 | 2.07 | 0.77 |
| 7:5A:1105:TYR:HB2 | 7:5A:1166:LEU:N | 1.99 | 0.77 |
| 7:5B:1105:TYR:HB2 | 7:5B:1166:LEU:N | 1.99 | 0.77 |
| 9:7A:11:TYR:OH | 9:7B:27:GLY:N | 2.16 | 0.77 |
| 1:DE:402:ARG:CD | 7:5B:777:ALA:CB | 2.61 | 0.77 |
| 2:ED:177:ASP:O | 1:EE:352:LYS:HA | 1.84 | 0.77 |
| 1:EE:101:ASN:ND2 | 2:EF:252:LYS:CG | 2.47 | 0.77 |
| 1:FC:423:GLU:CD | 7:5A:1256:ARG:HH22 | 1.91 | 0.77 |
| 1:FE:101:ASN:HD22 | 2:FF:252:LYS:HG3 | 1.47 | 0.77 |
| 1:GE:222:PRO:CG | 2:GF:324:LYS:HD3 | 2.14 | 0.77 |
| 1:HE:415:GLU:HG2 | 5:3A:235:LEU:HB3 | 1.65 | 0.77 |
| 1:JC:282:TYR:OH | 10:8Z:17:UNK:C | 2.31 | 0.77 |
| 1:JE:124:LYS:CD | 1:KE:284:GLU:OE1 | 2.32 | 0.77 |
| 1:KC:359:PRO:HB3 | 6:4A:299:TYR:HE2 | 1.44 | 0.77 |
| 2:LF:55:THR:CB | 2:MF:283:ALA:HA | 2.14 | 0.77 |
| 7:5A:1430:GLN:OE1 | 7:5A:1430:GLN:HA | 1.84 | 0.77 |
| 7:5C:1105:TYR:HB2 | 7:5C:1166:LEU:N | 1.99 | 0.77 |
| 9:7E:7:LEU:HD22 | 9:7F:27:GLY:HA2 | 1.52 | 0.77 |
| 9:7E:7:LEU:HD21 | 9:7F:27:GLY:C | 2.09 | 0.77 |
| 2:CB:212:PHE:CZ | 1:CC:326:LYS:CD | 2.19 | 0.77 |
| 1:DC:101:ASN:ND2 | 2:DD:252:LYS:CG | 2.47 | 0.77 |
| 1:GE:370:LYS:HE3 | 10:8R:18:UNK:N | 1.98 | 0.77 |
| 1:HC:415:GLU:CG | 5:3C:235:LEU:HB3 | 2.12 | 0.77 |
| 2:KF:217:LEU:CD2 | 6:4D:263:CYS:SG | 2.67 | 0.77 |
| 2:MB:86:ARG:HE | 2:MB:87:PRO:HD2 | 1.49 | 0.77 |
| 4:2A:16:GLN:C | 4:2A:19:MET:HB2 | 2.08 | 0.77 |
| 4:2B:16:GLN:C | 4:2B:19:MET:HB2 | 2.08 | 0.77 |
| 4:2C:16:GLN:C | 4:2C:19:MET:HB2 | 2.08 | 0.77 |
| 5:3B:230:ILE:CG2 | 5:3B:332:MET:SD | 2.73 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5B:1355:GLN:O | 7:5B:1358:LYS:HG3 | 1.83 | 0.77 |
| 9:7A:42:LEU:HD12 | 9:7B:39:GLY:CA | 2.11 | 0.77 |
| 1:AA:11:GLN:OE1 | 2:AB:245:GLN:O | 2.01 | 0.77 |
| 2:AF:227:HIS:HE1 | 6:4A:135:LEU:HD12 | 1.48 | 0.77 |
| 1:IA:402:ARG:HH22 | 7:5C:1418:GLN:CA | 1.97 | 0.77 |
| 1:LC:89:PRO:CG | 1:MC:280:LYS:NZ | 2.48 | 0.77 |
| 2:MD:86:ARG:HE | 2:MD:87:PRO:HD2 | 1.49 | 0.77 |
| 2:MF:86:ARG:HE | 2:MF:87:PRO:HD2 | 1.49 | 0.77 |
| 5:3A:230:ILE:CG2 | 5:3A:332:MET:SD | 2.73 | 0.77 |
| 6:4A:163:GLN:HA | 6:4A:163:GLN:OE1 | 1.82 | 0.77 |
| 7:5C:1253:ILE:HD11 | 9:7F:20:LEU:HD13 | 1.67 | 0.77 |
| 7:5C:1266:TYR:CA | 7:5C:1269:ASP:OD2 | 2.24 | 0.77 |
| 2:CD:87:PRO:CD | 2:DD:281:TYR:CZ | 2.68 | 0.77 |
| 1:DA:101:ASN:HD22 | 2:DB:252:LYS:CD | 1.96 | 0.77 |
| 1:DA:414:GLU:OE2 | 7:5C:789:LYS:CE | 2.32 | 0.77 |
| 2:GF:58:ARG:NH2 | 2:HF:281:TYR:CE1 | 2.53 | 0.77 |
| 1:HC:11:GLN:NE2 | 2:HD:247:ASN:OD1 | 2.18 | 0.77 |
| 2:JB:86:ARG:HE | 2:JB:87:PRO:HD2 | 1.49 | 0.77 |
| 2:JD:86:ARG:HE | 2:JD:87:PRO:HD2 | 1.49 | 0.77 |
| 2:KD:125:GLU:CG | 2:LD:336:LYS:HZ3 | 1.65 | 0.77 |
| 2:KF:276:ARG:NH1 | 6:4D:271:GLU:C | 2.42 | 0.77 |
| 2:LF:379:LYS:HZ1 | 4:2B:166:ILE:HB | 1.47 | 0.77 |
| 6:4B:163:GLN:HA | 6:4B:163:GLN:OE1 | 1.82 | 0.77 |
| 6:4D:163:GLN:HA | 6:4D:163:GLN:OE1 | 1.82 | 0.77 |
| 7:5A:842:LEU:HD23 | 7:5A:843:LEU:HD22 | 1.65 | 0.77 |
| 7:5C:1430:GLN:HA | 7:5C:1430:GLN:OE1 | 1.84 | 0.77 |
| 2:BB:177:ASP:CG | 1:BC:353:VAL:HG13 | 1.99 | 0.77 |
| 1:DE:222:PRO:CG | 2:DF:324:LYS:HD3 | 2.15 | 0.77 |
| 1:GC:11:GLN:NE2 | 2:GD:247:ASN:OD1 | 2.18 | 0.77 |
| 2:HF:86:ARG:HE | 2:HF:87:PRO:HD2 | 1.49 | 0.77 |
| 2:ID:220:PRO:HD2 | 1:IE:326:LYS:HE2 | 1.67 | 0.77 |
| 2:JF:86:ARG:HE | 2:JF:87:PRO:HD2 | 1.49 | 0.77 |
| 2:LB:331:LEU:CD1 | 4:2C:42:PHE:CE1 | 2.67 | 0.77 |
| 1:LC:60:LYS:HD3 | 1:MC:283:HIS:CG | 2.19 | 0.77 |
| 5:3C:230:ILE:CG2 | 5:3C:332:MET:SD | 2.73 | 0.77 |
| 6:4D:151:ARG:HG2 | 6:4D:151:ARG:NH1 | 1.94 | 0.77 |
| 7:5A:1355:GLN:O | 7:5A:1358:LYS:HG3 | 1.83 | 0.77 |
| 7:5B:842:LEU:HD23 | 7:5B:843:LEU:HD22 | 1.65 | 0.77 |
| 9:7A:39:GLY:CA | 9:7B:43:LEU:HD21 | 2.14 | 0.77 |
| 2:BD:220:PRO:O | 1:BE:324:VAL:HG13 | 1.84 | 0.77 |
| 2:CF:87:PRO:HD2 | 2:DF:281:TYR:CD2 | 2.20 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:DE:222:PRO:CD | 2:DF:324:LYS:HD3 | 2.15 | 0.77 |
| 1:EC:396:ASP:OD1 | 7:5A:821:LEU:HD11 | 1.83 | 0.77 |
| 2:GD:220:PRO:HD2 | 1:GE:326:LYS:HE2 | 1.67 | 0.77 |
| 2:HD:86:ARG:HE | 2:HD:87:PRO:HD2 | 1.49 | 0.77 |
| 2:LB:212:PHE:CZ | 1:LC:326:LYS:CD | 2.18 | 0.77 |
| 2:LD:274:THR:O | 6:4B:228:LEU:HD22 | 1.83 | 0.77 |
| 2:LF:270:PHE:CE2 | 6:4D:226:ILE:HG23 | 2.20 | 0.77 |
| 6:4C:163:GLN:HA | 6:4C:163:GLN:OE1 | 1.82 | 0.77 |
| 7:5C:842:LEU:HD23 | 7:5C:843:LEU:HD22 | 1.65 | 0.77 |
| 2:BB:220:PRO:HD2 | 1:BC:326:LYS:HE2 | 1.67 | 0.77 |
| 2:LD:340:TYR:CD1 | 4:2A:147:PHE:CA | 2.68 | 0.77 |
| 1:MA:279:GLU:OE1 | 6:4C:106:ALA:C | 2.28 | 0.77 |
| 5:3B:229:PHE:CD2 | 5:3B:331:GLN:CB | 2.68 | 0.77 |
| 9:7C:39:GLY:CA | 9:7D:43:LEU:HD21 | 2.14 | 0.77 |
| 2:AF:223:GLY:O | 6:4A:131:VAL:N | 2.03 | 0.76 |
| 1:CA:222:PRO:CD | 2:CB:324:LYS:HD3 | 2.13 | 0.76 |
| 1:DA:101:ASN:CG | 2:DB:252:LYS:HD2 | 2.06 | 0.76 |
| 2:ED:177:ASP:O | 1:EE:352:LYS:CD | 2.31 | 0.76 |
| 2:ED:178:THR:HG23 | 1:EE:258:ASN:ND2 | 1.99 | 0.76 |
| 1:FA:56:THR:O | 1:GA:285:GLN:CA | 2.32 | 0.76 |
| 1:FA:101:ASN:ND2 | 2:FB:252:LYS:CG | 2.48 | 0.76 |
| 1:FA:419:SER:HB3 | 7:5C:1256:ARG:HG2 | 1.67 | 0.76 |
| 2:HB:86:ARG:HE | 2:HB:87:PRO:HD2 | 1.49 | 0.76 |
| 1:IC:402:ARG:CZ | 7:5A:1417:GLN:CG | 2.51 | 0.76 |
| 2:JD:220:PRO:HD2 | 1:JE:326:LYS:HG2 | 1.67 | 0.76 |
| 2:KD:276:ARG:HH21 | 6:4B:265:TYR:CB | 1.97 | 0.76 |
| 2:LD:310:TYR:HE2 | 4:2A:147:PHE:CZ | 2.03 | 0.76 |
| 2:MB:110:ALA:O | 3:1A:61:HIS:HB2 | 1.82 | 0.76 |
| 6:4B:151:ARG:HG2 | 6:4B:151:ARG:NH1 | 1.94 | 0.76 |
| 7:5A:1266:TYR:CA | 7:5A:1269:ASP:OD2 | 2.24 | 0.76 |
| 7:5B:1275:ILE:HD13 | 9:7D:11:TYR:OH | 1.85 | 0.76 |
| 7:5C:1355:GLN:O | 7:5C:1358:LYS:HG3 | 1.83 | 0.76 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:CA | 2.15 | 0.76 |
| 2:AD:55:THR:HG23 | 2:BD:283:ALA:HB2 | 1.65 | 0.76 |
| 2:AD:220:PRO:HD2 | 1:AE:326:LYS:HG2 | 1.67 | 0.76 |
| 2:AF:361:LEU:CD2 | 6:4A:144:LEU:HD12 | 2.15 | 0.76 |
| 1:BA:101:ASN:HD22 | 2:BB:252:LYS:CG | 1.96 | 0.76 |
| 2:BD:212:PHE:CZ | 1:BE:326:LYS:CD | 2.23 | 0.76 |
| 2:KD:220:PRO:HD2 | 1:KE:326:LYS:HG2 | 1.67 | 0.76 |
| 5:3A:229:PHE:CD2 | 5:3A:331:GLN:CB | 2.68 | 0.76 |
| 2:BB:177:ASP:OD1 | 1:BC:353:VAL:HG12 | 1.77 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CF:87:PRO:HD2 | 2:DF:281:TYR:CZ | 2.19 | 0.76 |
| 1:GA:56:THR:OG1 | 1:HA:284:GLU:HA | 1.84 | 0.76 |
| 1:GE:71:GLU:OE1 | 2:GF:247:ASN:ND2 | 2.18 | 0.76 |
| 1:IC:11:GLN:NE2 | 2:ID:247:ASN:OD1 | 2.18 | 0.76 |
| 1:JA:89:PRO:N | 1:KA:283:HIS:CE1 | 2.35 | 0.76 |
| 1:JE:87:PHE:O | 1:KE:283:HIS:NE2 | 2.16 | 0.76 |
| 2:KB:220:PRO:HD2 | 1:KC:326:LYS:HE2 | 1.66 | 0.76 |
| 1:KC:11:GLN:NE2 | 2:KD:247:ASN:OD1 | 2.18 | 0.76 |
| 2:KD:125:GLU:HG3 | 2:LD:336:LYS:HE2 | 1.62 | 0.76 |
| 1:ME:222:PRO:CG | 2:MF:324:LYS:HD3 | 2.14 | 0.76 |
| 7:5A:1475:PHE:CZ | 7:5A:1565:GLU:CD | 2.63 | 0.76 |
| 7:5B:1245:GLY:C | 9:7D:12:GLU:CD | 2.52 | 0.76 |
| 7:5B:1475:PHE:CZ | 7:5B:1565:GLU:CD | 2.63 | 0.76 |
| 7:5C:1105:TYR:HB2 | 7:5C:1166:LEU:H | 1.49 | 0.76 |
| 7:5C:1475:PHE:CZ | 7:5C:1565:GLU:CD | 2.63 | 0.76 |
| 1:AE:71:GLU:OE1 | 2:AF:247:ASN:ND2 | 2.18 | 0.76 |
| 1:CA:101:ASN:HD22 | 2:CB:252:LYS:CG | 1.97 | 0.76 |
| 2:EB:208:TYR:OH | 1:EC:325:PRO:HB2 | 1.85 | 0.76 |
| 2:FF:106:TYR:O | 7:5B:1298:LYS:CE | 2.33 | 0.76 |
| 2:GB:55:THR:HG21 | 2:HB:284:LEU:N | 2.00 | 0.76 |
| 2:HD:261:PRO:CG | 5:3C:337:ARG:HH21 | 1.99 | 0.76 |
| 4:2A:16:GLN:O | 4:2A:19:MET:C | 2.28 | 0.76 |
| 4:2B:16:GLN:O | 4:2B:19:MET:C | 2.28 | 0.76 |
| 1:AC:11:GLN:NE2 | 2:AD:247:ASN:OD1 | 2.18 | 0.76 |
| 2:CB:397:TRP:CE3 | 1:CC:257:THR:HG23 | 2.20 | 0.76 |
| 2:CD:87:PRO:HD2 | 2:DD:281:TYR:CD2 | 2.20 | 0.76 |
| 2:CD:212:PHE:CZ | 1:CE:326:LYS:CD | 2.22 | 0.76 |
| 1:FA:101:ASN:HD22 | 2:FB:252:LYS:CG | 1.98 | 0.76 |
| 1:FE:402:ARG:CD | 7:5B:1259:TYR:CD2 | 2.67 | 0.76 |
| 2:HB:220:PRO:HD2 | 1:HC:326:LYS:HE2 | 1.66 | 0.76 |
| 2:HD:220:PRO:HD2 | 1:HE:326:LYS:HG2 | 1.68 | 0.76 |
| 2:KB:86:ARG:HE | 2:KB:87:PRO:HD2 | 1.49 | 0.76 |
| 2:KD:86:ARG:HE | 2:KD:87:PRO:HD2 | 1.49 | 0.76 |
| 2:LB:98:GLY:HA2 | 1:LC:254:GLU:HG3 | 1.67 | 0.76 |
| 1:LC:89:PRO:HD3 | 1:MC:280:LYS:CE | 2.15 | 0.76 |
| 2:LD:224:ASP:HA | 6:4B:219:ASN:OD1 | 1.85 | 0.76 |
| 4:2C:16:GLN:O | 4:2C:19:MET:C | 2.28 | 0.76 |
| 5:3C:229:PHE:CD2 | 5:3C:331:GLN:CB | 2.68 | 0.76 |
| 6:4A:151:ARG:HG2 | 6:4A:151:ARG:NH1 | 1.94 | 0.76 |
| 7:5A:1105:TYR:HB2 | 7:5A:1166:LEU:H | 1.49 | 0.76 |
| 7:5A:1348:LYS:HD3 | 7:5A:1348:LYS:N | 2.00 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5A:1548:VAL:CG1 | 7:5A:1569:GLU:HB2 | 2.11 | 0.76 |
| 7:5C:1348:LYS:HD3 | 7:5C:1348:LYS:N | 2.00 | 0.76 |
| 2:DB:178:THR:HG23 | 1:DC:258:ASN:ND2 | 2.00 | 0.76 |
| 2:FB:212:PHE:CE2 | 1:FC:326:LYS:HD3 | 2.18 | 0.76 |
| 1:FC:101:ASN:HD22 | 2:FD:252:LYS:CG | 1.98 | 0.76 |
| 2:FF:428:ALA:HB1 | 7:5B:1080:PHE:CZ | 2.21 | 0.76 |
| 2:GD:220:PRO:HD2 | 1:GE:326:LYS:HG2 | 1.68 | 0.76 |
| 1:KC:88:HIS:CA | 1:LC:284:GLU:HB3 | 1.95 | 0.76 |
| 2:KD:159:TYR:CE2 | 4:2A:35:VAL:O | 2.39 | 0.76 |
| 1:LA:89:PRO:CD | 1:MA:280:LYS:CD | 2.62 | 0.76 |
| 7:5B:836:ARG:HH11 | 7:5B:836:ARG:CB | 1.98 | 0.76 |
| 7:5B:1348:LYS:HD3 | 7:5B:1348:LYS:N | 2.00 | 0.76 |
| 7:5C:1407:GLN:O | 7:5C:1407:GLN:NE2 | 2.19 | 0.76 |
| 2:AD:361:LEU:HD22 | 6:4C:144:LEU:HD13 | 1.67 | 0.76 |
| 2:CB:87:PRO:HD2 | 2:DB:281:TYR:CD2 | 2.20 | 0.76 |
| 2:DD:177:ASP:O | 1:DE:352:LYS:HA | 1.85 | 0.76 |
| 2:ED:220:PRO:HD2 | 1:EE:326:LYS:CE | 2.16 | 0.76 |
| 2:EF:125:GLU:CB | 7:5B:903:PHE:CD2 | 2.66 | 0.76 |
| 2:FD:100:ASN:HB2 | 1:FE:257:THR:HG21 | 1.66 | 0.76 |
| 1:HE:71:GLU:OE1 | 2:HF:247:ASN:ND2 | 2.18 | 0.76 |
| 2:ID:220:PRO:HD2 | 1:IE:326:LYS:HG2 | 1.68 | 0.76 |
| 1:IE:71:GLU:OE1 | 2:IF:247:ASN:ND2 | 2.18 | 0.76 |
| 1:IE:402:ARG:NH2 | 7:5B:1418:GLN:HA | 2.01 | 0.76 |
| 1:JA:89:PRO:CG | 1:KA:279:GLU:C | 2.58 | 0.76 |
| 2:KF:86:ARG:HE | 2:KF:87:PRO:HD2 | 1.49 | 0.76 |
| 2:LB:331:LEU:HD11 | 4:2C:42:PHE:HE1 | 1.51 | 0.76 |
| 2:LD:397:TRP:HE3 | 1:LE:257:THR:HG22 | 1.43 | 0.76 |
| 5:3B:232:ALA:HB2 | 5:3B:336:ASN:N | 2.00 | 0.76 |
| 7:5A:1407:GLN:O | 7:5A:1407:GLN:NE2 | 2.19 | 0.76 |
| 7:5B:1407:GLN:O | 7:5B:1407:GLN:NE2 | 2.19 | 0.76 |
| 7:5C:773:ARG:O | 7:5C:773:ARG:NE | 2.19 | 0.76 |
| 7:5C:1425:LYS:HZ1 | 7:5C:1429:GLN:HB2 | 1.48 | 0.76 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:CA | 2.15 | 0.76 |
| 1:CC:222:PRO:CG | 2:CD:324:LYS:HD3 | 2.15 | 0.76 |
| 1:GA:89:PRO:CG | 1:HA:280:LYS:CE | 2.63 | 0.76 |
| 1:HC:222:PRO:CG | 2:HD:324:LYS:HD3 | 2.16 | 0.76 |
| 2:HF:160:PRO:HB3 | 5:3A:330:ARG:NH2 | 2.00 | 0.76 |
| 1:JC:11:GLN:NE2 | 2:JD:247:ASN:OD1 | 2.18 | 0.76 |
| 2:LB:340:TYR:CG | 4:2C:147:PHE:HB3 | 2.21 | 0.76 |
| 2:LB:340:TYR:HB2 | 4:2C:147:PHE:HB2 | 1.68 | 0.76 |
| 2:LD:270:PHE:CE2 | 6:4B:226:ILE:HG23 | 2.20 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MB:221:THR:HG21 | 6:4A:189:ARG:HH22 | 0.67 | 0.76 |
| 1:ME:282:TYR:CD2 | 6:4B:104:ARG:CD | 2.54 | 0.76 |
| 6:4D:289:LYS:HE3 | 6:4D:289:LYS:CA | 2.08 | 0.76 |
| 7:5B:1105:TYR:HB2 | 7:5B:1166:LEU:H | 1.49 | 0.76 |
| 7:5B:1266:TYR:CA | 7:5B:1269:ASP:OD2 | 2.24 | 0.76 |
| 7:5C:1271:ILE:HA | 9:7E:20:LEU:HD21 | 1.64 | 0.76 |
| 2:AB:220:PRO:HD2 | 1:AC:326:LYS:HE2 | 1.66 | 0.76 |
| 1:CA:101:ASN:CG | 2:CB:252:LYS:HD2 | 2.06 | 0.76 |
| 2:FB:220:PRO:O | 1:FC:324:VAL:HG11 | 1.86 | 0.76 |
| 1:IA:60:LYS:HZ2 | 1:JA:283:HIS:CD2 | 2.03 | 0.76 |
| 1:IC:222:PRO:CG | 2:ID:324:LYS:HD3 | 2.16 | 0.76 |
| 2:JB:220:PRO:HD2 | 1:JC:326:LYS:HE2 | 1.66 | 0.76 |
| 1:JC:222:PRO:CG | 2:JD:324:LYS:HD3 | 2.16 | 0.76 |
| 1:KC:85:GLN:OE1 | 1:LC:282:TYR:CA | 2.34 | 0.76 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CH2 | 2.54 | 0.76 |
| 1:MA:101:ASN:HD22 | 2:MB:252:LYS:HD2 | 1.38 | 0.76 |
| 5:3A:232:ALA:HB2 | 5:3A:336:ASN:N | 2.00 | 0.76 |
| 5:3C:232:ALA:HB2 | 5:3C:336:ASN:N | 2.00 | 0.76 |
| 7:5A:773:ARG:O | 7:5A:773:ARG:NE | 2.19 | 0.76 |
| 7:5B:1524:PHE:HE1 | 7:5B:1571:MET:CE | 1.99 | 0.76 |
| 9:7A:14:SER:O | 9:7B:35:ILE:CG1 | 2.34 | 0.76 |
| 2:AD:220:PRO:HD2 | 1:AE:326:LYS:HE2 | 1.67 | 0.76 |
| 1:EC:101:ASN:HD21 | 2:ED:252:LYS:HD2 | 0.93 | 0.76 |
| 1:FC:177:VAL:HG21 | 7:5A:915:PHE:HE2 | 1.44 | 0.76 |
| 2:ID:86:ARG:HE | 2:ID:87:PRO:HD2 | 1.49 | 0.76 |
| 2:ID:87:PRO:HD2 | 2:JD:281:TYR:CE2 | 2.20 | 0.76 |
| 2:KD:125:GLU:CB | 2:LD:336:LYS:HE2 | 2.14 | 0.76 |
| 2:LB:224:ASP:CA | 6:4A:219:ASN:OD1 | 2.22 | 0.76 |
| 1:ME:404:PHE:CE2 | 2:MF:345:ILE:CD1 | 2.70 | 0.76 |
| 7:5A:836:ARG:HH11 | 7:5A:836:ARG:CB | 1.98 | 0.76 |
| 7:5A:839:GLU:HA | 8:6A:109:ILE:N | 2.01 | 0.76 |
| 7:5B:840:GLY:C | 8:6B:109:ILE:HD11 | 1.63 | 0.76 |
| 1:BA:71:GLU:OE1 | 2:BB:247:ASN:ND2 | 2.20 | 0.75 |
| 2:CB:87:PRO:CD | 2:DB:281:TYR:CZ | 2.69 | 0.75 |
| 1:DA:101:ASN:HD22 | 2:DB:252:LYS:CG | 1.97 | 0.75 |
| 2:DD:177:ASP:OD2 | 1:DE:248:LEU:HD21 | 1.86 | 0.75 |
| 1:FE:101:ASN:CG | 2:FF:252:LYS:HD2 | 2.09 | 0.75 |
| 1:GA:89:PRO:CG | 1:HA:280:LYS:NZ | 2.47 | 0.75 |
| 1:GC:89:PRO:HG3 | 1:HC:280:LYS:CD | 2.15 | 0.75 |
| 2:IB:86:ARG:HE | 2:IB:87:PRO:HD2 | 1.50 | 0.75 |
| 1:IE:402:ARG:NH2 | 7:5B:1418:GLN:CA | 2.43 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JE:71:GLU:OE1 | 2:JF:247:ASN:ND2 | 2.18 | 0.75 |
| 1:KE:71:GLU:OE1 | 2:KF:247:ASN:ND2 | 2.18 | 0.75 |
| 6:4C:151:ARG:HG2 | 6:4C:151:ARG:NH1 | 1.94 | 0.75 |
| 7:5A:1374:ASP:HA | 7:5A:1377:LYS:HE2 | 1.68 | 0.75 |
| 7:5B:773:ARG:O | 7:5B:773:ARG:NE | 2.19 | 0.75 |
| 7:5C:1152:GLU:OE1 | 8:6C:66:ARG:NH1 | 2.18 | 0.75 |
| 7:5C:1374:ASP:HA | 7:5C:1377:LYS:HE2 | 1.68 | 0.75 |
| 1:BE:101:ASN:HD22 | 2:BF:252:LYS:CG | 1.98 | 0.75 |
| 2:EB:85:PHE:O | 2:FB:281:TYR:OH | 2.04 | 0.75 |
| 1:EC:402:ARG:CZ | 7:5A:824:ARG:HH22 | 1.99 | 0.75 |
| 1:IA:71:GLU:OE1 | 2:IB:247:ASN:ND2 | 2.19 | 0.75 |
| 1:LC:60:LYS:CD | 1:MC:283:HIS:CD2 | 2.70 | 0.75 |
| 1:MA:101:ASN:HD21 | 2:MB:252:LYS:HD2 | 0.94 | 0.75 |
| 4:2C:16:GLN:C | 4:2C:19:MET:N | 2.45 | 0.75 |
| 7:5A:1524:PHE:HE1 | 7:5A:1571:MET:CE | 1.99 | 0.75 |
| 1:AC:222:PRO:CG | 2:AD:324:LYS:HD3 | 2.16 | 0.75 |
| 2:BB:220:PRO:O | 1:BC:324:VAL:HG11 | 1.86 | 0.75 |
| 1:FC:56:THR:CA | 1:GC:285:GLN:HB3 | 2.16 | 0.75 |
| 2:HD:86:ARG:HA | 2:ID:281:TYR:CE1 | 2.21 | 0.75 |
| 2:IF:86:ARG:HE | 2:IF:87:PRO:HD2 | 1.49 | 0.75 |
| 2:KD:276:ARG:NH2 | 6:4B:265:TYR:CA | 2.45 | 0.75 |
| 2:LB:86:ARG:HE | 2:LB:87:PRO:HD2 | 1.49 | 0.75 |
| 2:LB:177:ASP:OD2 | 1:LC:248:LEU:HD23 | 1.86 | 0.75 |
| 2:LB:296:ALA:CB | 4:2C:149:ILE:HG21 | 2.14 | 0.75 |
| 2:LF:86:ARG:HE | 2:LF:87:PRO:HD2 | 1.49 | 0.75 |
| 1:ME:101:ASN:HD21 | 2:MF:252:LYS:CD | 1.72 | 0.75 |
| 4:2A:16:GLN:C | 4:2A:19:MET:N | 2.45 | 0.75 |
| 4:2B:16:GLN:C | 4:2B:19:MET:N | 2.45 | 0.75 |
| 7:5B:1374:ASP:HA | 7:5B:1377:LYS:HE2 | 1.68 | 0.75 |
| 7:5C:836:ARG:HH11 | 7:5C:836:ARG:CB | 1.98 | 0.75 |
| 9:7A:39:GLY:CA | 9:7B:43:LEU:HD11 | 2.16 | 0.75 |
| 2:BD:177:ASP:O | 1:BE:352:LYS:CD | 2.29 | 0.75 |
| 2:CD:220:PRO:CD | 1:CE:326:LYS:HE2 | 2.16 | 0.75 |
| 1:CE:71:GLU:OE1 | 2:CF:247:ASN:ND2 | 2.19 | 0.75 |
| 1:EA:222:PRO:CD | 2:EB:324:LYS:HD3 | 2.15 | 0.75 |
| 1:EA:430:LYS:HZ2 | 7:5C:834:ASN:CB | 1.99 | 0.75 |
| 2:EB:220:PRO:HD2 | 1:EC:326:LYS:CE | 2.17 | 0.75 |
| 1:FC:101:ASN:HD22 | 2:FD:252:LYS:CD | 1.99 | 0.75 |
| 2:JD:220:PRO:HD2 | 1:JE:326:LYS:HE2 | 1.67 | 0.75 |
| 2:LB:220:PRO:HD2 | 1:LC:326:LYS:HG2 | 1.69 | 0.75 |
| 2:MB:78:ALA:HB3 | 6:4A:178:HIS:NE2 | 2.02 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1436:ARG:HH11 | 7:5A:1436:ARG:HB3 | 1.50 | 0.75 |
| 7:5B:842:LEU:N | 7:5B:842:LEU:HD13 | 2.02 | 0.75 |
| 7:5B:1436:ARG:HH11 | 7:5B:1436:ARG:HB3 | 1.50 | 0.75 |
| 7:5C:1524:PHE:HE1 | 7:5C:1571:MET:CE | 1.99 | 0.75 |
| 9:7C:14:SER:O | 9:7D:35:ILE:CG1 | 2.34 | 0.75 |
| 1:AC:308:ARG:O | 3:1C:56:ASN:OD1 | 2.05 | 0.75 |
| 1:AE:342:GLN:HE21 | 3:1A:55:HIS:CD2 | 2.01 | 0.75 |
| 2:BD:177:ASP:OD1 | 1:BE:353:VAL:HG12 | 1.77 | 0.75 |
| 1:DC:400:ALA:O | 7:5A:775:PRO:HB3 | 1.83 | 0.75 |
| 2:ED:208:TYR:OH | 1:EE:325:PRO:HB2 | 1.87 | 0.75 |
| 1:FC:207:GLU:OE1 | 7:5A:915:PHE:HD2 | 1.68 | 0.75 |
| 1:GC:89:PRO:HG3 | 1:HC:280:LYS:CE | 2.16 | 0.75 |
| 1:GC:222:PRO:CG | 2:GD:324:LYS:HD3 | 2.16 | 0.75 |
| 2:HD:220:PRO:HD2 | 1:HE:326:LYS:HE2 | 1.67 | 0.75 |
| 1:IA:282:TYR:CE1 | 10:8V:15:UNK:HA | 2.22 | 0.75 |
| 2:LD:86:ARG:HE | 2:LD:87:PRO:HD2 | 1.49 | 0.75 |
| 2:LD:224:ASP:CA | 6:4B:219:ASN:OD1 | 2.24 | 0.75 |
| 1:LE:60:LYS:HD3 | 1:ME:283:HIS:CD2 | 2.22 | 0.75 |
| 7:5A:844:PHE:CD2 | 7:5A:849:ARG:HD2 | 2.22 | 0.75 |
| 7:5A:1548:VAL:CG1 | 7:5A:1565:GLU:C | 2.57 | 0.75 |
| 7:5B:844:PHE:CD2 | 7:5B:849:ARG:HD2 | 2.22 | 0.75 |
| 7:5B:1367:LYS:HA | 7:5B:1367:LYS:HE3 | 1.66 | 0.75 |
| 7:5C:842:LEU:N | 7:5C:842:LEU:HD13 | 2.02 | 0.75 |
| 7:5C:844:PHE:CD2 | 7:5C:849:ARG:HD2 | 2.22 | 0.75 |
| 7:5C:1548:VAL:CG1 | 7:5C:1569:GLU:HB2 | 2.11 | 0.75 |
| 1:AA:71:GLU:OE1 | 2:AB:247:ASN:ND2 | 2.19 | 0.75 |
| 2:EB:54:ALA:HA | 2:FB:283:ALA:CB | 2.11 | 0.75 |
| 2:ED:55:THR:CG2 | 2:FD:284:LEU:H | 2.00 | 0.75 |
| 2:FF:55:THR:H | 2:GF:283:ALA:CB | 1.97 | 0.75 |
| 2:FF:428:ALA:CB | 7:5B:1080:PHE:CZ | 2.67 | 0.75 |
| 1:GA:71:GLU:OE1 | 2:GB:247:ASN:ND2 | 2.19 | 0.75 |
| 1:JE:89:PRO:CG | 1:KE:280:LYS:CG | 2.54 | 0.75 |
| 1:KE:84:ARG:CZ | 1:LE:283:HIS:NE2 | 2.50 | 0.75 |
| 2:LD:55:THR:HG23 | 2:MD:283:ALA:HA | 0.77 | 0.75 |
| 1:MA:279:GLU:HG3 | 6:4C:110:LYS:HE2 | 1.68 | 0.75 |
| 6:4C:244:GLU:CD | 6:4C:284:LEU:HD11 | 2.12 | 0.75 |
| 7:5A:842:LEU:N | 7:5A:842:LEU:HD13 | 2.02 | 0.75 |
| 7:5A:1152:GLU:CD | 8:6A:66:ARG:HH12 | 1.95 | 0.75 |
| 7:5A:1367:LYS:HE3 | 7:5A:1367:LYS:HA | 1.66 | 0.75 |
| 7:5B:880:ILE:HD11 | 7:5B:1047:LEU:HD23 | 1.69 | 0.75 |
| 7:5B:1548:VAL:CG1 | 7:5B:1565:GLU:C | 2.57 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5C:1267:CYS:SG | 9:7E:8:ARG:CD | 2.74 | 0.75 |
| 7:5C:1436:ARG:HH11 | 7:5C:1436:ARG:HB3 | 1.50 | 0.75 |
| 7:5C:1548:VAL:CG1 | 7:5C:1565:GLU:C | 2.57 | 0.75 |
| 1:BA:11:GLN:OE1 | 2:BB:245:GLN:O | 2.04 | 0.75 |
| 2:DB:177:ASP:CB | 1:DC:353:VAL:HG12 | 2.17 | 0.75 |
| 2:EF:125:GLU:CD | 7:5B:903:PHE:HE2 | 1.94 | 0.75 |
| 1:FC:89:PRO:CA | 1:GC:280:LYS:NZ | 2.50 | 0.75 |
| 1:IE:279:GLU:CD | 10:8X:22:UNK:CA | 2.53 | 0.75 |
| 2:KF:125:GLU:CD | 2:LF:332:ASN:ND2 | 2.45 | 0.75 |
| 2:LB:221:THR:CG2 | 6:4A:220:GLY:H | 2.00 | 0.75 |
| 6:4A:244:GLU:CD | 6:4A:284:LEU:HD11 | 2.11 | 0.75 |
| 7:5C:1367:LYS:HA | 7:5C:1367:LYS:HE3 | 1.66 | 0.75 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:HD13 | 0.75 | 0.75 |
| 9:7C:39:GLY:CA | 9:7D:43:LEU:HD11 | 2.16 | 0.75 |
| 2:AD:40:SER:HG | 6:4C:152:PHE:HE2 | 0.79 | 0.75 |
| 2:AD:217:LEU:HD22 | 6:4C:132:LYS:CD | 2.15 | 0.75 |
| 2:AD:227:HIS:HE1 | 6:4C:135:LEU:HD12 | 1.51 | 0.75 |
| 1:FE:60:LYS:HD3 | 1:GE:283:HIS:CD2 | 2.22 | 0.75 |
| 1:GE:60:LYS:HD3 | 1:HE:283:HIS:CG | 2.22 | 0.75 |
| 1:HA:71:GLU:OE1 | 2:HB:247:ASN:ND2 | 2.19 | 0.75 |
| 1:JA:89:PRO:HG2 | 1:KA:279:GLU:C | 2.10 | 0.75 |
| 2:KB:32:PRO:HG2 | 6:4A:279:LEU:HD21 | 1.68 | 0.75 |
| 1:LC:222:PRO:HG3 | 2:LD:324:LYS:CD | 2.15 | 0.75 |
| 6:4B:244:GLU:CD | 6:4B:284:LEU:HD11 | 2.11 | 0.75 |
| 7:5A:880:ILE:HD11 | 7:5A:1047:LEU:HD23 | 1.69 | 0.75 |
| 9:7E:7:LEU:CD2 | 9:7F:30:ARG:HE | 1.99 | 0.75 |
| 1:BE:71:GLU:OE1 | 2:BF:247:ASN:ND2 | 2.20 | 0.75 |
| 2:DB:179:VAL:CG2 | 1:DC:258:ASN:HA | 2.17 | 0.75 |
| 1:EE:419:SER:OG | 7:5B:830:VAL:HG21 | 1.85 | 0.75 |
| 1:GA:11:GLN:NE2 | 2:GB:247:ASN:OD1 | 2.20 | 0.75 |
| 1:GC:60:LYS:HD3 | 1:HC:283:HIS:CA | 2.16 | 0.75 |
| 1:HA:11:GLN:NE2 | 2:HB:247:ASN:OD1 | 2.20 | 0.75 |
| 1:IE:60:LYS:NZ | 1:JE:283:HIS:NE2 | 2.35 | 0.75 |
| 1:KA:86:LEU:C | 1:LA:283:HIS:O | 2.30 | 0.75 |
| 2:KB:87:PRO:HG2 | 2:LB:282:ARG:HG2 | 1.63 | 0.75 |
| 1:KE:372:MET:HB3 | 6:4B:299:TYR:HE1 | 1.48 | 0.75 |
| 1:MC:101:ASN:HD21 | 2:MD:252:LYS:CD | 1.72 | 0.75 |
| 6:4D:244:GLU:CD | 6:4D:284:LEU:HD11 | 2.11 | 0.75 |
| 7:5A:1284:PHE:CE1 | 9:7A:12:GLU:CB | 2.67 | 0.75 |
| 7:5B:1474:LEU:HD22 | 7:5B:1576:ILE:CD1 | 2.16 | 0.75 |
| 7:5C:880:ILE:HD11 | 7:5C:1047:LEU:HD23 | 1.69 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:7A:30:ARG:NH1 | 9:7B:3:GLN:CG | 2.49 | 0.75 |
| 2:DD:397:TRP:HE3 | 1:DE:257:THR:HG22 | 1.43 | 0.74 |
| 2:KB:130:LEU:HB2 | 4:2C:37:GLY:HA2 | 1.68 | 0.74 |
| 1:KC:222:PRO:CG | 2:KD:324:LYS:HD3 | 2.16 | 0.74 |
| 2:KD:220:PRO:HD2 | 1:KE:326:LYS:HE2 | 1.67 | 0.74 |
| 2:LB:221:THR:HG21 | 6:4A:220:GLY:N | 2.01 | 0.74 |
| 2:LD:310:TYR:CE2 | 4:2A:147:PHE:CE2 | 2.75 | 0.74 |
| 2:LF:55:THR:CG2 | 2:MF:283:ALA:HB1 | 2.16 | 0.74 |
| 2:LF:306:ARG:NH2 | 4:2B:149:ILE:CG2 | 2.50 | 0.74 |
| 2:BD:179:VAL:CG2 | 1:BE:258:ASN:HA | 2.17 | 0.74 |
| 1:DC:71:GLU:OE1 | 2:DD:247:ASN:ND2 | 2.20 | 0.74 |
| 1:DE:101:ASN:HD22 | 2:DF:252:LYS:CD | 1.96 | 0.74 |
| 1:EA:393:HIS:CE1 | 7:5C:814:LYS:HG3 | 2.22 | 0.74 |
| 2:EB:177:ASP:OD2 | 1:EC:248:LEU:HD21 | 1.86 | 0.74 |
| 1:EC:430:LYS:HZ3 | 7:5A:834:ASN:ND2 | 1.27 | 0.74 |
| 2:ED:55:THR:HG21 | 2:FD:284:LEU:H | 1.52 | 0.74 |
| 1:HE:410:GLY:C | 5:3A:329:ARG:NH2 | 2.44 | 0.74 |
| 1:HE:420:GLU:OE1 | 5:3A:215:TYR:CE2 | 2.41 | 0.74 |
| 1:JA:71:GLU:OE1 | 2:JB:247:ASN:ND2 | 2.19 | 0.74 |
| 1:KA:71:GLU:OE1 | 2:KB:247:ASN:ND2 | 2.19 | 0.74 |
| 2:LD:221:THR:HG21 | 6:4B:220:GLY:N | 2.02 | 0.74 |
| 6:4D:111:GLU:HB3 | 6:4D:114:GLU:OE2 | 1.86 | 0.74 |
| 7:5C:1474:LEU:HD22 | 7:5C:1576:ILE:CD1 | 2.16 | 0.74 |
| 2:AB:220:PRO:O | 1:AC:324:VAL:HG11 | 1.88 | 0.74 |
| 2:AF:322:SER:N | 6:4A:156:PHE:CE2 | 2.56 | 0.74 |
| 2:GB:83:GLN:O | 2:HB:281:TYR:OH | 2.05 | 0.74 |
| 1:GC:409:VAL:CG1 | 5:3C:383:GLU:OE1 | 2.35 | 0.74 |
| 1:JE:88:HIS:ND1 | 1:KE:280:LYS:HD3 | 2.01 | 0.74 |
| 2:KD:83:GLN:HA | 2:LD:281:TYR:CD1 | 2.22 | 0.74 |
| 1:LC:221:ARG:HH11 | 2:LD:324:LYS:N | 1.86 | 0.74 |
| 2:LF:306:ARG:CZ | 4:2B:151:VAL:HG21 | 2.18 | 0.74 |
| 7:5A:1474:LEU:HD22 | 7:5A:1576:ILE:CD1 | 2.16 | 0.74 |
| 7:5A:1562:LEU:HD12 | 7:5A:1562:LEU:N | 2.02 | 0.74 |
| 7:5B:1562:LEU:HD12 | 7:5B:1562:LEU:N | 2.02 | 0.74 |
| 7:5C:1562:LEU:HD12 | 7:5C:1562:LEU:N | 2.02 | 0.74 |
| 9:7E:42:LEU:CD1 | 9:7F:39:GLY:CA | 2.65 | 0.74 |
| 2:AF:357:PRO:HD2 | 6:4A:151:ARG:HD2 | 1.69 | 0.74 |
| 1:BC:71:GLU:OE1 | 2:BD:247:ASN:ND2 | 2.21 | 0.74 |
| 2:DD:177:ASP:CB | 1:DE:353:VAL:HG12 | 2.18 | 0.74 |
| 1:GA:60:LYS:HD3 | 1:HA:283:HIS:CB | 2.18 | 0.74 |
| 1:JE:90:GLU:CB | 1:KE:280:LYS:HD2 | 1.82 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KB:87:PRO:HG2 | 2:LB:282:ARG:HD2 | 1.70 | 0.74 |
| 6:4B:111:GLU:HB3 | 6:4B:114:GLU:OE2 | 1.86 | 0.74 |
| 7:5B:1275:ILE:HG21 | 9:7D:11:TYR:OH | 1.86 | 0.74 |
| 7:5B:1565:GLU:CB | 7:5B:1568:LYS:HB2 | 2.05 | 0.74 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:HD13 | 0.75 | 0.74 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:CG1 | 2.17 | 0.74 |
| 9:7C:30:ARG:NH1 | 9:7D:3:GLN:CG | 2.49 | 0.74 |
| 1:DE:101:ASN:CG | 2:DF:252:LYS:HD2 | 2.08 | 0.74 |
| 2:FB:106:TYR:O | 7:5C:1298:LYS:CE | 2.34 | 0.74 |
| 1:FE:423:GLU:CD | 7:5B:1256:ARG:HH22 | 1.95 | 0.74 |
| 1:GE:56:THR:OG1 | 1:HE:284:GLU:C | 2.30 | 0.74 |
| 2:HB:220:PRO:O | 1:HC:324:VAL:HG11 | 1.88 | 0.74 |
| 1:IA:58:ALA:HB3 | 10:8Y:13:UNK:HA | 0.79 | 0.74 |
| 2:IB:220:PRO:HD2 | 1:IC:326:LYS:HG2 | 1.69 | 0.74 |
| 2:JB:220:PRO:HD2 | 1:JC:326:LYS:HG2 | 1.69 | 0.74 |
| 1:KE:85:GLN:CD | 1:LE:282:TYR:HB2 | 2.12 | 0.74 |
| 2:LB:397:TRP:CE3 | 1:LC:257:THR:HG23 | 2.21 | 0.74 |
| 2:LF:294:PHE:HD2 | 4:2B:147:PHE:HZ | 1.32 | 0.74 |
| 4:2A:16:GLN:C | 4:2A:19:MET:H | 1.96 | 0.74 |
| 4:2B:16:GLN:C | 4:2B:19:MET:H | 1.96 | 0.74 |
| 4:2C:16:GLN:C | 4:2C:19:MET:H | 1.96 | 0.74 |
| 7:5A:1565:GLU:CB | 7:5A:1568:LYS:HB2 | 2.05 | 0.74 |
| 7:5B:1089:PHE:CD1 | 7:5B:1101:LEU:HD22 | 2.21 | 0.74 |
| 7:5C:1089:PHE:CD1 | 7:5C:1101:LEU:HD22 | 2.21 | 0.74 |
| 2:CF:86:ARG:N | 2:DF:281:TYR:CE1 | 2.54 | 0.74 |
| 2:DB:397:TRP:CE3 | 1:DC:257:THR:HG23 | 2.22 | 0.74 |
| 2:EB:157:GLU:CD | 7:5C:935:LYS:HZ1 | 1.84 | 0.74 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:HD3 | 1.67 | 0.74 |
| 2:GB:220:PRO:O | 1:GC:324:VAL:HG11 | 1.88 | 0.74 |
| 2:IB:220:PRO:O | 1:IC:324:VAL:HG11 | 1.88 | 0.74 |
| 1:IC:279:GLU:OE2 | 10:8W:22:UNK:CB | 2.35 | 0.74 |
| 2:IF:86:ARG:NH1 | 2:JF:281:TYR:CA | 2.48 | 0.74 |
| 2:KB:220:PRO:O | 1:KC:324:VAL:HG11 | 1.88 | 0.74 |
| 2:KB:220:PRO:HD2 | 1:KC:326:LYS:HG2 | 1.69 | 0.74 |
| 1:LA:245:ASP:OD1 | 6:4C:216:ARG:CZ | 2.35 | 0.74 |
| 1:LC:60:LYS:HD2 | 6:4A:101:ARG:NH1 | 2.01 | 0.74 |
| 2:LD:55:THR:HG23 | 2:MD:283:ALA:C | 2.08 | 0.74 |
| 1:LE:60:LYS:HE3 | 6:4B:101:ARG:NH1 | 2.03 | 0.74 |
| 2:MD:78:ALA:CB | 6:4B:178:HIS:CD2 | 2.70 | 0.74 |
| 6:4A:111:GLU:HB3 | 6:4A:114:GLU:OE2 | 1.86 | 0.74 |
| 7:5B:1572:LEU:HG | 7:5B:1576:ILE:HD12 | 1.69 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5C:1565:GLU:CB | 7:5C:1568:LYS:HB2 | 2.05 | 0.74 |
| 2:BD:177:ASP:CB | 1:BE:353:VAL:HG12 | 2.17 | 0.74 |
| 1:EA:62:VAL:CG2 | 1:FA:283:HIS:O | 2.36 | 0.74 |
| 1:EE:101:ASN:HD21 | 2:EF:252:LYS:CD | 1.76 | 0.74 |
| 1:IA:279:GLU:OE2 | 10:8V:22:UNK:CA | 2.35 | 0.74 |
| 2:IF:86:ARG:CA | 2:JF:281:TYR:HE1 | 2.00 | 0.74 |
| 2:KB:87:PRO:CG | 2:LB:282:ARG:CD | 2.63 | 0.74 |
| 2:KF:276:ARG:HH21 | 6:4D:265:TYR:CB | 1.99 | 0.74 |
| 2:LD:306:ARG:HH21 | 4:2A:149:ILE:HG22 | 1.48 | 0.74 |
| 1:LE:89:PRO:CD | 1:ME:280:LYS:CD | 2.64 | 0.74 |
| 1:MA:279:GLU:OE1 | 6:4C:107:MET:CA | 2.36 | 0.74 |
| 1:ME:279:GLU:O | 6:4B:107:MET:CB | 2.35 | 0.74 |
| 7:5A:1089:PHE:CD1 | 7:5A:1101:LEU:HD22 | 2.21 | 0.74 |
| 7:5A:1572:LEU:HG | 7:5A:1576:ILE:HD12 | 1.69 | 0.74 |
| 7:5C:880:ILE:CD1 | 7:5C:1047:LEU:HD23 | 2.18 | 0.74 |
| 7:5C:1572:LEU:HG | 7:5C:1576:ILE:CD1 | 2.18 | 0.74 |
| 2:AB:220:PRO:HD2 | 1:AC:326:LYS:HG2 | 1.69 | 0.74 |
| 1:CE:60:LYS:HZ3 | 1:DE:283:HIS:CD2 | 2.04 | 0.74 |
| 2:DD:212:PHE:CE2 | 1:DE:326:LYS:HD3 | 2.15 | 0.74 |
| 1:FE:101:ASN:ND2 | 2:FF:252:LYS:CG | 2.50 | 0.74 |
| 2:HB:220:PRO:HD2 | 1:HC:326:LYS:HG2 | 1.69 | 0.74 |
| 2:HD:397:TRP:CB | 1:HE:256:GLN:HE22 | 2.00 | 0.74 |
| 1:IA:11:GLN:NE2 | 2:IB:247:ASN:OD1 | 2.20 | 0.74 |
| 1:JA:11:GLN:NE2 | 2:JB:247:ASN:OD1 | 2.20 | 0.74 |
| 2:KB:215:LEU:HD12 | 6:4A:267:ILE:HG22 | 1.60 | 0.74 |
| 2:LB:390:ARG:CD | 1:LC:439:THR:HG21 | 2.18 | 0.74 |
| 7:5A:880:ILE:CD1 | 7:5A:1047:LEU:HD23 | 2.18 | 0.74 |
| 7:5A:1487:ASN:HB3 | 7:5A:1568:LYS:NZ | 2.03 | 0.74 |
| 7:5A:1572:LEU:HG | 7:5A:1576:ILE:CD1 | 2.18 | 0.74 |
| 7:5B:1487:ASN:HB3 | 7:5B:1568:LYS:NZ | 2.03 | 0.74 |
| 7:5C:1487:ASN:HB3 | 7:5C:1568:LYS:NZ | 2.03 | 0.74 |
| 7:5C:1491:LEU:CD2 | 7:5C:1495:PHE:CG | 2.60 | 0.74 |
| 2:BD:178:THR:HG23 | 1:BE:258:ASN:ND2 | 2.00 | 0.74 |
| 2:EF:157:GLU:HA | 7:5B:945:LYS:NZ | 2.02 | 0.74 |
| 1:KA:11:GLN:NE2 | 2:KB:247:ASN:OD1 | 2.20 | 0.74 |
| 2:LD:221:THR:CG2 | 6:4B:220:GLY:H | 2.01 | 0.74 |
| 6:4C:111:GLU:HB3 | 6:4C:114:GLU:OE2 | 1.86 | 0.74 |
| 7:5B:880:ILE:CD1 | 7:5B:1047:LEU:HD23 | 2.17 | 0.74 |
| 1:AC:141:VAL:HG11 | 1:AC:172:TYR:HD1 | 1.53 | 0.74 |
| 2:BB:178:THR:HG23 | 1:BC:258:ASN:ND2 | 2.01 | 0.74 |
| 2:BD:212:PHE:CE2 | 1:BE:326:LYS:HD3 | 2.17 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:220:PRO:CD | 1:CC:326:LYS:HE2 | 2.17 | 0.74 |
| 1:CC:222:PRO:CD | 2:CD:324:LYS:HD3 | 2.16 | 0.74 |
| 1:DA:141:VAL:HG11 | 1:DA:172:TYR:HD1 | 1.53 | 0.74 |
| 1:EC:101:ASN:HD21 | 2:ED:252:LYS:CD | 1.68 | 0.74 |
| 1:EE:393:HIS:HE1 | 7:5B:814:LYS:HG3 | 1.52 | 0.74 |
| 1:JC:141:VAL:HG11 | 1:JC:172:TYR:HD1 | 1.53 | 0.74 |
| 2:JD:179:VAL:CG2 | 1:JE:258:ASN:HA | 2.18 | 0.74 |
| 1:JE:91:GLN:N | 1:KE:280:LYS:HZ1 | 1.85 | 0.74 |
| 1:LA:141:VAL:HG11 | 1:LA:172:TYR:HD1 | 1.53 | 0.74 |
| 2:LB:274:THR:O | 6:4A:228:LEU:HD22 | 1.84 | 0.74 |
| 2:LB:331:LEU:HD21 | 4:2C:42:PHE:CZ | 0.64 | 0.74 |
| 7:5A:1548:VAL:C | 7:5A:1566:GLU:HG2 | 2.13 | 0.74 |
| 7:5C:1491:LEU:HA | 7:5C:1495:PHE:CB | 2.13 | 0.74 |
| 7:5C:1572:LEU:HG | 7:5C:1576:ILE:HD12 | 1.69 | 0.74 |
| 1:AA:141:VAL:HG11 | 1:AA:172:TYR:HD1 | 1.53 | 0.73 |
| 2:AD:179:VAL:CG2 | 1:AE:258:ASN:HA | 2.18 | 0.73 |
| 1:AE:141:VAL:HG11 | 1:AE:172:TYR:HD1 | 1.53 | 0.73 |
| 1:AE:283:HIS:C | 2:MB:54:ALA:HB1 | 2.12 | 0.73 |
| 1:DC:141:VAL:HG11 | 1:DC:172:TYR:HD1 | 1.53 | 0.73 |
| 1:DE:141:VAL:HG11 | 1:DE:172:TYR:HD1 | 1.53 | 0.73 |
| 2:GD:179:VAL:CG2 | 1:GE:258:ASN:HA | 2.18 | 0.73 |
| 1:HC:141:VAL:HG11 | 1:HC:172:TYR:HD1 | 1.53 | 0.73 |
| 1:HC:401:LYS:CE | 2:HD:344:TRP:CZ3 | 2.62 | 0.73 |
| 1:JA:141:VAL:HG11 | 1:JA:172:TYR:HD1 | 1.53 | 0.73 |
| 2:KB:217:LEU:CG | 6:4A:263:CYS:SG | 2.74 | 0.73 |
| 2:KD:124:ALA:O | 4:2A:38:VAL:HG13 | 1.88 | 0.73 |
| 2:KF:77:ARG:C | 2:LF:281:TYR:OH | 2.31 | 0.73 |
| 1:LA:60:LYS:HD3 | 1:MA:283:HIS:CD2 | 2.23 | 0.73 |
| 1:LA:89:PRO:CG | 1:MA:280:LYS:HZ2 | 2.01 | 0.73 |
| 1:LC:89:PRO:HD3 | 1:MC:280:LYS:HZ1 | 1.35 | 0.73 |
| 1:LC:141:VAL:HG11 | 1:LC:172:TYR:HD1 | 1.53 | 0.73 |
| 2:LF:18:ALA:HB3 | 6:4D:217:ASN:ND2 | 2.02 | 0.73 |
| 7:5B:1548:VAL:C | 7:5B:1566:GLU:HG2 | 2.13 | 0.73 |
| 7:5B:1572:LEU:HG | 7:5B:1576:ILE:CD1 | 2.18 | 0.73 |
| 7:5C:1491:LEU:CD2 | 7:5C:1495:PHE:CE1 | 2.71 | 0.73 |
| 7:5C:1548:VAL:C | 7:5C:1566:GLU:HG2 | 2.13 | 0.73 |
| 1:AA:11:GLN:NE2 | 2:AB:247:ASN:OD1 | 2.20 | 0.73 |
| 1:CC:11:GLN:NE2 | 2:CD:247:ASN:OD1 | 2.21 | 0.73 |
| 1:DA:11:GLN:NE2 | 2:DB:247:ASN:OD1 | 2.21 | 0.73 |
| 1:DE:101:ASN:HD22 | 2:DF:252:LYS:CG | 2.00 | 0.73 |
| 2:ED:177:ASP:OD1 | 1:EE:353:VAL:HG12 | 1.76 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:GD:412:GLU:OE2 | 7:5A:1323:MET:HE2 | 1.87 | 0.73 |
| 1:HE:141:VAL:HG11 | 1:HE:172:TYR:HD1 | 1.53 | 0.73 |
| 1:HE:415:GLU:CG | 5:3A:235:LEU:HB3 | 2.17 | 0.73 |
| 2:JD:86:ARG:NE | 2:KD:281:TYR:CD2 | 2.55 | 0.73 |
| 2:JD:397:TRP:CB | 1:JE:256:GLN:HE22 | 2.00 | 0.73 |
| 1:JE:141:VAL:HG11 | 1:JE:172:TYR:HD1 | 1.53 | 0.73 |
| 1:KA:141:VAL:HG11 | 1:KA:172:TYR:HD1 | 1.53 | 0.73 |
| 1:KC:141:VAL:HG11 | 1:KC:172:TYR:HD1 | 1.53 | 0.73 |
| 1:LA:401:LYS:NZ | 2:LB:344:TRP:CE3 | 2.56 | 0.73 |
| 2:LB:178:THR:HG23 | 1:LC:258:ASN:ND2 | 2.02 | 0.73 |
| 2:LB:270:PHE:CE2 | 6:4A:226:ILE:HG23 | 2.22 | 0.73 |
| 7:5A:841:VAL:CG2 | 8:6A:11:PRO:CA | 2.66 | 0.73 |
| 7:5A:1491:LEU:CD2 | 7:5A:1495:PHE:CG | 2.60 | 0.73 |
| 7:5A:1491:LEU:HA | 7:5A:1495:PHE:CB | 2.13 | 0.73 |
| 7:5B:1491:LEU:HA | 7:5B:1495:PHE:CB | 2.13 | 0.73 |
| 2:DB:86:ARG:CA | 2:EB:281:TYR:CZ | 2.60 | 0.73 |
| 2:DB:177:ASP:O | 1:DC:352:LYS:HA | 1.88 | 0.73 |
| 1:EE:141:VAL:HG11 | 1:EE:172:TYR:HD1 | 1.53 | 0.73 |
| 1:FE:60:LYS:HD3 | 1:GE:283:HIS:CA | 2.14 | 0.73 |
| 1:FE:207:GLU:OE1 | 7:5B:915:PHE:HD2 | 1.70 | 0.73 |
| 1:HA:141:VAL:HG11 | 1:HA:172:TYR:HD1 | 1.54 | 0.73 |
| 1:KC:79:ARG:O | 1:LC:280:LYS:CE | 2.32 | 0.73 |
| 2:KD:397:TRP:CB | 1:KE:256:GLN:HE22 | 2.00 | 0.73 |
| 2:LB:331:LEU:CD2 | 4:2C:42:PHE:HZ | 0.35 | 0.73 |
| 1:LE:35:GLN:NE2 | 6:4B:101:ARG:HB2 | 2.02 | 0.73 |
| 1:LE:141:VAL:HG11 | 1:LE:172:TYR:HD1 | 1.54 | 0.73 |
| 1:MA:224:TYR:HE2 | 2:MB:246:LEU:HD11 | 1.53 | 0.73 |
| 1:MA:279:GLU:O | 6:4C:107:MET:CB | 2.34 | 0.73 |
| 7:5A:827:GLU:CG | 7:5A:849:ARG:NH2 | 2.52 | 0.73 |
| 7:5A:1491:LEU:CD2 | 7:5A:1495:PHE:CE1 | 2.71 | 0.73 |
| 7:5B:827:GLU:CG | 7:5B:849:ARG:NH2 | 2.52 | 0.73 |
| 7:5C:1374:ASP:OD1 | 7:5C:1374:ASP:N | 2.20 | 0.73 |
| 1:CA:71:GLU:OE1 | 2:CB:247:ASN:ND2 | 2.21 | 0.73 |
| 1:DC:101:ASN:HD22 | 2:DD:252:LYS:CD | 1.98 | 0.73 |
| 1:EA:141:VAL:HG11 | 1:EA:172:TYR:HD1 | 1.53 | 0.73 |
| 2:GB:220:PRO:HD2 | 1:GC:326:LYS:HG2 | 1.69 | 0.73 |
| 2:HD:179:VAL:CG2 | 1:HE:258:ASN:HA | 2.18 | 0.73 |
| 2:ID:179:VAL:CG2 | 1:IE:258:ASN:HA | 2.18 | 0.73 |
| 2:LD:391:ARG:HG3 | 1:LE:346:TRP:CD1 | 2.23 | 0.73 |
| 2:LF:379:LYS:HZ1 | 4:2B:166:ILE:CA | 2.01 | 0.73 |
| 1:MA:279:GLU:HB3 | 6:4C:110:LYS:HE3 | 1.70 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MF:78:ALA:CB | 6:4D:178:HIS:NE2 | 2.51 | 0.73 |
| 5:3B:224:ASP:H | 5:3B:335:LYS:NZ | 1.86 | 0.73 |
| 7:5B:1089:PHE:CD1 | 7:5B:1101:LEU:HD21 | 2.22 | 0.73 |
| 7:5C:827:GLU:CG | 7:5C:849:ARG:NH2 | 2.52 | 0.73 |
| 7:5C:1521:PHE:CA | 7:5C:1567:PHE:CE2 | 2.60 | 0.73 |
| 1:AC:401:LYS:CE | 2:AD:344:TRP:CZ3 | 2.62 | 0.73 |
| 2:BB:220:PRO:O | 1:BC:324:VAL:HG13 | 1.86 | 0.73 |
| 1:BC:11:GLN:OE1 | 2:BD:245:GLN:O | 2.06 | 0.73 |
| 1:EC:141:VAL:HG11 | 1:EC:172:TYR:HD1 | 1.54 | 0.73 |
| 1:FA:222:PRO:HG2 | 2:FB:324:LYS:HD3 | 1.69 | 0.73 |
| 2:KD:179:VAL:CG2 | 1:KE:258:ASN:HA | 2.18 | 0.73 |
| 1:KE:85:GLN:CA | 1:LE:283:HIS:CD2 | 2.71 | 0.73 |
| 1:KE:141:VAL:HG11 | 1:KE:172:TYR:HD1 | 1.54 | 0.73 |
| 2:LF:274:THR:O | 6:4D:228:LEU:HD22 | 1.88 | 0.73 |
| 1:MA:372:MET:CE | 6:4C:96:VAL:C | 2.43 | 0.73 |
| 2:MB:111:GLU:HA | 3:1A:62:SER:HA | 1.69 | 0.73 |
| 1:MC:404:PHE:CE2 | 2:MD:345:ILE:CD1 | 2.72 | 0.73 |
| 2:MD:391:ARG:HG3 | 1:ME:346:TRP:CD1 | 2.23 | 0.73 |
| 7:5A:1347:LEU:HB2 | 7:5A:1348:LYS:HE2 | 1.70 | 0.73 |
| 7:5B:1425:LYS:HZ1 | 7:5B:1429:GLN:HB2 | 1.50 | 0.73 |
| 7:5C:1347:LEU:HB2 | 7:5C:1348:LYS:HE2 | 1.70 | 0.73 |
| 7:5C:1474:LEU:HD22 | 7:5C:1576:ILE:HD13 | 1.70 | 0.73 |
| 2:AF:223:GLY:C | 6:4A:131:VAL:CB | 2.62 | 0.73 |
| 1:DE:400:ALA:HA | 7:5B:775:PRO:HB3 | 1.71 | 0.73 |
| 1:EE:101:ASN:HD22 | 2:EF:252:LYS:CG | 1.99 | 0.73 |
| 1:FA:55:GLU:O | 1:GA:285:GLN:OE1 | 2.06 | 0.73 |
| 1:FC:56:THR:OG1 | 1:GC:284:GLU:C | 2.31 | 0.73 |
| 2:FD:178:THR:HG23 | 1:FE:258:ASN:ND2 | 2.02 | 0.73 |
| 1:GC:60:LYS:NZ | 1:HC:283:HIS:ND1 | 2.37 | 0.73 |
| 2:GF:83:GLN:O | 2:HF:281:TYR:OH | 2.07 | 0.73 |
| 1:HC:416:GLY:HA2 | 5:3C:238:ILE:HD11 | 1.69 | 0.73 |
| 1:JE:282:TYR:CZ | 10:9A:17:UNK:CB | 2.72 | 0.73 |
| 2:LB:227:HIS:ND1 | 6:4A:226:ILE:HG13 | 2.01 | 0.73 |
| 1:LE:222:PRO:HD2 | 2:LF:324:LYS:CB | 2.17 | 0.73 |
| 2:MD:179:VAL:CG2 | 1:ME:258:ASN:HA | 2.19 | 0.73 |
| 5:3A:224:ASP:H | 5:3A:335:LYS:NZ | 1.86 | 0.73 |
| 7:5A:1374:ASP:OD1 | 7:5A:1374:ASP:N | 2.20 | 0.73 |
| 7:5A:1521:PHE:CZ | 7:5A:1571:MET:HG2 | 2.23 | 0.73 |
| 7:5A:1521:PHE:CA | 7:5A:1567:PHE:CE2 | 2.60 | 0.73 |
| 7:5B:1482:SER:CA | 7:5B:1485:LYS:HB2 | 2.16 | 0.73 |
| 7:5B:1491:LEU:CD2 | 7:5B:1495:PHE:CE1 | 2.71 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5C:1089:PHE:CD1 | 7:5C:1101:LEU:HD21 | 2.22 | 0.73 |
| 1:CA:141:VAL:HG11 | 1:CA:172:TYR:HD1 | 1.53 | 0.73 |
| 1:DE:71:GLU:OE1 | 2:DF:247:ASN:ND2 | 2.22 | 0.73 |
| 2:EB:177:ASP:O | 1:EC:352:LYS:HA | 1.88 | 0.73 |
| 1:EC:222:PRO:CG | 2:ED:324:LYS:HD3 | 2.17 | 0.73 |
| 1:EC:401:LYS:CE | 2:ED:344:TRP:CZ3 | 2.60 | 0.73 |
| 1:FA:207:GLU:OE1 | 7:5C:915:PHE:CD2 | 2.40 | 0.73 |
| 2:FB:84:LEU:O | 2:GB:281:TYR:HE1 | 1.70 | 0.73 |
| 1:FC:141:VAL:HG11 | 1:FC:172:TYR:HD1 | 1.53 | 0.73 |
| 2:FD:208:TYR:OH | 1:FE:325:PRO:HB2 | 1.88 | 0.73 |
| 1:FE:141:VAL:HG11 | 1:FE:172:TYR:HD1 | 1.54 | 0.73 |
| 1:LA:224:TYR:HE2 | 2:LB:246:LEU:HD11 | 1.53 | 0.73 |
| 2:LD:98:GLY:CA | 1:LE:254:GLU:HG2 | 2.18 | 0.73 |
| 7:5A:1265:ALA:O | 7:5A:1269:ASP:CG | 2.32 | 0.73 |
| 7:5B:1265:ALA:O | 7:5B:1269:ASP:CG | 2.32 | 0.73 |
| 7:5B:1347:LEU:HB2 | 7:5B:1348:LYS:HE2 | 1.70 | 0.73 |
| 7:5B:1521:PHE:CZ | 7:5B:1571:MET:HG2 | 2.23 | 0.73 |
| 7:5C:1265:ALA:O | 7:5C:1269:ASP:CG | 2.32 | 0.73 |
| 7:5C:1521:PHE:CZ | 7:5C:1571:MET:HG2 | 2.23 | 0.73 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:CG1 | 2.17 | 0.73 |
| 9:7C:30:ARG:HH12 | 9:7D:3:GLN:CB | 2.02 | 0.73 |
| 2:CD:397:TRP:CE3 | 1:CE:257:THR:HG23 | 2.23 | 0.73 |
| 1:GA:89:PRO:CG | 1:HA:280:LYS:CD | 2.65 | 0.73 |
| 2:GD:397:TRP:CB | 1:GE:256:GLN:HE22 | 2.00 | 0.73 |
| 2:KB:127:CYS:HB2 | 4:2C:38:VAL:HG21 | 1.68 | 0.73 |
| 2:LB:98:GLY:C | 1:LC:254:GLU:HG2 | 2.14 | 0.73 |
| 2:LD:224:ASP:CA | 6:4B:219:ASN:CG | 2.62 | 0.73 |
| 1:MA:11:GLN:NE2 | 2:MB:247:ASN:OD1 | 2.22 | 0.73 |
| 6:4A:244:GLU:O | 6:4A:247:LYS:HG2 | 1.88 | 0.73 |
| 7:5A:1089:PHE:CD1 | 7:5A:1101:LEU:HD21 | 2.22 | 0.73 |
| 7:5A:1271:ILE:CA | 9:7A:20:LEU:HD21 | 1.77 | 0.73 |
| 7:5A:1482:SER:CA | 7:5A:1485:LYS:HB2 | 2.16 | 0.73 |
| 7:5A:1548:VAL:HG13 | 7:5A:1569:GLU:HB2 | 1.69 | 0.73 |
| 7:5B:1126:PRO:CD | 8:6B:246:TYR:OH | 2.35 | 0.73 |
| 7:5B:1491:LEU:CD2 | 7:5B:1495:PHE:CG | 2.60 | 0.73 |
| 7:5B:1510:ASN:O | 7:5B:1558:LYS:HB3 | 1.88 | 0.73 |
| 7:5B:1521:PHE:CA | 7:5B:1567:PHE:CE2 | 2.60 | 0.73 |
| 7:5C:1548:VAL:HG13 | 7:5C:1569:GLU:HB2 | 1.69 | 0.73 |
| 8:6C:146:ILE:HD12 | 8:6C:183:LEU:HB3 | 1.70 | 0.73 |
| 9:7A:30:ARG:HH12 | 9:7B:3:GLN:CB | 2.02 | 0.73 |
| 9:7C:35:ILE:HG21 | 9:7D:42:LEU:O | 1.87 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CC:141:VAL:HG11 | 1:CC:172:TYR:HD1 | 1.53 | 0.73 |
| 2:DB:212:PHE:CE2 | 1:DC:326:LYS:HD3 | 2.14 | 0.73 |
| 1:DC:101:ASN:HD22 | 2:DD:252:LYS:CG | 2.00 | 0.73 |
| 1:FA:89:PRO:HG3 | 1:GA:280:LYS:CE | 2.18 | 0.73 |
| 1:FA:100:ALA:HB1 | 2:FB:252:LYS:HA | 1.70 | 0.73 |
| 1:FA:141:VAL:HG11 | 1:FA:172:TYR:HD1 | 1.53 | 0.73 |
| 2:FB:177:ASP:HA | 1:FC:353:VAL:HG12 | 1.71 | 0.73 |
| 2:FB:212:PHE:CZ | 1:FC:326:LYS:CD | 2.40 | 0.73 |
| 1:HE:404:PHE:HE2 | 2:HF:345:ILE:CD1 | 2.02 | 0.73 |
| 2:ID:86:ARG:CB | 2:JD:281:TYR:CE1 | 2.71 | 0.73 |
| 2:JB:220:PRO:O | 1:JC:324:VAL:HG11 | 1.88 | 0.73 |
| 2:KD:220:PRO:O | 1:KE:324:VAL:HG11 | 1.89 | 0.73 |
| 2:MB:220:PRO:O | 1:MC:324:VAL:CG1 | 2.37 | 0.73 |
| 5:3C:224:ASP:H | 5:3C:335:LYS:NZ | 1.87 | 0.73 |
| 6:4C:244:GLU:O | 6:4C:247:LYS:HG2 | 1.88 | 0.73 |
| 7:5A:840:GLY:C | 8:6A:109:ILE:HD11 | 1.53 | 0.73 |
| 7:5B:1374:ASP:OD1 | 7:5B:1374:ASP:N | 2.20 | 0.73 |
| 7:5B:1548:VAL:HG13 | 7:5B:1569:GLU:HB2 | 1.69 | 0.73 |
| 9:7E:35:ILE:CG2 | 9:7F:42:LEU:C | 2.61 | 0.73 |
| 2:AB:55:THR:HG21 | 2:BB:283:ALA:HA | 1.71 | 0.73 |
| 2:AD:220:PRO:O | 1:AE:324:VAL:HG11 | 1.89 | 0.73 |
| 2:CD:212:PHE:CE2 | 1:CE:326:LYS:HD3 | 2.17 | 0.73 |
| 2:EF:125:GLU:HG2 | 7:5B:903:PHE:HD2 | 1.48 | 0.73 |
| 1:FE:101:ASN:HD22 | 2:FF:252:LYS:CD | 2.00 | 0.73 |
| 2:HD:220:PRO:O | 1:HE:324:VAL:HG11 | 1.89 | 0.73 |
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:CB | 2.17 | 0.73 |
| 2:KD:221:THR:CB | 6:4B:261:SER:C | 2.54 | 0.73 |
| 2:LF:215:LEU:HD13 | 6:4D:225:PRO:HB3 | 1.71 | 0.73 |
| 1:MA:279:GLU:CB | 6:4C:110:LYS:CE | 2.66 | 0.73 |
| 7:5A:841:VAL:N | 8:6A:109:ILE:HD11 | 2.01 | 0.73 |
| 7:5A:1474:LEU:HD22 | 7:5A:1576:ILE:HD13 | 1.70 | 0.73 |
| 7:5A:1510:ASN:O | 7:5A:1558:LYS:HB3 | 1.88 | 0.73 |
| 9:7A:35:ILE:HG21 | 9:7B:42:LEU:O | 1.87 | 0.73 |
| 9:7A:38:LEU:CD2 | 9:7B:42:LEU:HD13 | 2.19 | 0.73 |
| 2:AD:284:LEU:HD11 | 6:4C:144:LEU:HD13 | 1.67 | 0.72 |
| 1:AE:404:PHE:HE2 | 2:AF:345:ILE:CD1 | 2.02 | 0.72 |
| 1:CA:11:GLN:NE2 | 2:CB:247:ASN:OD1 | 2.22 | 0.72 |
| 1:GA:141:VAL:HG11 | 1:GA:172:TYR:HD1 | 1.53 | 0.72 |
| 2:GB:86:ARG:HH22 | 2:HB:281:TYR:CE2 | 1.46 | 0.72 |
| 2:ID:220:PRO:O | 1:IE:324:VAL:HG11 | 1.89 | 0.72 |
| 1:LA:401:LYS:NZ | 2:LB:344:TRP:CH2 | 2.57 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:4B:244:GLU:O | 6:4B:247:LYS:HG2 | 1.88 | 0.72 |
| 6:4D:251:TYR:CE2 | 6:4D:280:VAL:HG11 | 2.24 | 0.72 |
| 7:5C:1243:ASP:CG | 9:7F:8:ARG:NH1 | 2.45 | 0.72 |
| 2:CD:179:VAL:CG2 | 1:CE:258:ASN:HA | 2.19 | 0.72 |
| 1:CE:141:VAL:HG11 | 1:CE:172:TYR:HD1 | 1.53 | 0.72 |
| 1:DA:60:LYS:CD | 1:EA:283:HIS:CD2 | 2.60 | 0.72 |
| 1:FC:60:LYS:HD2 | 1:GC:283:HIS:HD2 | 1.51 | 0.72 |
| 2:ID:397:TRP:CB | 1:IE:256:GLN:HE22 | 2.00 | 0.72 |
| 1:ME:404:PHE:HE2 | 2:MF:345:ILE:HD12 | 1.51 | 0.72 |
| 6:4B:251:TYR:CE2 | 6:4B:280:VAL:HG11 | 2.24 | 0.72 |
| 6:4D:244:GLU:O | 6:4D:247:LYS:HG2 | 1.88 | 0.72 |
| 1:BE:11:GLN:OE1 | 2:BF:245:GLN:O | 2.07 | 0.72 |
| 2:CB:86:ARG:CB | 2:DB:281:TYR:HE1 | 1.83 | 0.72 |
| 2:CB:178:THR:HG23 | 1:CC:258:ASN:ND2 | 2.01 | 0.72 |
| 2:CD:177:ASP:O | 1:CE:352:LYS:CD | 2.30 | 0.72 |
| 2:ED:157:GLU:OE1 | 7:5A:935:LYS:CE | 2.36 | 0.72 |
| 1:FA:89:PRO:CG | 1:GA:280:LYS:CE | 2.67 | 0.72 |
| 1:GC:141:VAL:HG11 | 1:GC:172:TYR:HD1 | 1.53 | 0.72 |
| 2:LB:231:ALA:HB2 | 6:4A:226:ILE:HD13 | 0.73 | 0.72 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CE3 | 2.57 | 0.72 |
| 2:LD:177:ASP:OD2 | 1:LE:353:VAL:CG1 | 2.37 | 0.72 |
| 2:MF:78:ALA:CB | 6:4D:178:HIS:CD2 | 2.72 | 0.72 |
| 7:5A:1152:GLU:CD | 8:6A:66:ARG:NH1 | 2.46 | 0.72 |
| 7:5C:1510:ASN:O | 7:5C:1558:LYS:HB3 | 1.88 | 0.72 |
| 9:7D:12:GLU:HA | 9:7D:16:THR:HG1 | 1.54 | 0.72 |
| 1:CE:11:GLN:NE2 | 2:CF:247:ASN:OD1 | 2.22 | 0.72 |
| 1:DA:402:ARG:HH21 | 7:5C:777:ALA:HB3 | 1.54 | 0.72 |
| 1:DC:101:ASN:CG | 2:DD:252:LYS:HD2 | 2.09 | 0.72 |
| 1:EC:401:LYS:HE3 | 2:ED:344:TRP:CZ3 | 2.24 | 0.72 |
| 1:FA:101:ASN:HD22 | 2:FB:252:LYS:CD | 1.98 | 0.72 |
| 1:FA:222:PRO:CG | 2:FB:324:LYS:CD | 2.66 | 0.72 |
| 2:GD:220:PRO:O | 1:GE:324:VAL:HG11 | 1.89 | 0.72 |
| 1:GE:141:VAL:HG11 | 1:GE:172:TYR:HD1 | 1.53 | 0.72 |
| 1:HC:71:GLU:OE1 | 2:HD:247:ASN:ND2 | 2.22 | 0.72 |
| 1:HE:159:VAL:CG2 | 5:3A:209:ARG:NE | 2.50 | 0.72 |
| 1:KE:404:PHE:HE2 | 2:KF:345:ILE:CD1 | 2.02 | 0.72 |
| 1:LA:222:PRO:HD2 | 2:LB:324:LYS:CB | 2.20 | 0.72 |
| 2:LB:223:GLY:HA3 | 6:4A:219:ASN:HA | 1.69 | 0.72 |
| 2:LB:224:ASP:CA | 6:4A:219:ASN:CG | 2.62 | 0.72 |
| 6:4A:251:TYR:CE2 | 6:4A:280:VAL:HG11 | 2.24 | 0.72 |
| 7:5B:1474:LEU:HD22 | 7:5B:1576:ILE:HD13 | 1.70 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5C:1552:LYS:HZ1 | 7:5C:1563:SER:HB3 | 1.52 | 0.72 |
| 2:AD:361:LEU:CD2 | 6:4C:144:LEU:HD12 | 2.18 | 0.72 |
| 2:AF:322:SER:N | 6:4A:156:PHE:HE2 | 1.86 | 0.72 |
| 2:DB:397:TRP:HE3 | 1:DC:257:THR:CG2 | 1.98 | 0.72 |
| 2:DD:220:PRO:HD2 | 1:DE:326:LYS:CG | 2.17 | 0.72 |
| 1:EE:393:HIS:CE1 | 7:5B:814:LYS:CG | 2.70 | 0.72 |
| 1:FA:89:PRO:CD | 1:GA:280:LYS:HZ2 | 2.01 | 0.72 |
| 2:GD:55:THR:H | 2:HD:283:ALA:CA | 2.01 | 0.72 |
| 1:GE:11:GLN:NE2 | 2:GF:247:ASN:OD1 | 2.23 | 0.72 |
| 1:IC:71:GLU:OE1 | 2:ID:247:ASN:ND2 | 2.22 | 0.72 |
| 1:JE:404:PHE:HE2 | 2:JF:345:ILE:CD1 | 2.02 | 0.72 |
| 1:LC:222:PRO:HD2 | 2:LD:324:LYS:CB | 2.19 | 0.72 |
| 1:LE:222:PRO:HD2 | 2:LF:324:LYS:CD | 2.15 | 0.72 |
| 2:MD:220:PRO:O | 1:ME:324:VAL:CG1 | 2.38 | 0.72 |
| 7:5C:1378:GLN:CA | 7:5C:1381:ILE:HD13 | 2.18 | 0.72 |
| 9:7C:38:LEU:CD2 | 9:7D:42:LEU:HD13 | 2.19 | 0.72 |
| 9:7E:11:TYR:HE1 | 9:7F:26:LEU:CG | 2.02 | 0.72 |
| 2:AF:361:LEU:HD22 | 6:4A:144:LEU:HD13 | 1.70 | 0.72 |
| 1:BE:222:PRO:CD | 2:BF:324:LYS:HD3 | 2.18 | 0.72 |
| 2:CD:177:ASP:CB | 1:CE:353:VAL:HG12 | 2.20 | 0.72 |
| 2:DD:208:TYR:OH | 1:DE:325:PRO:HB2 | 1.90 | 0.72 |
| 1:EE:101:ASN:HD22 | 2:EF:252:LYS:CD | 1.99 | 0.72 |
| 2:HB:177:ASP:CB | 1:HC:353:VAL:HG12 | 2.20 | 0.72 |
| 1:HE:410:GLY:CA | 5:3A:329:ARG:HH21 | 2.03 | 0.72 |
| 2:JB:177:ASP:CB | 1:JC:353:VAL:HG12 | 2.20 | 0.72 |
| 2:JF:88:ASP:CG | 2:KF:278:SER:OG | 2.33 | 0.72 |
| 2:MD:177:ASP:CG | 1:ME:353:VAL:HG13 | 2.10 | 0.72 |
| 1:ME:372:MET:HE2 | 6:4B:96:VAL:CA | 2.19 | 0.72 |
| 6:4C:251:TYR:CE2 | 6:4C:280:VAL:HG11 | 2.24 | 0.72 |
| 7:5A:1378:GLN:CA | 7:5A:1381:ILE:HD13 | 2.18 | 0.72 |
| 7:5B:801:LEU:HD23 | 7:5B:801:LEU:N | 2.04 | 0.72 |
| 7:5B:1378:GLN:CA | 7:5B:1381:ILE:HD13 | 2.18 | 0.72 |
| 2:AB:177:ASP:CB | 1:AC:353:VAL:HG12 | 2.20 | 0.72 |
| 2:EB:55:THR:HG21 | 2:FB:284:LEU:H | 1.54 | 0.72 |
| 2:ED:179:VAL:CG2 | 1:EE:258:ASN:HA | 2.20 | 0.72 |
| 1:FC:404:PHE:HE2 | 2:FD:345:ILE:CD1 | 2.03 | 0.72 |
| 1:FE:419:SER:HB2 | 7:5B:1256:ARG:HE | 0.61 | 0.72 |
| 1:HE:11:GLN:NE2 | 2:HF:247:ASN:OD1 | 2.23 | 0.72 |
| 1:JC:90:GLU:HG2 | 1:KC:280:LYS:HD2 | 1.68 | 0.72 |
| 1:KA:88:HIS:CG | 1:LA:284:GLU:HB2 | 2.24 | 0.72 |
| 2:KB:177:ASP:CB | 1:KC:353:VAL:HG12 | 2.20 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:KC:71:GLU:OE1 | 2:KD:247:ASN:ND2 | 2.22 | 0.72 |
| 2:KF:215:LEU:CD1 | 6:4D:267:ILE:CG2 | 2.65 | 0.72 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:HG2 | 1.85 | 0.72 |
| 8:6A:146:ILE:HD12 | 8:6A:183:LEU:HB3 | 1.70 | 0.72 |
| 2:CF:87:PRO:CD | 2:DF:281:TYR:CZ | 2.73 | 0.72 |
| 2:DB:208:TYR:OH | 1:DC:325:PRO:HB2 | 1.90 | 0.72 |
| 1:EA:426:ALA:CB | 7:5C:833:PHE:HB2 | 2.18 | 0.72 |
| 1:FA:177:VAL:HG21 | 7:5C:915:PHE:HE2 | 1.44 | 0.72 |
| 1:FE:419:SER:OG | 7:5B:1256:ARG:HD3 | 1.89 | 0.72 |
| 1:GC:71:GLU:OE1 | 2:GD:247:ASN:ND2 | 2.22 | 0.72 |
| 1:IC:60:LYS:HZ2 | 1:JC:283:HIS:CD2 | 2.08 | 0.72 |
| 2:JD:220:PRO:O | 1:JE:324:VAL:HG11 | 1.89 | 0.72 |
| 1:KA:85:GLN:HE22 | 1:LA:282:TYR:HB3 | 1.44 | 0.72 |
| 2:LD:179:VAL:CG2 | 1:LE:258:ASN:CA | 2.67 | 0.72 |
| 1:LE:222:PRO:HG3 | 2:LF:324:LYS:HD2 | 1.70 | 0.72 |
| 7:5A:1316:LEU:HA | 7:5A:1319:HIS:HB2 | 1.72 | 0.72 |
| 1:AC:71:GLU:OE1 | 2:AD:247:ASN:ND2 | 2.22 | 0.72 |
| 1:EA:401:LYS:CE | 2:EB:344:TRP:CZ3 | 2.64 | 0.72 |
| 1:FE:101:ASN:HD22 | 2:FF:252:LYS:CG | 2.02 | 0.72 |
| 2:IF:424:GLN:HE22 | 7:5B:1413:GLN:CD | 1.71 | 0.72 |
| 2:LB:177:ASP:OD1 | 1:LC:353:VAL:HG12 | 1.74 | 0.72 |
| 2:LF:340:TYR:CG | 4:2B:147:PHE:CB | 2.72 | 0.72 |
| 6:4C:289:LYS:HE3 | 6:4C:289:LYS:CA | 2.08 | 0.72 |
| 7:5C:1105:TYR:HB3 | 7:5C:1166:LEU:N | 2.03 | 0.72 |
| 7:5C:1316:LEU:HA | 7:5C:1319:HIS:HB2 | 1.72 | 0.72 |
| 9:7E:11:TYR:HE1 | 9:7F:26:LEU:CD2 | 1.99 | 0.72 |
| 1:DA:400:ALA:O | 7:5C:775:PRO:HB3 | 1.90 | 0.72 |
| 2:KB:276:ARG:HH21 | 6:4A:265:TYR:CB | 2.02 | 0.72 |
| 2:KF:83:GLN:OE1 | 2:LF:281:TYR:CD1 | 2.23 | 0.72 |
| 6:4A:289:LYS:HE3 | 6:4A:289:LYS:CA | 2.08 | 0.72 |
| 7:5A:801:LEU:HD23 | 7:5A:801:LEU:N | 2.04 | 0.72 |
| 7:5A:1105:TYR:HB3 | 7:5A:1166:LEU:N | 2.03 | 0.72 |
| 7:5B:1105:TYR:HB3 | 7:5B:1166:LEU:N | 2.03 | 0.72 |
| 7:5B:1316:LEU:HA | 7:5B:1319:HIS:HB2 | 1.72 | 0.72 |
| 2:BB:212:PHE:CZ | 1:BC:326:LYS:CD | 2.24 | 0.71 |
| 2:ED:177:ASP:OD2 | 1:EE:248:LEU:HD21 | 1.89 | 0.71 |
| 1:GE:404:PHE:HE2 | 2:GF:345:ILE:CD1 | 2.02 | 0.71 |
| 1:JE:11:GLN:NE2 | 2:JF:247:ASN:OD1 | 2.23 | 0.71 |
| 7:5A:829:GLY:HA2 | 8:6A:109:ILE:CG2 | 2.20 | 0.71 |
| 7:5B:1436:ARG:HH11 | 7:5B:1436:ARG:CG | 2.02 | 0.71 |
| 7:5C:836:ARG:HH11 | 7:5C:836:ARG:CG | 2.03 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:6B:146:ILE:HD12 | 8:6B:183:LEU:HB3 | 1.70 | 0.71 |
| 1:IA:141:VAL:HG11 | 1:IA:172:TYR:HD1 | 1.54 | 0.71 |
| 1:JC:91:GLN:N | 1:KC:280:LYS:HZ1 | 1.88 | 0.71 |
| 2:JD:177:ASP:CB | 1:JE:353:VAL:HG12 | 2.20 | 0.71 |
| 1:KE:85:GLN:OE1 | 1:LE:282:TYR:CA | 2.38 | 0.71 |
| 1:LE:401:LYS:NZ | 2:LF:344:TRP:CE3 | 2.58 | 0.71 |
| 1:MC:279:GLU:HB3 | 6:4A:110:LYS:HE3 | 1.70 | 0.71 |
| 7:5A:1275:ILE:HD13 | 9:7B:11:TYR:OH | 1.89 | 0.71 |
| 7:5A:1284:PHE:CZ | 9:7A:12:GLU:OE1 | 2.43 | 0.71 |
| 7:5A:1424:GLN:HE21 | 7:5A:1424:GLN:C | 1.98 | 0.71 |
| 7:5B:1246:LEU:N | 9:7D:12:GLU:OE2 | 2.23 | 0.71 |
| 7:5B:1424:GLN:HE21 | 7:5B:1424:GLN:C | 1.98 | 0.71 |
| 9:7E:30:ARG:NH1 | 9:7F:3:GLN:CA | 2.44 | 0.71 |
| 1:FE:402:ARG:NH2 | 7:5B:1262:GLU:OE1 | 2.23 | 0.71 |
| 2:GB:177:ASP:CB | 1:GC:353:VAL:HG12 | 2.20 | 0.71 |
| 2:HD:177:ASP:CB | 1:HE:353:VAL:HG12 | 2.20 | 0.71 |
| 1:IC:141:VAL:HG11 | 1:IC:172:TYR:HD1 | 1.53 | 0.71 |
| 1:IE:404:PHE:HE2 | 2:IF:345:ILE:CD1 | 2.02 | 0.71 |
| 2:LD:231:ALA:HB1 | 6:4B:226:ILE:HD13 | 1.70 | 0.71 |
| 4:2A:164:ARG:NH1 | 4:2A:164:ARG:HB2 | 2.05 | 0.71 |
| 4:2C:164:ARG:NH1 | 4:2C:164:ARG:HB2 | 2.05 | 0.71 |
| 7:5A:836:ARG:HH11 | 7:5A:836:ARG:CG | 2.03 | 0.71 |
| 7:5A:1436:ARG:HH11 | 7:5A:1436:ARG:CG | 2.02 | 0.71 |
| 7:5C:1424:GLN:HE21 | 7:5C:1424:GLN:C | 1.98 | 0.71 |
| 7:5C:1436:ARG:NE | 7:5C:1436:ARG:O | 2.23 | 0.71 |
| 2:AD:177:ASP:CB | 1:AE:353:VAL:HG12 | 2.20 | 0.71 |
| 2:AD:397:TRP:CB | 1:AE:256:GLN:HE22 | 2.00 | 0.71 |
| 2:AF:55:THR:HG23 | 2:BF:283:ALA:HB2 | 1.70 | 0.71 |
| 2:AF:361:LEU:CD2 | 6:4A:144:LEU:CD1 | 2.65 | 0.71 |
| 1:BA:141:VAL:HG11 | 1:BA:172:TYR:HD1 | 1.53 | 0.71 |
| 1:BE:141:VAL:HG11 | 1:BE:172:TYR:HD1 | 1.53 | 0.71 |
| 2:EB:125:GLU:CG | 7:5C:903:PHE:CD2 | 2.63 | 0.71 |
| 1:IE:11:GLN:NE2 | 2:IF:247:ASN:OD1 | 2.23 | 0.71 |
| 1:JC:124:LYS:CD | 1:KC:284:GLU:OE1 | 2.39 | 0.71 |
| 2:KB:87:PRO:CD | 2:LB:282:ARG:CG | 2.61 | 0.71 |
| 2:KD:54:ALA:CA | 2:LD:285:THR:CG2 | 2.68 | 0.71 |
| 2:KD:177:ASP:CB | 1:KE:353:VAL:HG12 | 2.20 | 0.71 |
| 1:LA:222:PRO:HG3 | 2:LB:324:LYS:CD | 2.19 | 0.71 |
| 1:LE:89:PRO:HG2 | 1:ME:280:LYS:HD2 | 1.71 | 0.71 |
| 7:5A:1436:ARG:NE | 7:5A:1436:ARG:O | 2.23 | 0.71 |
| 7:5B:1436:ARG:NE | 7:5B:1436:ARG:O | 2.23 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5C:801:LEU:HD23 | 7:5C:801:LEU:N | 2.04 | 0.71 |
| 9:7C:15:VAL:CA | 9:7D:35:ILE:HD12 | 2.02 | 0.71 |
| 1:BC:141:VAL:HG11 | 1:BC:172:TYR:HD1 | 1.53 | 0.71 |
| 2:DF:86:ARG:N | 2:EF:281:TYR:CE1 | 2.58 | 0.71 |
| 1:EA:396:ASP:CG | 7:5C:821:LEU:HD11 | 2.16 | 0.71 |
| 1:FA:207:GLU:OE1 | 7:5C:915:PHE:HD2 | 1.74 | 0.71 |
| 1:FE:222:PRO:HD2 | 2:FF:324:LYS:HD3 | 1.71 | 0.71 |
| 2:IB:177:ASP:CB | 1:IC:353:VAL:HG12 | 2.20 | 0.71 |
| 2:ID:98:GLY:CA | 1:IE:254:GLU:CG | 2.48 | 0.71 |
| 1:IE:279:GLU:CD | 10:8X:22:UNK:HA | 2.09 | 0.71 |
| 1:JC:71:GLU:OE1 | 2:JD:247:ASN:ND2 | 2.22 | 0.71 |
| 4:2B:164:ARG:NH1 | 4:2B:164:ARG:HB2 | 2.05 | 0.71 |
| 6:4B:289:LYS:HE3 | 6:4B:289:LYS:CA | 2.08 | 0.71 |
| 7:5C:1436:ARG:HH11 | 7:5C:1436:ARG:CG | 2.02 | 0.71 |
| 2:EB:157:GLU:OE1 | 7:5C:935:LYS:CE | 2.38 | 0.71 |
| 2:FB:177:ASP:CA | 1:FC:353:VAL:HG12 | 2.20 | 0.71 |
| 2:FB:208:TYR:OH | 1:FC:325:PRO:HB2 | 1.91 | 0.71 |
| 2:GB:179:VAL:CG2 | 1:GC:258:ASN:HA | 2.21 | 0.71 |
| 1:KE:11:GLN:NE2 | 2:KF:247:ASN:OD1 | 2.23 | 0.71 |
| 2:KF:276:ARG:NH2 | 6:4D:266:ASN:N | 2.38 | 0.71 |
| 1:MC:141:VAL:HG11 | 1:MC:172:TYR:HD1 | 1.53 | 0.71 |
| 1:MC:224:TYR:HE2 | 2:MD:246:LEU:HD11 | 1.56 | 0.71 |
| 1:ME:141:VAL:HG11 | 1:ME:172:TYR:HD1 | 1.54 | 0.71 |
| 6:4D:107:MET:HG3 | 6:4D:110:LYS:HE3 | 1.71 | 0.71 |
| 7:5B:836:ARG:HH11 | 7:5B:836:ARG:CG | 2.03 | 0.71 |
| 7:5B:1416:LYS:HA | 7:5B:1416:LYS:HZ3 | 1.53 | 0.71 |
| 7:5C:1541:ILE:HG12 | 7:5C:1574:ILE:CD1 | 2.21 | 0.71 |
| 1:CC:71:GLU:OE1 | 2:CD:247:ASN:ND2 | 2.24 | 0.71 |
| 1:EA:430:LYS:HZ3 | 7:5C:834:ASN:ND2 | 1.23 | 0.71 |
| 2:EF:157:GLU:HA | 7:5B:945:LYS:HZ3 | 1.55 | 0.71 |
| 1:FA:89:PRO:CD | 1:GA:280:LYS:CE | 2.64 | 0.71 |
| 2:GB:55:THR:HG22 | 2:HB:283:ALA:HB1 | 1.70 | 0.71 |
| 1:IE:141:VAL:HG11 | 1:IE:172:TYR:HD1 | 1.54 | 0.71 |
| 2:JB:179:VAL:CG2 | 1:JC:258:ASN:HA | 2.21 | 0.71 |
| 2:KB:162:ARG:HG3 | 4:2C:36:THR:HB | 1.72 | 0.71 |
| 2:KD:276:ARG:NH2 | 6:4B:266:ASN:N | 2.39 | 0.71 |
| 2:LD:276:ARG:NH1 | 6:4B:229:GLU:CA | 2.33 | 0.71 |
| 1:ME:279:GLU:OE1 | 6:4B:106:ALA:C | 2.33 | 0.71 |
| 6:4C:107:MET:HG3 | 6:4C:110:LYS:HE3 | 1.71 | 0.71 |
| 7:5A:1541:ILE:HG12 | 7:5A:1574:ILE:CD1 | 2.21 | 0.71 |
| 7:5B:1152:GLU:CD | 8:6B:66:ARG:HH12 | 1.98 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5C:1544:ILE:C | 7:5C:1570:ALA:CA | 2.49 | 0.71 |
| 2:CD:177:ASP:O | 1:CE:352:LYS:HA | 1.90 | 0.71 |
| 1:EC:426:ALA:CB | 7:5A:833:PHE:HB2 | 2.20 | 0.71 |
| 1:FA:101:ASN:HD21 | 2:FB:252:LYS:CD | 1.82 | 0.71 |
| 1:FE:207:GLU:OE1 | 7:5B:915:PHE:CB | 2.36 | 0.71 |
| 2:GD:177:ASP:CB | 1:GE:353:VAL:HG12 | 2.20 | 0.71 |
| 1:GE:56:THR:O | 1:HE:285:GLN:HA | 1.89 | 0.71 |
| 1:HC:410:GLY:CA | 5:3C:329:ARG:HH21 | 2.03 | 0.71 |
| 1:IE:393:HIS:HB3 | 5:3A:308:PHE:HE2 | 1.55 | 0.71 |
| 1:JE:89:PRO:CD | 1:KE:280:LYS:HA | 2.20 | 0.71 |
| 1:KC:85:GLN:NE2 | 1:LC:282:TYR:HB2 | 2.03 | 0.71 |
| 6:4A:107:MET:HG3 | 6:4A:110:LYS:HE3 | 1.72 | 0.71 |
| 7:5A:1487:ASN:HB3 | 7:5A:1568:LYS:CD | 2.21 | 0.71 |
| 7:5A:1552:LYS:HZ1 | 7:5A:1563:SER:HB3 | 1.53 | 0.71 |
| 8:6A:136:LEU:HD23 | 8:6A:140:GLN:HB2 | 1.71 | 0.71 |
| 9:7E:7:LEU:CD2 | 9:7F:27:GLY:HA3 | 2.01 | 0.71 |
| 2:AB:179:VAL:CG2 | 1:AC:258:ASN:HA | 2.21 | 0.71 |
| 1:AE:11:GLN:NE2 | 2:AF:247:ASN:OD1 | 2.23 | 0.71 |
| 1:BC:222:PRO:CD | 2:BD:324:LYS:HD3 | 2.19 | 0.71 |
| 2:CB:220:PRO:HD2 | 1:CC:326:LYS:CG | 2.20 | 0.71 |
| 2:DD:397:TRP:CE3 | 1:DE:257:THR:HG23 | 2.25 | 0.71 |
| 2:GD:54:ALA:HB1 | 2:HD:281:TYR:O | 1.90 | 0.71 |
| 2:HD:98:GLY:CA | 1:HE:254:GLU:CG | 2.48 | 0.71 |
| 2:IB:179:VAL:CG2 | 1:IC:258:ASN:HA | 2.21 | 0.71 |
| 1:LE:60:LYS:NZ | 1:ME:283:HIS:CG | 2.58 | 0.71 |
| 1:MA:141:VAL:HG11 | 1:MA:172:TYR:HD1 | 1.53 | 0.71 |
| 1:MC:404:PHE:HE2 | 2:MD:345:ILE:HD12 | 1.54 | 0.71 |
| 7:5A:1425:LYS:HZ1 | 7:5A:1429:GLN:HB2 | 1.53 | 0.71 |
| 7:5B:1541:ILE:HG12 | 7:5B:1574:ILE:CD1 | 2.21 | 0.71 |
| 7:5C:1487:ASN:HB3 | 7:5C:1568:LYS:CD | 2.21 | 0.71 |
| 8:6C:136:LEU:HD23 | 8:6C:140:GLN:HB2 | 1.71 | 0.71 |
| 2:FB:212:PHE:HZ | 1:FC:326:LYS:CE | 2.04 | 0.71 |
| 2:HB:98:GLY:CA | 1:HC:254:GLU:CG | 2.48 | 0.71 |
| 1:IA:279:GLU:HA | 10:8V:22:UNK:CB | 2.21 | 0.71 |
| 1:IC:393:HIS:HB3 | 5:3C:308:PHE:CE2 | 2.25 | 0.71 |
| 2:IF:56:GLY:H | 10:9A:36:UNK:HA | 1.56 | 0.71 |
| 2:JD:86:ARG:NH1 | 2:KD:280:GLN:O | 2.24 | 0.71 |
| 1:KE:85:GLN:CD | 1:LE:282:TYR:CB | 2.64 | 0.71 |
| 2:LB:55:THR:HG23 | 2:MB:283:ALA:C | 2.10 | 0.71 |
| 2:LB:379:LYS:CA | 4:2C:166:ILE:HD13 | 1.76 | 0.71 |
| 7:5A:1089:PHE:CE1 | 7:5A:1101:LEU:CD2 | 2.74 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:841:VAL:HG23 | 8:6C:11:PRO:HG3 | 1.71 | 0.71 |
| 7:5C:1089:PHE:CE1 | 7:5C:1101:LEU:CD2 | 2.74 | 0.71 |
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:HG2 | 1.85 | 0.71 |
| 8:6B:136:LEU:HD23 | 8:6B:140:GLN:HB2 | 1.72 | 0.71 |
| 1:FE:404:PHE:HE2 | 2:FF:345:ILE:CD1 | 2.04 | 0.70 |
| 2:HB:179:VAL:CG2 | 1:HC:258:ASN:HA | 2.21 | 0.70 |
| 1:IC:401:LYS:CE | 2:ID:344:TRP:CZ3 | 2.62 | 0.70 |
| 2:ID:177:ASP:CB | 1:IE:353:VAL:HG12 | 2.20 | 0.70 |
| 2:ID:178:THR:HG23 | 1:IE:258:ASN:ND2 | 2.05 | 0.70 |
| 1:KE:85:GLN:HG2 | 1:LE:283:HIS:HD2 | 1.55 | 0.70 |
| 2:LB:55:THR:HG23 | 2:MB:283:ALA:HA | 0.71 | 0.70 |
| 1:LC:35:GLN:HE21 | 6:4A:101:ARG:HB2 | 1.54 | 0.70 |
| 7:5A:1416:LYS:HA | 7:5A:1416:LYS:HZ3 | 1.53 | 0.70 |
| 1:AC:342:GLN:NE2 | 3:1C:55:HIS:CE1 | 2.58 | 0.70 |
| 2:CB:86:ARG:CG | 2:DB:281:TYR:CE1 | 2.39 | 0.70 |
| 1:EC:426:ALA:HB3 | 7:5A:833:PHE:HB2 | 1.73 | 0.70 |
| 2:FB:332:ASN:CG | 7:5C:909:ASN:HD21 | 1.99 | 0.70 |
| 2:HD:178:THR:HG23 | 1:HE:258:ASN:ND2 | 2.06 | 0.70 |
| 2:JD:178:THR:HG23 | 1:JE:258:ASN:ND2 | 2.05 | 0.70 |
| 2:KB:54:ALA:HA | 2:LB:285:THR:HG22 | 1.72 | 0.70 |
| 1:LA:89:PRO:HG2 | 1:MA:280:LYS:HD2 | 1.73 | 0.70 |
| 6:4C:285:ARG:HB3 | 6:4C:285:ARG:HH11 | 1.53 | 0.70 |
| 7:5B:1521:PHE:CE1 | 7:5B:1570:ALA:HB3 | 2.26 | 0.70 |
| 2:ED:125:GLU:CB | 7:5A:903:PHE:CD2 | 2.72 | 0.70 |
| 2:FD:331:LEU:HD22 | 7:5A:915:PHE:CE2 | 2.25 | 0.70 |
| 2:FD:332:ASN:ND2 | 7:5A:909:ASN:OD1 | 2.24 | 0.70 |
| 2:GD:178:THR:HG23 | 1:GE:258:ASN:ND2 | 2.05 | 0.70 |
| 2:KD:178:THR:HG23 | 1:KE:258:ASN:ND2 | 2.05 | 0.70 |
| 1:KE:85:GLN:HA | 1:LE:283:HIS:HA | 0.79 | 0.70 |
| 1:LA:60:LYS:NZ | 1:MA:283:HIS:CG | 2.52 | 0.70 |
| 2:LB:54:ALA:CB | 2:MB:281:TYR:O | 2.40 | 0.70 |
| 2:LD:223:GLY:HA3 | 6:4B:219:ASN:HA | 1.71 | 0.70 |
| 2:LD:294:PHE:HD2 | 4:2A:147:PHE:CZ | 2.09 | 0.70 |
| 1:LE:60:LYS:CD | 6:4B:101:ARG:CZ | 2.54 | 0.70 |
| 6:4A:285:ARG:HB3 | 6:4A:285:ARG:HH11 | 1.53 | 0.70 |
| 7:5A:1521:PHE:CE1 | 7:5A:1570:ALA:HB3 | 2.26 | 0.70 |
| 7:5B:874:GLN:HB2 | 8:6B:59:LYS:HZ2 | 1.53 | 0.70 |
| 7:5C:1521:PHE:CE1 | 7:5C:1570:ALA:HB3 | 2.26 | 0.70 |
| 1:DA:401:LYS:HE2 | 2:DB:344:TRP:CE3 | 2.24 | 0.70 |
| 1:FC:419:SER:HB2 | 7:5A:1256:ARG:HE | 0.64 | 0.70 |
| 2:GD:86:ARG:NH2 | 2:HD:281:TYR:CE2 | 2.47 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HB:212:PHE:CZ | 1:HC:326:LYS:CD | 2.31 | 0.70 |
| 1:HC:420:GLU:OE1 | 5:3C:215:TYR:CE1 | 2.43 | 0.70 |
| 2:IB:362:LYS:NZ | 10:8V:36:UNK:O | 2.21 | 0.70 |
| 2:KB:179:VAL:CG2 | 1:KC:258:ASN:HA | 2.21 | 0.70 |
| 1:KE:359:PRO:HB3 | 6:4B:299:TYR:CZ | 2.25 | 0.70 |
| 2:KF:276:ARG:CZ | 6:4D:271:GLU:C | 2.59 | 0.70 |
| 2:LD:227:HIS:ND1 | 6:4B:226:ILE:HG13 | 2.04 | 0.70 |
| 1:LE:224:TYR:CE2 | 2:LF:246:LEU:HD11 | 2.24 | 0.70 |
| 1:ME:11:GLN:NE2 | 2:MF:247:ASN:OD1 | 2.25 | 0.70 |
| 6:4C:184:GLU:HA | 6:4C:184:GLU:OE1 | 1.90 | 0.70 |
| 7:5A:1436:ARG:HH11 | 7:5A:1436:ARG:CB | 2.05 | 0.70 |
| 7:5B:1521:PHE:CE1 | 7:5B:1570:ALA:CB | 2.74 | 0.70 |
| 7:5C:1436:ARG:HH11 | 7:5C:1436:ARG:CB | 2.05 | 0.70 |
| 7:5C:1521:PHE:CE1 | 7:5C:1570:ALA:CB | 2.74 | 0.70 |
| 2:AD:40:SER:HB2 | 6:4C:152:PHE:CD2 | 2.25 | 0.70 |
| 1:CE:282:TYR:CE2 | 10:8F:18:UNK:CA | 2.72 | 0.70 |
| 1:HE:416:GLY:CA | 5:3A:238:ILE:HD11 | 2.21 | 0.70 |
| 2:KB:227:HIS:HB3 | 6:4A:267:ILE:HD11 | 1.73 | 0.70 |
| 1:KE:62:VAL:CG2 | 1:LE:285:GLN:HB3 | 2.21 | 0.70 |
| 2:LB:379:LYS:HZ1 | 4:2C:166:ILE:N | 1.88 | 0.70 |
| 7:5A:1089:PHE:CE1 | 7:5A:1101:LEU:HD22 | 2.26 | 0.70 |
| 7:5A:1521:PHE:CE1 | 7:5A:1570:ALA:CB | 2.74 | 0.70 |
| 7:5B:1089:PHE:CE1 | 7:5B:1101:LEU:CD2 | 2.74 | 0.70 |
| 7:5B:1436:ARG:HH11 | 7:5B:1436:ARG:CB | 2.05 | 0.70 |
| 7:5C:1089:PHE:CE1 | 7:5C:1101:LEU:HD22 | 2.26 | 0.70 |
| 9:7E:7:LEU:CD2 | 9:7F:27:GLY:C | 2.63 | 0.70 |
| 1:DE:282:TYR:CD2 | 10:8I:18:UNK:CB | 2.74 | 0.70 |
| 2:IB:5:VAL:HG12 | 2:IB:62:ARG:HD3 | 1.74 | 0.70 |
| 2:JB:88:ASP:CB | 2:KB:278:SER:OG | 2.36 | 0.70 |
| 2:KB:215:LEU:HD13 | 6:4A:267:ILE:CB | 2.20 | 0.70 |
| 2:KF:77:ARG:CG | 2:LF:281:TYR:OH | 2.33 | 0.70 |
| 1:LA:245:ASP:CG | 6:4C:216:ARG:HE | 1.99 | 0.70 |
| 2:LD:306:ARG:HH12 | 4:2A:151:VAL:CG2 | 2.03 | 0.70 |
| 2:MB:111:GLU:CG | 3:1A:62:SER:HA | 2.22 | 0.70 |
| 7:5B:1089:PHE:CE1 | 7:5B:1101:LEU:HD22 | 2.26 | 0.70 |
| 2:AD:212:PHE:CZ | 1:AE:326:LYS:CD | 2.34 | 0.70 |
| 1:DC:222:PRO:HD2 | 2:DD:324:LYS:HD3 | 1.72 | 0.70 |
| 2:DD:220:PRO:HD2 | 1:DE:326:LYS:CE | 2.20 | 0.70 |
| 1:FA:207:GLU:OE1 | 7:5C:915:PHE:CB | 2.38 | 0.70 |
| 1:FA:404:PHE:CE2 | 2:FB:345:ILE:CD1 | 2.74 | 0.70 |
| 1:FE:222:PRO:CG | 2:FF:324:LYS:CD | 2.69 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:FF:55:THR:CG2 | 2:GF:284:LEU:N | 2.53 | 0.70 |
| 2:HD:5:VAL:HG12 | 2:HD:62:ARG:HD3 | 1.74 | 0.70 |
| 2:ID:5:VAL:HG12 | 2:ID:62:ARG:HD3 | 1.74 | 0.70 |
| 2:JB:5:VAL:HG12 | 2:JB:62:ARG:HD3 | 1.74 | 0.70 |
| 2:JD:5:VAL:HG12 | 2:JD:62:ARG:HD3 | 1.74 | 0.70 |
| 2:KF:276:ARG:HH22 | 6:4D:266:ASN:H | 1.40 | 0.70 |
| 2:KF:276:ARG:NE | 6:4D:265:TYR:HB2 | 2.07 | 0.70 |
| 1:LA:407:TRP:CE3 | 2:LB:255:VAL:HG22 | 2.20 | 0.70 |
| 1:MA:372:MET:HE2 | 6:4C:96:VAL:CA | 2.22 | 0.70 |
| 6:4A:134:LEU:C | 6:4A:134:LEU:HD12 | 2.17 | 0.70 |
| 6:4B:285:ARG:HB3 | 6:4B:285:ARG:HH11 | 1.53 | 0.70 |
| 6:4C:134:LEU:C | 6:4C:134:LEU:HD12 | 2.17 | 0.70 |
| 6:4D:293:ASP:HA | 6:4D:296:ASN:HB2 | 1.74 | 0.70 |
| 10:8G:38:UNK:C | 10:8H:1:UNK:CA | 2.69 | 0.70 |
| 1:EA:404:PHE:HE2 | 2:EB:345:ILE:CD1 | 2.05 | 0.70 |
| 2:HB:5:VAL:HG12 | 2:HB:62:ARG:HD3 | 1.74 | 0.70 |
| 1:HE:282:TYR:CE1 | 10:8U:15:UNK:O | 2.44 | 0.70 |
| 1:IC:402:ARG:HH21 | 7:5A:1417:GLN:HG3 | 1.37 | 0.70 |
| 2:IF:5:VAL:HG12 | 2:IF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:IF:87:PRO:HD2 | 2:JF:281:TYR:CE2 | 2.26 | 0.70 |
| 1:LE:221:ARG:HH11 | 2:LF:324:LYS:N | 1.90 | 0.70 |
| 6:4B:134:LEU:C | 6:4B:134:LEU:HD12 | 2.17 | 0.70 |
| 6:4B:293:ASP:HA | 6:4B:296:ASN:HB2 | 1.74 | 0.70 |
| 6:4C:115:LYS:HA | 6:4C:118:ILE:HD12 | 1.74 | 0.70 |
| 7:5A:1544:ILE:C | 7:5A:1570:ALA:CA | 2.49 | 0.70 |
| 7:5C:866:TYR:HB2 | 7:5C:954:ILE:CG2 | 2.22 | 0.70 |
| 7:5C:1381:ILE:HD12 | 7:5C:1381:ILE:N | 2.05 | 0.70 |
| 10:8D:38:UNK:C | 10:8E:1:UNK:CA | 2.69 | 0.70 |
| 10:8J:38:UNK:C | 10:8K:1:UNK:CA | 2.69 | 0.70 |
| 2:CB:5:VAL:HG12 | 2:CB:62:ARG:HD3 | 1.74 | 0.70 |
| 2:CD:86:ARG:N | 2:DD:281:TYR:CE1 | 2.59 | 0.70 |
| 1:CE:11:GLN:OE1 | 2:CF:245:GLN:O | 2.09 | 0.70 |
| 2:DB:5:VAL:HG12 | 2:DB:62:ARG:HD3 | 1.74 | 0.70 |
| 1:EA:101:ASN:HD21 | 2:EB:252:LYS:HD2 | 0.87 | 0.70 |
| 1:EC:105:ARG:NH1 | 2:ED:251:ARG:HD3 | 2.07 | 0.70 |
| 2:FF:5:VAL:HG12 | 2:FF:62:ARG:HD3 | 1.74 | 0.70 |
| 1:IE:393:HIS:CB | 5:3A:308:PHE:CE2 | 2.75 | 0.70 |
| 1:JC:401:LYS:CE | 2:JD:344:TRP:CZ3 | 2.62 | 0.70 |
| 2:JF:85:PHE:HB3 | 2:KF:281:TYR:OH | 1.91 | 0.70 |
| 2:KB:77:ARG:HG2 | 2:LB:281:TYR:CE2 | 2.18 | 0.70 |
| 2:KD:212:PHE:CZ | 1:KE:326:LYS:CD | 2.34 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KF:5:VAL:HG12 | 2:KF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:KF:276:ARG:NH2 | 6:4D:265:TYR:HA | 2.05 | 0.70 |
| 2:LB:220:PRO:O | 1:LC:324:VAL:CG1 | 2.39 | 0.70 |
| 1:LE:401:LYS:NZ | 2:LF:344:TRP:CH2 | 2.60 | 0.70 |
| 2:LF:5:VAL:HG12 | 2:LF:62:ARG:HD3 | 1.74 | 0.70 |
| 1:MA:279:GLU:CD | 6:4C:106:ALA:HB3 | 2.17 | 0.70 |
| 2:MB:179:VAL:CG2 | 1:MC:258:ASN:HA | 2.22 | 0.70 |
| 2:MF:5:VAL:HG12 | 2:MF:62:ARG:HD3 | 1.74 | 0.70 |
| 6:4A:115:LYS:HA | 6:4A:118:ILE:HD12 | 1.74 | 0.70 |
| 6:4A:184:GLU:HA | 6:4A:184:GLU:OE1 | 1.90 | 0.70 |
| 6:4A:293:ASP:HA | 6:4A:296:ASN:HB2 | 1.74 | 0.70 |
| 6:4B:115:LYS:HA | 6:4B:118:ILE:HD12 | 1.74 | 0.70 |
| 7:5A:866:TYR:HB2 | 7:5A:954:ILE:CG2 | 2.22 | 0.70 |
| 7:5A:1253:ILE:HD11 | 9:7B:20:LEU:HD13 | 1.72 | 0.70 |
| 7:5A:1381:ILE:HD12 | 7:5A:1381:ILE:N | 2.04 | 0.70 |
| 7:5B:1275:ILE:HG21 | 9:7D:11:TYR:HH | 1.57 | 0.70 |
| 7:5C:874:GLN:CB | 8:6C:59:LYS:HZ3 | 2.04 | 0.70 |
| 7:5C:890:ILE:HD13 | 7:5C:1072:PHE:CE1 | 2.27 | 0.70 |
| 9:7A:30:ARG:NH1 | 9:7B:3:GLN:CB | 2.54 | 0.70 |
| 10:8M:38:UNK:C | 10:8N:1:UNK:CA | 2.69 | 0.70 |
| 2:AD:178:THR:HG23 | 1:AE:258:ASN:ND2 | 2.05 | 0.70 |
| 2:BD:86:ARG:CA | 2:CD:281:TYR:CE1 | 2.61 | 0.70 |
| 2:BF:5:VAL:HG12 | 2:BF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:DD:5:VAL:HG12 | 2:DD:62:ARG:HD3 | 1.74 | 0.70 |
| 2:DF:5:VAL:HG12 | 2:DF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:ED:5:VAL:HG12 | 2:ED:62:ARG:HD3 | 1.74 | 0.70 |
| 2:EF:5:VAL:HG12 | 2:EF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:FB:5:VAL:HG12 | 2:FB:62:ARG:HD3 | 1.74 | 0.70 |
| 2:FD:5:VAL:HG12 | 2:FD:62:ARG:HD3 | 1.74 | 0.70 |
| 2:FD:177:ASP:O | 1:FE:352:LYS:HA | 1.92 | 0.70 |
| 1:FE:60:LYS:CE | 1:GE:283:HIS:CD2 | 2.75 | 0.70 |
| 2:GD:212:PHE:CZ | 1:GE:326:LYS:CD | 2.34 | 0.70 |
| 2:HB:397:TRP:CB | 1:HC:256:GLN:HE22 | 2.04 | 0.70 |
| 2:HF:5:VAL:HG12 | 2:HF:62:ARG:HD3 | 1.74 | 0.70 |
| 2:IB:178:THR:HG23 | 1:IC:258:ASN:ND2 | 2.06 | 0.70 |
| 2:JF:5:VAL:HG12 | 2:JF:62:ARG:HD3 | 1.74 | 0.70 |
| 1:KA:124:LYS:CD | 1:LA:290:GLU:HA | 2.21 | 0.70 |
| 2:KD:5:VAL:HG12 | 2:KD:62:ARG:HD3 | 1.74 | 0.70 |
| 1:LC:407:TRP:CE3 | 2:LD:255:VAL:HG22 | 2.22 | 0.70 |
| 2:LD:5:VAL:HG12 | 2:LD:62:ARG:HD3 | 1.74 | 0.70 |
| 2:LD:77:ARG:NH1 | 6:4B:204:ARG:HH22 | 1.86 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4C:293:ASP:HA | 6:4C:296:ASN:HB2 | 1.74 | 0.70 |
| 6:4D:115:LYS:HA | 6:4D:118:ILE:HD12 | 1.74 | 0.70 |
| 6:4D:134:LEU:C | 6:4D:134:LEU:HD12 | 2.17 | 0.70 |
| 7:5B:866:TYR:HB2 | 7:5B:954:ILE:CG2 | 2.22 | 0.70 |
| 7:5B:1423:LYS:HA | 7:5B:1423:LYS:HZ3 | 1.57 | 0.70 |
| 9:7A:18:VAL:HG11 | 9:7A:42:LEU:CD2 | 2.21 | 0.70 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:CG | 2.22 | 0.70 |
| 10:8A:38:UNK:C | 10:8B:1:UNK:CA | 2.70 | 0.70 |
| 2:AD:223:GLY:HA3 | 6:4C:131:VAL:CB | 2.17 | 0.69 |
| 2:BD:5:VAL:HG12 | 2:BD:62:ARG:HD3 | 1.74 | 0.69 |
| 2:CD:5:VAL:HG12 | 2:CD:62:ARG:HD3 | 1.74 | 0.69 |
| 2:CF:5:VAL:HG12 | 2:CF:62:ARG:HD3 | 1.74 | 0.69 |
| 1:FA:404:PHE:HE2 | 2:FB:345:ILE:HD12 | 1.56 | 0.69 |
| 2:GB:212:PHE:CE2 | 1:GC:326:LYS:HD3 | 2.22 | 0.69 |
| 2:GF:86:ARG:NH2 | 2:HF:281:TYR:CD2 | 2.45 | 0.69 |
| 1:HA:278:ALA:CB | 10:8S:22:UNK:N | 2.55 | 0.69 |
| 2:KD:54:ALA:CA | 2:LD:285:THR:HG22 | 2.22 | 0.69 |
| 2:KD:83:GLN:HA | 2:LD:281:TYR:CE1 | 2.27 | 0.69 |
| 2:KD:87:PRO:HG2 | 2:LD:282:ARG:HG2 | 1.72 | 0.69 |
| 2:LB:5:VAL:HG12 | 2:LB:62:ARG:HD3 | 1.74 | 0.69 |
| 1:ME:372:MET:CE | 6:4B:96:VAL:CA | 2.70 | 0.69 |
| 7:5A:890:ILE:HD13 | 7:5A:1072:PHE:CE1 | 2.27 | 0.69 |
| 7:5B:890:ILE:HD13 | 7:5B:1072:PHE:CE1 | 2.27 | 0.69 |
| 7:5B:1152:GLU:OE2 | 8:6B:66:ARG:NH2 | 2.24 | 0.69 |
| 7:5B:1381:ILE:HD12 | 7:5B:1381:ILE:N | 2.05 | 0.69 |
| 9:7C:30:ARG:NH1 | 9:7D:3:GLN:CB | 2.54 | 0.69 |
| 9:7E:35:ILE:HG23 | 9:7F:42:LEU:O | 1.90 | 0.69 |
| 9:7E:36:GLN:HA | 9:7F:43:LEU:HD22 | 1.71 | 0.69 |
| 10:8P:38:UNK:C | 10:8Q:1:UNK:CA | 2.69 | 0.69 |
| 2:AB:5:VAL:HG12 | 2:AB:62:ARG:HD3 | 1.74 | 0.69 |
| 2:AF:5:VAL:HG12 | 2:AF:62:ARG:HD3 | 1.74 | 0.69 |
| 2:BD:177:ASP:O | 1:BE:352:LYS:HA | 1.92 | 0.69 |
| 2:BD:208:TYR:OH | 1:BE:325:PRO:HB2 | 1.92 | 0.69 |
| 2:CF:86:ARG:HH11 | 2:DF:281:TYR:HA | 1.53 | 0.69 |
| 2:DB:177:ASP:OD1 | 1:DC:353:VAL:HG12 | 1.75 | 0.69 |
| 1:EE:404:PHE:HE2 | 2:EF:345:ILE:HD12 | 1.56 | 0.69 |
| 2:EF:55:THR:N | 2:FF:283:ALA:HB2 | 2.06 | 0.69 |
| 2:FB:331:LEU:HD21 | 7:5C:915:PHE:CZ | 2.25 | 0.69 |
| 2:FF:332:ASN:CG | 7:5B:909:ASN:HD21 | 2.01 | 0.69 |
| 2:GB:5:VAL:HG12 | 2:GB:62:ARG:HD3 | 1.74 | 0.69 |
| 2:HB:178:THR:HG23 | 1:HC:258:ASN:ND2 | 2.06 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:IC:282:TYR:CG | 10:8W:15:UNK:HA | 2.28 | 0.69 |
| 2:JB:178:THR:HG23 | 1:JC:258:ASN:ND2 | 2.06 | 0.69 |
| 1:LC:60:LYS:HD3 | 1:MC:283:HIS:HA | 1.74 | 0.69 |
| 2:LD:215:LEU:HD13 | 6:4B:225:PRO:HB3 | 1.74 | 0.69 |
| 2:MD:5:VAL:HG12 | 2:MD:62:ARG:HD3 | 1.74 | 0.69 |
| 10:8Y:38:UNK:C | 10:8Z:1:UNK:CA | 2.70 | 0.69 |
| 2:AD:5:VAL:HG12 | 2:AD:62:ARG:HD3 | 1.74 | 0.69 |
| 1:AE:401:LYS:CE | 2:AF:344:TRP:CZ3 | 2.67 | 0.69 |
| 2:BB:5:VAL:HG12 | 2:BB:62:ARG:HD3 | 1.74 | 0.69 |
| 1:DE:402:ARG:HE | 7:5B:777:ALA:CB | 2.02 | 0.69 |
| 1:DE:404:PHE:HE2 | 2:DF:345:ILE:CD1 | 2.05 | 0.69 |
| 1:EA:396:ASP:OD1 | 7:5C:821:LEU:HD11 | 1.91 | 0.69 |
| 2:EB:5:VAL:HG12 | 2:EB:62:ARG:HD3 | 1.74 | 0.69 |
| 1:EE:402:ARG:CZ | 7:5B:824:ARG:NH2 | 2.54 | 0.69 |
| 2:EF:54:ALA:HA | 2:FF:283:ALA:CB | 2.21 | 0.69 |
| 1:GC:224:TYR:HE2 | 2:GD:246:LEU:HD11 | 1.57 | 0.69 |
| 2:GD:5:VAL:HG12 | 2:GD:62:ARG:HD3 | 1.74 | 0.69 |
| 2:KB:5:VAL:HG12 | 2:KB:62:ARG:HD3 | 1.74 | 0.69 |
| 2:KB:217:LEU:HD13 | 6:4A:263:CYS:SG | 2.33 | 0.69 |
| 2:LB:212:PHE:HZ | 1:LC:326:LYS:CE | 2.04 | 0.69 |
| 1:LE:222:PRO:HD3 | 2:LF:324:LYS:HD3 | 1.65 | 0.69 |
| 2:LF:224:ASP:CA | 6:4D:219:ASN:OD1 | 2.32 | 0.69 |
| 2:MB:397:TRP:CD2 | 1:MC:256:GLN:O | 2.25 | 0.69 |
| 6:4B:184:GLU:HA | 6:4B:184:GLU:OE1 | 1.90 | 0.69 |
| 6:4D:285:ARG:HB3 | 6:4D:285:ARG:HH11 | 1.53 | 0.69 |
| 7:5A:1276:GLU:HG2 | 9:7B:7:LEU:HD12 | 1.73 | 0.69 |
| 7:5B:1490:LYS:HA | 7:5B:1494:LEU:HB3 | 1.74 | 0.69 |
| 7:5C:841:VAL:HG21 | 8:6C:11:PRO:HA | 1.74 | 0.69 |
| 1:BC:11:GLN:NE2 | 2:BD:247:ASN:OD1 | 2.25 | 0.69 |
| 2:CB:86:ARG:N | 2:DB:281:TYR:CE1 | 2.58 | 0.69 |
| 2:CB:177:ASP:O | 1:CC:352:LYS:HA | 1.92 | 0.69 |
| 1:CE:282:TYR:HE2 | 10:8F:18:UNK:CA | 2.04 | 0.69 |
| 1:DA:402:ARG:CZ | 7:5C:777:ALA:HB1 | 2.18 | 0.69 |
| 2:GB:178:THR:HG23 | 1:GC:258:ASN:ND2 | 2.06 | 0.69 |
| 1:GC:60:LYS:CD | 1:HC:283:HIS:CG | 2.76 | 0.69 |
| 2:GF:5:VAL:HG12 | 2:GF:62:ARG:HD3 | 1.74 | 0.69 |
| 2:KB:178:THR:HG23 | 1:KC:258:ASN:ND2 | 2.06 | 0.69 |
| 2:KD:125:GLU:O | 4:2A:38:VAL:HA | 1.93 | 0.69 |
| 2:KF:276:ARG:HH21 | 6:4D:265:TYR:HB2 | 1.57 | 0.69 |
| 1:LE:404:PHE:CE1 | 2:LF:259:PRO:HA | 2.28 | 0.69 |
| 2:MB:5:VAL:HG12 | 2:MB:62:ARG:HD3 | 1.74 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:4C:139:ASP:OD2 | 6:4C:140:PRO:CD | 2.40 | 0.69 |
| 7:5B:1544:ILE:CA | 7:5B:1573:ARG:CD | 2.39 | 0.69 |
| 7:5C:1524:PHE:HE1 | 7:5C:1571:MET:HE2 | 1.55 | 0.69 |
| 10:8S:38:UNK:C | 10:8T:1:UNK:CA | 2.70 | 0.69 |
| 2:AD:362:LYS:CG | 6:4C:146:ILE:HB | 2.14 | 0.69 |
| 2:CD:178:THR:HG23 | 1:CE:258:ASN:ND2 | 2.04 | 0.69 |
| 2:GB:98:GLY:CA | 1:GC:254:GLU:CG | 2.48 | 0.69 |
| 1:HC:416:GLY:CA | 5:3C:238:ILE:HD11 | 2.23 | 0.69 |
| 1:HE:278:ALA:HB3 | 10:8U:22:UNK:CB | 2.21 | 0.69 |
| 1:IC:60:LYS:NZ | 1:JC:283:HIS:CD2 | 2.60 | 0.69 |
| 1:IE:282:TYR:OH | 10:8X:17:UNK:CB | 2.37 | 0.69 |
| 1:KC:401:LYS:CE | 2:KD:344:TRP:CZ3 | 2.62 | 0.69 |
| 1:KE:85:GLN:OE1 | 1:LE:283:HIS:N | 2.25 | 0.69 |
| 2:LB:77:ARG:HH12 | 6:4A:204:ARG:HH22 | 1.40 | 0.69 |
| 1:LC:89:PRO:CG | 1:MC:280:LYS:HZ1 | 2.06 | 0.69 |
| 2:LD:179:VAL:HG21 | 1:LE:258:ASN:C | 2.16 | 0.69 |
| 2:MB:391:ARG:HG3 | 1:MC:346:TRP:CD1 | 2.27 | 0.69 |
| 7:5B:1524:PHE:HE1 | 7:5B:1571:MET:HE2 | 1.54 | 0.69 |
| 7:5C:1243:ASP:HB3 | 9:7F:8:ARG:NH1 | 2.07 | 0.69 |
| 7:5C:1490:LYS:HA | 7:5C:1494:LEU:HB3 | 1.74 | 0.69 |
| 2:CD:86:ARG:CB | 2:DD:281:TYR:HE1 | 1.85 | 0.69 |
| 1:GA:224:TYR:HE2 | 2:GB:246:LEU:HD11 | 1.57 | 0.69 |
| 2:JB:397:TRP:CB | 1:JC:256:GLN:HE22 | 2.04 | 0.69 |
| 1:JC:91:GLN:H | 1:KC:280:LYS:HZ2 | 0.73 | 0.69 |
| 2:KB:397:TRP:CB | 1:KC:256:GLN:HE22 | 2.04 | 0.69 |
| 2:KF:339:SER:HB2 | 7:5B:1504:ARG:NH1 | 2.07 | 0.69 |
| 6:4A:139:ASP:OD2 | 6:4A:140:PRO:CD | 2.40 | 0.69 |
| 6:4D:184:GLU:HA | 6:4D:184:GLU:OE1 | 1.91 | 0.69 |
| 7:5A:1490:LYS:HA | 7:5A:1494:LEU:HB3 | 1.74 | 0.69 |
| 7:5B:1552:LYS:HZ1 | 7:5B:1563:SER:HB3 | 1.54 | 0.69 |
| 9:7A:7:LEU:HD22 | 9:7B:27:GLY:HA3 | 0.70 | 0.69 |
| 9:7C:7:LEU:HD22 | 9:7D:27:GLY:HA3 | 0.70 | 0.69 |
| 2:AD:321:MET:C | 6:4C:156:PHE:CD2 | 2.70 | 0.69 |
| 1:BA:222:PRO:CD | 2:BB:324:LYS:HD3 | 2.22 | 0.69 |
| 2:BB:177:ASP:CB | 1:BC:353:VAL:HG12 | 2.22 | 0.69 |
| 2:DD:85:PHE:C | 2:ED:281:TYR:CZ | 2.71 | 0.69 |
| 2:DD:86:ARG:CA | 2:ED:281:TYR:CZ | 2.66 | 0.69 |
| 1:FC:178:SER:OG | 2:FD:347:ASN:HB3 | 1.92 | 0.69 |
| 1:FE:178:SER:OG | 2:FF:347:ASN:HB3 | 1.92 | 0.69 |
| 2:GD:58:ARG:NH2 | 2:HD:281:TYR:OH | 2.26 | 0.69 |
| 1:GE:60:LYS:HD2 | 1:HE:283:HIS:CD2 | 2.28 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LA:222:PRO:HG3 | 2:LB:324:LYS:HD2 | 1.73 | 0.69 |
| 2:LF:224:ASP:HA | 6:4D:219:ASN:OD1 | 1.92 | 0.69 |
| 1:MC:11:GLN:NE2 | 2:MD:247:ASN:OD1 | 2.26 | 0.69 |
| 1:MC:100:ALA:HB1 | 2:MD:252:LYS:HA | 1.74 | 0.69 |
| 1:MC:282:TYR:CD2 | 6:4A:104:ARG:CD | 2.62 | 0.69 |
| 6:4B:139:ASP:OD2 | 6:4B:140:PRO:CD | 2.40 | 0.69 |
| 7:5A:1126:PRO:CD | 8:6A:246:TYR:OH | 2.40 | 0.69 |
| 7:5C:1544:ILE:CD1 | 7:5C:1574:ILE:CG1 | 2.61 | 0.69 |
| 9:7D:18:VAL:HG12 | 9:7D:42:LEU:HD23 | 1.72 | 0.69 |
| 9:7E:18:VAL:HG21 | 9:7F:35:ILE:HG21 | 1.75 | 0.69 |
| 2:CB:177:ASP:CB | 1:CC:353:VAL:HG12 | 2.23 | 0.69 |
| 1:DA:402:ARG:HE | 7:5C:777:ALA:HB2 | 1.45 | 0.69 |
| 1:EE:62:VAL:HG21 | 1:FE:283:HIS:O | 1.93 | 0.69 |
| 1:EE:404:PHE:CE2 | 2:EF:345:ILE:CD1 | 2.75 | 0.69 |
| 1:FC:207:GLU:OE1 | 7:5A:915:PHE:CB | 2.38 | 0.69 |
| 2:GD:98:GLY:CA | 1:GE:254:GLU:CG | 2.48 | 0.69 |
| 1:HE:419:SER:HG | 5:3A:238:ILE:CD1 | 2.04 | 0.69 |
| 2:IB:397:TRP:CB | 1:IC:256:GLN:HE22 | 2.04 | 0.69 |
| 2:JB:86:ARG:NH1 | 2:KB:280:GLN:O | 2.26 | 0.69 |
| 1:JC:89:PRO:HG2 | 1:KC:280:LYS:CG | 2.20 | 0.69 |
| 2:JD:88:ASP:HB2 | 2:KD:278:SER:CB | 2.22 | 0.69 |
| 2:KD:159:TYR:CE2 | 4:2A:35:VAL:C | 2.68 | 0.69 |
| 2:KD:276:ARG:CZ | 6:4B:271:GLU:O | 2.34 | 0.69 |
| 2:KF:118:ASP:CG | 4:2B:148:ASN:HD21 | 2.00 | 0.69 |
| 2:LB:337:ASN:HD21 | 4:2C:148:ASN:HB2 | 1.57 | 0.69 |
| 4:2C:162:GLN:HA | 4:2C:162:GLN:NE2 | 2.04 | 0.69 |
| 6:4D:139:ASP:OD2 | 6:4D:140:PRO:CD | 2.40 | 0.69 |
| 7:5A:1524:PHE:HE1 | 7:5A:1571:MET:HE2 | 1.55 | 0.69 |
| 7:5B:1544:ILE:C | 7:5B:1570:ALA:CA | 2.49 | 0.69 |
| 7:5C:1416:LYS:HA | 7:5C:1416:LYS:HZ3 | 1.54 | 0.69 |
| 9:7F:18:VAL:HG12 | 9:7F:42:LEU:HD23 | 1.72 | 0.69 |
| 2:AB:178:THR:HG23 | 1:AC:258:ASN:ND2 | 2.06 | 0.69 |
| 1:BA:11:GLN:NE2 | 2:BB:247:ASN:OD1 | 2.26 | 0.69 |
| 1:BC:401:LYS:CE | 2:BD:344:TRP:CZ3 | 2.68 | 0.69 |
| 2:BD:220:PRO:CD | 1:BE:326:LYS:HE2 | 2.22 | 0.69 |
| 2:EB:54:ALA:CB | 2:FB:281:TYR:O | 2.41 | 0.69 |
| 2:EB:178:THR:HG23 | 1:EC:258:ASN:ND2 | 2.05 | 0.69 |
| 1:FC:419:SER:OG | 7:5A:1256:ARG:HD3 | 1.93 | 0.69 |
| 1:GA:60:LYS:CD | 1:HA:283:HIS:CD2 | 2.76 | 0.69 |
| 1:IC:278:ALA:CB | 10:8W:21:UNK:CA | 2.71 | 0.69 |
| 1:IE:393:HIS:HB3 | 5:3A:308:PHE:CD2 | 2.28 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JC:90:GLU:HG2 | 1:KC:280:LYS:HB3 | 1.74 | 0.69 |
| 4:2A:16:GLN:CB | 4:2A:19:MET:HB2 | 2.22 | 0.69 |
| 4:2A:162:GLN:HA | 4:2A:162:GLN:NE2 | 2.05 | 0.69 |
| 4:2C:16:GLN:CB | 4:2C:19:MET:HB2 | 2.22 | 0.69 |
| 5:3C:224:ASP:N | 5:3C:335:LYS:NZ | 2.41 | 0.69 |
| 9:7A:11:TYR:CE1 | 9:7B:26:LEU:CG | 2.71 | 0.69 |
| 9:7C:39:GLY:HA3 | 9:7D:43:LEU:HG | 1.74 | 0.69 |
| 1:AE:342:GLN:HE22 | 3:1A:55:HIS:CE1 | 2.06 | 0.69 |
| 1:EA:396:ASP:CG | 7:5C:817:LEU:HD23 | 2.18 | 0.69 |
| 1:EC:430:LYS:NZ | 7:5A:834:ASN:ND2 | 0.71 | 0.69 |
| 1:FC:56:THR:O | 1:GC:285:GLN:HA | 1.93 | 0.69 |
| 1:IC:389:SER:HB2 | 5:3C:307:LYS:CB | 2.23 | 0.69 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:CD | 2.70 | 0.69 |
| 1:LC:404:PHE:CE1 | 2:LD:259:PRO:HA | 2.28 | 0.69 |
| 2:LF:306:ARG:HH21 | 4:2B:149:ILE:HG22 | 1.58 | 0.69 |
| 2:MD:221:THR:CG2 | 6:4B:189:ARG:HH12 | 2.05 | 0.69 |
| 4:2B:162:GLN:HA | 4:2B:162:GLN:NE2 | 2.05 | 0.69 |
| 7:5B:1548:VAL:CG1 | 7:5B:1569:GLU:HB2 | 2.11 | 0.69 |
| 9:7C:11:TYR:CE1 | 9:7D:26:LEU:CB | 2.41 | 0.69 |
| 1:BA:404:PHE:HE2 | 2:BB:345:ILE:CD1 | 2.05 | 0.68 |
| 1:DC:404:PHE:HE2 | 2:DD:345:ILE:CD1 | 2.06 | 0.68 |
| 1:EC:430:LYS:HZ2 | 7:5A:834:ASN:CB | 2.05 | 0.68 |
| 2:GB:397:TRP:CB | 1:GC:256:GLN:HE22 | 2.04 | 0.68 |
| 2:ID:87:PRO:HD2 | 2:JD:281:TYR:CZ | 2.27 | 0.68 |
| 1:KE:85:GLN:HG2 | 1:LE:283:HIS:CD2 | 2.28 | 0.68 |
| 5:3B:233:ASP:H | 5:3B:336:ASN:HD21 | 1.40 | 0.68 |
| 7:5A:841:VAL:HG23 | 8:6A:11:PRO:HG3 | 1.75 | 0.68 |
| 7:5B:839:GLU:CD | 8:6B:107:PRO:O | 2.36 | 0.68 |
| 1:CA:11:GLN:OE1 | 2:CB:245:GLN:O | 2.10 | 0.68 |
| 1:DE:400:ALA:C | 7:5B:775:PRO:CB | 2.63 | 0.68 |
| 1:FA:60:LYS:CD | 1:GA:283:HIS:HD2 | 1.98 | 0.68 |
| 2:LD:55:THR:HG21 | 2:MD:284:LEU:N | 2.05 | 0.68 |
| 2:LF:77:ARG:NH1 | 6:4D:204:ARG:HH22 | 1.84 | 0.68 |
| 1:MA:372:MET:CE | 6:4C:96:VAL:CA | 2.72 | 0.68 |
| 1:ME:224:TYR:HE2 | 2:MF:246:LEU:HD11 | 1.59 | 0.68 |
| 4:2B:16:GLN:CB | 4:2B:19:MET:HB2 | 2.22 | 0.68 |
| 6:4B:107:MET:HG3 | 6:4B:110:LYS:HE3 | 1.72 | 0.68 |
| 7:5A:1544:ILE:CA | 7:5A:1573:ARG:CD | 2.39 | 0.68 |
| 7:5B:1434:LYS:HA | 7:5B:1434:LYS:HE3 | 1.75 | 0.68 |
| 7:5C:1482:SER:CA | 7:5C:1485:LYS:HB2 | 2.16 | 0.68 |
| 9:7B:18:VAL:HG12 | 9:7B:42:LEU:HD23 | 1.72 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:DE:400:ALA:O | 7:5B:775:PRO:CA | 2.40 | 0.68 |
| 1:FC:222:PRO:CG | 2:FD:324:LYS:CD | 2.68 | 0.68 |
| 2:ID:424:GLN:CD | 7:5A:1413:GLN:HE22 | 1.81 | 0.68 |
| 1:IE:389:SER:HB3 | 5:3A:307:LYS:HD3 | 1.73 | 0.68 |
| 1:JA:279:GLU:OE1 | 10:8Y:22:UNK:CB | 2.42 | 0.68 |
| 2:LB:55:THR:CG2 | 2:MB:283:ALA:HB1 | 2.19 | 0.68 |
| 1:LC:60:LYS:HD3 | 1:MC:283:HIS:CB | 2.22 | 0.68 |
| 1:MA:279:GLU:CG | 6:4C:110:LYS:CE | 2.70 | 0.68 |
| 2:MD:177:ASP:O | 1:ME:352:LYS:CD | 2.33 | 0.68 |
| 5:3A:233:ASP:H | 5:3A:336:ASN:HD21 | 1.40 | 0.68 |
| 7:5A:843:LEU:O | 7:5A:843:LEU:HD23 | 1.93 | 0.68 |
| 8:6C:202:GLU:OE2 | 8:6C:218:LEU:HB2 | 1.93 | 0.68 |
| 10:8V:38:UNK:C | 10:8W:1:UNK:CA | 2.70 | 0.68 |
| 2:AB:55:THR:CG2 | 2:BB:283:ALA:CB | 2.69 | 0.68 |
| 1:AC:224:TYR:HE2 | 2:AD:246:LEU:HD11 | 1.57 | 0.68 |
| 1:CE:222:PRO:HD2 | 2:CF:324:LYS:HD3 | 1.75 | 0.68 |
| 1:EE:430:LYS:HZ3 | 7:5B:834:ASN:ND2 | 1.19 | 0.68 |
| 1:HC:224:TYR:HE2 | 2:HD:246:LEU:HD11 | 1.57 | 0.68 |
| 2:HD:177:ASP:O | 1:HE:352:LYS:CD | 2.34 | 0.68 |
| 2:IB:86:ARG:CA | 2:JB:281:TYR:HE1 | 2.04 | 0.68 |
| 2:IB:87:PRO:HD2 | 2:JB:281:TYR:CE2 | 2.27 | 0.68 |
| 1:JC:224:TYR:HE2 | 2:JD:246:LEU:HD11 | 1.57 | 0.68 |
| 1:KA:224:TYR:HE2 | 2:KB:246:LEU:HD11 | 1.57 | 0.68 |
| 1:LA:407:TRP:HE3 | 2:LB:255:VAL:HG13 | 1.55 | 0.68 |
| 2:LB:179:VAL:CG2 | 1:LC:258:ASN:CA | 2.72 | 0.68 |
| 1:LC:222:PRO:HG3 | 2:LD:324:LYS:HD2 | 1.73 | 0.68 |
| 2:LD:390:ARG:HD2 | 1:LE:439:THR:HG21 | 1.74 | 0.68 |
| 1:ME:279:GLU:OE2 | 6:4B:106:ALA:CB | 2.41 | 0.68 |
| 7:5A:1434:LYS:HA | 7:5A:1434:LYS:HE3 | 1.75 | 0.68 |
| 7:5B:843:LEU:O | 7:5B:843:LEU:HD23 | 1.93 | 0.68 |
| 7:5B:1401:LYS:HD3 | 7:5B:1401:LYS:N | 2.07 | 0.68 |
| 7:5C:843:LEU:O | 7:5C:843:LEU:HD23 | 1.94 | 0.68 |
| 7:5C:1243:ASP:CB | 9:7F:8:ARG:HH12 | 2.05 | 0.68 |
| 8:6A:202:GLU:OE2 | 8:6A:218:LEU:HB2 | 1.93 | 0.68 |
| 9:7E:18:VAL:HG11 | 9:7E:42:LEU:CD2 | 2.21 | 0.68 |
| 2:AD:356:ILE:CD1 | 6:4C:152:PHE:CE1 | 2.69 | 0.68 |
| 1:EA:282:TYR:CD2 | 10:8J:18:UNK:CB | 2.74 | 0.68 |
| 2:FD:212:PHE:HZ | 1:FE:326:LYS:CE | 2.06 | 0.68 |
| 1:LC:401:LYS:NZ | 2:LD:344:TRP:CZ3 | 2.60 | 0.68 |
| 1:LE:245:ASP:OD1 | 6:4B:216:ARG:CZ | 2.42 | 0.68 |
| 2:LF:224:ASP:CA | 6:4D:219:ASN:CG | 2.67 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LF:306:ARG:NH1 | 4:2B:151:VAL:HG21 | 2.07 | 0.68 |
| 2:MD:178:THR:HG23 | 1:ME:258:ASN:ND2 | 2.06 | 0.68 |
| 4:2A:16:GLN:O | 4:2A:19:MET:CA | 2.42 | 0.68 |
| 4:2B:16:GLN:O | 4:2B:19:MET:CA | 2.42 | 0.68 |
| 6:4C:291:LYS:HA | 6:4C:294:LEU:HD12 | 1.75 | 0.68 |
| 2:AF:226:ASN:HD21 | 13:AF:501:GDP:HN1 | 1.42 | 0.68 |
| 1:DC:11:GLN:OE1 | 2:DD:245:GLN:O | 2.12 | 0.68 |
| 1:HA:222:PRO:CD | 2:HB:324:LYS:HD3 | 2.24 | 0.68 |
| 1:HA:401:LYS:CE | 2:HB:344:TRP:CZ3 | 2.67 | 0.68 |
| 2:IB:212:PHE:CZ | 1:IC:326:LYS:CD | 2.31 | 0.68 |
| 2:JF:88:ASP:CG | 2:KF:278:SER:HG | 2.01 | 0.68 |
| 1:KA:359:PRO:HB3 | 6:4C:299:TYR:HE2 | 1.53 | 0.68 |
| 1:LA:35:GLN:NE2 | 6:4C:101:ARG:HB2 | 2.07 | 0.68 |
| 2:LB:331:LEU:CG | 4:2C:42:PHE:HE1 | 2.07 | 0.68 |
| 2:LF:306:ARG:CZ | 4:2B:149:ILE:CG2 | 2.71 | 0.68 |
| 4:2C:16:GLN:O | 4:2C:19:MET:CA | 2.42 | 0.68 |
| 6:4A:291:LYS:HA | 6:4A:294:LEU:HD12 | 1.75 | 0.68 |
| 6:4B:291:LYS:HA | 6:4B:294:LEU:HD12 | 1.75 | 0.68 |
| 6:4D:291:LYS:HA | 6:4D:294:LEU:HD12 | 1.75 | 0.68 |
| 7:5C:1434:LYS:HA | 7:5C:1434:LYS:HE3 | 1.75 | 0.68 |
| 8:6B:202:GLU:OE2 | 8:6B:218:LEU:HB2 | 1.93 | 0.68 |
| 9:7C:11:TYR:CG | 9:7D:23:LEU:HD22 | 2.29 | 0.68 |
| 2:AB:226:ASN:HD21 | 13:AB:501:GDP:HN1 | 1.42 | 0.68 |
| 2:AD:226:ASN:HD21 | 13:AD:501:GDP:HN1 | 1.42 | 0.68 |
| 1:BE:11:GLN:NE2 | 2:BF:247:ASN:OD1 | 2.27 | 0.68 |
| 1:FA:402:ARG:NH2 | 7:5C:1262:GLU:OE1 | 2.27 | 0.68 |
| 1:GA:60:LYS:NZ | 1:HA:283:HIS:ND1 | 2.37 | 0.68 |
| 1:HA:224:TYR:HE2 | 2:HB:246:LEU:HD11 | 1.57 | 0.68 |
| 2:HB:177:ASP:O | 1:HC:352:LYS:CD | 2.35 | 0.68 |
| 1:HC:410:GLY:C | 5:3C:329:ARG:HH22 | 2.01 | 0.68 |
| 1:IA:60:LYS:NZ | 1:JA:283:HIS:NE2 | 2.41 | 0.68 |
| 2:KD:125:GLU:CB | 2:LD:336:LYS:CE | 2.71 | 0.68 |
| 2:KF:221:THR:CB | 6:4D:261:SER:O | 2.41 | 0.68 |
| 1:LC:222:PRO:HD3 | 2:LD:324:LYS:HD3 | 1.65 | 0.68 |
| 7:5A:1401:LYS:HD3 | 7:5A:1401:LYS:N | 2.07 | 0.68 |
| 7:5B:826:LEU:HB3 | 7:5B:840:GLY:O | 1.93 | 0.68 |
| 7:5B:1544:ILE:C | 7:5B:1573:ARG:HD2 | 2.18 | 0.68 |
| 7:5C:1401:LYS:HD3 | 7:5C:1401:LYS:N | 2.07 | 0.68 |
| 9:7A:11:TYR:CG | 9:7B:23:LEU:HD22 | 2.29 | 0.68 |
| 2:DB:220:PRO:HD2 | 1:DC:326:LYS:CE | 2.22 | 0.68 |
| 1:DC:101:ASN:HD21 | 2:DD:252:LYS:HD2 | 0.86 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:EE:100:ALA:HB1 | 2:EF:252:LYS:HA | 1.76 | 0.68 |
| 1:FA:178:SER:OG | 2:FB:347:ASN:HB3 | 1.94 | 0.68 |
| 1:GA:222:PRO:CD | 2:GB:324:LYS:HD3 | 2.24 | 0.68 |
| 1:IA:222:PRO:CD | 2:IB:324:LYS:HD3 | 2.24 | 0.68 |
| 1:IA:224:TYR:HE2 | 2:IB:246:LEU:HD11 | 1.57 | 0.68 |
| 1:JA:222:PRO:CD | 2:JB:324:LYS:HD3 | 2.24 | 0.68 |
| 1:LC:89:PRO:CD | 1:MC:280:LYS:CE | 2.72 | 0.68 |
| 5:3C:233:ASP:H | 5:3C:336:ASN:HD21 | 1.39 | 0.68 |
| 7:5A:1495:PHE:CE2 | 7:5A:1562:LEU:HD22 | 2.29 | 0.68 |
| 7:5A:1577:LYS:HA | 7:5A:1577:LYS:CE | 2.22 | 0.68 |
| 7:5B:1495:PHE:CE2 | 7:5B:1562:LEU:HD22 | 2.29 | 0.68 |
| 7:5B:1573:ARG:C | 7:5B:1577:LYS:HB2 | 2.15 | 0.68 |
| 7:5B:1577:LYS:CE | 7:5B:1577:LYS:HA | 2.22 | 0.68 |
| 7:5C:1544:ILE:CA | 7:5C:1573:ARG:CD | 2.39 | 0.68 |
| 7:5C:1577:LYS:CE | 7:5C:1577:LYS:HA | 2.22 | 0.68 |
| 1:AA:401:LYS:CE | 2:AB:344:TRP:CZ3 | 2.67 | 0.68 |
| 1:GE:409:VAL:CB | 5:3A:383:GLU:OE1 | 2.42 | 0.68 |
| 2:KB:126:GLY:O | 4:2C:39:ALA:HB2 | 1.92 | 0.68 |
| 1:LC:60:LYS:HD2 | 1:MC:283:HIS:CD2 | 2.29 | 0.68 |
| 1:LE:76:ASP:OD2 | 1:LE:79:ARG:NH2 | 2.27 | 0.68 |
| 2:LF:227:HIS:ND1 | 6:4D:226:ILE:HG13 | 2.08 | 0.68 |
| 7:5A:826:LEU:HB3 | 7:5A:840:GLY:O | 1.93 | 0.68 |
| 7:5A:1544:ILE:C | 7:5A:1573:ARG:HD2 | 2.18 | 0.68 |
| 7:5C:826:LEU:HB3 | 7:5C:840:GLY:O | 1.93 | 0.68 |
| 9:7A:39:GLY:HA3 | 9:7B:43:LEU:HG | 1.74 | 0.68 |
| 1:DE:11:GLN:OE1 | 2:DF:245:GLN:O | 2.12 | 0.68 |
| 2:ED:54:ALA:HA | 2:FD:283:ALA:CB | 2.17 | 0.68 |
| 1:EE:76:ASP:OD2 | 1:EE:79:ARG:NH2 | 2.27 | 0.68 |
| 2:FD:106:TYR:CE1 | 7:5A:1295:LYS:N | 2.60 | 0.68 |
| 1:FE:419:SER:C | 7:5B:1256:ARG:NH2 | 2.51 | 0.68 |
| 1:GC:60:LYS:HD3 | 1:HC:283:HIS:HB3 | 1.76 | 0.68 |
| 1:HA:404:PHE:HE2 | 2:HB:345:ILE:CD1 | 2.07 | 0.68 |
| 1:IC:60:LYS:NZ | 1:JC:283:HIS:NE2 | 2.40 | 0.68 |
| 1:KA:404:PHE:HE2 | 2:KB:345:ILE:CD1 | 2.07 | 0.68 |
| 2:LB:179:VAL:HG21 | 1:LC:258:ASN:C | 2.18 | 0.68 |
| 1:MA:279:GLU:O | 6:4C:107:MET:HG2 | 1.46 | 0.68 |
| 7:5C:1495:PHE:CE2 | 7:5C:1562:LEU:HD22 | 2.29 | 0.68 |
| 7:5C:1544:ILE:C | 7:5C:1573:ARG:HD2 | 2.18 | 0.68 |
| 1:BA:76:ASP:OD2 | 1:BA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:DC:282:TYR:CD2 | 10:8H:18:UNK:CB | 2.76 | 0.67 |
| 1:EC:76:ASP:OD2 | 1:EC:79:ARG:NH2 | 2.27 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EE:222:PRO:HD2 | 2:EF:324:LYS:HD3 | 1.75 | 0.67 |
| 2:FF:332:ASN:ND2 | 7:5B:909:ASN:OD1 | 2.27 | 0.67 |
| 1:GA:76:ASP:OD2 | 1:GA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:GC:76:ASP:OD2 | 1:GC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:IB:87:PRO:HD2 | 2:JB:281:TYR:CZ | 2.29 | 0.67 |
| 1:JE:279:GLU:OE1 | 10:9A:22:UNK:CA | 2.41 | 0.67 |
| 1:KA:76:ASP:OD2 | 1:KA:79:ARG:NH2 | 2.27 | 0.67 |
| 2:KB:83:GLN:HA | 2:LB:281:TYR:CE1 | 2.29 | 0.67 |
| 1:KC:76:ASP:OD2 | 1:KC:79:ARG:NH2 | 2.27 | 0.67 |
| 1:KE:76:ASP:OD2 | 1:KE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:KE:85:GLN:C | 1:LE:283:HIS:HA | 2.18 | 0.67 |
| 1:KE:359:PRO:CG | 6:4B:299:TYR:CE2 | 2.77 | 0.67 |
| 2:KF:221:THR:CB | 6:4D:261:SER:C | 2.63 | 0.67 |
| 1:LC:76:ASP:OD2 | 1:LC:79:ARG:NH2 | 2.27 | 0.67 |
| 9:7C:12:GLU:HA | 9:7C:16:THR:OG1 | 1.94 | 0.67 |
| 9:7C:18:VAL:HG11 | 9:7C:42:LEU:CD2 | 2.21 | 0.67 |
| 1:AA:76:ASP:OD2 | 1:AA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:AA:404:PHE:HE2 | 2:AB:345:ILE:CD1 | 2.07 | 0.67 |
| 2:AB:397:TRP:CB | 1:AC:256:GLN:HE22 | 2.04 | 0.67 |
| 1:BC:76:ASP:OD2 | 1:BC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:CD:208:TYR:OH | 1:CE:325:PRO:HB2 | 1.94 | 0.67 |
| 1:DA:60:LYS:CD | 1:EA:283:HIS:HD2 | 1.92 | 0.67 |
| 1:EA:76:ASP:OD2 | 1:EA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:FC:282:TYR:CD2 | 10:8N:18:UNK:CB | 2.73 | 0.67 |
| 1:FE:76:ASP:OD2 | 1:FE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:GE:76:ASP:OD2 | 1:GE:79:ARG:NH2 | 2.27 | 0.67 |
| 2:HD:226:ASN:HD21 | 13:HD:501:GDP:HN1 | 1.42 | 0.67 |
| 1:HE:410:GLY:C | 5:3A:329:ARG:HH22 | 2.02 | 0.67 |
| 1:IC:389:SER:HB2 | 5:3C:307:LYS:HB3 | 1.74 | 0.67 |
| 1:JA:76:ASP:OD2 | 1:JA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:JA:224:TYR:HE2 | 2:JB:246:LEU:HD11 | 1.57 | 0.67 |
| 1:JA:404:PHE:HE2 | 2:JB:345:ILE:CD1 | 2.07 | 0.67 |
| 2:KD:221:THR:CB | 6:4B:261:SER:O | 2.41 | 0.67 |
| 1:KE:62:VAL:HG22 | 1:LE:285:GLN:HB3 | 1.74 | 0.67 |
| 2:LF:226:ASN:HD21 | 13:LF:501:GDP:HN1 | 1.42 | 0.67 |
| 1:MA:76:ASP:OD2 | 1:MA:79:ARG:NH2 | 2.27 | 0.67 |
| 6:4A:164:ARG:HB3 | 6:4A:164:ARG:HH11 | 1.57 | 0.67 |
| 6:4B:164:ARG:HB3 | 6:4B:164:ARG:HH11 | 1.57 | 0.67 |
| 6:4D:179:ARG:HH11 | 6:4D:179:ARG:HG2 | 1.59 | 0.67 |
| 7:5A:1565:GLU:HB3 | 7:5A:1568:LYS:HD2 | 1.75 | 0.67 |
| 7:5C:1565:GLU:HB3 | 7:5C:1568:LYS:HD2 | 1.75 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:224:TYR:HE2 | 2:AB:246:LEU:HD11 | 1.57 | 0.67 |
| 1:DA:402:ARG:NE | 7:5C:777:ALA:HB1 | 2.05 | 0.67 |
| 2:DD:85:PHE:O | 2:ED:281:TYR:CZ | 2.46 | 0.67 |
| 1:DE:76:ASP:OD2 | 1:DE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:EE:105:ARG:NH1 | 2:EF:251:ARG:HD3 | 2.10 | 0.67 |
| 2:EF:85:PHE:O | 2:FF:281:TYR:OH | 2.12 | 0.67 |
| 1:FC:76:ASP:OD2 | 1:FC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:FF:55:THR:HG23 | 2:GF:283:ALA:C | 2.19 | 0.67 |
| 1:HA:76:ASP:OD2 | 1:HA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:HA:282:TYR:CD1 | 10:8S:15:UNK:HA | 2.29 | 0.67 |
| 2:HB:226:ASN:HD21 | 13:HB:501:GDP:HN1 | 1.42 | 0.67 |
| 1:HE:101:ASN:HD21 | 2:HF:252:LYS:HD2 | 0.84 | 0.67 |
| 2:HF:226:ASN:HD21 | 13:HF:501:GDP:HN1 | 1.42 | 0.67 |
| 2:IB:391:ARG:HG3 | 1:IC:346:TRP:CD1 | 2.30 | 0.67 |
| 1:IE:101:ASN:HD21 | 2:IF:252:LYS:HD2 | 0.84 | 0.67 |
| 1:JE:101:ASN:HD21 | 2:JF:252:LYS:HD2 | 0.84 | 0.67 |
| 2:KD:217:LEU:CD2 | 6:4B:263:CYS:HG | 2.01 | 0.67 |
| 1:KE:101:ASN:HD21 | 2:KF:252:LYS:HD2 | 0.84 | 0.67 |
| 1:LA:76:ASP:OD2 | 1:LA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:MC:372:MET:HE2 | 6:4A:96:VAL:H | 1.58 | 0.67 |
| 6:4D:164:ARG:HB3 | 6:4D:164:ARG:HH11 | 1.57 | 0.67 |
| 7:5A:1573:ARG:C | 7:5A:1577:LYS:HB2 | 2.16 | 0.67 |
| 1:AA:222:PRO:CD | 2:AB:324:LYS:HD3 | 2.24 | 0.67 |
| 1:AC:76:ASP:OD2 | 1:AC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:AD:217:LEU:HD22 | 6:4C:132:LYS:HD3 | 1.75 | 0.67 |
| 1:BE:76:ASP:OD2 | 1:BE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:CC:76:ASP:OD2 | 1:CC:79:ARG:NH2 | 2.27 | 0.67 |
| 1:CE:76:ASP:OD2 | 1:CE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:FA:76:ASP:OD2 | 1:FA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:FC:71:GLU:CD | 2:FD:247:ASN:ND2 | 2.52 | 0.67 |
| 1:GC:60:LYS:HD2 | 1:HC:283:HIS:CD2 | 2.30 | 0.67 |
| 1:HC:76:ASP:OD2 | 1:HC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:HD:212:PHE:CZ | 1:HE:326:LYS:CD | 2.34 | 0.67 |
| 1:IC:76:ASP:OD2 | 1:IC:79:ARG:NH2 | 2.27 | 0.67 |
| 1:IE:76:ASP:OD2 | 1:IE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:IE:393:HIS:CB | 5:3A:308:PHE:HE2 | 2.06 | 0.67 |
| 1:JA:282:TYR:CD2 | 10:8Y:15:UNK:O | 2.47 | 0.67 |
| 1:JE:90:GLU:HG2 | 1:KE:280:LYS:HD2 | 1.76 | 0.67 |
| 2:JF:87:PRO:HG2 | 2:KF:278:SER:HA | 1.76 | 0.67 |
| 1:KA:222:PRO:CD | 2:KB:324:LYS:HD3 | 2.24 | 0.67 |
| 1:LC:407:TRP:HE3 | 2:LD:255:VAL:HG13 | 1.55 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:LD:226:ASN:HD21 | 13:LD:501:GDP:HN1 | 1.42 | 0.67 |
| 2:LF:221:THR:HG21 | 6:4D:220:GLY:N | 2.10 | 0.67 |
| 1:MC:76:ASP:OD2 | 1:MC:79:ARG:NH2 | 2.27 | 0.67 |
| 1:ME:76:ASP:OD2 | 1:ME:79:ARG:NH2 | 2.27 | 0.67 |
| 6:4B:179:ARG:HH11 | 6:4B:179:ARG:HG2 | 1.59 | 0.67 |
| 7:5A:1547:SER:O | 7:5A:1569:GLU:CD | 2.36 | 0.67 |
| 7:5B:1548:VAL:HG11 | 7:5B:1566:GLU:C | 2.18 | 0.67 |
| 7:5B:1565:GLU:HB3 | 7:5B:1568:LYS:HD2 | 1.75 | 0.67 |
| 7:5C:1332:GLN:CA | 7:5C:1332:GLN:HE21 | 2.07 | 0.67 |
| 7:5C:1547:SER:O | 7:5C:1569:GLU:CD | 2.36 | 0.67 |
| 1:CA:76:ASP:OD2 | 1:CA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:CC:11:GLN:OE1 | 2:CD:245:GLN:O | 2.12 | 0.67 |
| 2:CF:86:ARG:N | 2:DF:281:TYR:HE1 | 1.91 | 0.67 |
| 1:DC:76:ASP:OD2 | 1:DC:79:ARG:NH2 | 2.27 | 0.67 |
| 1:EA:105:ARG:NH1 | 2:EB:251:ARG:HD3 | 2.10 | 0.67 |
| 2:FD:220:PRO:O | 1:FE:324:VAL:HG13 | 1.93 | 0.67 |
| 1:GA:404:PHE:HE2 | 2:GB:345:ILE:CD1 | 2.07 | 0.67 |
| 2:GF:416:ASN:ND2 | 7:5B:1327:LYS:HE3 | 2.08 | 0.67 |
| 1:HE:76:ASP:OD2 | 1:HE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:CB | 2.56 | 0.67 |
| 1:IC:224:TYR:HE2 | 2:ID:246:LEU:HD11 | 1.57 | 0.67 |
| 1:JC:76:ASP:OD2 | 1:JC:79:ARG:NH2 | 2.27 | 0.67 |
| 2:LD:390:ARG:CD | 1:LE:439:THR:HG21 | 2.24 | 0.67 |
| 2:MB:226:ASN:HD21 | 13:MB:502:GDP:HN1 | 1.42 | 0.67 |
| 1:ME:279:GLU:O | 6:4B:107:MET:HG2 | 1.38 | 0.67 |
| 6:4C:164:ARG:HB3 | 6:4C:164:ARG:HH11 | 1.57 | 0.67 |
| 6:4D:221:MET:SD | 6:4D:222:PRO:HD2 | 2.33 | 0.67 |
| 7:5A:1332:GLN:HE21 | 7:5A:1332:GLN:CA | 2.07 | 0.67 |
| 7:5B:1392:LEU:C | 7:5B:1392:LEU:HD13 | 2.19 | 0.67 |
| 7:5C:1491:LEU:HD11 | 7:5C:1495:PHE:HE1 | 1.57 | 0.67 |
| 2:AB:391:ARG:HG3 | 1:AC:346:TRP:CD1 | 2.30 | 0.67 |
| 1:AE:76:ASP:OD2 | 1:AE:79:ARG:NH2 | 2.27 | 0.67 |
| 1:AE:101:ASN:HD21 | 2:AF:252:LYS:HD2 | 0.84 | 0.67 |
| 1:BE:404:PHE:HE2 | 2:BF:345:ILE:CD1 | 2.07 | 0.67 |
| 2:BF:226:ASN:HD21 | 13:BF:501:GDP:HN1 | 1.42 | 0.67 |
| 1:GE:101:ASN:HD21 | 2:GF:252:LYS:HD2 | 0.84 | 0.67 |
| 1:IA:76:ASP:OD2 | 1:IA:79:ARG:NH2 | 2.27 | 0.67 |
| 2:JB:226:ASN:HD21 | 13:JB:501:GDP:HN1 | 1.42 | 0.67 |
| 2:JB:391:ARG:HG3 | 1:JC:346:TRP:CD1 | 2.30 | 0.67 |
| 2:KB:397:TRP:CD2 | 1:KC:256:GLN:O | 2.30 | 0.67 |
| 2:LF:55:THR:HG23 | 2:MF:283:ALA:C | 2.16 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MD:226:ASN:HD21 | 13:MD:502:GDP:HN1 | 1.42 | 0.67 |
| 6:4D:285:ARG:HH11 | 6:4D:285:ARG:C | 2.03 | 0.67 |
| 7:5B:1332:GLN:CA | 7:5B:1332:GLN:HE21 | 2.07 | 0.67 |
| 7:5B:1547:SER:O | 7:5B:1569:GLU:CD | 2.36 | 0.67 |
| 1:DA:76:ASP:OD2 | 1:DA:79:ARG:NH2 | 2.27 | 0.67 |
| 1:DA:222:PRO:HD2 | 2:DB:324:LYS:HD3 | 1.74 | 0.67 |
| 2:EB:179:VAL:CG2 | 1:EC:258:ASN:HA | 2.25 | 0.67 |
| 1:EC:404:PHE:CE2 | 2:ED:345:ILE:CD1 | 2.76 | 0.67 |
| 2:FB:390:ARG:CD | 1:FC:439:THR:HG21 | 2.24 | 0.67 |
| 1:GE:224:TYR:HE2 | 2:GF:246:LEU:HD11 | 1.59 | 0.67 |
| 1:HE:370:LYS:HG3 | 10:8U:18:UNK:N | 2.04 | 0.67 |
| 1:JE:76:ASP:OD2 | 1:JE:79:ARG:NH2 | 2.27 | 0.67 |
| 2:KB:276:ARG:NH2 | 6:4A:266:ASN:N | 2.41 | 0.67 |
| 1:KC:224:TYR:HE2 | 2:KD:246:LEU:HD11 | 1.57 | 0.67 |
| 2:LB:226:ASN:HD21 | 13:LB:501:GDP:HN1 | 1.42 | 0.67 |
| 1:MC:372:MET:CE | 6:4A:96:VAL:C | 2.51 | 0.67 |
| 6:4A:110:LYS:HE2 | 6:4A:113:ILE:HD11 | 1.74 | 0.67 |
| 6:4A:179:ARG:HH11 | 6:4A:179:ARG:HG2 | 1.59 | 0.67 |
| 6:4B:110:LYS:HE2 | 6:4B:113:ILE:HD11 | 1.75 | 0.67 |
| 6:4B:285:ARG:HH11 | 6:4B:285:ARG:C | 2.03 | 0.67 |
| 7:5A:1392:LEU:C | 7:5A:1392:LEU:HD13 | 2.19 | 0.67 |
| 7:5C:1426:GLU:OE2 | 7:5C:1426:GLU:HA | 1.95 | 0.67 |
| 7:5C:1548:VAL:HG11 | 7:5C:1566:GLU:C | 2.18 | 0.67 |
| 1:DA:71:GLU:OE1 | 2:DB:247:ASN:ND2 | 2.28 | 0.67 |
| 1:DC:414:GLU:OE2 | 7:5A:789:LYS:NZ | 2.27 | 0.67 |
| 2:DD:179:VAL:CG2 | 1:DE:258:ASN:O | 2.33 | 0.67 |
| 1:DE:222:PRO:HD2 | 2:DF:324:LYS:HD3 | 1.75 | 0.67 |
| 2:EB:177:ASP:OD1 | 1:EC:353:VAL:HG12 | 1.81 | 0.67 |
| 2:HB:391:ARG:HG3 | 1:HC:346:TRP:CD1 | 2.30 | 0.67 |
| 2:JD:226:ASN:HD21 | 13:JD:501:GDP:HN1 | 1.42 | 0.67 |
| 2:KF:221:THR:CG2 | 6:4D:261:SER:CA | 2.49 | 0.67 |
| 2:LD:178:THR:HG23 | 1:LE:258:ASN:ND2 | 2.07 | 0.67 |
| 1:MA:282:TYR:CD1 | 6:4C:98:PRO:HB3 | 2.29 | 0.67 |
| 6:4A:285:ARG:HH11 | 6:4A:285:ARG:C | 2.03 | 0.67 |
| 6:4B:221:MET:SD | 6:4B:222:PRO:HD2 | 2.33 | 0.67 |
| 6:4C:221:MET:SD | 6:4C:222:PRO:HD2 | 2.33 | 0.67 |
| 6:4C:285:ARG:HH11 | 6:4C:285:ARG:C | 2.03 | 0.67 |
| 6:4D:110:LYS:HE2 | 6:4D:113:ILE:HD11 | 1.75 | 0.67 |
| 7:5C:1573:ARG:C | 7:5C:1577:LYS:HB2 | 2.16 | 0.67 |
| 2:BD:226:ASN:HD21 | 13:BD:501:GDP:HN1 | 1.42 | 0.67 |
| 2:DD:397:TRP:HE3 | 1:DE:257:THR:CG2 | 2.01 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HB:148:GLY:O | 2:HB:152:ILE:HG12 | 1.95 | 0.67 |
| 2:IF:86:ARG:CB | 2:JF:281:TYR:CE1 | 2.77 | 0.67 |
| 1:JE:90:GLU:C | 1:KE:280:LYS:NZ | 2.27 | 0.67 |
| 2:KB:215:LEU:HD13 | 6:4A:267:ILE:HG22 | 0.68 | 0.67 |
| 1:LA:60:LYS:HD3 | 1:MA:283:HIS:HA | 1.76 | 0.67 |
| 2:LB:55:THR:HG21 | 2:MB:284:LEU:N | 2.09 | 0.67 |
| 2:LB:148:GLY:O | 2:LB:152:ILE:HG12 | 1.95 | 0.67 |
| 1:LC:84:ARG:NH1 | 6:4A:108:LYS:CE | 2.45 | 0.67 |
| 2:LD:148:GLY:O | 2:LD:152:ILE:HG12 | 1.95 | 0.67 |
| 2:LF:148:GLY:O | 2:LF:152:ILE:HG12 | 1.95 | 0.67 |
| 7:5A:1426:GLU:OE2 | 7:5A:1426:GLU:HA | 1.95 | 0.67 |
| 7:5A:1548:VAL:HG11 | 7:5A:1566:GLU:C | 2.18 | 0.67 |
| 7:5C:1152:GLU:CD | 8:6C:66:ARG:NH2 | 2.53 | 0.67 |
| 7:5C:1392:LEU:C | 7:5C:1392:LEU:HD13 | 2.19 | 0.67 |
| 7:5C:1482:SER:O | 7:5C:1486:THR:N | 2.21 | 0.67 |
| 9:7C:7:LEU:HD23 | 9:7D:30:ARG:HE | 1.58 | 0.67 |
| 1:AC:404:PHE:HE2 | 2:AD:345:ILE:CD1 | 2.09 | 0.67 |
| 2:DB:220:PRO:HD2 | 1:DC:326:LYS:CG | 2.23 | 0.67 |
| 1:EC:398:MET:SD | 2:ED:345:ILE:CG1 | 2.79 | 0.67 |
| 2:ED:86:ARG:CA | 2:FD:281:TYR:CE1 | 2.78 | 0.67 |
| 1:EE:426:ALA:CB | 7:5B:833:PHE:CD1 | 2.51 | 0.67 |
| 1:HC:404:PHE:HE2 | 2:HD:345:ILE:CD1 | 2.08 | 0.67 |
| 2:HD:148:GLY:O | 2:HD:152:ILE:HG12 | 1.95 | 0.67 |
| 2:HF:148:GLY:O | 2:HF:152:ILE:HG12 | 1.95 | 0.67 |
| 1:IE:401:LYS:CE | 2:IF:344:TRP:CZ3 | 2.67 | 0.67 |
| 1:IE:402:ARG:HE | 7:5B:1417:GLN:HG3 | 1.58 | 0.67 |
| 2:JD:177:ASP:O | 1:JE:352:LYS:CD | 2.34 | 0.67 |
| 2:KB:148:GLY:O | 2:KB:152:ILE:HG12 | 1.95 | 0.67 |
| 2:KB:391:ARG:HG3 | 1:KC:346:TRP:CD1 | 2.30 | 0.67 |
| 2:KD:148:GLY:O | 2:KD:152:ILE:HG12 | 1.95 | 0.67 |
| 2:KF:148:GLY:O | 2:KF:152:ILE:HG12 | 1.95 | 0.67 |
| 1:LC:60:LYS:NZ | 1:MC:283:HIS:CG | 2.53 | 0.67 |
| 1:MC:279:GLU:O | 6:4A:107:MET:HG2 | 1.44 | 0.67 |
| 2:MD:111:GLU:HA | 3:1B:62:SER:HA | 1.76 | 0.67 |
| 6:4A:221:MET:SD | 6:4A:222:PRO:HD2 | 2.33 | 0.67 |
| 6:4C:179:ARG:HH11 | 6:4C:179:ARG:HG2 | 1.59 | 0.67 |
| 7:5A:1491:LEU:HD11 | 7:5A:1495:PHE:HE1 | 1.57 | 0.67 |
| 8:6A:20:LYS:NZ | 8:6A:101:GLU:OE1 | 2.26 | 0.67 |
| 9:7A:7:LEU:HD23 | 9:7B:30:ARG:HE | 1.58 | 0.67 |
| 9:7A:12:GLU:HA | 9:7A:16:THR:OG1 | 1.94 | 0.67 |
| 2:BB:86:ARG:CA | 2:CB:281:TYR:CE1 | 2.67 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:DD:176:SER:OG | 1:DE:349:THR:OG1 | 2.11 | 0.66 |
| 2:DD:220:PRO:CD | 1:DE:326:LYS:HG2 | 2.24 | 0.66 |
| 2:EB:148:GLY:O | 2:EB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:ED:148:GLY:O | 2:ED:152:ILE:HG12 | 1.95 | 0.66 |
| 2:ED:220:PRO:HD2 | 1:EE:326:LYS:CG | 2.25 | 0.66 |
| 2:FD:331:LEU:HD21 | 7:5A:915:PHE:CZ | 2.30 | 0.66 |
| 1:HE:224:TYR:HE2 | 2:HF:246:LEU:HD11 | 1.59 | 0.66 |
| 2:ID:148:GLY:O | 2:ID:152:ILE:HG12 | 1.95 | 0.66 |
| 2:IF:148:GLY:O | 2:IF:152:ILE:HG12 | 1.95 | 0.66 |
| 2:JD:86:ARG:HH12 | 2:KD:280:GLN:HB3 | 1.56 | 0.66 |
| 2:JF:226:ASN:HD21 | 13:JF:501:GDP:HN1 | 1.42 | 0.66 |
| 1:KA:85:GLN:HA | 1:LA:283:HIS:N | 2.09 | 0.66 |
| 1:KC:359:PRO:HG3 | 6:4A:299:TYR:CD2 | 2.31 | 0.66 |
| 1:MA:404:PHE:CE2 | 2:MB:345:ILE:CD1 | 2.78 | 0.66 |
| 2:MD:111:GLU:CG | 3:1B:62:SER:HA | 2.20 | 0.66 |
| 2:MF:226:ASN:HD21 | 13:MF:502:GDP:HN1 | 1.42 | 0.66 |
| 6:4C:110:LYS:HE2 | 6:4C:113:ILE:HD11 | 1.74 | 0.66 |
| 9:7E:12:GLU:HA | 9:7E:16:THR:OG1 | 1.94 | 0.66 |
| 1:BA:401:LYS:CE | 2:BB:344:TRP:CZ3 | 2.68 | 0.66 |
| 2:BB:226:ASN:HD21 | 13:BB:501:GDP:HN1 | 1.42 | 0.66 |
| 2:DB:148:GLY:O | 2:DB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:DD:148:GLY:O | 2:DD:152:ILE:HG12 | 1.95 | 0.66 |
| 1:DE:11:GLN:NE2 | 2:DF:247:ASN:OD1 | 2.28 | 0.66 |
| 2:EF:148:GLY:O | 2:EF:152:ILE:HG12 | 1.95 | 0.66 |
| 2:FD:332:ASN:CG | 7:5A:909:ASN:HD21 | 2.04 | 0.66 |
| 2:GB:148:GLY:O | 2:GB:152:ILE:HG12 | 1.95 | 0.66 |
| 1:GC:60:LYS:HD3 | 1:HC:283:HIS:HA | 1.76 | 0.66 |
| 1:GE:60:LYS:HD3 | 1:HE:283:HIS:HA | 1.75 | 0.66 |
| 2:IB:148:GLY:O | 2:IB:152:ILE:HG12 | 1.95 | 0.66 |
| 1:KE:88:HIS:HA | 1:LE:284:GLU:CA | 2.24 | 0.66 |
| 2:KF:226:ASN:HD21 | 13:KF:501:GDP:HN1 | 1.42 | 0.66 |
| 2:MF:148:GLY:O | 2:MF:152:ILE:HG12 | 1.95 | 0.66 |
| 7:5C:1399:LYS:O | 7:5C:1399:LYS:HG2 | 1.94 | 0.66 |
| 7:5C:1524:PHE:CE1 | 7:5C:1571:MET:HE2 | 2.29 | 0.66 |
| 7:5C:1533:GLU:CD | 7:5C:1604:ALA:HB1 | 2.20 | 0.66 |
| 9:7A:10:TYR:HE2 | 9:7B:26:LEU:HG | 1.60 | 0.66 |
| 2:BB:208:TYR:OH | 1:BC:325:PRO:HB2 | 1.95 | 0.66 |
| 2:CB:148:GLY:O | 2:CB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:CB:208:TYR:OH | 1:CC:325:PRO:HB2 | 1.94 | 0.66 |
| 1:CE:60:LYS:NZ | 1:DE:283:HIS:CE1 | 2.63 | 0.66 |
| 2:CF:86:ARG:CB | 2:DF:281:TYR:HE1 | 1.90 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:DF:148:GLY:O | 2:DF:152:ILE:HG12 | 1.95 | 0.66 |
| 1:FA:423:GLU:CD | 7:5C:1256:ARG:HH22 | 1.99 | 0.66 |
| 1:GE:60:LYS:NZ | 1:HE:283:HIS:ND1 | 2.40 | 0.66 |
| 2:HD:397:TRP:CD2 | 1:HE:256:GLN:O | 2.31 | 0.66 |
| 1:IA:404:PHE:HE2 | 2:IB:345:ILE:CD1 | 2.07 | 0.66 |
| 2:JB:177:ASP:O | 1:JC:352:LYS:CD | 2.35 | 0.66 |
| 2:JF:148:GLY:O | 2:JF:152:ILE:HG12 | 1.95 | 0.66 |
| 2:KF:83:GLN:HA | 2:LF:281:TYR:CE1 | 2.30 | 0.66 |
| 1:LA:60:LYS:HD2 | 1:MA:283:HIS:CD2 | 2.28 | 0.66 |
| 2:LB:390:ARG:HD2 | 1:LC:439:THR:HG21 | 1.75 | 0.66 |
| 1:LE:407:TRP:HE3 | 2:LF:255:VAL:HG13 | 1.57 | 0.66 |
| 2:MD:148:GLY:O | 2:MD:152:ILE:HG12 | 1.95 | 0.66 |
| 6:4A:242:ARG:O | 6:4A:247:LYS:HE3 | 1.94 | 0.66 |
| 7:5A:1524:PHE:CE1 | 7:5A:1571:MET:HE2 | 2.29 | 0.66 |
| 7:5A:1533:GLU:CD | 7:5A:1604:ALA:HB1 | 2.20 | 0.66 |
| 7:5B:1399:LYS:O | 7:5B:1399:LYS:HG2 | 1.93 | 0.66 |
| 7:5B:1426:GLU:OE2 | 7:5B:1426:GLU:HA | 1.95 | 0.66 |
| 2:AF:40:SER:CB | 6:4A:152:PHE:CE2 | 2.74 | 0.66 |
| 2:CD:148:GLY:O | 2:CD:152:ILE:HG12 | 1.95 | 0.66 |
| 2:CF:148:GLY:O | 2:CF:152:ILE:HG12 | 1.95 | 0.66 |
| 2:EF:157:GLU:OE1 | 7:5B:935:LYS:CE | 2.43 | 0.66 |
| 2:FB:148:GLY:O | 2:FB:152:ILE:HG12 | 1.95 | 0.66 |
| 1:FC:224:TYR:HE2 | 2:FD:246:LEU:HD11 | 1.58 | 0.66 |
| 2:FF:148:GLY:O | 2:FF:152:ILE:HG12 | 1.95 | 0.66 |
| 2:GB:391:ARG:HG3 | 1:GC:346:TRP:CD1 | 2.30 | 0.66 |
| 2:GD:148:GLY:O | 2:GD:152:ILE:HG12 | 1.95 | 0.66 |
| 2:GF:148:GLY:O | 2:GF:152:ILE:HG12 | 1.95 | 0.66 |
| 1:IA:402:ARG:CZ | 7:5C:1417:GLN:CB | 2.73 | 0.66 |
| 2:IF:226:ASN:HD21 | 13:IF:501:GDP:HN1 | 1.42 | 0.66 |
| 2:JD:148:GLY:O | 2:JD:152:ILE:HG12 | 1.95 | 0.66 |
| 1:LE:222:PRO:HG2 | 2:LF:324:LYS:CB | 2.25 | 0.66 |
| 2:MB:148:GLY:O | 2:MB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:MB:221:THR:CG2 | 6:4A:189:ARG:HH12 | 2.08 | 0.66 |
| 6:4B:242:ARG:O | 6:4B:247:LYS:HE3 | 1.94 | 0.66 |
| 7:5B:1353:GLU:HB3 | 7:5B:1357:LYS:HE3 | 1.77 | 0.66 |
| 7:5B:1524:PHE:CE1 | 7:5B:1571:MET:HE2 | 2.29 | 0.66 |
| 9:7E:14:SER:O | 9:7F:35:ILE:HD11 | 1.95 | 0.66 |
| 2:CD:220:PRO:HD2 | 1:CE:326:LYS:CE | 2.26 | 0.66 |
| 2:CF:226:ASN:HD21 | 13:CF:501:GDP:HN1 | 1.42 | 0.66 |
| 1:DE:101:ASN:HD21 | 2:DF:252:LYS:HD2 | 0.85 | 0.66 |
| 1:EC:100:ALA:HB1 | 2:ED:252:LYS:HA | 1.77 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:EC:396:ASP:CG | 7:5A:821:LEU:HD11 | 2.20 | 0.66 |
| 2:ED:100:ASN:HB2 | 1:EE:257:THR:HG21 | 1.78 | 0.66 |
| 1:EE:393:HIS:ND1 | 7:5B:814:LYS:CG | 2.59 | 0.66 |
| 2:FD:148:GLY:O | 2:FD:152:ILE:HG12 | 1.95 | 0.66 |
| 1:HC:159:VAL:HG22 | 5:3C:209:ARG:HH21 | 1.58 | 0.66 |
| 1:HE:415:GLU:HG3 | 5:3A:235:LEU:HB2 | 1.74 | 0.66 |
| 2:JB:148:GLY:O | 2:JB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:KD:226:ASN:HD21 | 13:KD:501:GDP:HN1 | 1.42 | 0.66 |
| 2:KF:125:GLU:O | 4:2B:38:VAL:HA | 1.94 | 0.66 |
| 1:LA:222:PRO:CG | 2:LB:324:LYS:HD2 | 2.24 | 0.66 |
| 2:LB:223:GLY:C | 6:4A:219:ASN:CG | 2.59 | 0.66 |
| 2:LB:391:ARG:O | 1:LC:262:TYR:OH | 2.14 | 0.66 |
| 1:LC:224:TYR:CE2 | 2:LD:246:LEU:HD11 | 2.29 | 0.66 |
| 1:ME:100:ALA:HB1 | 2:MF:252:LYS:HA | 1.77 | 0.66 |
| 2:MF:221:THR:CG2 | 6:4D:189:ARG:NH2 | 2.08 | 0.66 |
| 4:2A:112:GLU:OE2 | 4:2A:115:LEU:CD1 | 2.44 | 0.66 |
| 4:2B:112:GLU:OE2 | 4:2B:115:LEU:CD1 | 2.44 | 0.66 |
| 4:2C:112:GLU:OE2 | 4:2C:115:LEU:CD1 | 2.44 | 0.66 |
| 6:4C:242:ARG:O | 6:4C:247:LYS:HE3 | 1.94 | 0.66 |
| 6:4D:242:ARG:O | 6:4D:247:LYS:HE3 | 1.94 | 0.66 |
| 7:5A:1353:GLU:HB3 | 7:5A:1357:LYS:HE3 | 1.77 | 0.66 |
| 7:5A:1482:SER:O | 7:5A:1486:THR:N | 2.21 | 0.66 |
| 7:5B:1491:LEU:HD11 | 7:5B:1495:PHE:HE1 | 1.57 | 0.66 |
| 2:AB:220:PRO:O | 1:AC:324:VAL:HG13 | 1.95 | 0.66 |
| 2:AD:397:TRP:CD2 | 1:AE:256:GLN:O | 2.31 | 0.66 |
| 1:BA:101:ASN:HD21 | 2:BB:252:LYS:HD2 | 0.84 | 0.66 |
| 2:BB:148:GLY:O | 2:BB:152:ILE:HG12 | 1.95 | 0.66 |
| 2:BD:148:GLY:O | 2:BD:152:ILE:HG12 | 1.95 | 0.66 |
| 1:CE:98:ASP:OD1 | 1:CE:99:ALA:N | 2.29 | 0.66 |
| 1:CE:224:TYR:HE2 | 2:CF:246:LEU:HD11 | 1.59 | 0.66 |
| 2:DF:226:ASN:HD21 | 13:DF:501:GDP:HN1 | 1.42 | 0.66 |
| 1:EA:11:GLN:NE2 | 2:EB:247:ASN:OD1 | 2.29 | 0.66 |
| 1:EA:222:PRO:HD2 | 2:EB:324:LYS:HD3 | 1.77 | 0.66 |
| 1:FA:85:GLN:O | 1:GA:283:HIS:CE1 | 2.49 | 0.66 |
| 2:ID:226:ASN:HD21 | 13:ID:501:GDP:HN1 | 1.42 | 0.66 |
| 1:JE:401:LYS:CE | 2:JF:344:TRP:CZ3 | 2.67 | 0.66 |
| 1:KC:79:ARG:HG2 | 1:LC:280:LYS:NZ | 2.00 | 0.66 |
| 1:KC:404:PHE:HE2 | 2:KD:345:ILE:CD1 | 2.09 | 0.66 |
| 1:MC:279:GLU:O | 6:4A:107:MET:CB | 2.43 | 0.66 |
| 6:4C:266:ASN:HB2 | 6:4C:273:ARG:NH1 | 2.11 | 0.66 |
| 7:5A:1399:LYS:HG2 | 7:5A:1399:LYS:O | 1.94 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1533:GLU:CD | 7:5B:1604:ALA:HB1 | 2.20 | 0.66 |
| 7:5C:1353:GLU:HB3 | 7:5C:1357:LYS:HE3 | 1.77 | 0.66 |
| 8:6C:131:ASP:H | 8:6C:136:LEU:HD12 | 1.60 | 0.66 |
| 1:AC:98:ASP:OD1 | 1:AC:99:ALA:N | 2.29 | 0.66 |
| 2:BF:86:ARG:CA | 2:CF:281:TYR:CE1 | 2.61 | 0.66 |
| 1:CA:98:ASP:OD1 | 1:CA:99:ALA:N | 2.29 | 0.66 |
| 1:CA:101:ASN:HD21 | 2:CB:252:LYS:HD2 | 0.83 | 0.66 |
| 1:CC:98:ASP:OD1 | 1:CC:99:ALA:N | 2.29 | 0.66 |
| 1:FC:98:ASP:OD1 | 1:FC:99:ALA:N | 2.29 | 0.66 |
| 1:FC:222:PRO:HD2 | 2:FD:324:LYS:HD3 | 1.77 | 0.66 |
| 1:FE:98:ASP:OD1 | 1:FE:99:ALA:N | 2.29 | 0.66 |
| 1:GA:56:THR:O | 1:HA:285:GLN:HB3 | 1.96 | 0.66 |
| 1:GA:98:ASP:OD1 | 1:GA:99:ALA:N | 2.29 | 0.66 |
| 1:GE:60:LYS:CD | 1:HE:283:HIS:HB3 | 2.21 | 0.66 |
| 1:HC:278:ALA:HB2 | 10:8T:21:UNK:CB | 2.26 | 0.66 |
| 1:JA:88:HIS:O | 1:KA:280:LYS:NZ | 2.25 | 0.66 |
| 1:JC:98:ASP:OD1 | 1:JC:99:ALA:N | 2.29 | 0.66 |
| 1:JC:404:PHE:HE2 | 2:JD:345:ILE:CD1 | 2.08 | 0.66 |
| 1:LA:47:ASP:OD1 | 6:4C:203:LYS:NZ | 2.27 | 0.66 |
| 1:LC:60:LYS:CD | 6:4A:101:ARG:NH2 | 2.42 | 0.66 |
| 2:LD:397:TRP:CE3 | 1:LE:257:THR:HG23 | 2.27 | 0.66 |
| 1:MA:372:MET:HE2 | 6:4C:96:VAL:H | 1.56 | 0.66 |
| 6:4A:266:ASN:HB2 | 6:4A:273:ARG:NH1 | 2.11 | 0.66 |
| 1:AA:98:ASP:OD1 | 1:AA:99:ALA:N | 2.29 | 0.66 |
| 1:AE:98:ASP:OD1 | 1:AE:99:ALA:N | 2.29 | 0.66 |
| 1:BA:98:ASP:OD1 | 1:BA:99:ALA:N | 2.29 | 0.66 |
| 1:BC:404:PHE:HE2 | 2:BD:345:ILE:CD1 | 2.08 | 0.66 |
| 2:CD:220:PRO:HD2 | 1:CE:326:LYS:CG | 2.25 | 0.66 |
| 2:CD:226:ASN:HD21 | 13:CD:501:GDP:HN1 | 1.42 | 0.66 |
| 1:CE:101:ASN:HD21 | 2:CF:252:LYS:HD2 | 0.83 | 0.66 |
| 1:EC:430:LYS:HZ1 | 7:5A:834:ASN:HD21 | 0.78 | 0.66 |
| 1:FA:98:ASP:OD1 | 1:FA:99:ALA:N | 2.29 | 0.66 |
| 2:FB:331:LEU:HD21 | 7:5C:915:PHE:CE1 | 2.30 | 0.66 |
| 1:FE:71:GLU:CD | 2:FF:247:ASN:ND2 | 2.54 | 0.66 |
| 2:GB:58:ARG:NH2 | 2:HB:281:TYR:CZ | 2.64 | 0.66 |
| 1:GC:98:ASP:OD1 | 1:GC:99:ALA:N | 2.29 | 0.66 |
| 1:GE:98:ASP:OD1 | 1:GE:99:ALA:N | 2.29 | 0.66 |
| 1:IA:328:VAL:HG11 | 1:IA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:IC:404:PHE:HE2 | 2:ID:345:ILE:CD1 | 2.09 | 0.66 |
| 2:JD:177:ASP:OD1 | 1:JE:353:VAL:HG12 | 1.84 | 0.66 |
| 1:JE:98:ASP:OD1 | 1:JE:99:ALA:N | 2.29 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:2B:12:LEU:HD23 | 4:2B:20:LYS:CB | 2.21 | 0.66 |
| 7:5C:1423:LYS:HA | 7:5C:1423:LYS:HE2 | 1.76 | 0.66 |
| 7:5C:1572:LEU:HD11 | 7:5C:1576:ILE:HD11 | 1.78 | 0.66 |
| 9:7A:18:VAL:HG11 | 9:7A:42:LEU:HD22 | 1.77 | 0.66 |
| 1:BC:98:ASP:OD1 | 1:BC:99:ALA:N | 2.29 | 0.66 |
| 2:BF:148:GLY:O | 2:BF:152:ILE:HG12 | 1.95 | 0.66 |
| 1:DA:224:TYR:HE2 | 2:DB:246:LEU:HD11 | 1.61 | 0.66 |
| 2:DD:226:ASN:HD21 | 13:DD:501:GDP:HN1 | 1.42 | 0.66 |
| 2:EB:397:TRP:CD2 | 1:EC:256:GLN:O | 2.31 | 0.66 |
| 1:FA:328:VAL:HG11 | 1:FA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:FE:328:VAL:HG11 | 1:FE:353:VAL:HG21 | 1.78 | 0.66 |
| 1:HA:278:ALA:HB2 | 10:8S:21:UNK:CB | 2.26 | 0.66 |
| 1:HA:328:VAL:HG11 | 1:HA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:JA:98:ASP:OD1 | 1:JA:99:ALA:N | 2.29 | 0.66 |
| 1:JA:328:VAL:HG11 | 1:JA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:KE:90:GLU:N | 1:LE:284:GLU:OE1 | 2.28 | 0.66 |
| 1:KE:328:VAL:HG11 | 1:KE:353:VAL:HG21 | 1.78 | 0.66 |
| 1:LA:98:ASP:OD1 | 1:LA:99:ALA:N | 2.29 | 0.66 |
| 2:MB:178:THR:HG23 | 1:MC:258:ASN:ND2 | 2.07 | 0.66 |
| 1:MC:328:VAL:HG11 | 1:MC:353:VAL:HG21 | 1.78 | 0.66 |
| 2:MF:221:THR:CG2 | 6:4D:189:ARG:HH12 | 2.08 | 0.66 |
| 6:4B:266:ASN:HB2 | 6:4B:273:ARG:NH1 | 2.11 | 0.66 |
| 7:5A:1105:TYR:HE2 | 7:5A:1258:ARG:HH22 | 1.44 | 0.66 |
| 7:5A:1267:CYS:SG | 9:7A:8:ARG:CD | 2.84 | 0.66 |
| 7:5A:1423:LYS:HA | 7:5A:1423:LYS:HE2 | 1.77 | 0.66 |
| 7:5B:1423:LYS:HA | 7:5B:1423:LYS:HE2 | 1.76 | 0.66 |
| 7:5B:1482:SER:O | 7:5B:1486:THR:N | 2.21 | 0.66 |
| 9:7C:11:TYR:HE1 | 9:7D:26:LEU:CD2 | 1.89 | 0.66 |
| 2:BD:87:PRO:HD2 | 2:CD:281:TYR:CE2 | 2.30 | 0.66 |
| 1:CA:222:PRO:HD2 | 2:CB:324:LYS:HD3 | 1.76 | 0.66 |
| 1:DC:11:GLN:NE2 | 2:DD:247:ASN:OD1 | 2.29 | 0.66 |
| 1:DE:98:ASP:OD1 | 1:DE:99:ALA:N | 2.29 | 0.66 |
| 1:EA:328:VAL:HG11 | 1:EA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:EE:328:VAL:HG11 | 1:EE:353:VAL:HG21 | 1.78 | 0.66 |
| 1:FC:89:PRO:N | 1:GC:280:LYS:HZ1 | 1.86 | 0.66 |
| 1:FC:328:VAL:HG11 | 1:FC:353:VAL:HG21 | 1.78 | 0.66 |
| 1:FE:404:PHE:HE2 | 2:FF:345:ILE:HD12 | 1.61 | 0.66 |
| 1:FE:422:ARG:NE | 7:5B:1170:THR:CB | 2.57 | 0.66 |
| 1:HA:98:ASP:OD1 | 1:HA:99:ALA:N | 2.29 | 0.66 |
| 1:HC:98:ASP:OD1 | 1:HC:99:ALA:N | 2.29 | 0.66 |
| 1:HC:328:VAL:HG11 | 1:HC:353:VAL:HG21 | 1.78 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:IE:328:VAL:HG11 | 1:IE:353:VAL:HG21 | 1.78 | 0.66 |
| 1:KA:98:ASP:OD1 | 1:KA:99:ALA:N | 2.29 | 0.66 |
| 1:KA:328:VAL:HG11 | 1:KA:353:VAL:HG21 | 1.78 | 0.66 |
| 2:KB:226:ASN:HD21 | 13:KB:501:GDP:HN1 | 1.42 | 0.66 |
| 1:KC:98:ASP:OD1 | 1:KC:99:ALA:N | 2.29 | 0.66 |
| 1:KE:98:ASP:OD1 | 1:KE:99:ALA:N | 2.29 | 0.66 |
| 1:LA:328:VAL:HG11 | 1:LA:353:VAL:HG21 | 1.78 | 0.66 |
| 1:MA:100:ALA:HB1 | 2:MB:252:LYS:HA | 1.77 | 0.66 |
| 1:MA:328:VAL:HG11 | 1:MA:353:VAL:HG21 | 1.78 | 0.66 |
| 4:2A:12:LEU:HD23 | 4:2A:20:LYS:CB | 2.21 | 0.66 |
| 7:5B:1105:TYR:HE2 | 7:5B:1258:ARG:HH22 | 1.44 | 0.66 |
| 7:5B:1572:LEU:HD11 | 7:5B:1576:ILE:HD11 | 1.78 | 0.66 |
| 7:5C:1105:TYR:HE2 | 7:5C:1258:ARG:HH22 | 1.44 | 0.66 |
| 9:7F:12:GLU:O | 9:7F:16:THR:OG1 | 2.14 | 0.66 |
| 1:AA:60:LYS:HD3 | 1:BA:283:HIS:CD2 | 2.30 | 0.65 |
| 1:BE:328:VAL:HG11 | 1:BE:353:VAL:HG21 | 1.78 | 0.65 |
| 2:CB:226:ASN:HD21 | 13:CB:501:GDP:HN1 | 1.42 | 0.65 |
| 1:DC:98:ASP:OD1 | 1:DC:99:ALA:N | 2.29 | 0.65 |
| 1:DE:400:ALA:CA | 7:5B:775:PRO:HB3 | 2.26 | 0.65 |
| 1:EC:328:VAL:HG11 | 1:EC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:FA:56:THR:CA | 1:GA:285:GLN:CB | 2.63 | 0.65 |
| 1:FA:224:TYR:HE2 | 2:FB:246:LEU:HD11 | 1.61 | 0.65 |
| 2:GD:177:ASP:OD1 | 1:GE:353:VAL:HG12 | 1.84 | 0.65 |
| 1:GE:56:THR:OG1 | 1:HE:285:GLN:N | 2.29 | 0.65 |
| 1:HA:101:ASN:HD21 | 2:HB:252:LYS:HD2 | 0.82 | 0.65 |
| 2:IB:226:ASN:HD21 | 13:IB:501:GDP:HN1 | 1.42 | 0.65 |
| 1:IC:328:VAL:HG11 | 1:IC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:JA:101:ASN:HD21 | 2:JB:252:LYS:HD2 | 0.82 | 0.65 |
| 2:JB:208:TYR:OH | 1:JC:325:PRO:HB2 | 1.96 | 0.65 |
| 1:JC:328:VAL:HG11 | 1:JC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:KA:87:PHE:C | 1:LA:283:HIS:O | 2.40 | 0.65 |
| 1:KC:328:VAL:HG11 | 1:KC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:LA:404:PHE:CE1 | 2:LB:259:PRO:HA | 2.32 | 0.65 |
| 2:LB:212:PHE:CE2 | 1:LC:326:LYS:HD3 | 2.17 | 0.65 |
| 1:LC:98:ASP:OD1 | 1:LC:99:ALA:N | 2.29 | 0.65 |
| 1:ME:328:VAL:HG11 | 1:ME:353:VAL:HG21 | 1.78 | 0.65 |
| 1:ME:372:MET:HE2 | 6:4B:96:VAL:H | 1.56 | 0.65 |
| 4:2C:171:VAL:HB | 4:2C:176:ARG:HH21 | 1.61 | 0.65 |
| 6:4D:266:ASN:HB2 | 6:4D:273:ARG:NH1 | 2.11 | 0.65 |
| 7:5A:1572:LEU:HD11 | 7:5A:1576:ILE:HD11 | 1.78 | 0.65 |
| 7:5B:1425:LYS:NZ | 7:5B:1429:GLN:HB2 | 2.11 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:7C:35:ILE:HG22 | 9:7D:43:LEU:HA | 1.78 | 0.65 |
| 2:AD:356:ILE:CD1 | 6:4C:152:PHE:HE1 | 2.07 | 0.65 |
| 1:AE:328:VAL:HG11 | 1:AE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:BA:224:TYR:HE2 | 2:BB:246:LEU:HD11 | 1.61 | 0.65 |
| 1:BA:328:VAL:HG11 | 1:BA:353:VAL:HG21 | 1.78 | 0.65 |
| 1:BC:328:VAL:HG11 | 1:BC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:BE:98:ASP:OD1 | 1:BE:99:ALA:N | 2.29 | 0.65 |
| 1:DA:328:VAL:HG11 | 1:DA:353:VAL:HG21 | 1.78 | 0.65 |
| 1:DC:328:VAL:HG11 | 1:DC:353:VAL:HG21 | 1.78 | 0.65 |
| 2:ED:125:GLU:CD | 7:5A:903:PHE:HE2 | 2.03 | 0.65 |
| 2:FF:226:ASN:HD21 | 13:FF:501:GDP:HN1 | 1.42 | 0.65 |
| 1:JE:328:VAL:HG11 | 1:JE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:KE:401:LYS:CE | 2:KF:344:TRP:CZ3 | 2.67 | 0.65 |
| 2:KF:159:TYR:CE2 | 4:2B:35:VAL:C | 2.74 | 0.65 |
| 1:LC:328:VAL:HG11 | 1:LC:353:VAL:HG21 | 1.78 | 0.65 |
| 4:2A:171:VAL:HB | 4:2A:176:ARG:HH21 | 1.61 | 0.65 |
| 7:5A:1425:LYS:NZ | 7:5A:1429:GLN:HB2 | 2.11 | 0.65 |
| 7:5B:1416:LYS:HD3 | 7:5B:1416:LYS:O | 1.96 | 0.65 |
| 7:5C:1247:LYS:HE2 | 7:5C:1248:LEU:HG | 1.77 | 0.65 |
| 7:5C:1425:LYS:NZ | 7:5C:1429:GLN:HB2 | 2.11 | 0.65 |
| 9:7C:10:TYR:HE2 | 9:7D:26:LEU:HG | 1.60 | 0.65 |
| 1:AA:328:VAL:HG11 | 1:AA:353:VAL:HG21 | 1.78 | 0.65 |
| 1:AC:328:VAL:HG11 | 1:AC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:BE:101:ASN:HD21 | 2:BF:252:LYS:HD2 | 0.83 | 0.65 |
| 2:DB:226:ASN:HD21 | 13:DB:501:GDP:HN1 | 1.41 | 0.65 |
| 2:EB:125:GLU:CB | 7:5C:903:PHE:CD2 | 2.79 | 0.65 |
| 1:EE:98:ASP:OD1 | 1:EE:99:ALA:N | 2.29 | 0.65 |
| 2:FD:54:ALA:CB | 2:GD:281:TYR:O | 2.44 | 0.65 |
| 2:FD:55:THR:HG23 | 2:GD:283:ALA:CB | 2.26 | 0.65 |
| 2:FD:226:ASN:HD21 | 13:FD:502:GDP:HN1 | 1.42 | 0.65 |
| 1:GC:404:PHE:HE2 | 2:GD:345:ILE:CD1 | 2.09 | 0.65 |
| 1:GE:328:VAL:HG11 | 1:GE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:HE:98:ASP:OD1 | 1:HE:99:ALA:N | 2.29 | 0.65 |
| 1:IA:101:ASN:HD21 | 2:IB:252:LYS:HD2 | 0.82 | 0.65 |
| 1:IE:98:ASP:OD1 | 1:IE:99:ALA:N | 2.29 | 0.65 |
| 1:JE:89:PRO:HG2 | 1:KE:280:LYS:HG2 | 1.68 | 0.65 |
| 2:KD:276:ARG:HH22 | 6:4B:266:ASN:H | 1.43 | 0.65 |
| 1:KE:224:TYR:HE2 | 2:KF:246:LEU:HD11 | 1.59 | 0.65 |
| 1:KE:359:PRO:HG3 | 6:4B:299:TYR:CE2 | 2.31 | 0.65 |
| 2:LB:55:THR:CG2 | 2:MB:284:LEU:H | 2.09 | 0.65 |
| 1:LC:60:LYS:HD3 | 1:MC:283:HIS:CD2 | 2.30 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LE:98:ASP:OD1 | 1:LE:99:ALA:N | 2.29 | 0.65 |
| 1:LE:328:VAL:HG11 | 1:LE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:ME:404:PHE:CE2 | 2:MF:345:ILE:HD11 | 2.31 | 0.65 |
| 6:4D:151:ARG:HH11 | 6:4D:151:ARG:CG | 2.08 | 0.65 |
| 7:5B:912:VAL:HG11 | 7:5B:918:ILE:HG13 | 1.78 | 0.65 |
| 9:7C:11:TYR:CE1 | 9:7D:26:LEU:CG | 2.71 | 0.65 |
| 2:AD:391:ARG:HG3 | 1:AE:346:TRP:CD1 | 2.31 | 0.65 |
| 1:AE:224:TYR:HE2 | 2:AF:246:LEU:HD11 | 1.59 | 0.65 |
| 2:AF:148:GLY:O | 2:AF:152:ILE:HG12 | 1.95 | 0.65 |
| 1:CA:404:PHE:HE2 | 2:CB:345:ILE:CD1 | 2.09 | 0.65 |
| 2:CB:179:VAL:CG2 | 1:CC:258:ASN:CA | 2.75 | 0.65 |
| 1:DA:98:ASP:OD1 | 1:DA:99:ALA:N | 2.29 | 0.65 |
| 1:DE:328:VAL:HG11 | 1:DE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:EA:402:ARG:CZ | 7:5C:824:ARG:NH2 | 2.58 | 0.65 |
| 2:EF:55:THR:HG23 | 2:FF:283:ALA:CB | 2.25 | 0.65 |
| 1:GA:101:ASN:HD21 | 2:GB:252:LYS:HD2 | 0.82 | 0.65 |
| 1:GA:328:VAL:HG11 | 1:GA:353:VAL:HG21 | 1.78 | 0.65 |
| 1:GC:328:VAL:HG11 | 1:GC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:HE:328:VAL:HG11 | 1:HE:353:VAL:HG21 | 1.78 | 0.65 |
| 1:IC:279:GLU:HA | 10:8W:22:UNK:CB | 2.26 | 0.65 |
| 1:IE:224:TYR:HE2 | 2:IF:246:LEU:HD11 | 1.59 | 0.65 |
| 1:MA:105:ARG:NH1 | 2:MB:251:ARG:HD3 | 2.11 | 0.65 |
| 2:MB:390:ARG:HD2 | 1:MC:439:THR:HG21 | 1.77 | 0.65 |
| 4:2C:12:LEU:HD23 | 4:2C:20:LYS:CB | 2.22 | 0.65 |
| 7:5A:1416:LYS:HD3 | 7:5A:1416:LYS:O | 1.97 | 0.65 |
| 7:5B:839:GLU:HA | 8:6B:109:ILE:N | 2.11 | 0.65 |
| 7:5C:773:ARG:C | 7:5C:775:PRO:CD | 2.67 | 0.65 |
| 7:5C:1416:LYS:HD3 | 7:5C:1416:LYS:O | 1.97 | 0.65 |
| 7:5C:1482:SER:HA | 7:5C:1485:LYS:CB | 2.21 | 0.65 |
| 2:AD:148:GLY:O | 2:AD:152:ILE:HG12 | 1.95 | 0.65 |
| 1:CA:224:TYR:HE2 | 2:CB:246:LEU:HD11 | 1.60 | 0.65 |
| 2:CB:176:SER:OG | 1:CC:349:THR:OG1 | 2.12 | 0.65 |
| 1:CE:328:VAL:HG11 | 1:CE:353:VAL:HG21 | 1.78 | 0.65 |
| 2:DD:60:VAL:HG21 | 2:ED:281:TYR:CD1 | 2.31 | 0.65 |
| 1:EC:98:ASP:OD1 | 1:EC:99:ALA:N | 2.29 | 0.65 |
| 2:FD:397:TRP:CB | 1:FE:256:GLN:HE22 | 2.07 | 0.65 |
| 2:GB:226:ASN:HD21 | 13:GB:501:GDP:HN1 | 1.42 | 0.65 |
| 1:HC:415:GLU:HG3 | 5:3C:235:LEU:HB2 | 1.73 | 0.65 |
| 1:IC:98:ASP:OD1 | 1:IC:99:ALA:N | 2.29 | 0.65 |
| 1:JE:224:TYR:HE2 | 2:JF:246:LEU:HD11 | 1.59 | 0.65 |
| 1:KA:101:ASN:HD21 | 2:KB:252:LYS:HD2 | 0.82 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:KF:125:GLU:CD | 2:LF:336:LYS:NZ | 2.54 | 0.65 |
| 2:LB:228:LEU:HD23 | 6:4A:225:PRO:HG2 | 1.79 | 0.65 |
| 1:ME:98:ASP:OD1 | 1:ME:99:ALA:N | 2.29 | 0.65 |
| 4:2B:171:VAL:HB | 4:2B:176:ARG:HH21 | 1.61 | 0.65 |
| 6:4B:151:ARG:HH11 | 6:4B:151:ARG:CG | 2.08 | 0.65 |
| 6:4D:266:ASN:HD22 | 6:4D:273:ARG:NH1 | 1.95 | 0.65 |
| 7:5A:912:VAL:HG11 | 7:5A:918:ILE:HG13 | 1.78 | 0.65 |
| 7:5A:1443:LYS:C | 7:5A:1443:LYS:HD2 | 2.21 | 0.65 |
| 7:5B:1487:ASN:HB3 | 7:5B:1568:LYS:CD | 2.21 | 0.65 |
| 7:5C:912:VAL:HG11 | 7:5C:918:ILE:HG13 | 1.78 | 0.65 |
| 7:5C:1443:LYS:C | 7:5C:1443:LYS:HD2 | 2.21 | 0.65 |
| 9:7A:35:ILE:HG22 | 9:7B:43:LEU:HA | 1.78 | 0.65 |
| 1:AA:101:ASN:HD21 | 2:AB:252:LYS:HD2 | 0.82 | 0.65 |
| 2:AB:148:GLY:O | 2:AB:152:ILE:HG12 | 1.95 | 0.65 |
| 1:CA:328:VAL:HG11 | 1:CA:353:VAL:HG21 | 1.78 | 0.65 |
| 1:EC:430:LYS:HZ1 | 7:5A:834:ASN:ND2 | 0.60 | 0.65 |
| 2:EF:226:ASN:HD21 | 13:EF:501:GDP:HN1 | 1.42 | 0.65 |
| 1:FC:100:ALA:HB1 | 2:FD:252:LYS:HA | 1.77 | 0.65 |
| 2:GD:391:ARG:HG3 | 1:GE:346:TRP:CD1 | 2.31 | 0.65 |
| 1:IA:401:LYS:CE | 2:IB:344:TRP:CZ3 | 2.67 | 0.65 |
| 2:IF:56:GLY:HA2 | 10:9A:36:UNK:HA | 1.79 | 0.65 |
| 2:LF:221:THR:CG2 | 6:4D:220:GLY:H | 2.09 | 0.65 |
| 2:MD:221:THR:CG2 | 6:4B:189:ARG:NH2 | 2.18 | 0.65 |
| 6:4A:266:ASN:HD22 | 6:4A:273:ARG:NH1 | 1.95 | 0.65 |
| 6:4B:266:ASN:HD22 | 6:4B:273:ARG:NH1 | 1.95 | 0.65 |
| 6:4C:266:ASN:HD22 | 6:4C:273:ARG:NH1 | 1.95 | 0.65 |
| 7:5A:773:ARG:C | 7:5A:775:PRO:CD | 2.67 | 0.65 |
| 7:5B:1443:LYS:C | 7:5B:1443:LYS:HD2 | 2.22 | 0.65 |
| 9:7B:12:GLU:O | 9:7B:16:THR:OG1 | 2.14 | 0.65 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:HD11 | 1.78 | 0.65 |
| 1:BE:60:LYS:NZ | 1:CE:283:HIS:NE2 | 2.45 | 0.65 |
| 2:CB:220:PRO:CD | 1:CC:326:LYS:HG2 | 2.26 | 0.65 |
| 1:EA:402:ARG:HE | 7:5C:824:ARG:HH22 | 1.40 | 0.65 |
| 2:EB:226:ASN:HD21 | 13:EB:501:GDP:HN1 | 1.42 | 0.65 |
| 2:FB:177:ASP:O | 1:FC:352:LYS:HA | 1.97 | 0.65 |
| 2:FB:226:ASN:HD21 | 13:FB:502:GDP:HN1 | 1.42 | 0.65 |
| 1:FC:222:PRO:HG2 | 2:FD:324:LYS:HD3 | 1.78 | 0.65 |
| 1:FC:419:SER:C | 7:5A:1256:ARG:NH2 | 2.54 | 0.65 |
| 1:GA:370:LYS:CG | 10:8P:17:UNK:C | 2.68 | 0.65 |
| 2:GB:212:PHE:CZ | 1:GC:326:LYS:CD | 2.31 | 0.65 |
| 1:HC:419:SER:HG | 5:3C:238:ILE:CD1 | 2.08 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KD:276:ARG:HH21 | 6:4B:265:TYR:HB2 | 1.62 | 0.65 |
| 2:LB:215:LEU:HD13 | 6:4A:225:PRO:HB3 | 1.79 | 0.65 |
| 5:3B:224:ASP:N | 5:3B:335:LYS:NZ | 2.41 | 0.65 |
| 6:4A:151:ARG:HH11 | 6:4A:151:ARG:CG | 2.08 | 0.65 |
| 7:5A:1247:LYS:HE2 | 7:5A:1248:LEU:HG | 1.77 | 0.65 |
| 7:5B:773:ARG:C | 7:5B:775:PRO:CD | 2.67 | 0.65 |
| 9:7D:12:GLU:O | 9:7D:16:THR:OG1 | 2.14 | 0.65 |
| 1:CC:328:VAL:HG11 | 1:CC:353:VAL:HG21 | 1.78 | 0.65 |
| 1:EA:98:ASP:OD1 | 1:EA:99:ALA:N | 2.29 | 0.65 |
| 2:GB:220:PRO:O | 1:GC:324:VAL:HG13 | 1.95 | 0.65 |
| 2:GD:226:ASN:HD21 | 13:GD:501:GDP:HN1 | 1.42 | 0.65 |
| 2:GF:226:ASN:HD21 | 13:GF:501:GDP:HN1 | 1.42 | 0.65 |
| 2:ID:391:ARG:HG3 | 1:IE:346:TRP:CD1 | 2.31 | 0.65 |
| 2:JD:391:ARG:HG3 | 1:JE:346:TRP:CD1 | 2.31 | 0.65 |
| 2:LD:177:ASP:OD2 | 1:LE:248:LEU:HD23 | 1.97 | 0.65 |
| 1:MC:105:ARG:NH1 | 2:MD:251:ARG:HD3 | 2.11 | 0.65 |
| 5:3A:224:ASP:N | 5:3A:335:LYS:NZ | 2.41 | 0.65 |
| 6:4D:230:TYR:OH | 6:4D:240:LYS:HG2 | 1.96 | 0.65 |
| 7:5A:839:GLU:HA | 7:5A:839:GLU:OE1 | 1.97 | 0.65 |
| 7:5A:1535:ILE:HG12 | 7:5A:1574:ILE:C | 2.21 | 0.65 |
| 7:5B:839:GLU:HA | 7:5B:839:GLU:OE1 | 1.97 | 0.65 |
| 7:5B:1535:ILE:HG12 | 7:5B:1574:ILE:C | 2.21 | 0.65 |
| 7:5C:839:GLU:OE1 | 7:5C:839:GLU:HA | 1.97 | 0.65 |
| 7:5C:1535:ILE:HG12 | 7:5C:1574:ILE:C | 2.21 | 0.65 |
| 8:6A:131:ASP:H | 8:6A:136:LEU:HD12 | 1.60 | 0.65 |
| 2:AF:356:ILE:CD1 | 6:4A:152:PHE:HE1 | 2.09 | 0.65 |
| 2:ED:226:ASN:HD21 | 13:ED:502:GDP:HN1 | 1.42 | 0.65 |
| 1:EE:430:LYS:NZ | 7:5B:834:ASN:ND2 | 0.69 | 0.65 |
| 1:FC:282:TYR:CZ | 10:8N:18:UNK:CB | 2.74 | 0.65 |
| 1:FC:404:PHE:HE2 | 2:FD:345:ILE:HD12 | 1.62 | 0.65 |
| 2:FD:220:PRO:HD2 | 1:FE:326:LYS:HG2 | 1.78 | 0.65 |
| 1:GA:60:LYS:HD2 | 1:HA:283:HIS:CD2 | 2.32 | 0.65 |
| 2:GB:208:TYR:OH | 1:GC:325:PRO:HB2 | 1.96 | 0.65 |
| 2:JB:177:ASP:OD1 | 1:JC:353:VAL:HG12 | 1.84 | 0.65 |
| 2:JB:212:PHE:CZ | 1:JC:326:LYS:CD | 2.31 | 0.65 |
| 2:JB:220:PRO:O | 1:JC:324:VAL:HG13 | 1.95 | 0.65 |
| 2:KD:391:ARG:HG3 | 1:KE:346:TRP:CD1 | 2.31 | 0.65 |
| 2:LD:55:THR:CG2 | 2:MD:284:LEU:N | 2.60 | 0.65 |
| 1:MA:404:PHE:HE2 | 2:MB:345:ILE:HD12 | 1.61 | 0.65 |
| 6:4B:154:LYS:HB2 | 6:4B:154:LYS:HZ3 | 1.62 | 0.65 |
| 6:4B:230:TYR:OH | 6:4B:240:LYS:HG2 | 1.95 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5A:1565:GLU:OE1 | 7:5A:1569:GLU:HB2 | 1.97 | 0.65 |
| 7:5B:1565:GLU:OE1 | 7:5B:1569:GLU:HB2 | 1.97 | 0.65 |
| 7:5C:1565:GLU:OE1 | 7:5C:1569:GLU:HB2 | 1.97 | 0.65 |
| 8:6C:20:LYS:NZ | 8:6C:101:GLU:OE1 | 2.26 | 0.65 |
| 9:7C:35:ILE:O | 9:7D:43:LEU:CD2 | 2.44 | 0.65 |
| 9:7E:38:LEU:CD2 | 9:7F:42:LEU:HD13 | 2.21 | 0.65 |
| 1:AE:60:LYS:HD3 | 1:BE:283:HIS:CD2 | 2.31 | 0.65 |
| 1:BC:224:TYR:HE2 | 2:BD:246:LEU:HD11 | 1.62 | 0.65 |
| 1:CE:105:ARG:NH1 | 2:CF:251:ARG:HD3 | 2.12 | 0.65 |
| 2:EB:157:GLU:OE1 | 7:5C:935:LYS:NZ | 2.30 | 0.65 |
| 1:EE:396:ASP:O | 7:5B:817:LEU:HD11 | 1.97 | 0.65 |
| 1:IA:98:ASP:OD1 | 1:IA:99:ALA:N | 2.29 | 0.65 |
| 2:ID:212:PHE:CZ | 1:IE:326:LYS:CD | 2.34 | 0.65 |
| 2:LB:276:ARG:NH1 | 6:4A:229:GLU:CA | 2.38 | 0.65 |
| 1:MC:71:GLU:CD | 2:MD:247:ASN:ND2 | 2.54 | 0.65 |
| 7:5A:1482:SER:HA | 7:5A:1485:LYS:CB | 2.21 | 0.65 |
| 7:5B:1247:LYS:HE2 | 7:5B:1248:LEU:HG | 1.77 | 0.65 |
| 8:6B:131:ASP:H | 8:6B:136:LEU:HD12 | 1.60 | 0.65 |
| 2:CD:87:PRO:HD3 | 2:DD:281:TYR:CE2 | 2.32 | 0.64 |
| 1:DA:176:GLN:O | 2:DB:347:ASN:ND2 | 2.28 | 0.64 |
| 2:FD:401:GLU:N | 7:5A:1293:VAL:HG21 | 2.12 | 0.64 |
| 1:JA:279:GLU:CG | 10:8Y:22:UNK:HA | 2.27 | 0.64 |
| 1:JC:89:PRO:HG2 | 1:KC:280:LYS:CB | 2.26 | 0.64 |
| 2:KB:55:THR:HG21 | 2:LB:363:MET:HE1 | 0.67 | 0.64 |
| 1:KC:87:PHE:O | 1:LC:283:HIS:C | 2.40 | 0.64 |
| 2:LB:306:ARG:CZ | 4:2C:149:ILE:HG21 | 2.17 | 0.64 |
| 2:LD:310:TYR:CE2 | 4:2A:147:PHE:CZ | 2.84 | 0.64 |
| 1:MA:98:ASP:OD1 | 1:MA:99:ALA:N | 2.29 | 0.64 |
| 6:4C:151:ARG:HH11 | 6:4C:151:ARG:CG | 2.08 | 0.64 |
| 2:AD:284:LEU:CD1 | 6:4C:144:LEU:CD1 | 2.42 | 0.64 |
| 2:BB:397:TRP:CB | 1:BC:256:GLN:HE22 | 2.08 | 0.64 |
| 2:CB:86:ARG:HH11 | 2:DB:281:TYR:HA | 1.59 | 0.64 |
| 1:FC:402:ARG:NH2 | 7:5A:1262:GLU:OE1 | 2.29 | 0.64 |
| 2:GB:177:ASP:OD1 | 1:GC:353:VAL:HG12 | 1.84 | 0.64 |
| 2:IB:220:PRO:O | 1:IC:324:VAL:HG13 | 1.95 | 0.64 |
| 2:JD:86:ARG:HE | 2:KD:281:TYR:HD2 | 1.44 | 0.64 |
| 1:MC:98:ASP:OD1 | 1:MC:99:ALA:N | 2.29 | 0.64 |
| 1:MC:279:GLU:OE1 | 6:4A:106:ALA:C | 2.40 | 0.64 |
| 6:4A:132:LYS:HE2 | 6:4A:132:LYS:CA | 2.27 | 0.64 |
| 6:4A:230:TYR:OH | 6:4A:240:LYS:HG2 | 1.95 | 0.64 |
| 6:4B:132:LYS:HE2 | 6:4B:132:LYS:CA | 2.27 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4C:132:LYS:HE2 | 6:4C:132:LYS:CA | 2.27 | 0.64 |
| 7:5C:1243:ASP:CB | 9:7F:8:ARG:NH1 | 2.60 | 0.64 |
| 7:5C:1325:ARG:HD3 | 7:5C:1325:ARG:N | 2.11 | 0.64 |
| 9:7C:15:VAL:CG1 | 9:7D:35:ILE:HD12 | 2.16 | 0.64 |
| 2:AD:320:ARG:HH12 | 6:4C:152:PHE:C | 2.06 | 0.64 |
| 1:BC:101:ASN:HD21 | 2:BD:252:LYS:HD2 | 0.83 | 0.64 |
| 1:EC:404:PHE:HE2 | 2:ED:345:ILE:HD12 | 1.62 | 0.64 |
| 1:EC:430:LYS:NZ | 7:5A:834:ASN:HD21 | 1.17 | 0.64 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:HD2 | 2.26 | 0.64 |
| 2:IB:208:TYR:OH | 1:IC:325:PRO:HB2 | 1.96 | 0.64 |
| 1:IC:278:ALA:HB3 | 10:8W:21:UNK:CA | 2.26 | 0.64 |
| 2:ID:424:GLN:HE21 | 7:5A:1413:GLN:CD | 1.71 | 0.64 |
| 1:JA:124:LYS:HD2 | 1:KA:284:GLU:OE1 | 1.97 | 0.64 |
| 2:KB:54:ALA:HA | 2:LB:285:THR:CG2 | 2.27 | 0.64 |
| 2:LD:221:THR:CG2 | 6:4B:220:GLY:N | 2.60 | 0.64 |
| 2:MD:78:ALA:HB1 | 6:4B:178:HIS:CD2 | 2.32 | 0.64 |
| 6:4B:287:ASP:OD2 | 6:4B:287:ASP:N | 2.30 | 0.64 |
| 6:4C:230:TYR:OH | 6:4C:240:LYS:HG2 | 1.95 | 0.64 |
| 6:4C:286:ASP:O | 6:4C:289:LYS:HB3 | 1.98 | 0.64 |
| 6:4D:132:LYS:HE2 | 6:4D:132:LYS:CA | 2.27 | 0.64 |
| 7:5A:1423:LYS:HA | 7:5A:1423:LYS:HZ3 | 1.62 | 0.64 |
| 2:AB:208:TYR:OH | 1:AC:325:PRO:HB2 | 1.96 | 0.64 |
| 2:BF:87:PRO:HD2 | 2:CF:281:TYR:CE2 | 2.32 | 0.64 |
| 2:CB:179:VAL:HG21 | 1:CC:258:ASN:C | 2.21 | 0.64 |
| 1:CC:404:PHE:HE2 | 2:CD:345:ILE:CD1 | 2.10 | 0.64 |
| 2:ED:179:VAL:CG2 | 1:EE:258:ASN:O | 2.35 | 0.64 |
| 1:FA:87:PHE:O | 1:GA:280:LYS:NZ | 2.30 | 0.64 |
| 1:FA:105:ARG:NH1 | 2:FB:251:ARG:HD3 | 2.13 | 0.64 |
| 2:FF:54:ALA:HA | 2:GF:283:ALA:CB | 2.25 | 0.64 |
| 2:HD:391:ARG:HG3 | 1:HE:346:TRP:CD1 | 2.31 | 0.64 |
| 2:IB:212:PHE:CE2 | 1:IC:326:LYS:HD3 | 2.22 | 0.64 |
| 1:JA:88:HIS:CE1 | 1:KA:280:LYS:HB3 | 2.33 | 0.64 |
| 1:JA:401:LYS:CE | 2:JB:344:TRP:CZ3 | 2.67 | 0.64 |
| 1:KA:245:ASP:HB2 | 6:4C:253:ARG:HE | 1.62 | 0.64 |
| 2:KF:159:TYR:CE2 | 4:2B:35:VAL:O | 2.51 | 0.64 |
| 1:LA:47:ASP:OD1 | 6:4C:203:LYS:HE3 | 1.97 | 0.64 |
| 2:MB:177:ASP:O | 1:MC:352:LYS:CD | 2.36 | 0.64 |
| 4:2B:162:GLN:HE21 | 4:2B:162:GLN:CA | 2.03 | 0.64 |
| 5:3B:230:ILE:C | 5:3B:332:MET:HG2 | 2.22 | 0.64 |
| 7:5A:1253:ILE:HD12 | 7:5A:1261:ALA:HB1 | 1.80 | 0.64 |
| 7:5A:1325:ARG:HD3 | 7:5A:1325:ARG:N | 2.11 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5B:1253:ILE:HD12 | 7:5B:1261:ALA:HB1 | 1.80 | 0.64 |
| 7:5B:1482:SER:HA | 7:5B:1485:LYS:CB | 2.21 | 0.64 |
| 7:5C:1253:ILE:HD12 | 7:5C:1261:ALA:HB1 | 1.80 | 0.64 |
| 7:5C:1423:LYS:HA | 7:5C:1423:LYS:HZ3 | 1.62 | 0.64 |
| 9:7A:35:ILE:O | 9:7B:43:LEU:CD2 | 2.44 | 0.64 |
| 9:7C:18:VAL:HG11 | 9:7C:42:LEU:HD22 | 1.77 | 0.64 |
| 9:7C:39:GLY:C | 9:7D:43:LEU:HD11 | 2.23 | 0.64 |
| 9:7E:7:LEU:HG | 9:7F:30:ARG:HH21 | 1.61 | 0.64 |
| 2:AD:322:SER:H | 6:4C:156:PHE:HE2 | 1.42 | 0.64 |
| 2:CB:220:PRO:HD2 | 1:CC:326:LYS:CE | 2.27 | 0.64 |
| 1:EC:222:PRO:CD | 2:ED:324:LYS:HD3 | 2.26 | 0.64 |
| 1:FC:207:GLU:CD | 7:5A:915:PHE:CD2 | 2.76 | 0.64 |
| 2:HB:208:TYR:OH | 1:HC:325:PRO:HB2 | 1.96 | 0.64 |
| 1:HE:419:SER:CB | 5:3A:238:ILE:HD12 | 2.27 | 0.64 |
| 2:KB:208:TYR:OH | 1:KC:325:PRO:HB2 | 1.96 | 0.64 |
| 2:KB:212:PHE:CZ | 1:KC:326:LYS:CD | 2.31 | 0.64 |
| 2:KB:220:PRO:O | 1:KC:324:VAL:HG13 | 1.95 | 0.64 |
| 2:KD:177:ASP:O | 1:KE:352:LYS:CD | 2.34 | 0.64 |
| 1:KE:79:ARG:O | 1:LE:280:LYS:CE | 2.41 | 0.64 |
| 2:LB:220:PRO:O | 1:LC:324:VAL:HG13 | 1.97 | 0.64 |
| 1:LC:245:ASP:OD1 | 6:4A:216:ARG:NE | 2.30 | 0.64 |
| 6:4A:286:ASP:O | 6:4A:289:LYS:HB3 | 1.98 | 0.64 |
| 6:4D:287:ASP:OD2 | 6:4D:287:ASP:N | 2.30 | 0.64 |
| 7:5B:1246:LEU:O | 7:5B:1250:VAL:HG23 | 1.96 | 0.64 |
| 7:5C:1246:LEU:O | 7:5C:1250:VAL:HG23 | 1.96 | 0.64 |
| 7:5C:1524:PHE:CE1 | 7:5C:1571:MET:CE | 2.81 | 0.64 |
| 9:7A:39:GLY:C | 9:7B:43:LEU:HD11 | 2.23 | 0.64 |
| 9:7E:18:VAL:HG11 | 9:7E:42:LEU:HD22 | 1.77 | 0.64 |
| 2:AF:356:ILE:CD1 | 6:4A:152:PHE:CE1 | 2.75 | 0.64 |
| 1:CC:60:LYS:HZ3 | 1:DC:283:HIS:CD2 | 2.11 | 0.64 |
| 1:EA:426:ALA:HB3 | 7:5C:833:PHE:HB2 | 1.79 | 0.64 |
| 1:EE:426:ALA:CB | 7:5B:833:PHE:HD1 | 2.00 | 0.64 |
| 1:FA:222:PRO:HG3 | 2:FB:324:LYS:HD3 | 1.74 | 0.64 |
| 1:HC:288:VAL:HG11 | 1:HC:327:ASP:HB3 | 1.79 | 0.64 |
| 1:HE:288:VAL:HG11 | 1:HE:327:ASP:HB3 | 1.79 | 0.64 |
| 2:KB:177:ASP:O | 1:KC:352:LYS:CD | 2.35 | 0.64 |
| 2:LB:306:ARG:HE | 4:2C:149:ILE:CB | 2.05 | 0.64 |
| 1:LC:60:LYS:HE3 | 6:4A:101:ARG:NH1 | 2.11 | 0.64 |
| 5:3A:230:ILE:C | 5:3A:332:MET:HG2 | 2.22 | 0.64 |
| 7:5A:1524:PHE:CE1 | 7:5A:1571:MET:CE | 2.81 | 0.64 |
| 7:5B:1524:PHE:CE1 | 7:5B:1571:MET:CE | 2.81 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:7A:11:TYR:CE1 | 9:7B:26:LEU:CB | 2.41 | 0.64 |
| 9:7E:35:ILE:O | 9:7F:43:LEU:HD23 | 1.98 | 0.64 |
| 2:AD:320:ARG:CD | 6:4C:153:ASP:O | 2.45 | 0.64 |
| 2:BD:100:ASN:HB2 | 1:BE:257:THR:HG21 | 1.79 | 0.64 |
| 2:BF:100:ASN:ND2 | 2:BF:401:GLU:OE2 | 2.31 | 0.64 |
| 1:DA:288:VAL:HG11 | 1:DA:327:ASP:HB3 | 1.79 | 0.64 |
| 1:DC:288:VAL:HG11 | 1:DC:327:ASP:HB3 | 1.79 | 0.64 |
| 1:DE:288:VAL:HG11 | 1:DE:327:ASP:HB3 | 1.79 | 0.64 |
| 1:FA:422:ARG:CZ | 7:5C:1170:THR:C | 2.68 | 0.64 |
| 2:FB:391:ARG:O | 1:FC:262:TYR:OH | 2.14 | 0.64 |
| 2:FD:177:ASP:HA | 1:FE:353:VAL:HG12 | 1.80 | 0.64 |
| 1:HA:288:VAL:HG11 | 1:HA:327:ASP:HB3 | 1.79 | 0.64 |
| 2:HB:220:PRO:O | 1:HC:324:VAL:HG13 | 1.95 | 0.64 |
| 1:KA:87:PHE:N | 1:LA:283:HIS:O | 2.31 | 0.64 |
| 2:KD:125:GLU:CG | 2:LD:336:LYS:HE2 | 2.21 | 0.64 |
| 2:KD:273:LEU:HG | 6:4B:268:LEU:HD21 | 1.75 | 0.64 |
| 2:LB:55:THR:CG2 | 2:MB:284:LEU:N | 2.61 | 0.64 |
| 2:LB:221:THR:HG23 | 6:4A:219:ASN:HD22 | 1.63 | 0.64 |
| 2:MB:100:ASN:HB2 | 1:MC:257:THR:HG21 | 1.79 | 0.64 |
| 8:6C:14:ARG:NE | 8:6C:89:ILE:HG23 | 2.13 | 0.64 |
| 9:7A:11:TYR:CD2 | 9:7B:23:LEU:HD22 | 2.33 | 0.64 |
| 9:7C:11:TYR:CD2 | 9:7D:23:LEU:HD22 | 2.33 | 0.64 |
| 2:AD:321:MET:C | 6:4C:156:PHE:HD2 | 2.05 | 0.64 |
| 1:CC:101:ASN:HD21 | 2:CD:252:LYS:HD2 | 0.81 | 0.64 |
| 1:CE:178:SER:OG | 2:CF:347:ASN:HB3 | 1.97 | 0.64 |
| 2:DB:179:VAL:CG2 | 1:DC:258:ASN:O | 2.37 | 0.64 |
| 1:DE:401:LYS:CE | 2:DF:344:TRP:CZ3 | 2.71 | 0.64 |
| 2:DF:100:ASN:ND2 | 2:DF:401:GLU:OE2 | 2.31 | 0.64 |
| 2:EB:100:ASN:ND2 | 2:EB:401:GLU:OE2 | 2.31 | 0.64 |
| 2:EB:177:ASP:O | 1:EC:352:LYS:CD | 2.36 | 0.64 |
| 2:ED:100:ASN:ND2 | 2:ED:401:GLU:OE2 | 2.31 | 0.64 |
| 1:FC:288:VAL:HG11 | 1:FC:327:ASP:HB3 | 1.79 | 0.64 |
| 1:FE:224:TYR:HE2 | 2:FF:246:LEU:HD11 | 1.61 | 0.64 |
| 1:IE:279:GLU:HA | 10:8X:22:UNK:CB | 2.28 | 0.64 |
| 2:KB:86:ARG:CG | 2:LB:288:GLU:CD | 2.68 | 0.64 |
| 1:LA:60:LYS:HD3 | 1:MA:283:HIS:CB | 2.28 | 0.64 |
| 1:LA:288:VAL:HG11 | 1:LA:327:ASP:HB3 | 1.79 | 0.64 |
| 2:LB:221:THR:CG2 | 6:4A:220:GLY:N | 2.60 | 0.64 |
| 1:LE:245:ASP:CG | 6:4B:216:ARG:HE | 2.05 | 0.64 |
| 1:LE:288:VAL:HG11 | 1:LE:327:ASP:HB3 | 1.80 | 0.64 |
| 5:3B:221:VAL:HG13 | 5:3B:230:ILE:HG23 | 1.80 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:3C:230:ILE:C | 5:3C:332:MET:HG2 | 2.22 | 0.64 |
| 6:4B:286:ASP:O | 6:4B:289:LYS:HB3 | 1.98 | 0.64 |
| 7:5A:1246:LEU:O | 7:5A:1250:VAL:HG23 | 1.96 | 0.64 |
| 7:5C:1491:LEU:HD13 | 7:5C:1495:PHE:HD1 | 0.53 | 0.64 |
| 8:6B:20:LYS:NZ | 8:6B:101:GLU:OE1 | 2.26 | 0.64 |
| 2:BB:179:VAL:CG2 | 1:BC:258:ASN:CA | 2.76 | 0.64 |
| 2:BD:100:ASN:ND2 | 2:BD:401:GLU:OE2 | 2.31 | 0.64 |
| 2:CD:100:ASN:ND2 | 2:CD:401:GLU:OE2 | 2.31 | 0.64 |
| 2:CF:100:ASN:ND2 | 2:CF:401:GLU:OE2 | 2.31 | 0.64 |
| 2:DD:100:ASN:ND2 | 2:DD:401:GLU:OE2 | 2.31 | 0.64 |
| 2:EF:100:ASN:ND2 | 2:EF:401:GLU:OE2 | 2.31 | 0.64 |
| 1:FA:288:VAL:HG11 | 1:FA:327:ASP:HB3 | 1.80 | 0.64 |
| 2:FB:54:ALA:HB1 | 2:GB:282:ARG:C | 2.22 | 0.64 |
| 2:FD:100:ASN:ND2 | 2:FD:401:GLU:OE2 | 2.31 | 0.64 |
| 1:FE:288:VAL:HG11 | 1:FE:327:ASP:HB3 | 1.80 | 0.64 |
| 2:FF:100:ASN:ND2 | 2:FF:401:GLU:OE2 | 2.31 | 0.64 |
| 2:FF:106:TYR:CE1 | 7:5B:1295:LYS:N | 2.64 | 0.64 |
| 1:IA:279:GLU:HG2 | 10:8V:22:UNK:HA | 1.78 | 0.64 |
| 1:IC:401:LYS:HE3 | 2:ID:344:TRP:CZ3 | 2.33 | 0.64 |
| 1:LC:288:VAL:HG11 | 1:LC:327:ASP:HB3 | 1.80 | 0.64 |
| 2:LD:228:LEU:HD21 | 6:4B:225:PRO:CG | 2.28 | 0.64 |
| 1:LE:407:TRP:CE3 | 2:LF:255:VAL:HG22 | 2.26 | 0.64 |
| 4:2A:162:GLN:HE21 | 4:2A:162:GLN:CA | 2.03 | 0.64 |
| 5:3A:221:VAL:HG13 | 5:3A:230:ILE:HG23 | 1.80 | 0.64 |
| 6:4C:154:LYS:HB2 | 6:4C:154:LYS:HZ3 | 1.63 | 0.64 |
| 6:4D:286:ASP:O | 6:4D:289:LYS:HB3 | 1.98 | 0.64 |
| 7:5B:1325:ARG:HD3 | 7:5B:1325:ARG:N | 2.11 | 0.64 |
| 1:BA:288:VAL:HG11 | 1:BA:327:ASP:HB3 | 1.79 | 0.64 |
| 2:BB:100:ASN:ND2 | 2:BB:401:GLU:OE2 | 2.31 | 0.64 |
| 1:CA:105:ARG:NH1 | 2:CB:251:ARG:HD3 | 2.13 | 0.64 |
| 2:CB:100:ASN:ND2 | 2:CB:401:GLU:OE2 | 2.31 | 0.64 |
| 1:CC:105:ARG:NH1 | 2:CD:251:ARG:HD3 | 2.13 | 0.64 |
| 1:DA:401:LYS:CE | 2:DB:344:TRP:CZ3 | 2.72 | 0.64 |
| 2:DB:100:ASN:ND2 | 2:DB:401:GLU:OE2 | 2.31 | 0.64 |
| 2:DD:179:VAL:HG21 | 1:DE:258:ASN:C | 2.22 | 0.64 |
| 1:EC:11:GLN:NE2 | 2:ED:247:ASN:OD1 | 2.31 | 0.64 |
| 2:FB:100:ASN:ND2 | 2:FB:401:GLU:OE2 | 2.31 | 0.64 |
| 2:FB:397:TRP:CH2 | 1:FC:255:PHE:O | 2.45 | 0.64 |
| 2:FD:220:PRO:CD | 1:FE:326:LYS:HE2 | 2.26 | 0.64 |
| 1:FE:207:GLU:CD | 7:5B:915:PHE:CD2 | 2.76 | 0.64 |
| 1:GA:56:THR:OG1 | 1:HA:284:GLU:CA | 2.45 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HB:397:TRP:CD2 | 1:HC:256:GLN:O | 2.30 | 0.64 |
| 2:HF:100:ASN:ND2 | 2:HF:401:GLU:OE2 | 2.31 | 0.64 |
| 1:JA:288:VAL:HG11 | 1:JA:327:ASP:HB3 | 1.79 | 0.64 |
| 1:JC:401:LYS:HE3 | 2:JD:344:TRP:CZ3 | 2.33 | 0.64 |
| 1:JE:288:VAL:HG11 | 1:JE:327:ASP:HB3 | 1.79 | 0.64 |
| 1:KA:401:LYS:CE | 2:KB:344:TRP:CZ3 | 2.67 | 0.64 |
| 1:KC:401:LYS:HE3 | 2:KD:344:TRP:CZ3 | 2.33 | 0.64 |
| 2:KF:272:PRO:C | 6:4D:268:LEU:HD21 | 2.19 | 0.64 |
| 2:LB:228:LEU:HD21 | 6:4A:225:PRO:CG | 2.28 | 0.64 |
| 2:LD:221:THR:HG23 | 6:4B:219:ASN:HD22 | 1.62 | 0.64 |
| 2:LF:100:ASN:ND2 | 2:LF:401:GLU:OE2 | 2.31 | 0.64 |
| 2:MB:78:ALA:CB | 6:4A:178:HIS:CD2 | 2.80 | 0.64 |
| 2:MB:100:ASN:ND2 | 2:MB:401:GLU:OE2 | 2.31 | 0.64 |
| 7:5A:1030:PHE:CE2 | 7:5A:1034:ILE:HD11 | 2.33 | 0.64 |
| 7:5A:1491:LEU:HD13 | 7:5A:1495:PHE:HD1 | 0.53 | 0.64 |
| 7:5B:1030:PHE:CE2 | 7:5B:1034:ILE:HD11 | 2.33 | 0.64 |
| 7:5B:1332:GLN:HE21 | 7:5B:1332:GLN:N | 1.96 | 0.64 |
| 8:6A:14:ARG:NE | 8:6A:89:ILE:HG23 | 2.13 | 0.64 |
| 1:BC:288:VAL:HG11 | 1:BC:327:ASP:HB3 | 1.79 | 0.63 |
| 2:CD:176:SER:OG | 1:CE:349:THR:OG1 | 2.16 | 0.63 |
| 1:EC:430:LYS:NZ | 7:5A:834:ASN:HD22 | 0.36 | 0.63 |
| 1:FC:105:ARG:NH1 | 2:FD:251:ARG:HD3 | 2.13 | 0.63 |
| 1:GA:60:LYS:CD | 1:HA:283:HIS:CG | 2.81 | 0.63 |
| 2:GB:55:THR:CG2 | 2:HB:284:LEU:N | 2.58 | 0.63 |
| 1:HC:420:GLU:OE1 | 5:3C:215:TYR:CE2 | 2.51 | 0.63 |
| 2:HD:100:ASN:ND2 | 2:HD:401:GLU:OE2 | 2.31 | 0.63 |
| 2:IB:424:GLN:NE2 | 7:5C:1413:GLN:NE2 | 0.75 | 0.63 |
| 2:JB:177:ASP:OD2 | 1:JC:248:LEU:HD23 | 1.97 | 0.63 |
| 1:JC:87:PHE:O | 1:KC:283:HIS:NE2 | 2.29 | 0.63 |
| 1:JC:288:VAL:HG11 | 1:JC:327:ASP:HB3 | 1.79 | 0.63 |
| 2:KB:273:LEU:HA | 6:4A:268:LEU:HG | 1.73 | 0.63 |
| 2:LB:222:TYR:CD2 | 1:LC:247:ALA:HB1 | 2.34 | 0.63 |
| 2:LB:379:LYS:CE | 4:2C:164:ARG:O | 2.46 | 0.63 |
| 2:LD:100:ASN:ND2 | 2:LD:401:GLU:OE2 | 2.31 | 0.63 |
| 2:LD:228:LEU:HD23 | 6:4B:225:PRO:HG2 | 1.80 | 0.63 |
| 2:LF:231:ALA:HB1 | 6:4D:226:ILE:HD13 | 1.74 | 0.63 |
| 4:2C:162:GLN:HE21 | 4:2C:162:GLN:CA | 2.03 | 0.63 |
| 5:3C:221:VAL:HG13 | 5:3C:230:ILE:HG23 | 1.80 | 0.63 |
| 7:5A:1332:GLN:HE21 | 7:5A:1332:GLN:N | 1.97 | 0.63 |
| 7:5B:1491:LEU:HD13 | 7:5B:1495:PHE:HD1 | 0.53 | 0.63 |
| 7:5C:1552:LYS:HZ1 | 7:5C:1563:SER:CA | 2.09 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:6B:14:ARG:NE | 8:6B:89:ILE:HG23 | 2.13 | 0.63 |
| 9:7C:15:VAL:CB | 9:7D:35:ILE:HD12 | 2.24 | 0.63 |
| 2:BB:177:ASP:O | 1:BC:352:LYS:HA | 1.98 | 0.63 |
| 1:BE:288:VAL:HG11 | 1:BE:327:ASP:HB3 | 1.80 | 0.63 |
| 1:EA:419:SER:OG | 7:5C:830:VAL:HG21 | 1.96 | 0.63 |
| 2:GB:100:ASN:ND2 | 2:GB:401:GLU:OE2 | 2.31 | 0.63 |
| 2:GF:100:ASN:ND2 | 2:GF:401:GLU:OE2 | 2.31 | 0.63 |
| 2:HB:100:ASN:ND2 | 2:HB:401:GLU:OE2 | 2.31 | 0.63 |
| 2:KF:118:ASP:CG | 4:2B:148:ASN:ND2 | 2.55 | 0.63 |
| 2:LB:100:ASN:ND2 | 2:LB:401:GLU:OE2 | 2.31 | 0.63 |
| 1:MC:372:MET:HE2 | 6:4A:96:VAL:CA | 2.28 | 0.63 |
| 2:MD:100:ASN:ND2 | 2:MD:401:GLU:OE2 | 2.31 | 0.63 |
| 2:MD:397:TRP:CB | 1:ME:256:GLN:HE22 | 2.08 | 0.63 |
| 7:5B:1524:PHE:HD1 | 7:5B:1567:PHE:CZ | 2.07 | 0.63 |
| 7:5C:1030:PHE:CE2 | 7:5C:1034:ILE:HD11 | 2.33 | 0.63 |
| 7:5C:1524:PHE:HE1 | 7:5C:1571:MET:SD | 2.22 | 0.63 |
| 9:7C:10:TYR:CZ | 9:7D:34:PRO:HB3 | 2.32 | 0.63 |
| 2:BB:179:VAL:HG21 | 1:BC:258:ASN:C | 2.22 | 0.63 |
| 2:CD:86:ARG:HH11 | 2:DD:281:TYR:HA | 1.60 | 0.63 |
| 2:CF:87:PRO:HD3 | 2:DF:281:TYR:CE2 | 2.33 | 0.63 |
| 2:GD:100:ASN:ND2 | 2:GD:401:GLU:OE2 | 2.31 | 0.63 |
| 1:GE:288:VAL:HG11 | 1:GE:327:ASP:HB3 | 1.79 | 0.63 |
| 2:HB:86:ARG:HA | 2:IB:281:TYR:CE1 | 2.33 | 0.63 |
| 2:IB:100:ASN:ND2 | 2:IB:401:GLU:OE2 | 2.31 | 0.63 |
| 1:JE:89:PRO:HG2 | 1:KE:280:LYS:CB | 2.28 | 0.63 |
| 2:KF:100:ASN:ND2 | 2:KF:401:GLU:OE2 | 2.31 | 0.63 |
| 2:KF:128:ASP:C | 4:2B:38:VAL:HG23 | 2.24 | 0.63 |
| 1:LA:60:LYS:NZ | 1:MA:283:HIS:CE1 | 2.66 | 0.63 |
| 2:LB:178:THR:HA | 1:LC:352:LYS:HD3 | 1.80 | 0.63 |
| 2:LB:227:HIS:HD1 | 6:4A:226:ILE:HG13 | 1.63 | 0.63 |
| 2:MD:177:ASP:CG | 1:ME:353:VAL:HG11 | 2.06 | 0.63 |
| 7:5A:1524:PHE:HE1 | 7:5A:1571:MET:SD | 2.22 | 0.63 |
| 7:5B:1491:LEU:CA | 7:5B:1495:PHE:CB | 2.62 | 0.63 |
| 7:5C:1332:GLN:HE21 | 7:5C:1332:GLN:N | 1.97 | 0.63 |
| 9:7A:10:TYR:CZ | 9:7B:34:PRO:HB3 | 2.32 | 0.63 |
| 2:AB:100:ASN:ND2 | 2:AB:401:GLU:OE2 | 2.31 | 0.63 |
| 2:AB:397:TRP:CD2 | 1:AC:256:GLN:O | 2.30 | 0.63 |
| 1:CC:222:PRO:HD2 | 2:CD:324:LYS:HD3 | 1.78 | 0.63 |
| 1:EC:402:ARG:CZ | 7:5A:824:ARG:NH2 | 2.62 | 0.63 |
| 1:EE:178:SER:OG | 2:EF:347:ASN:HB3 | 1.98 | 0.63 |
| 2:FD:177:ASP:CA | 1:FE:353:VAL:HG12 | 2.28 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KD:100:ASN:ND2 | 2:KD:401:GLU:OE2 | 2.31 | 0.63 |
| 2:MF:100:ASN:ND2 | 2:MF:401:GLU:OE2 | 2.31 | 0.63 |
| 7:5B:1253:ILE:HD11 | 9:7D:20:LEU:HD13 | 1.81 | 0.63 |
| 7:5C:1548:VAL:CG1 | 7:5C:1566:GLU:N | 2.61 | 0.63 |
| 1:CC:224:TYR:HE2 | 2:CD:246:LEU:HD11 | 1.61 | 0.63 |
| 1:GA:288:VAL:HG11 | 1:GA:327:ASP:HB3 | 1.79 | 0.63 |
| 1:GC:288:VAL:HG11 | 1:GC:327:ASP:HB3 | 1.79 | 0.63 |
| 1:HC:401:LYS:HE3 | 2:HD:344:TRP:CZ3 | 2.33 | 0.63 |
| 2:IB:100:ASN:HB2 | 1:IC:257:THR:HG21 | 1.81 | 0.63 |
| 2:ID:100:ASN:ND2 | 2:ID:401:GLU:OE2 | 2.31 | 0.63 |
| 2:JF:86:ARG:NH1 | 2:KF:280:GLN:CB | 2.36 | 0.63 |
| 2:KB:100:ASN:ND2 | 2:KB:401:GLU:OE2 | 2.31 | 0.63 |
| 1:LC:176:GLN:HE22 | 4:2A:42:PHE:CB | 2.10 | 0.63 |
| 7:5A:1524:PHE:HD1 | 7:5A:1567:PHE:CZ | 2.07 | 0.63 |
| 7:5B:1524:PHE:HE1 | 7:5B:1571:MET:SD | 2.22 | 0.63 |
| 2:AF:217:LEU:HD23 | 6:4A:132:LYS:HG2 | 1.77 | 0.63 |
| 2:BD:179:VAL:HG21 | 1:BE:258:ASN:C | 2.23 | 0.63 |
| 1:CA:178:SER:OG | 2:CB:347:ASN:HB3 | 1.98 | 0.63 |
| 1:CE:404:PHE:HE2 | 2:CF:345:ILE:CD1 | 2.11 | 0.63 |
| 2:DB:60:VAL:HG21 | 2:EB:281:TYR:CD1 | 2.34 | 0.63 |
| 1:EE:288:VAL:HG11 | 1:EE:327:ASP:HB3 | 1.79 | 0.63 |
| 2:GD:178:THR:HB | 2:GD:181:GLU:HG3 | 1.81 | 0.63 |
| 1:HE:222:PRO:CD | 2:HF:324:LYS:HD3 | 2.29 | 0.63 |
| 2:IF:56:GLY:N | 10:9A:36:UNK:HA | 2.12 | 0.63 |
| 2:IF:100:ASN:ND2 | 2:IF:401:GLU:OE2 | 2.31 | 0.63 |
| 2:KB:82:GLY:C | 2:LB:281:TYR:CE1 | 2.76 | 0.63 |
| 2:KB:177:ASP:OD2 | 1:KC:248:LEU:HD23 | 1.97 | 0.63 |
| 2:LD:54:ALA:CB | 2:MD:281:TYR:O | 2.47 | 0.63 |
| 4:2B:164:ARG:HH11 | 4:2B:164:ARG:HG2 | 1.63 | 0.63 |
| 7:5A:1548:VAL:CG1 | 7:5A:1566:GLU:N | 2.61 | 0.63 |
| 7:5B:1383:GLU:OE1 | 7:5B:1383:GLU:N | 2.32 | 0.63 |
| 7:5C:1524:PHE:HD1 | 7:5C:1567:PHE:CZ | 2.07 | 0.63 |
| 2:AD:100:ASN:ND2 | 2:AD:401:GLU:OE2 | 2.31 | 0.63 |
| 2:DB:86:ARG:N | 2:EB:281:TYR:HE1 | 1.95 | 0.63 |
| 2:DD:179:VAL:CG2 | 1:DE:258:ASN:CA | 2.77 | 0.63 |
| 1:EC:288:VAL:HG11 | 1:EC:327:ASP:HB3 | 1.79 | 0.63 |
| 1:GA:89:PRO:CG | 1:HA:280:LYS:HZ2 | 2.08 | 0.63 |
| 2:GB:100:ASN:HB2 | 1:GC:257:THR:HG21 | 1.81 | 0.63 |
| 2:GB:178:THR:HB | 2:GB:181:GLU:HG3 | 1.81 | 0.63 |
| 1:GC:401:LYS:CE | 2:GD:344:TRP:CZ3 | 2.62 | 0.63 |
| 2:GF:178:THR:HB | 2:GF:181:GLU:HG3 | 1.81 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:ID:100:ASN:HB2 | 1:IE:257:THR:HG21 | 1.81 | 0.63 |
| 2:ID:178:THR:HB | 2:ID:181:GLU:HG3 | 1.81 | 0.63 |
| 1:IE:222:PRO:CD | 2:IF:324:LYS:HD3 | 2.29 | 0.63 |
| 1:JA:89:PRO:HG2 | 1:KA:280:LYS:N | 2.14 | 0.63 |
| 1:KA:79:ARG:HD2 | 1:LA:280:LYS:HD2 | 1.81 | 0.63 |
| 2:KF:272:PRO:O | 6:4D:268:LEU:HD23 | 1.89 | 0.63 |
| 2:MB:177:ASP:O | 1:MC:352:LYS:HA | 1.98 | 0.63 |
| 7:5A:1383:GLU:OE1 | 7:5A:1383:GLU:N | 2.32 | 0.63 |
| 2:AD:55:THR:CG2 | 2:BD:283:ALA:CB | 2.73 | 0.63 |
| 2:BF:85:PHE:O | 2:CF:281:TYR:OH | 2.16 | 0.63 |
| 2:BF:178:THR:HB | 2:BF:181:GLU:HG3 | 1.81 | 0.63 |
| 1:CE:60:LYS:HZ3 | 1:DE:283:HIS:CE1 | 2.16 | 0.63 |
| 1:FA:402:ARG:CD | 7:5C:1259:TYR:CD2 | 2.75 | 0.63 |
| 1:FE:422:ARG:CZ | 7:5B:1170:THR:CA | 2.76 | 0.63 |
| 2:GD:100:ASN:HB2 | 1:GE:257:THR:HG21 | 1.81 | 0.63 |
| 2:IB:177:ASP:OD2 | 1:IC:248:LEU:HD23 | 1.97 | 0.63 |
| 2:IB:178:THR:HB | 2:IB:181:GLU:HG3 | 1.81 | 0.63 |
| 2:IF:178:THR:HB | 2:IF:181:GLU:HG3 | 1.81 | 0.63 |
| 1:JE:222:PRO:CD | 2:JF:324:LYS:HD3 | 2.29 | 0.63 |
| 1:JE:370:LYS:HE2 | 10:9A:17:UNK:CB | 2.24 | 0.63 |
| 2:KB:212:PHE:CE2 | 1:KC:326:LYS:HD3 | 2.22 | 0.63 |
| 1:KE:222:PRO:CD | 2:KF:324:LYS:HD3 | 2.29 | 0.63 |
| 2:LD:177:ASP:CG | 1:LE:353:VAL:HG13 | 2.16 | 0.63 |
| 2:LF:274:THR:O | 6:4D:228:LEU:HD21 | 1.90 | 0.63 |
| 4:2A:164:ARG:HH11 | 4:2A:164:ARG:HG2 | 1.63 | 0.63 |
| 4:2C:164:ARG:HG2 | 4:2C:164:ARG:HH11 | 1.63 | 0.63 |
| 7:5B:1436:ARG:HH11 | 7:5B:1436:ARG:HG3 | 1.63 | 0.63 |
| 7:5B:1548:VAL:CG1 | 7:5B:1566:GLU:N | 2.61 | 0.63 |
| 7:5C:1142:PHE:HD1 | 7:5C:1146:LEU:HD12 | 1.63 | 0.63 |
| 7:5C:1436:ARG:HH11 | 7:5C:1436:ARG:HG3 | 1.63 | 0.63 |
| 1:AE:288:VAL:HG11 | 1:AE:327:ASP:HB3 | 1.79 | 0.63 |
| 2:BB:178:THR:HB | 2:BB:181:GLU:HG3 | 1.81 | 0.63 |
| 2:BD:178:THR:HB | 2:BD:181:GLU:HG3 | 1.81 | 0.63 |
| 2:CD:178:THR:HB | 2:CD:181:GLU:HG3 | 1.81 | 0.63 |
| 1:CE:176:GLN:O | 2:CF:347:ASN:ND2 | 2.31 | 0.63 |
| 1:EA:288:VAL:HG11 | 1:EA:327:ASP:HB3 | 1.79 | 0.63 |
| 2:FD:54:ALA:HA | 2:GD:283:ALA:HB3 | 1.78 | 0.63 |
| 1:FE:60:LYS:CD | 1:GE:283:HIS:HD2 | 2.09 | 0.63 |
| 2:JF:100:ASN:ND2 | 2:JF:401:GLU:OE2 | 2.31 | 0.63 |
| 1:LA:60:LYS:HZ3 | 1:MA:283:HIS:CE1 | 2.17 | 0.63 |
| 1:LE:60:LYS:NZ | 1:ME:283:HIS:CE1 | 2.67 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MD:178:THR:HB | 2:MD:181:GLU:HG3 | 1.81 | 0.63 |
| 7:5A:1436:ARG:HH11 | 7:5A:1436:ARG:HG3 | 1.63 | 0.63 |
| 7:5A:1552:LYS:HZ1 | 7:5A:1563:SER:CA | 2.10 | 0.63 |
| 7:5C:1355:GLN:C | 7:5C:1358:LYS:HG3 | 2.15 | 0.63 |
| 7:5C:1383:GLU:OE1 | 7:5C:1383:GLU:N | 2.32 | 0.63 |
| 1:AC:342:GLN:HE21 | 3:1C:55:HIS:CD2 | 2.09 | 0.62 |
| 1:AC:401:LYS:HE3 | 2:AD:344:TRP:CZ3 | 2.33 | 0.62 |
| 2:AD:55:THR:HG21 | 2:BD:283:ALA:HA | 1.80 | 0.62 |
| 2:AF:100:ASN:ND2 | 2:AF:401:GLU:OE2 | 2.31 | 0.62 |
| 2:CF:178:THR:HB | 2:CF:181:GLU:HG3 | 1.81 | 0.62 |
| 1:DA:11:GLN:OE1 | 2:DB:245:GLN:O | 2.16 | 0.62 |
| 2:EB:212:PHE:HZ | 1:EC:326:LYS:CE | 2.10 | 0.62 |
| 1:FA:419:SER:C | 7:5C:1256:ARG:NH2 | 2.57 | 0.62 |
| 2:FD:397:TRP:CD2 | 1:FE:256:GLN:O | 2.13 | 0.62 |
| 1:IA:60:LYS:NZ | 1:JA:283:HIS:CD2 | 2.65 | 0.62 |
| 2:IB:86:ARG:CB | 2:JB:281:TYR:CE1 | 2.78 | 0.62 |
| 2:JD:86:ARG:CZ | 2:KD:280:GLN:CA | 2.77 | 0.62 |
| 2:JD:208:TYR:OH | 1:JE:325:PRO:HB2 | 1.99 | 0.62 |
| 1:KC:88:HIS:CG | 1:LC:284:GLU:HB2 | 2.32 | 0.62 |
| 2:KF:276:ARG:NH2 | 6:4D:265:TYR:CA | 2.55 | 0.62 |
| 9:7A:10:TYR:CE2 | 9:7B:34:PRO:HB3 | 2.34 | 0.62 |
| 1:AA:288:VAL:HG11 | 1:AA:327:ASP:HB3 | 1.79 | 0.62 |
| 1:AC:288:VAL:HG11 | 1:AC:327:ASP:HB3 | 1.80 | 0.62 |
| 2:AD:220:PRO:O | 1:AE:324:VAL:HG13 | 1.98 | 0.62 |
| 1:DC:178:SER:OG | 2:DD:347:ASN:HB3 | 1.98 | 0.62 |
| 2:EF:222:TYR:O | 2:EF:226:ASN:ND2 | 2.28 | 0.62 |
| 2:FB:177:ASP:CG | 1:FC:353:VAL:HG13 | 1.94 | 0.62 |
| 1:GE:222:PRO:CD | 2:GF:324:LYS:HD3 | 2.29 | 0.62 |
| 2:GF:309:ARG:NH2 | 2:GF:426:GLN:O | 2.32 | 0.62 |
| 2:IB:222:TYR:O | 2:IB:226:ASN:ND2 | 2.27 | 0.62 |
| 2:ID:87:PRO:CD | 2:JD:281:TYR:CE2 | 2.83 | 0.62 |
| 2:JD:100:ASN:ND2 | 2:JD:401:GLU:OE2 | 2.31 | 0.62 |
| 2:LB:274:THR:H | 6:4A:228:LEU:HD21 | 1.64 | 0.62 |
| 2:LB:309:ARG:NH2 | 2:LB:426:GLN:O | 2.32 | 0.62 |
| 2:LF:274:THR:HG23 | 6:4D:228:LEU:HD22 | 1.81 | 0.62 |
| 2:MB:178:THR:HB | 2:MB:181:GLU:HG3 | 1.81 | 0.62 |
| 7:5A:1142:PHE:HD1 | 7:5A:1146:LEU:HD12 | 1.63 | 0.62 |
| 7:5A:1491:LEU:CA | 7:5A:1495:PHE:CB | 2.62 | 0.62 |
| 7:5C:1126:PRO:HG2 | 8:6C:246:TYR:OH | 1.99 | 0.62 |
| 2:AB:177:ASP:CG | 1:AC:353:VAL:HG11 | 1.96 | 0.62 |
| 2:AD:357:PRO:O | 6:4C:151:ARG:CZ | 2.47 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:178:THR:HB | 2:CB:181:GLU:HG3 | 1.81 | 0.62 |
| 1:CE:288:VAL:HG11 | 1:CE:327:ASP:HB3 | 1.80 | 0.62 |
| 2:CF:86:ARG:HB2 | 2:DF:281:TYR:CE1 | 2.31 | 0.62 |
| 1:DA:178:SER:OG | 2:DB:347:ASN:HB3 | 1.98 | 0.62 |
| 2:ED:309:ARG:NH2 | 2:ED:426:GLN:O | 2.32 | 0.62 |
| 1:FA:56:THR:OG1 | 1:GA:285:GLN:CA | 2.47 | 0.62 |
| 1:GC:401:LYS:HE3 | 2:GD:344:TRP:CZ3 | 2.33 | 0.62 |
| 1:HC:101:ASN:HD21 | 2:HD:252:LYS:HD2 | 0.79 | 0.62 |
| 1:IC:279:GLU:CD | 10:8W:22:UNK:CA | 2.71 | 0.62 |
| 2:JD:177:ASP:OD2 | 1:JE:248:LEU:HD23 | 1.99 | 0.62 |
| 2:KD:276:ARG:NH2 | 6:4B:271:GLU:C | 2.52 | 0.62 |
| 2:LB:228:LEU:CD2 | 6:4A:225:PRO:HG2 | 2.30 | 0.62 |
| 2:LB:296:ALA:HB3 | 4:2C:149:ILE:CG2 | 1.97 | 0.62 |
| 2:LF:224:ASP:CA | 6:4D:219:ASN:ND2 | 2.62 | 0.62 |
| 2:LF:306:ARG:NH2 | 4:2B:149:ILE:HG22 | 2.14 | 0.62 |
| 7:5A:1263:GLN:OE1 | 9:7A:8:ARG:NH1 | 2.32 | 0.62 |
| 7:5A:1355:GLN:C | 7:5A:1358:LYS:HG3 | 2.15 | 0.62 |
| 8:6C:107:PRO:HA | 8:6C:118:GLU:OE1 | 1.99 | 0.62 |
| 9:7C:10:TYR:CE2 | 9:7D:34:PRO:HB3 | 2.34 | 0.62 |
| 2:BD:85:PHE:O | 2:CD:281:TYR:OH | 2.16 | 0.62 |
| 1:FA:402:ARG:HH11 | 7:5C:1259:TYR:HD2 | 1.46 | 0.62 |
| 2:FF:331:LEU:HD22 | 7:5B:915:PHE:CE2 | 2.33 | 0.62 |
| 2:HB:177:ASP:OD2 | 1:HC:248:LEU:HD23 | 1.97 | 0.62 |
| 2:HD:177:ASP:OD1 | 1:HE:353:VAL:HG12 | 1.84 | 0.62 |
| 2:HD:212:PHE:HZ | 1:HE:326:LYS:HD3 | 0.54 | 0.62 |
| 2:LF:54:ALA:CB | 2:MF:281:TYR:O | 2.48 | 0.62 |
| 1:MA:288:VAL:HG11 | 1:MA:327:ASP:HB3 | 1.79 | 0.62 |
| 2:MF:178:THR:HB | 2:MF:181:GLU:HG3 | 1.81 | 0.62 |
| 7:5B:1142:PHE:HD1 | 7:5B:1146:LEU:HD12 | 1.63 | 0.62 |
| 7:5B:1355:GLN:C | 7:5B:1358:LYS:HG3 | 2.15 | 0.62 |
| 9:7E:12:GLU:CA | 9:7E:16:THR:OG1 | 2.46 | 0.62 |
| 2:AB:100:ASN:HB2 | 1:AC:257:THR:HG21 | 1.81 | 0.62 |
| 2:AF:40:SER:HG | 6:4A:152:PHE:HE2 | 0.65 | 0.62 |
| 2:BB:212:PHE:CE2 | 1:BC:326:LYS:HD3 | 2.20 | 0.62 |
| 1:CA:288:VAL:HG11 | 1:CA:327:ASP:HB3 | 1.80 | 0.62 |
| 1:CC:370:LYS:HE3 | 10:8E:17:UNK:CB | 2.20 | 0.62 |
| 2:EB:100:ASN:HB2 | 1:EC:257:THR:HG21 | 1.81 | 0.62 |
| 1:EC:282:TYR:CD2 | 10:8K:18:UNK:CB | 2.81 | 0.62 |
| 2:ED:157:GLU:HA | 7:5A:945:LYS:NZ | 2.13 | 0.62 |
| 2:ED:177:ASP:C | 1:EE:352:LYS:HA | 2.25 | 0.62 |
| 1:FA:100:ALA:HB1 | 2:FB:252:LYS:CA | 2.29 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FE:419:SER:CB | 7:5B:1256:ARG:CG | 2.77 | 0.62 |
| 1:GA:89:PRO:HD3 | 1:HA:280:LYS:CE | 2.24 | 0.62 |
| 2:GD:208:TYR:OH | 1:GE:325:PRO:HB2 | 1.99 | 0.62 |
| 2:GD:220:PRO:O | 1:GE:324:VAL:HG13 | 1.98 | 0.62 |
| 1:IA:108:TYR:HA | 1:IA:112:LYS:HE3 | 1.81 | 0.62 |
| 1:IC:108:TYR:HA | 1:IC:112:LYS:HE3 | 1.81 | 0.62 |
| 2:ID:177:ASP:OD1 | 1:IE:353:VAL:HG12 | 1.84 | 0.62 |
| 2:KD:178:THR:HB | 2:KD:181:GLU:HG3 | 1.81 | 0.62 |
| 2:KF:158:GLU:CA | 4:2B:34:ASN:CB | 2.48 | 0.62 |
| 2:KF:178:THR:HB | 2:KF:181:GLU:HG3 | 1.81 | 0.62 |
| 2:LB:228:LEU:HD21 | 6:4A:225:PRO:CB | 2.28 | 0.62 |
| 2:LD:306:ARG:CZ | 4:2A:149:ILE:HG21 | 2.22 | 0.62 |
| 1:LE:60:LYS:HD2 | 1:ME:283:HIS:CD2 | 2.31 | 0.62 |
| 1:MC:288:VAL:HG11 | 1:MC:327:ASP:HB3 | 1.79 | 0.62 |
| 5:3C:232:ALA:HB2 | 5:3C:335:LYS:C | 2.25 | 0.62 |
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:HG3 | 1.99 | 0.62 |
| 8:6A:107:PRO:HA | 8:6A:118:GLU:OE1 | 1.99 | 0.62 |
| 9:7A:12:GLU:CA | 9:7A:16:THR:OG1 | 2.46 | 0.62 |
| 1:AC:60:LYS:HD3 | 1:BC:283:HIS:CD2 | 2.34 | 0.62 |
| 1:AC:101:ASN:HD21 | 2:AD:252:LYS:HD2 | 0.79 | 0.62 |
| 2:AF:321:MET:C | 6:4A:156:PHE:CD2 | 2.78 | 0.62 |
| 1:CC:288:VAL:HG11 | 1:CC:327:ASP:HB3 | 1.80 | 0.62 |
| 2:EB:309:ARG:NH2 | 2:EB:426:GLN:O | 2.32 | 0.62 |
| 2:FB:178:THR:HB | 2:FB:181:GLU:HG3 | 1.81 | 0.62 |
| 1:FC:402:ARG:CZ | 7:5A:1259:TYR:HA | 2.30 | 0.62 |
| 2:GB:55:THR:CA | 2:HB:283:ALA:HB2 | 2.26 | 0.62 |
| 2:GB:177:ASP:OD2 | 1:GC:248:LEU:HD23 | 1.97 | 0.62 |
| 1:GC:101:ASN:HD21 | 2:GD:252:LYS:HD2 | 0.79 | 0.62 |
| 2:GD:309:ARG:NH2 | 2:GD:426:GLN:O | 2.32 | 0.62 |
| 1:HA:108:TYR:HA | 1:HA:112:LYS:HE3 | 1.81 | 0.62 |
| 1:HE:404:PHE:HE2 | 2:HF:345:ILE:HD12 | 1.65 | 0.62 |
| 2:JB:86:ARG:CZ | 2:KB:281:TYR:N | 2.56 | 0.62 |
| 2:JB:100:ASN:ND2 | 2:JB:401:GLU:OE2 | 2.31 | 0.62 |
| 2:JB:100:ASN:HB2 | 1:JC:257:THR:HG21 | 1.81 | 0.62 |
| 1:JC:101:ASN:HD21 | 2:JD:252:LYS:HD2 | 0.79 | 0.62 |
| 2:LB:55:THR:CG2 | 2:MB:283:ALA:C | 2.72 | 0.62 |
| 2:LD:215:LEU:CD1 | 6:4B:225:PRO:HB3 | 2.29 | 0.62 |
| 2:LD:274:THR:O | 6:4B:228:LEU:HD21 | 1.94 | 0.62 |
| 2:LF:223:GLY:HA3 | 6:4D:219:ASN:HA | 1.80 | 0.62 |
| 1:MC:404:PHE:CE2 | 2:MD:345:ILE:HD11 | 2.35 | 0.62 |
| 1:ME:288:VAL:HG11 | 1:ME:327:ASP:HB3 | 1.80 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AD:179:VAL:CG2 | 1:AE:258:ASN:CA | 2.78 | 0.62 |
| 2:CB:179:VAL:CG2 | 1:CC:258:ASN:O | 2.37 | 0.62 |
| 2:DB:176:SER:OG | 1:DC:349:THR:OG1 | 2.16 | 0.62 |
| 2:DF:178:THR:HB | 2:DF:181:GLU:HG3 | 1.81 | 0.62 |
| 1:EA:401:LYS:HE3 | 2:EB:344:TRP:CZ3 | 2.34 | 0.62 |
| 1:EC:419:SER:OG | 7:5A:830:VAL:HG21 | 1.99 | 0.62 |
| 2:ED:157:GLU:OE1 | 7:5A:935:LYS:NZ | 2.32 | 0.62 |
| 2:FB:54:ALA:HB1 | 2:GB:283:ALA:N | 2.13 | 0.62 |
| 2:GB:309:ARG:NH2 | 2:GB:426:GLN:O | 2.32 | 0.62 |
| 1:HC:108:TYR:HA | 1:HC:112:LYS:HE3 | 1.81 | 0.62 |
| 2:ID:177:ASP:O | 1:IE:352:LYS:CD | 2.34 | 0.62 |
| 1:KA:108:TYR:HA | 1:KA:112:LYS:HE3 | 1.81 | 0.62 |
| 2:KD:125:GLU:HB2 | 2:LD:336:LYS:HE2 | 1.80 | 0.62 |
| 2:KD:177:ASP:OD2 | 1:KE:248:LEU:HD23 | 1.98 | 0.62 |
| 2:KF:125:GLU:HG2 | 2:LF:336:LYS:HZ1 | 1.58 | 0.62 |
| 2:LD:212:PHE:CZ | 1:LE:326:LYS:CD | 2.29 | 0.62 |
| 1:MC:372:MET:CE | 6:4A:96:VAL:CA | 2.78 | 0.62 |
| 2:MD:100:ASN:HB2 | 1:ME:257:THR:HG21 | 1.81 | 0.62 |
| 5:3A:232:ALA:HB2 | 5:3A:335:LYS:C | 2.25 | 0.62 |
| 7:5A:1077:ASN:HA | 7:5A:1083:THR:HG21 | 1.81 | 0.62 |
| 7:5B:1077:ASN:HA | 7:5B:1083:THR:HG21 | 1.81 | 0.62 |
| 7:5C:1491:LEU:CA | 7:5C:1495:PHE:CB | 2.62 | 0.62 |
| 8:6B:107:PRO:HA | 8:6B:118:GLU:OE1 | 1.99 | 0.62 |
| 1:AE:222:PRO:CD | 2:AF:324:LYS:HD3 | 2.29 | 0.62 |
| 2:AF:359:LYS:CA | 6:4A:151:ARG:HH22 | 1.98 | 0.62 |
| 1:BE:224:TYR:HE2 | 2:BF:246:LEU:HD11 | 1.65 | 0.62 |
| 1:DC:224:TYR:HE2 | 2:DD:246:LEU:HD11 | 1.65 | 0.62 |
| 2:DD:178:THR:HB | 2:DD:181:GLU:HG3 | 1.81 | 0.62 |
| 2:DF:55:THR:HG23 | 2:EF:283:ALA:HA | 1.81 | 0.62 |
| 2:EB:178:THR:HB | 2:EB:181:GLU:HG3 | 1.81 | 0.62 |
| 1:FA:419:SER:OG | 7:5C:1256:ARG:HD3 | 1.98 | 0.62 |
| 2:GB:177:ASP:O | 1:GC:352:LYS:CD | 2.35 | 0.62 |
| 2:GD:177:ASP:O | 1:GE:352:LYS:CD | 2.34 | 0.62 |
| 1:HE:108:TYR:HA | 1:HE:112:LYS:HE3 | 1.81 | 0.62 |
| 2:IB:177:ASP:O | 1:IC:352:LYS:CD | 2.35 | 0.62 |
| 1:IC:101:ASN:HD21 | 2:ID:252:LYS:HD2 | 0.79 | 0.62 |
| 2:ID:177:ASP:OD2 | 1:IE:248:LEU:HD23 | 1.99 | 0.62 |
| 1:IE:108:TYR:HA | 1:IE:112:LYS:HE3 | 1.81 | 0.62 |
| 2:JB:212:PHE:CE2 | 1:JC:326:LYS:HD3 | 2.22 | 0.62 |
| 1:JC:108:TYR:HA | 1:JC:112:LYS:HE3 | 1.81 | 0.62 |
| 1:JE:108:TYR:HA | 1:JE:112:LYS:HE3 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:JF:178:THR:HB | 2:JF:181:GLU:HG3 | 1.81 | 0.62 |
| 2:KB:178:THR:HB | 2:KB:181:GLU:HG3 | 1.81 | 0.62 |
| 2:KF:77:ARG:CD | 2:LF:281:TYR:CZ | 2.82 | 0.62 |
| 2:LB:231:ALA:HB1 | 6:4A:226:ILE:HD13 | 1.69 | 0.62 |
| 2:LF:178:THR:HB | 2:LF:181:GLU:HG3 | 1.81 | 0.62 |
| 2:LF:215:LEU:CD1 | 6:4D:225:PRO:HB3 | 2.29 | 0.62 |
| 5:3B:232:ALA:HB2 | 5:3B:335:LYS:C | 2.25 | 0.62 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:HG3 | 1.99 | 0.62 |
| 7:5B:1552:LYS:HZ1 | 7:5B:1563:SER:CA | 2.10 | 0.62 |
| 7:5C:1077:ASN:HA | 7:5C:1083:THR:HG22 | 1.81 | 0.62 |
| 9:7A:15:VAL:CB | 9:7B:35:ILE:HD12 | 2.24 | 0.62 |
| 2:AB:212:PHE:CZ | 1:AC:326:LYS:CD | 2.31 | 0.62 |
| 2:ED:179:VAL:HG21 | 1:EE:258:ASN:C | 2.25 | 0.62 |
| 1:FE:108:TYR:HA | 1:FE:112:LYS:HE3 | 1.81 | 0.62 |
| 2:GD:179:VAL:CG2 | 1:GE:258:ASN:CA | 2.78 | 0.62 |
| 1:GE:60:LYS:NZ | 1:HE:283:HIS:CG | 2.67 | 0.62 |
| 2:HB:100:ASN:HB2 | 1:HC:257:THR:HG21 | 1.81 | 0.62 |
| 2:HF:178:THR:HB | 2:HF:181:GLU:HG3 | 1.81 | 0.62 |
| 2:JD:178:THR:HB | 2:JD:181:GLU:HG3 | 1.81 | 0.62 |
| 1:JE:88:HIS:CE1 | 1:KE:280:LYS:HB3 | 2.35 | 0.62 |
| 2:KB:100:ASN:HB2 | 1:KC:257:THR:HG21 | 1.81 | 0.62 |
| 1:KC:108:TYR:HA | 1:KC:112:LYS:HE3 | 1.81 | 0.62 |
| 2:LD:223:GLY:C | 6:4B:219:ASN:CG | 2.63 | 0.62 |
| 2:MB:177:ASP:CB | 1:MC:353:VAL:HG12 | 2.30 | 0.62 |
| 2:MF:222:TYR:O | 2:MF:226:ASN:ND2 | 2.28 | 0.62 |
| 4:2C:71:LYS:HE3 | 4:2C:72:TYR:CZ | 2.35 | 0.62 |
| 6:4D:289:LYS:HA | 6:4D:289:LYS:CE | 2.25 | 0.62 |
| 7:5B:1376:GLN:HA | 7:5B:1379:LYS:HD2 | 1.80 | 0.62 |
| 7:5C:1077:ASN:HA | 7:5C:1083:THR:HG21 | 1.81 | 0.62 |
| 8:6B:177:TYR:CE1 | 8:6B:199:ILE:HD13 | 2.34 | 0.62 |
| 9:7C:18:VAL:HG12 | 9:7C:42:LEU:HD23 | 1.75 | 0.62 |
| 2:BB:87:PRO:HD2 | 2:CB:281:TYR:CE2 | 2.35 | 0.62 |
| 2:CB:86:ARG:HB2 | 2:DB:281:TYR:HE1 | 1.64 | 0.62 |
| 2:DD:100:ASN:HB2 | 1:DE:257:THR:HG21 | 1.82 | 0.62 |
| 2:ED:178:THR:HB | 2:ED:181:GLU:HG3 | 1.81 | 0.62 |
| 1:EE:71:GLU:CD | 2:EF:247:ASN:ND2 | 2.58 | 0.62 |
| 1:FA:207:GLU:CD | 7:5C:915:PHE:CD2 | 2.78 | 0.62 |
| 2:FD:178:THR:HB | 2:FD:181:GLU:HG3 | 1.81 | 0.62 |
| 2:FF:178:THR:HB | 2:FF:181:GLU:HG3 | 1.81 | 0.62 |
| 1:IA:402:ARG:HH21 | 7:5C:1417:GLN:HG3 | 1.28 | 0.62 |
| 2:ID:222:TYR:O | 2:ID:226:ASN:ND2 | 2.27 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:JA:108:TYR:HA | 1:JA:112:LYS:HE3 | 1.81 | 0.62 |
| 1:KC:85:GLN:HG2 | 1:LC:283:HIS:HD2 | 1.65 | 0.62 |
| 2:KD:179:VAL:CG2 | 1:KE:258:ASN:CA | 2.78 | 0.62 |
| 2:LB:306:ARG:HH21 | 4:2C:149:ILE:HG22 | 1.60 | 0.62 |
| 4:2A:71:LYS:HE3 | 4:2A:72:TYR:CZ | 2.35 | 0.62 |
| 4:2B:71:LYS:HE3 | 4:2B:72:TYR:CZ | 2.35 | 0.62 |
| 7:5A:1077:ASN:HA | 7:5A:1083:THR:HG22 | 1.81 | 0.62 |
| 7:5A:1376:GLN:HA | 7:5A:1379:LYS:HD2 | 1.80 | 0.62 |
| 7:5B:1113:ILE:HG12 | 7:5B:1157:THR:HG23 | 1.82 | 0.62 |
| 7:5C:839:GLU:CD | 8:6C:109:ILE:N | 2.29 | 0.62 |
| 8:6A:177:TYR:CE1 | 8:6A:199:ILE:HD13 | 2.34 | 0.62 |
| 8:6C:177:TYR:CE1 | 8:6C:199:ILE:HD13 | 2.34 | 0.62 |
| 2:AB:177:ASP:OD2 | 1:AC:248:LEU:HD23 | 1.97 | 0.61 |
| 2:AD:208:TYR:OH | 1:AE:325:PRO:HB2 | 1.99 | 0.61 |
| 2:AD:356:ILE:HG23 | 6:4C:152:PHE:CE1 | 2.35 | 0.61 |
| 1:AE:404:PHE:HE2 | 2:AF:345:ILE:HD12 | 1.65 | 0.61 |
| 2:BB:222:TYR:CD2 | 1:BC:247:ALA:HB1 | 2.35 | 0.61 |
| 2:CB:212:PHE:CE2 | 1:CC:326:LYS:HD3 | 2.18 | 0.61 |
| 1:DA:402:ARG:CD | 7:5C:777:ALA:CB | 2.75 | 0.61 |
| 13:ED:502:GDP:C8 | 1:EE:248:LEU:CD1 | 2.83 | 0.61 |
| 1:FE:422:ARG:CZ | 7:5B:1170:THR:C | 2.71 | 0.61 |
| 1:GC:108:TYR:HA | 1:GC:112:LYS:HE3 | 1.81 | 0.61 |
| 2:GD:177:ASP:OD2 | 1:GE:248:LEU:HD23 | 1.98 | 0.61 |
| 1:GE:108:TYR:HA | 1:GE:112:LYS:HE3 | 1.81 | 0.61 |
| 2:HD:177:ASP:OD2 | 1:HE:248:LEU:HD23 | 1.98 | 0.61 |
| 2:JF:86:ARG:NH2 | 2:KF:280:GLN:CG | 2.60 | 0.61 |
| 1:KA:288:VAL:HG11 | 1:KA:327:ASP:HB3 | 1.79 | 0.61 |
| 1:KE:288:VAL:HG11 | 1:KE:327:ASP:HB3 | 1.79 | 0.61 |
| 1:LC:35:GLN:NE2 | 6:4A:101:ARG:HB2 | 2.15 | 0.61 |
| 2:LD:228:LEU:CD2 | 6:4B:225:PRO:HG2 | 2.30 | 0.61 |
| 1:MC:279:GLU:OE2 | 6:4A:106:ALA:CB | 2.47 | 0.61 |
| 1:ME:71:GLU:CD | 2:MF:247:ASN:ND2 | 2.57 | 0.61 |
| 7:5A:1521:PHE:CZ | 7:5A:1570:ALA:HB3 | 2.34 | 0.61 |
| 7:5B:1268:LEU:HD21 | 9:7D:19:LEU:HD13 | 1.82 | 0.61 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:HG3 | 1.99 | 0.61 |
| 7:5C:1521:PHE:CZ | 7:5C:1570:ALA:HB3 | 2.34 | 0.61 |
| 9:7C:12:GLU:CA | 9:7C:16:THR:OG1 | 2.46 | 0.61 |
| 2:AD:100:ASN:HB2 | 1:AE:257:THR:HG21 | 1.81 | 0.61 |
| 2:CB:86:ARG:HA | 2:DB:281:TYR:OH | 1.96 | 0.61 |
| 2:DB:178:THR:HB | 2:DB:181:GLU:HG3 | 1.81 | 0.61 |
| 2:DF:85:PHE:O | 2:EF:281:TYR:CZ | 2.52 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FC:108:TYR:HA | 1:FC:112:LYS:HE3 | 1.81 | 0.61 |
| 1:FE:100:ALA:HB1 | 2:FF:252:LYS:HA | 1.81 | 0.61 |
| 2:HD:178:THR:HB | 2:HD:181:GLU:HG3 | 1.81 | 0.61 |
| 2:HD:208:TYR:OH | 1:HE:325:PRO:HB2 | 1.99 | 0.61 |
| 2:ID:179:VAL:CG2 | 1:IE:258:ASN:CA | 2.78 | 0.61 |
| 2:ID:208:TYR:OH | 1:IE:325:PRO:HB2 | 1.99 | 0.61 |
| 1:IE:288:VAL:HG11 | 1:IE:327:ASP:HB3 | 1.79 | 0.61 |
| 1:KC:85:GLN:HG2 | 1:LC:283:HIS:CD2 | 2.34 | 0.61 |
| 1:KC:101:ASN:HD21 | 2:KD:252:LYS:HD2 | 0.79 | 0.61 |
| 1:KC:288:VAL:HG11 | 1:KC:327:ASP:HB3 | 1.80 | 0.61 |
| 1:KE:108:TYR:HA | 1:KE:112:LYS:HE3 | 1.81 | 0.61 |
| 1:LA:108:TYR:HA | 1:LA:112:LYS:HE3 | 1.81 | 0.61 |
| 1:LC:60:LYS:HD3 | 1:MC:283:HIS:CA | 2.29 | 0.61 |
| 1:MC:108:TYR:HA | 1:MC:112:LYS:HE3 | 1.81 | 0.61 |
| 6:4A:215:LYS:O | 6:4A:215:LYS:HG3 | 2.01 | 0.61 |
| 6:4B:215:LYS:O | 6:4B:215:LYS:HG3 | 2.01 | 0.61 |
| 6:4C:215:LYS:HG3 | 6:4C:215:LYS:O | 2.01 | 0.61 |
| 7:5B:1521:PHE:CZ | 7:5B:1570:ALA:HB3 | 2.34 | 0.61 |
| 7:5B:1572:LEU:CD1 | 7:5B:1576:ILE:HD11 | 2.29 | 0.61 |
| 7:5C:1113:ILE:HG12 | 7:5C:1157:THR:HG23 | 1.82 | 0.61 |
| 7:5C:1572:LEU:CD1 | 7:5C:1576:ILE:HD11 | 2.29 | 0.61 |
| 9:7E:18:VAL:HG12 | 9:7E:42:LEU:HD23 | 1.75 | 0.61 |
| 2:BD:179:VAL:CG2 | 1:BE:258:ASN:CA | 2.78 | 0.61 |
| 1:DC:404:PHE:HE2 | 2:DD:345:ILE:HD12 | 1.65 | 0.61 |
| 1:DE:404:PHE:HE2 | 2:DF:345:ILE:HD12 | 1.65 | 0.61 |
| 1:FA:108:TYR:HA | 1:FA:112:LYS:HE3 | 1.81 | 0.61 |
| 2:FD:331:LEU:HD21 | 7:5A:915:PHE:CE1 | 2.35 | 0.61 |
| 1:GA:105:ARG:NH1 | 2:GB:251:ARG:HD3 | 2.16 | 0.61 |
| 1:GA:108:TYR:HA | 1:GA:112:LYS:HE3 | 1.81 | 0.61 |
| 1:IA:288:VAL:HG11 | 1:IA:327:ASP:HB3 | 1.79 | 0.61 |
| 1:IC:288:VAL:HG11 | 1:IC:327:ASP:HB3 | 1.80 | 0.61 |
| 2:JB:178:THR:HB | 2:JB:181:GLU:HG3 | 1.81 | 0.61 |
| 2:KD:87:PRO:CD | 2:LD:282:ARG:HG3 | 2.25 | 0.61 |
| 2:KD:100:ASN:HB2 | 1:KE:257:THR:HG21 | 1.81 | 0.61 |
| 2:KD:208:TYR:OH | 1:KE:325:PRO:HB2 | 1.99 | 0.61 |
| 1:LC:108:TYR:HA | 1:LC:112:LYS:HE3 | 1.81 | 0.61 |
| 2:LD:178:THR:HB | 2:LD:181:GLU:HG3 | 1.81 | 0.61 |
| 1:MA:108:TYR:HA | 1:MA:112:LYS:HE3 | 1.81 | 0.61 |
| 2:MB:390:ARG:CD | 1:MC:439:THR:HG21 | 2.30 | 0.61 |
| 1:ME:108:TYR:HA | 1:ME:112:LYS:HE3 | 1.81 | 0.61 |
| 6:4D:215:LYS:HG3 | 6:4D:215:LYS:O | 2.01 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1113:ILE:HG12 | 7:5A:1157:THR:HG23 | 1.82 | 0.61 |
| 7:5A:1572:LEU:CD1 | 7:5A:1576:ILE:HD11 | 2.29 | 0.61 |
| 7:5C:835:GLN:HE21 | 7:5C:835:GLN:CA | 2.13 | 0.61 |
| 7:5C:1267:CYS:SG | 9:7E:8:ARG:CZ | 2.87 | 0.61 |
| 7:5C:1376:GLN:HA | 7:5C:1379:LYS:HD2 | 1.80 | 0.61 |
| 1:AA:105:ARG:NH1 | 2:AB:251:ARG:HD3 | 2.16 | 0.61 |
| 2:AB:212:PHE:CE2 | 1:AC:326:LYS:HD3 | 2.22 | 0.61 |
| 2:BB:100:ASN:HB2 | 1:BC:257:THR:HG21 | 1.82 | 0.61 |
| 13:DD:501:GDP:C8 | 1:DE:248:LEU:CD1 | 2.83 | 0.61 |
| 1:EA:108:TYR:HA | 1:EA:112:LYS:HE3 | 1.81 | 0.61 |
| 1:EC:108:TYR:HA | 1:EC:112:LYS:HE3 | 1.81 | 0.61 |
| 1:EE:224:TYR:HE2 | 2:EF:246:LEU:HD11 | 1.65 | 0.61 |
| 2:EF:178:THR:HB | 2:EF:181:GLU:HG3 | 1.81 | 0.61 |
| 1:FE:222:PRO:HG2 | 2:FF:324:LYS:HD3 | 1.82 | 0.61 |
| 2:HB:178:THR:HB | 2:HB:181:GLU:HG3 | 1.81 | 0.61 |
| 2:IF:87:PRO:HD2 | 2:JF:281:TYR:CZ | 2.35 | 0.61 |
| 1:JE:404:PHE:HE2 | 2:JF:345:ILE:HD12 | 1.65 | 0.61 |
| 2:KB:276:ARG:NH2 | 6:4A:271:GLU:C | 2.46 | 0.61 |
| 2:KF:117:LEU:HD21 | 4:2B:144:ASN:OD1 | 2.00 | 0.61 |
| 2:LB:228:LEU:CD2 | 6:4A:225:PRO:CG | 2.78 | 0.61 |
| 7:5B:1077:ASN:HA | 7:5B:1083:THR:HG22 | 1.81 | 0.61 |
| 2:AF:362:LYS:HG2 | 6:4A:146:ILE:CB | 2.21 | 0.61 |
| 2:BD:397:TRP:CB | 1:BE:256:GLN:HE22 | 2.11 | 0.61 |
| 1:BE:222:PRO:HD2 | 2:BF:324:LYS:HD3 | 1.81 | 0.61 |
| 1:DC:400:ALA:HA | 7:5A:775:PRO:HB3 | 1.80 | 0.61 |
| 1:FA:222:PRO:HD2 | 2:FB:324:LYS:HD3 | 1.83 | 0.61 |
| 1:FC:404:PHE:CE2 | 2:FD:345:ILE:CD1 | 2.82 | 0.61 |
| 2:FD:55:THR:CB | 2:GD:283:ALA:HA | 2.30 | 0.61 |
| 1:GC:56:THR:O | 1:HC:285:GLN:CA | 2.48 | 0.61 |
| 2:HB:177:ASP:OD1 | 1:HC:353:VAL:HG12 | 1.84 | 0.61 |
| 1:HC:222:PRO:CD | 2:HD:324:LYS:HD3 | 2.31 | 0.61 |
| 2:HD:220:PRO:O | 1:HE:324:VAL:HG13 | 1.98 | 0.61 |
| 2:HF:261:PRO:HB2 | 5:3A:337:ARG:HH21 | 0.85 | 0.61 |
| 2:JD:73:MET:HA | 2:JD:76:VAL:HG12 | 1.83 | 0.61 |
| 2:KF:73:MET:HA | 2:KF:76:VAL:HG12 | 1.83 | 0.61 |
| 2:KF:276:ARG:CZ | 6:4D:271:GLU:O | 2.49 | 0.61 |
| 1:LA:224:TYR:CE2 | 2:LB:246:LEU:HD11 | 2.33 | 0.61 |
| 2:LB:178:THR:HB | 2:LB:181:GLU:HG3 | 1.81 | 0.61 |
| 1:LC:60:LYS:CD | 1:MC:283:HIS:CG | 2.83 | 0.61 |
| 2:LD:227:HIS:HD1 | 6:4B:226:ILE:HG13 | 1.65 | 0.61 |
| 1:LE:108:TYR:HA | 1:LE:112:LYS:HE3 | 1.81 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MD:177:ASP:CB | 1:ME:353:VAL:HG12 | 2.29 | 0.61 |
| 2:MF:221:THR:HB | 6:4D:189:ARG:NH1 | 2.15 | 0.61 |
| 7:5A:835:GLN:HE21 | 7:5A:835:GLN:CA | 2.13 | 0.61 |
| 7:5B:1367:LYS:HB2 | 7:5B:1367:LYS:HZ1 | 1.62 | 0.61 |
| 1:AA:108:TYR:HA | 1:AA:112:LYS:HE3 | 1.81 | 0.61 |
| 2:AF:178:THR:HB | 2:AF:181:GLU:HG3 | 1.81 | 0.61 |
| 2:BF:309:ARG:NH2 | 2:BF:426:GLN:O | 2.32 | 0.61 |
| 1:CA:176:GLN:O | 2:CB:347:ASN:ND2 | 2.32 | 0.61 |
| 1:DA:108:TYR:HA | 1:DA:112:LYS:HE3 | 1.81 | 0.61 |
| 1:EE:108:TYR:HA | 1:EE:112:LYS:HE3 | 1.81 | 0.61 |
| 1:FC:402:ARG:HD3 | 7:5A:1259:TYR:HB2 | 1.82 | 0.61 |
| 2:GB:54:ALA:CB | 2:HB:281:TYR:O | 2.48 | 0.61 |
| 1:GE:404:PHE:HE2 | 2:GF:345:ILE:HD12 | 1.65 | 0.61 |
| 1:HA:105:ARG:NH1 | 2:HB:251:ARG:HD3 | 2.16 | 0.61 |
| 1:HC:282:TYR:CD1 | 10:8T:15:UNK:HA | 2.35 | 0.61 |
| 1:HE:278:ALA:CB | 10:8U:22:UNK:CB | 2.78 | 0.61 |
| 1:IC:222:PRO:CD | 2:ID:324:LYS:HD3 | 2.31 | 0.61 |
| 2:JB:86:ARG:CD | 2:KB:281:TYR:CD2 | 2.43 | 0.61 |
| 2:JD:100:ASN:HB2 | 1:JE:257:THR:HG21 | 1.81 | 0.61 |
| 1:KA:105:ARG:NH1 | 2:KB:251:ARG:HD3 | 2.16 | 0.61 |
| 1:KA:359:PRO:CB | 6:4C:299:TYR:CE2 | 2.71 | 0.61 |
| 1:KC:88:HIS:CB | 1:LC:284:GLU:HB2 | 2.29 | 0.61 |
| 1:MA:71:GLU:CD | 2:MB:247:ASN:ND2 | 2.57 | 0.61 |
| 2:MF:73:MET:HA | 2:MF:76:VAL:HG12 | 1.83 | 0.61 |
| 6:4B:289:LYS:HA | 6:4B:289:LYS:CE | 2.25 | 0.61 |
| 7:5B:835:GLN:HE21 | 7:5B:835:GLN:CA | 2.13 | 0.61 |
| 7:5B:1272:ILE:CD1 | 9:7D:11:TYR:HD2 | 2.13 | 0.61 |
| 2:AB:177:ASP:O | 1:AC:352:LYS:CD | 2.35 | 0.61 |
| 1:AC:108:TYR:HA | 1:AC:112:LYS:HE3 | 1.81 | 0.61 |
| 2:AD:73:MET:HA | 2:AD:76:VAL:HG12 | 1.83 | 0.61 |
| 2:AD:177:ASP:O | 1:AE:352:LYS:CD | 2.34 | 0.61 |
| 2:AD:179:VAL:HG21 | 1:AE:258:ASN:C | 2.25 | 0.61 |
| 2:AF:73:MET:HA | 2:AF:76:VAL:HG12 | 1.83 | 0.61 |
| 2:BD:309:ARG:NH2 | 2:BD:426:GLN:O | 2.32 | 0.61 |
| 1:BE:108:TYR:HA | 1:BE:112:LYS:HE3 | 1.81 | 0.61 |
| 1:CA:108:TYR:HA | 1:CA:112:LYS:HE3 | 1.81 | 0.61 |
| 2:DB:100:ASN:HB2 | 1:DC:257:THR:HG21 | 1.83 | 0.61 |
| 2:DB:220:PRO:CD | 1:DC:326:LYS:HG2 | 2.30 | 0.61 |
| 2:HD:100:ASN:HB2 | 1:HE:257:THR:HG21 | 1.81 | 0.61 |
| 2:JB:73:MET:HA | 2:JB:76:VAL:HG12 | 1.83 | 0.61 |
| 1:JC:222:PRO:CD | 2:JD:324:LYS:HD3 | 2.31 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JE:128:ASN:HA | 1:KE:285:GLN:HE22 | 1.66 | 0.61 |
| 2:JF:73:MET:HA | 2:JF:76:VAL:HG12 | 1.83 | 0.61 |
| 2:KD:73:MET:HA | 2:KD:76:VAL:HG12 | 1.83 | 0.61 |
| 2:KD:126:GLY:O | 4:2A:39:ALA:HB2 | 2.00 | 0.61 |
| 1:ME:105:ARG:NH1 | 2:MF:251:ARG:HD3 | 2.15 | 0.61 |
| 7:5A:1367:LYS:HB2 | 7:5A:1367:LYS:HZ1 | 1.62 | 0.61 |
| 7:5A:1411:LYS:HD3 | 7:5A:1411:LYS:O | 2.00 | 0.61 |
| 7:5A:1490:LYS:HG3 | 7:5A:1494:LEU:CG | 2.30 | 0.61 |
| 7:5B:1411:LYS:HD3 | 7:5B:1411:LYS:O | 2.00 | 0.61 |
| 7:5B:1490:LYS:HG3 | 7:5B:1494:LEU:CG | 2.31 | 0.61 |
| 7:5C:1490:LYS:HG3 | 7:5C:1494:LEU:CG | 2.30 | 0.61 |
| 2:AB:73:MET:HA | 2:AB:76:VAL:HG12 | 1.83 | 0.61 |
| 2:AB:178:THR:HB | 2:AB:181:GLU:HG3 | 1.81 | 0.61 |
| 2:AD:178:THR:HB | 2:AD:181:GLU:HG3 | 1.81 | 0.61 |
| 1:BA:108:TYR:HA | 1:BA:112:LYS:HE3 | 1.81 | 0.61 |
| 1:BC:108:TYR:HA | 1:BC:112:LYS:HE3 | 1.81 | 0.61 |
| 1:CC:108:TYR:HA | 1:CC:112:LYS:HE3 | 1.81 | 0.61 |
| 2:DB:222:TYR:O | 2:DB:226:ASN:ND2 | 2.28 | 0.61 |
| 1:DC:108:TYR:HA | 1:DC:112:LYS:HE3 | 1.81 | 0.61 |
| 1:DC:401:LYS:CE | 2:DD:344:TRP:CZ3 | 2.73 | 0.61 |
| 2:DF:86:ARG:CB | 2:EF:281:TYR:CE1 | 2.83 | 0.61 |
| 2:ED:125:GLU:HG2 | 7:5A:903:PHE:HD2 | 1.58 | 0.61 |
| 1:EE:11:GLN:NE2 | 2:EF:247:ASN:OD1 | 2.34 | 0.61 |
| 1:GC:222:PRO:CD | 2:GD:324:LYS:HD3 | 2.31 | 0.61 |
| 2:IB:177:ASP:OD1 | 1:IC:353:VAL:HG12 | 1.84 | 0.61 |
| 2:IF:222:TYR:O | 2:IF:226:ASN:ND2 | 2.28 | 0.61 |
| 2:JD:220:PRO:O | 1:JE:324:VAL:HG13 | 1.98 | 0.61 |
| 2:LB:73:MET:HA | 2:LB:76:VAL:HG12 | 1.83 | 0.61 |
| 4:2A:164:ARG:HH11 | 4:2A:164:ARG:CG | 2.14 | 0.61 |
| 6:4D:131:VAL:O | 6:4D:131:VAL:HG13 | 2.01 | 0.61 |
| 7:5A:1548:VAL:HB | 7:5A:1566:GLU:O | 2.01 | 0.61 |
| 7:5C:1411:LYS:HD3 | 7:5C:1411:LYS:O | 2.00 | 0.61 |
| 7:5C:1548:VAL:HB | 7:5C:1566:GLU:O | 2.01 | 0.61 |
| 9:7A:10:TYR:OH | 9:7B:34:PRO:HB3 | 2.01 | 0.61 |
| 2:AB:222:TYR:O | 2:AB:226:ASN:ND2 | 2.27 | 0.61 |
| 2:AD:177:ASP:OD2 | 1:AE:248:LEU:HD23 | 1.98 | 0.61 |
| 1:AE:108:TYR:HA | 1:AE:112:LYS:HE3 | 1.81 | 0.61 |
| 1:CE:108:TYR:HA | 1:CE:112:LYS:HE3 | 1.81 | 0.61 |
| 2:EF:54:ALA:C | 2:FF:283:ALA:HB2 | 2.26 | 0.61 |
| 2:HD:179:VAL:CG2 | 1:HE:258:ASN:CA | 2.78 | 0.61 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:CB | 2.64 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:KB:73:MET:HA | 2:KB:76:VAL:HG12 | 1.83 | 0.61 |
| 1:KE:85:GLN:NE2 | 1:LE:282:TYR:HB2 | 2.13 | 0.61 |
| 2:KF:82:GLY:O | 2:LF:281:TYR:HE1 | 1.84 | 0.61 |
| 2:LB:228:LEU:HD21 | 6:4A:225:PRO:HB2 | 1.82 | 0.61 |
| 2:LB:331:LEU:HD22 | 4:2C:42:PHE:CZ | 1.10 | 0.61 |
| 2:LF:224:ASP:CG | 6:4D:219:ASN:ND2 | 2.54 | 0.61 |
| 6:4A:131:VAL:O | 6:4A:131:VAL:HG13 | 2.00 | 0.61 |
| 6:4B:131:VAL:O | 6:4B:131:VAL:HG13 | 2.00 | 0.61 |
| 6:4C:131:VAL:O | 6:4C:131:VAL:HG13 | 2.00 | 0.61 |
| 6:4D:101:ARG:HG3 | 6:4D:101:ARG:NH2 | 2.15 | 0.61 |
| 7:5B:1548:VAL:HB | 7:5B:1566:GLU:O | 2.01 | 0.61 |
| 7:5B:1577:LYS:HA | 7:5B:1577:LYS:HE3 | 1.81 | 0.61 |
| 7:5C:1367:LYS:HB2 | 7:5C:1367:LYS:HZ1 | 1.62 | 0.61 |
| 2:BB:309:ARG:NH2 | 2:BB:426:GLN:O | 2.32 | 0.61 |
| 1:DE:108:TYR:HA | 1:DE:112:LYS:HE3 | 1.81 | 0.61 |
| 1:EA:426:ALA:HB1 | 7:5C:833:PHE:HB2 | 1.83 | 0.61 |
| 1:FA:89:PRO:HD3 | 1:GA:280:LYS:HZ3 | 1.66 | 0.61 |
| 2:FB:401:GLU:N | 7:5C:1293:VAL:HG21 | 2.16 | 0.61 |
| 1:FC:11:GLN:NE2 | 2:FD:247:ASN:OD1 | 2.34 | 0.61 |
| 2:FD:390:ARG:CD | 1:FE:439:THR:HG21 | 2.31 | 0.61 |
| 1:FE:404:PHE:CE2 | 2:FF:345:ILE:CD1 | 2.83 | 0.61 |
| 2:GB:55:THR:HG1 | 2:HB:282:ARG:C | 2.02 | 0.61 |
| 2:GD:73:MET:HA | 2:GD:76:VAL:HG12 | 1.83 | 0.61 |
| 2:GD:409:THR:O | 7:5A:1330:ILE:HD13 | 2.00 | 0.61 |
| 2:GF:73:MET:HA | 2:GF:76:VAL:HG12 | 1.83 | 0.61 |
| 2:HB:73:MET:HA | 2:HB:76:VAL:HG12 | 1.83 | 0.61 |
| 2:HB:212:PHE:CE2 | 1:HC:326:LYS:HD3 | 2.22 | 0.61 |
| 2:HD:73:MET:HA | 2:HD:76:VAL:HG12 | 1.83 | 0.61 |
| 1:IA:105:ARG:NH1 | 2:IB:251:ARG:HD3 | 2.16 | 0.61 |
| 2:IF:73:MET:HA | 2:IF:76:VAL:HG12 | 1.83 | 0.61 |
| 2:JD:179:VAL:CG2 | 1:JE:258:ASN:CA | 2.78 | 0.61 |
| 2:JF:309:ARG:NH2 | 2:JF:426:GLN:O | 2.32 | 0.61 |
| 2:KF:125:GLU:CD | 2:LF:336:LYS:HZ3 | 2.09 | 0.61 |
| 2:LB:331:LEU:CD1 | 4:2C:42:PHE:HE1 | 2.09 | 0.61 |
| 2:LD:340:TYR:HB2 | 4:2A:147:PHE:HB2 | 1.81 | 0.61 |
| 2:LF:55:THR:HG21 | 2:MF:284:LEU:N | 2.13 | 0.61 |
| 2:MB:73:MET:HA | 2:MB:76:VAL:HG12 | 1.83 | 0.61 |
| 2:MD:73:MET:HA | 2:MD:76:VAL:HG12 | 1.83 | 0.61 |
| 4:2B:164:ARG:HH11 | 4:2B:164:ARG:CG | 2.14 | 0.61 |
| 4:2C:164:ARG:HB2 | 4:2C:164:ARG:CZ | 2.31 | 0.61 |
| 4:2C:164:ARG:HH11 | 4:2C:164:ARG:CG | 2.14 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5A:1412:LYS:HD3 | 7:5A:1412:LYS:C | 2.26 | 0.61 |
| 7:5C:1412:LYS:HD3 | 7:5C:1412:LYS:C | 2.26 | 0.61 |
| 9:7C:10:TYR:OH | 9:7D:34:PRO:HB3 | 2.01 | 0.61 |
| 9:7C:14:SER:C | 9:7D:35:ILE:CD1 | 2.66 | 0.61 |
| 2:BB:177:ASP:OD2 | 1:BC:248:LEU:HD23 | 1.98 | 0.60 |
| 1:EA:100:ALA:HB1 | 2:EB:252:LYS:HA | 1.83 | 0.60 |
| 1:EE:393:HIS:ND1 | 7:5B:814:LYS:HG2 | 2.16 | 0.60 |
| 1:EE:426:ALA:CB | 7:5B:833:PHE:CB | 2.79 | 0.60 |
| 2:FD:177:ASP:OD2 | 1:FE:248:LEU:HD23 | 1.99 | 0.60 |
| 2:HF:73:MET:HA | 2:HF:76:VAL:HG12 | 1.83 | 0.60 |
| 2:IB:73:MET:HA | 2:IB:76:VAL:HG12 | 1.83 | 0.60 |
| 2:ID:73:MET:HA | 2:ID:76:VAL:HG12 | 1.83 | 0.60 |
| 1:KC:222:PRO:CD | 2:KD:324:LYS:HD3 | 2.31 | 0.60 |
| 2:KD:220:PRO:O | 1:KE:324:VAL:HG13 | 1.98 | 0.60 |
| 1:LC:47:ASP:OD1 | 6:4A:203:LYS:NZ | 2.32 | 0.60 |
| 2:LD:73:MET:HA | 2:LD:76:VAL:HG12 | 1.83 | 0.60 |
| 2:LD:212:PHE:HZ | 1:LE:326:LYS:CG | 2.10 | 0.60 |
| 4:2A:164:ARG:HB2 | 4:2A:164:ARG:CZ | 2.31 | 0.60 |
| 4:2B:164:ARG:HB2 | 4:2B:164:ARG:CZ | 2.31 | 0.60 |
| 7:5A:1577:LYS:HA | 7:5A:1577:LYS:HE3 | 1.81 | 0.60 |
| 7:5B:1412:LYS:HD3 | 7:5B:1412:LYS:C | 2.26 | 0.60 |
| 9:7A:18:VAL:HG12 | 9:7A:42:LEU:HD23 | 1.75 | 0.60 |
| 1:AC:222:PRO:CD | 2:AD:324:LYS:HD3 | 2.31 | 0.60 |
| 2:BF:73:MET:HA | 2:BF:76:VAL:HG12 | 1.83 | 0.60 |
| 1:DC:402:ARG:HE | 7:5A:777:ALA:HB2 | 1.52 | 0.60 |
| 1:EE:430:LYS:NZ | 7:5B:834:ASN:HD22 | 0.48 | 0.60 |
| 2:FD:73:MET:HA | 2:FD:76:VAL:HG12 | 1.83 | 0.60 |
| 2:FD:391:ARG:O | 1:FE:262:TYR:OH | 2.18 | 0.60 |
| 2:GB:73:MET:HA | 2:GB:76:VAL:HG12 | 1.83 | 0.60 |
| 2:ID:220:PRO:O | 1:IE:324:VAL:HG13 | 1.98 | 0.60 |
| 1:IE:404:PHE:HE2 | 2:IF:345:ILE:HD12 | 1.65 | 0.60 |
| 1:JA:292:THR:HG21 | 1:JA:331:SER:HB3 | 1.83 | 0.60 |
| 2:KF:83:GLN:HA | 2:LF:281:TYR:CD1 | 2.37 | 0.60 |
| 2:LF:73:MET:HA | 2:LF:76:VAL:HG12 | 1.83 | 0.60 |
| 2:MD:179:VAL:HG21 | 1:ME:258:ASN:C | 2.25 | 0.60 |
| 6:4A:260:ARG:NH2 | 6:4A:295:LYS:HE2 | 2.16 | 0.60 |
| 6:4A:289:LYS:HA | 6:4A:289:LYS:CE | 2.25 | 0.60 |
| 7:5A:841:VAL:HG23 | 8:6A:11:PRO:CG | 2.31 | 0.60 |
| 7:5C:1548:VAL:CA | 7:5C:1569:GLU:CG | 2.78 | 0.60 |
| 7:5C:1552:LYS:HD2 | 7:5C:1566:GLU:OE1 | 2.01 | 0.60 |
| 2:CF:73:MET:HA | 2:CF:76:VAL:HG12 | 1.83 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:DA:101:ASN:HD21 | 2:DB:252:LYS:HD2 | 0.78 | 0.60 |
| 2:DD:73:MET:HA | 2:DD:76:VAL:HG12 | 1.83 | 0.60 |
| 2:DD:177:ASP:C | 1:DE:352:LYS:HA | 2.25 | 0.60 |
| 1:DE:224:TYR:HE2 | 2:DF:246:LEU:HD11 | 1.67 | 0.60 |
| 2:EB:86:ARG:CA | 2:FB:281:TYR:CE1 | 2.83 | 0.60 |
| 2:FB:397:TRP:CB | 1:FC:256:GLN:HE22 | 2.12 | 0.60 |
| 2:FF:73:MET:HA | 2:FF:76:VAL:HG12 | 1.83 | 0.60 |
| 2:IB:424:GLN:NE2 | 7:5C:1413:GLN:HE21 | 0.36 | 0.60 |
| 1:IC:58:ALA:HB3 | 10:8Z:13:UNK:HA | 0.64 | 0.60 |
| 1:IC:431:ASP:OD2 | 5:3C:61:SER:O | 2.18 | 0.60 |
| 1:JC:292:THR:HG21 | 1:JC:331:SER:HB3 | 1.83 | 0.60 |
| 2:MD:179:VAL:CG2 | 1:ME:258:ASN:CA | 2.79 | 0.60 |
| 4:2A:16:GLN:O | 4:2A:19:MET:N | 2.35 | 0.60 |
| 4:2B:16:GLN:O | 4:2B:19:MET:N | 2.35 | 0.60 |
| 5:3C:21:PHE:CD2 | 5:3C:24:MET:CE | 2.84 | 0.60 |
| 6:4C:260:ARG:NH2 | 6:4C:295:LYS:HE2 | 2.16 | 0.60 |
| 7:5A:872:GLU:OE1 | 8:6A:90:ARG:NH1 | 2.34 | 0.60 |
| 7:5C:1577:LYS:HA | 7:5C:1577:LYS:HE3 | 1.81 | 0.60 |
| 1:CA:104:ALA:HB2 | 1:CA:413:MET:HE2 | 1.84 | 0.60 |
| 1:CC:104:ALA:HB2 | 1:CC:413:MET:HE2 | 1.84 | 0.60 |
| 1:CC:176:GLN:O | 2:CD:347:ASN:ND2 | 2.33 | 0.60 |
| 1:CC:282:TYR:HE2 | 10:8E:18:UNK:CA | 2.13 | 0.60 |
| 2:EF:73:MET:HA | 2:EF:76:VAL:HG12 | 1.83 | 0.60 |
| 2:FB:73:MET:HA | 2:FB:76:VAL:HG12 | 1.83 | 0.60 |
| 2:FB:177:ASP:OD2 | 1:FC:248:LEU:HD23 | 2.00 | 0.60 |
| 1:FE:105:ARG:NH1 | 2:FF:251:ARG:HD3 | 2.17 | 0.60 |
| 1:GC:409:VAL:CG2 | 5:3C:383:GLU:OE1 | 2.47 | 0.60 |
| 1:GE:404:PHE:CE2 | 2:GF:345:ILE:CD1 | 2.84 | 0.60 |
| 2:ID:397:TRP:CD2 | 1:IE:256:GLN:O | 2.31 | 0.60 |
| 2:JD:212:PHE:CZ | 1:JE:326:LYS:CD | 2.34 | 0.60 |
| 2:JD:309:ARG:NH2 | 2:JD:426:GLN:O | 2.32 | 0.60 |
| 1:JE:104:ALA:HB2 | 1:JE:413:MET:HE2 | 1.84 | 0.60 |
| 1:JE:292:THR:HG21 | 1:JE:331:SER:HB3 | 1.83 | 0.60 |
| 2:KD:177:ASP:OD1 | 1:KE:353:VAL:HG12 | 1.84 | 0.60 |
| 2:KD:179:VAL:HG21 | 1:KE:258:ASN:C | 2.25 | 0.60 |
| 1:LA:104:ALA:HB2 | 1:LA:413:MET:HE2 | 1.84 | 0.60 |
| 2:LB:212:PHE:CZ | 1:LC:326:LYS:CE | 2.82 | 0.60 |
| 1:MA:104:ALA:HB2 | 1:MA:413:MET:HE2 | 1.84 | 0.60 |
| 1:MA:401:LYS:HE3 | 2:MB:344:TRP:CZ3 | 2.36 | 0.60 |
| 1:MC:100:ALA:HB1 | 2:MD:252:LYS:CA | 2.31 | 0.60 |
| 1:MC:104:ALA:HB2 | 1:MC:413:MET:HE2 | 1.84 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:ME:104:ALA:HB2 | 1:ME:413:MET:HE2 | 1.84 | 0.60 |
| 4:2C:16:GLN:O | 4:2C:19:MET:N | 2.35 | 0.60 |
| 6:4B:260:ARG:NH2 | 6:4B:295:LYS:HE2 | 2.16 | 0.60 |
| 7:5A:1552:LYS:HD2 | 7:5A:1566:GLU:OE1 | 2.01 | 0.60 |
| 7:5C:839:GLU:CD | 8:6C:109:ILE:HG13 | 2.27 | 0.60 |
| 9:7C:7:LEU:CD2 | 9:7D:27:GLY:O | 2.37 | 0.60 |
| 1:AE:104:ALA:HB2 | 1:AE:413:MET:HE2 | 1.84 | 0.60 |
| 1:BC:104:ALA:HB2 | 1:BC:413:MET:HE2 | 1.84 | 0.60 |
| 2:BD:73:MET:HA | 2:BD:76:VAL:HG12 | 1.83 | 0.60 |
| 2:BD:86:ARG:CA | 2:CD:281:TYR:HE1 | 2.15 | 0.60 |
| 1:BE:104:ALA:HB2 | 1:BE:413:MET:HE2 | 1.84 | 0.60 |
| 2:CD:73:MET:HA | 2:CD:76:VAL:HG12 | 1.83 | 0.60 |
| 1:CE:104:ALA:HB2 | 1:CE:413:MET:HE2 | 1.84 | 0.60 |
| 2:DD:222:TYR:O | 2:DD:226:ASN:ND2 | 2.28 | 0.60 |
| 2:DF:73:MET:HA | 2:DF:76:VAL:HG12 | 1.83 | 0.60 |
| 2:ED:73:MET:HA | 2:ED:76:VAL:HG12 | 1.83 | 0.60 |
| 2:FB:178:THR:HG23 | 1:FC:258:ASN:ND2 | 2.11 | 0.60 |
| 1:GC:60:LYS:CD | 1:HC:283:HIS:CD2 | 2.85 | 0.60 |
| 2:HD:177:ASP:O | 1:HE:352:LYS:HA | 2.02 | 0.60 |
| 2:HD:179:VAL:HG21 | 1:HE:258:ASN:C | 2.25 | 0.60 |
| 1:IA:104:ALA:HB2 | 1:IA:413:MET:HE2 | 1.84 | 0.60 |
| 1:IA:292:THR:HG21 | 1:IA:331:SER:HB3 | 1.83 | 0.60 |
| 1:IC:104:ALA:HB2 | 1:IC:413:MET:HE2 | 1.84 | 0.60 |
| 1:IC:292:THR:HG21 | 1:IC:331:SER:HB3 | 1.83 | 0.60 |
| 1:IE:404:PHE:CE2 | 2:IF:345:ILE:CD1 | 2.84 | 0.60 |
| 1:JC:104:ALA:HB2 | 1:JC:413:MET:HE2 | 1.84 | 0.60 |
| 2:JD:179:VAL:HG21 | 1:JE:258:ASN:C | 2.25 | 0.60 |
| 1:JE:401:LYS:HE3 | 2:JF:344:TRP:CZ3 | 2.37 | 0.60 |
| 1:JE:404:PHE:CE2 | 2:JF:345:ILE:CD1 | 2.84 | 0.60 |
| 1:KA:85:GLN:CD | 1:LA:282:TYR:HB3 | 2.15 | 0.60 |
| 1:KE:404:PHE:HE2 | 2:KF:345:ILE:HD12 | 1.65 | 0.60 |
| 2:LB:221:THR:HG23 | 6:4A:219:ASN:ND2 | 2.16 | 0.60 |
| 1:LC:222:PRO:HG2 | 2:LD:324:LYS:CB | 2.31 | 0.60 |
| 1:MA:292:THR:HG21 | 1:MA:331:SER:HB3 | 1.83 | 0.60 |
| 2:MB:111:GLU:CG | 3:1A:62:SER:HB2 | 2.31 | 0.60 |
| 6:4D:260:ARG:NH2 | 6:4D:295:LYS:HE2 | 2.16 | 0.60 |
| 7:5A:1548:VAL:CA | 7:5A:1569:GLU:CG | 2.78 | 0.60 |
| 7:5B:1552:LYS:HD2 | 7:5B:1566:GLU:OE1 | 2.01 | 0.60 |
| 9:7A:15:VAL:CG1 | 9:7B:35:ILE:CA | 2.76 | 0.60 |
| 1:AC:104:ALA:HB2 | 1:AC:413:MET:HE2 | 1.84 | 0.60 |
| 1:AE:404:PHE:CE2 | 2:AF:345:ILE:CD1 | 2.84 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BB:73:MET:HA | 2:BB:76:VAL:HG12 | 1.83 | 0.60 |
| 2:CB:73:MET:HA | 2:CB:76:VAL:HG12 | 1.83 | 0.60 |
| 1:CC:282:TYR:CE2 | 10:8E:18:UNK:CA | 2.82 | 0.60 |
| 2:DB:73:MET:HA | 2:DB:76:VAL:HG12 | 1.83 | 0.60 |
| 2:DB:179:VAL:HG21 | 1:DC:258:ASN:C | 2.25 | 0.60 |
| 2:DF:60:VAL:HG21 | 2:EF:281:TYR:CD1 | 2.35 | 0.60 |
| 1:FA:104:ALA:HB2 | 1:FA:413:MET:HE2 | 1.84 | 0.60 |
| 1:FE:60:LYS:HZ3 | 1:GE:283:HIS:CB | 2.12 | 0.60 |
| 1:FE:60:LYS:HD2 | 1:GE:283:HIS:CD2 | 2.35 | 0.60 |
| 1:FE:104:ALA:HB2 | 1:FE:413:MET:HE2 | 1.84 | 0.60 |
| 2:FF:54:ALA:HB1 | 2:GF:281:TYR:O | 2.00 | 0.60 |
| 2:GB:86:ARG:HH22 | 2:HB:281:TYR:CD2 | 1.04 | 0.60 |
| 1:HA:104:ALA:HB2 | 1:HA:413:MET:HE2 | 1.84 | 0.60 |
| 2:HB:177:ASP:O | 1:HC:352:LYS:HA | 2.02 | 0.60 |
| 1:HC:104:ALA:HB2 | 1:HC:413:MET:HE2 | 1.84 | 0.60 |
| 2:HD:261:PRO:HB2 | 5:3C:337:ARG:HH21 | 0.77 | 0.60 |
| 1:IE:104:ALA:HB2 | 1:IE:413:MET:HE2 | 1.84 | 0.60 |
| 1:IE:401:LYS:HE3 | 2:IF:344:TRP:CZ3 | 2.37 | 0.60 |
| 1:JA:104:ALA:HB2 | 1:JA:413:MET:HE2 | 1.84 | 0.60 |
| 2:JB:177:ASP:O | 1:JC:352:LYS:HA | 2.02 | 0.60 |
| 2:JD:177:ASP:O | 1:JE:352:LYS:HA | 2.02 | 0.60 |
| 1:KE:401:LYS:HE3 | 2:KF:344:TRP:CZ3 | 2.37 | 0.60 |
| 1:LC:104:ALA:HB2 | 1:LC:413:MET:HE2 | 1.84 | 0.60 |
| 1:MC:292:THR:HG21 | 1:MC:331:SER:HB3 | 1.83 | 0.60 |
| 2:MD:390:ARG:HD2 | 1:ME:439:THR:HG21 | 1.82 | 0.60 |
| 1:ME:292:THR:HG21 | 1:ME:331:SER:HB3 | 1.83 | 0.60 |
| 2:MF:221:THR:CG2 | 6:4D:189:ARG:NH1 | 2.65 | 0.60 |
| 5:3A:21:PHE:CD2 | 5:3A:24:MET:CE | 2.84 | 0.60 |
| 5:3C:21:PHE:CD2 | 5:3C:24:MET:HE2 | 2.36 | 0.60 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:HG2 | 1.85 | 0.60 |
| 7:5B:1276:GLU:HG2 | 9:7D:7:LEU:HD13 | 1.82 | 0.60 |
| 1:CC:178:SER:OG | 2:CD:347:ASN:HB3 | 2.01 | 0.60 |
| 2:EB:73:MET:HA | 2:EB:76:VAL:HG12 | 1.83 | 0.60 |
| 1:FC:104:ALA:HB2 | 1:FC:413:MET:HE2 | 1.84 | 0.60 |
| 1:HE:104:ALA:HB2 | 1:HE:413:MET:HE2 | 1.84 | 0.60 |
| 1:IC:393:HIS:HB3 | 5:3C:308:PHE:CD2 | 2.37 | 0.60 |
| 1:IE:292:THR:HG21 | 1:IE:331:SER:HB3 | 1.83 | 0.60 |
| 1:JA:88:HIS:HE1 | 1:KA:280:LYS:HB3 | 1.67 | 0.60 |
| 2:JB:86:ARG:HH12 | 2:KB:280:GLN:HB3 | 1.67 | 0.60 |
| 2:KB:177:ASP:O | 1:KC:352:LYS:HA | 2.02 | 0.60 |
| 2:KD:177:ASP:O | 1:KE:352:LYS:HA | 2.02 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:KF:276:ARG:NH2 | 6:4D:271:GLU:C | 2.58 | 0.60 |
| 1:LE:104:ALA:HB2 | 1:LE:413:MET:HE2 | 1.84 | 0.60 |
| 4:2A:164:ARG:HA | 4:2A:164:ARG:NE | 2.17 | 0.60 |
| 4:2B:164:ARG:HA | 4:2B:164:ARG:NE | 2.17 | 0.60 |
| 4:2C:164:ARG:HA | 4:2C:164:ARG:NE | 2.17 | 0.60 |
| 5:3B:21:PHE:CD2 | 5:3B:24:MET:HE2 | 2.36 | 0.60 |
| 7:5A:1579:LYS:O | 7:5A:1583:ASN:N | 2.32 | 0.60 |
| 1:AA:104:ALA:HB2 | 1:AA:413:MET:HE2 | 1.84 | 0.60 |
| 2:AD:222:TYR:O | 2:AD:226:ASN:ND2 | 2.27 | 0.60 |
| 2:BD:391:ARG:HG3 | 1:BE:346:TRP:CD1 | 2.36 | 0.60 |
| 2:HB:55:THR:HG23 | 2:IB:283:ALA:HA | 1.83 | 0.60 |
| 1:IC:279:GLU:OE2 | 10:8W:22:UNK:HA | 2.00 | 0.60 |
| 1:IE:282:TYR:CG | 10:8X:15:UNK:HA | 2.37 | 0.60 |
| 2:JB:309:ARG:NH2 | 2:JB:426:GLN:O | 2.32 | 0.60 |
| 2:JD:87:PRO:HG2 | 2:KD:278:SER:HA | 1.83 | 0.60 |
| 2:JD:88:ASP:CG | 2:KD:278:SER:OG | 2.45 | 0.60 |
| 1:KA:292:THR:HG21 | 1:KA:331:SER:HB3 | 1.83 | 0.60 |
| 1:KE:404:PHE:CE2 | 2:KF:345:ILE:CD1 | 2.84 | 0.60 |
| 2:KF:125:GLU:CB | 2:LF:336:LYS:HE2 | 2.31 | 0.60 |
| 2:LB:177:ASP:CG | 1:LC:353:VAL:HG11 | 2.12 | 0.60 |
| 1:LC:60:LYS:CE | 6:4A:101:ARG:NH1 | 2.65 | 0.60 |
| 2:LD:397:TRP:CD2 | 1:LE:256:GLN:O | 2.41 | 0.60 |
| 1:MC:282:TYR:CD1 | 6:4A:98:PRO:HB3 | 2.37 | 0.60 |
| 5:3A:21:PHE:CD2 | 5:3A:24:MET:HE2 | 2.36 | 0.60 |
| 6:4C:289:LYS:HA | 6:4C:289:LYS:CE | 2.25 | 0.60 |
| 7:5A:1404:LYS:C | 7:5A:1404:LYS:HE3 | 2.26 | 0.60 |
| 7:5B:1404:LYS:C | 7:5B:1404:LYS:HE3 | 2.26 | 0.60 |
| 7:5B:1548:VAL:CA | 7:5B:1569:GLU:CG | 2.78 | 0.60 |
| 7:5B:1579:LYS:O | 7:5B:1583:ASN:N | 2.32 | 0.60 |
| 7:5C:1404:LYS:C | 7:5C:1404:LYS:HE3 | 2.26 | 0.60 |
| 7:5C:1579:LYS:O | 7:5C:1583:ASN:N | 2.32 | 0.60 |
| 2:AB:177:ASP:O | 1:AC:352:LYS:HA | 2.02 | 0.60 |
| 1:BA:104:ALA:HB2 | 1:BA:413:MET:HE2 | 1.84 | 0.60 |
| 1:DC:105:ARG:NH1 | 2:DD:251:ARG:HD3 | 2.17 | 0.60 |
| 2:DF:309:ARG:NH2 | 2:DF:426:GLN:O | 2.32 | 0.60 |
| 1:EC:71:GLU:CD | 2:ED:247:ASN:ND2 | 2.59 | 0.60 |
| 1:FA:422:ARG:CZ | 7:5C:1170:THR:CA | 2.79 | 0.60 |
| 1:FC:402:ARG:HH11 | 7:5A:1259:TYR:HD2 | 1.48 | 0.60 |
| 1:FE:419:SER:HB3 | 7:5B:1256:ARG:CG | 2.29 | 0.60 |
| 1:HC:159:VAL:CG2 | 5:3C:209:ARG:NE | 2.58 | 0.60 |
| 2:ID:87:PRO:CD | 2:JD:281:TYR:CZ | 2.85 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:IF:56:GLY:CA | 10:9A:36:UNK:HA | 2.31 | 0.60 |
| 1:JA:105:ARG:NH1 | 2:JB:251:ARG:HD3 | 2.16 | 0.60 |
| 1:KC:292:THR:HG21 | 1:KC:331:SER:HB3 | 1.83 | 0.60 |
| 2:KD:212:PHE:CE2 | 1:KE:326:LYS:HD3 | 2.26 | 0.60 |
| 1:KE:292:THR:HG21 | 1:KE:331:SER:HB3 | 1.83 | 0.60 |
| 2:KF:126:GLY:O | 4:2B:39:ALA:N | 2.35 | 0.60 |
| 1:LA:60:LYS:CD | 1:MA:283:HIS:CG | 2.84 | 0.60 |
| 1:LC:56:THR:OG1 | 1:MC:284:GLU:HA | 2.02 | 0.60 |
| 2:LD:274:THR:H | 6:4B:228:LEU:HD21 | 1.65 | 0.60 |
| 3:1B:93:ILE:HD11 | 3:1B:104:VAL:HG21 | 1.84 | 0.60 |
| 6:4A:244:GLU:HG3 | 6:4A:284:LEU:CD1 | 2.22 | 0.60 |
| 2:AD:361:LEU:CD2 | 6:4C:144:LEU:CD1 | 2.69 | 0.60 |
| 2:CD:86:ARG:HA | 2:DD:281:TYR:OH | 1.98 | 0.60 |
| 1:DA:104:ALA:HB2 | 1:DA:413:MET:HE2 | 1.84 | 0.60 |
| 2:DD:397:TRP:CD2 | 1:DE:256:GLN:O | 2.35 | 0.60 |
| 1:EE:426:ALA:HB1 | 7:5B:833:PHE:CD1 | 2.37 | 0.60 |
| 1:GA:104:ALA:HB2 | 1:GA:413:MET:HE2 | 1.84 | 0.60 |
| 1:GC:402:ARG:HD2 | 5:3C:381:ASN:CG | 2.27 | 0.60 |
| 2:JB:87:PRO:HG2 | 2:KB:278:SER:HA | 1.84 | 0.60 |
| 1:JE:90:GLU:CG | 1:KE:280:LYS:HB3 | 2.30 | 0.60 |
| 2:KD:217:LEU:HD13 | 6:4B:263:CYS:SG | 2.42 | 0.60 |
| 1:LA:47:ASP:OD1 | 6:4C:203:LYS:CE | 2.50 | 0.60 |
| 2:LD:379:LYS:CE | 4:2A:164:ARG:O | 2.50 | 0.60 |
| 2:LD:394:PHE:CD1 | 1:LE:261:PRO:HA | 2.37 | 0.60 |
| 1:LE:292:THR:HG21 | 1:LE:331:SER:HB3 | 1.83 | 0.60 |
| 3:1A:93:ILE:HD11 | 3:1A:104:VAL:HG21 | 1.84 | 0.60 |
| 5:3B:21:PHE:CD2 | 5:3B:24:MET:CE | 2.84 | 0.60 |
| 6:4D:244:GLU:HG3 | 6:4D:284:LEU:CD1 | 2.22 | 0.60 |
| 6:4D:251:TYR:HB2 | 6:4D:288:TYR:CE2 | 2.36 | 0.60 |
| 9:7C:42:LEU:CD1 | 9:7D:39:GLY:HA3 | 2.32 | 0.60 |
| 1:AA:292:THR:HG21 | 1:AA:331:SER:HB3 | 1.83 | 0.59 |
| 1:AC:292:THR:HG21 | 1:AC:331:SER:HB3 | 1.83 | 0.59 |
| 2:AD:177:ASP:O | 1:AE:352:LYS:HA | 2.02 | 0.59 |
| 1:AE:292:THR:HG21 | 1:AE:331:SER:HB3 | 1.83 | 0.59 |
| 1:AE:401:LYS:HE3 | 2:AF:344:TRP:CZ3 | 2.37 | 0.59 |
| 1:GA:60:LYS:HD3 | 1:HA:283:HIS:CD2 | 2.36 | 0.59 |
| 1:GC:104:ALA:HB2 | 1:GC:413:MET:HE2 | 1.84 | 0.59 |
| 1:GC:402:ARG:HD2 | 5:3C:381:ASN:HD21 | 1.61 | 0.59 |
| 1:HE:401:LYS:HE3 | 2:HF:344:TRP:CZ3 | 2.37 | 0.59 |
| 1:HE:404:PHE:CE2 | 2:HF:345:ILE:CD1 | 2.84 | 0.59 |
| 1:KE:85:GLN:HA | 1:LE:283:HIS:CD2 | 2.35 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:LA:292:THR:HG21 | 1:LA:331:SER:HB3 | 1.83 | 0.59 |
| 1:LC:292:THR:HG21 | 1:LC:331:SER:HB3 | 1.83 | 0.59 |
| 2:LD:228:LEU:CD2 | 6:4B:225:PRO:CG | 2.80 | 0.59 |
| 1:LE:47:ASP:OD1 | 6:4B:203:LYS:HE3 | 2.00 | 0.59 |
| 6:4C:251:TYR:HB2 | 6:4C:288:TYR:CE2 | 2.36 | 0.59 |
| 7:5A:1276:GLU:HG2 | 9:7B:7:LEU:HD13 | 1.82 | 0.59 |
| 7:5A:1541:ILE:HG12 | 7:5A:1574:ILE:HD11 | 1.84 | 0.59 |
| 7:5C:1521:PHE:CE2 | 7:5C:1567:PHE:CG | 2.58 | 0.59 |
| 7:5C:1541:ILE:HG12 | 7:5C:1574:ILE:HD11 | 1.84 | 0.59 |
| 7:5C:1552:LYS:HD2 | 7:5C:1566:GLU:CD | 2.27 | 0.59 |
| 9:7E:14:SER:CB | 9:7F:34:PRO:HG3 | 2.30 | 0.59 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:CD1 | 2.32 | 0.59 |
| 2:BD:220:PRO:HD2 | 1:BE:326:LYS:CG | 2.32 | 0.59 |
| 2:DB:179:VAL:CG2 | 1:DC:258:ASN:CA | 2.80 | 0.59 |
| 1:DC:104:ALA:HB2 | 1:DC:413:MET:HE2 | 1.84 | 0.59 |
| 2:DD:309:ARG:NH2 | 2:DD:426:GLN:O | 2.32 | 0.59 |
| 1:DE:105:ARG:NH1 | 2:DF:251:ARG:HD3 | 2.17 | 0.59 |
| 1:FA:177:VAL:CG2 | 7:5C:915:PHE:CZ | 2.64 | 0.59 |
| 1:FA:422:ARG:HE | 7:5C:1170:THR:C | 2.10 | 0.59 |
| 2:FD:180:VAL:HG12 | 1:FE:258:ASN:OD1 | 2.01 | 0.59 |
| 1:FE:292:THR:HG21 | 1:FE:331:SER:HB3 | 1.83 | 0.59 |
| 2:FF:309:ARG:NH2 | 2:FF:426:GLN:O | 2.32 | 0.59 |
| 1:IA:401:LYS:HE3 | 2:IB:344:TRP:CZ3 | 2.37 | 0.59 |
| 1:JA:176:GLN:O | 2:JB:347:ASN:ND2 | 2.34 | 0.59 |
| 1:JC:89:PRO:CD | 1:KC:280:LYS:HA | 2.32 | 0.59 |
| 2:KB:273:LEU:CB | 6:4A:268:LEU:HG | 2.32 | 0.59 |
| 1:KC:84:ARG:NE | 1:LC:283:HIS:CE1 | 2.65 | 0.59 |
| 1:KC:127:ASP:OD2 | 1:LC:334:THR:HG23 | 2.02 | 0.59 |
| 2:KD:273:LEU:CB | 6:4B:268:LEU:CD2 | 2.73 | 0.59 |
| 2:LD:55:THR:CG2 | 2:MD:284:LEU:H | 2.10 | 0.59 |
| 2:LF:221:THR:HG23 | 6:4D:219:ASN:HD22 | 1.65 | 0.59 |
| 3:1C:93:ILE:HD11 | 3:1C:104:VAL:HG21 | 1.84 | 0.59 |
| 6:4B:251:TYR:HB2 | 6:4B:288:TYR:CE2 | 2.36 | 0.59 |
| 7:5B:1541:ILE:HG12 | 7:5B:1574:ILE:HD11 | 1.84 | 0.59 |
| 7:5C:1552:LYS:NZ | 7:5C:1563:SER:CA | 2.64 | 0.59 |
| 2:AD:281:TYR:CE1 | 1:MA:88:HIS:HA | 2.36 | 0.59 |
| 2:BD:220:PRO:HD2 | 1:BE:326:LYS:CE | 2.32 | 0.59 |
| 1:DE:178:SER:OG | 2:DF:347:ASN:HB3 | 2.01 | 0.59 |
| 2:DF:222:TYR:O | 2:DF:226:ASN:ND2 | 2.28 | 0.59 |
| 1:EE:60:LYS:HD3 | 1:FE:283:HIS:HA | 1.84 | 0.59 |
| 1:FC:292:THR:HG21 | 1:FC:331:SER:HB3 | 1.83 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:292:THR:HG21 | 1:HA:331:SER:HB3 | 1.83 | 0.59 |
| 1:IC:402:ARG:NH2 | 7:5A:1418:GLN:CA | 2.55 | 0.59 |
| 1:JA:401:LYS:HE3 | 2:JB:344:TRP:CZ3 | 2.37 | 0.59 |
| 1:KE:85:GLN:CG | 1:LE:283:HIS:HD2 | 2.15 | 0.59 |
| 1:KE:104:ALA:HB2 | 1:KE:413:MET:HE2 | 1.84 | 0.59 |
| 2:KF:125:GLU:CG | 2:LF:336:LYS:HE2 | 2.26 | 0.59 |
| 2:LF:379:LYS:HE3 | 4:2B:166:ILE:CG1 | 2.32 | 0.59 |
| 6:4B:244:GLU:HG3 | 6:4B:284:LEU:CD1 | 2.22 | 0.59 |
| 7:5A:907:PHE:CD2 | 7:5A:921:HIS:CD2 | 2.90 | 0.59 |
| 7:5A:1552:LYS:NZ | 7:5A:1563:SER:CA | 2.64 | 0.59 |
| 7:5B:907:PHE:CD2 | 7:5B:921:HIS:CD2 | 2.90 | 0.59 |
| 7:5B:1552:LYS:NZ | 7:5B:1563:SER:CA | 2.64 | 0.59 |
| 7:5C:907:PHE:CD2 | 7:5C:921:HIS:CD2 | 2.91 | 0.59 |
| 9:7A:30:ARG:CZ | 9:7B:3:GLN:HA | 2.22 | 0.59 |
| 9:7C:15:VAL:CG1 | 9:7D:35:ILE:CA | 2.76 | 0.59 |
| 1:DA:105:ARG:NH1 | 2:DB:251:ARG:HD3 | 2.17 | 0.59 |
| 1:DE:104:ALA:HB2 | 1:DE:413:MET:HE2 | 1.84 | 0.59 |
| 2:EF:157:GLU:CD | 7:5B:935:LYS:HZ1 | 1.95 | 0.59 |
| 1:FE:11:GLN:NE2 | 2:FF:247:ASN:OD1 | 2.35 | 0.59 |
| 1:GC:292:THR:HG21 | 1:GC:331:SER:HB3 | 1.83 | 0.59 |
| 2:GD:177:ASP:O | 1:GE:352:LYS:HA | 2.02 | 0.59 |
| 2:GD:179:VAL:HG21 | 1:GE:258:ASN:C | 2.25 | 0.59 |
| 1:GE:292:THR:HG21 | 1:GE:331:SER:HB3 | 1.83 | 0.59 |
| 1:HA:401:LYS:HE3 | 2:HB:344:TRP:CZ3 | 2.38 | 0.59 |
| 1:HC:292:THR:HG21 | 1:HC:331:SER:HB3 | 1.83 | 0.59 |
| 1:HE:282:TYR:CZ | 10:8U:19:UNK:N | 2.62 | 0.59 |
| 2:LB:215:LEU:CD1 | 6:4A:225:PRO:HB3 | 2.33 | 0.59 |
| 2:LB:224:ASP:CA | 6:4A:219:ASN:ND2 | 2.61 | 0.59 |
| 6:4A:251:TYR:HB2 | 6:4A:288:TYR:CE2 | 2.36 | 0.59 |
| 6:4C:195:ASN:HA | 6:4C:198:ASN:HD22 | 1.67 | 0.59 |
| 7:5A:1552:LYS:HD2 | 7:5A:1566:GLU:CD | 2.27 | 0.59 |
| 7:5B:1552:LYS:HD2 | 7:5B:1566:GLU:CD | 2.27 | 0.59 |
| 8:6A:146:ILE:HD12 | 8:6A:183:LEU:CB | 2.31 | 0.59 |
| 8:6B:146:ILE:HD12 | 8:6B:183:LEU:CB | 2.31 | 0.59 |
| 2:DB:309:ARG:NH2 | 2:DB:426:GLN:O | 2.32 | 0.59 |
| 2:DD:222:TYR:CD2 | 1:DE:247:ALA:HB1 | 2.37 | 0.59 |
| 1:EC:100:ALA:HB1 | 2:ED:252:LYS:CA | 2.32 | 0.59 |
| 1:EE:292:THR:HG21 | 1:EE:331:SER:HB3 | 1.83 | 0.59 |
| 2:FB:222:TYR:CE2 | 1:FC:325:PRO:HG2 | 2.38 | 0.59 |
| 1:FC:401:LYS:CE | 2:FD:344:TRP:CZ3 | 2.76 | 0.59 |
| 2:FD:309:ARG:NH2 | 2:FD:426:GLN:O | 2.32 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GC:105:ARG:NH1 | 2:GD:251:ARG:HD3 | 2.18 | 0.59 |
| 1:GE:104:ALA:HB2 | 1:GE:413:MET:HE2 | 1.84 | 0.59 |
| 2:HB:212:PHE:HZ | 1:HC:326:LYS:CE | 2.14 | 0.59 |
| 2:JF:86:ARG:NE | 2:KF:281:TYR:CD2 | 2.68 | 0.59 |
| 1:KA:401:LYS:HE3 | 2:KB:344:TRP:CZ3 | 2.38 | 0.59 |
| 2:KD:87:PRO:HG2 | 2:LD:282:ARG:CD | 2.31 | 0.59 |
| 2:KF:87:PRO:HG2 | 2:LF:282:ARG:HG2 | 1.83 | 0.59 |
| 2:LB:223:GLY:CA | 6:4A:219:ASN:ND2 | 2.65 | 0.59 |
| 2:LD:296:ALA:H | 4:2A:149:ILE:HA | 1.67 | 0.59 |
| 2:MF:78:ALA:HB1 | 6:4D:178:HIS:CD2 | 2.37 | 0.59 |
| 6:4A:195:ASN:HA | 6:4A:198:ASN:HD22 | 1.67 | 0.59 |
| 6:4D:168:PHE:HD1 | 6:4D:168:PHE:O | 1.85 | 0.59 |
| 6:4D:224:ASN:OD1 | 6:4D:225:PRO:HD2 | 2.02 | 0.59 |
| 9:7A:14:SER:C | 9:7B:35:ILE:CD1 | 2.66 | 0.59 |
| 1:DE:404:PHE:CE2 | 2:DF:345:ILE:CD1 | 2.85 | 0.59 |
| 1:EE:104:ALA:HB2 | 1:EE:413:MET:HE2 | 1.84 | 0.59 |
| 1:FA:292:THR:HG21 | 1:FA:331:SER:HB3 | 1.83 | 0.59 |
| 1:FA:422:ARG:NE | 7:5C:1170:THR:CB | 2.63 | 0.59 |
| 1:FE:177:VAL:CG2 | 7:5B:915:PHE:CZ | 2.62 | 0.59 |
| 2:GB:177:ASP:O | 1:GC:352:LYS:HA | 2.02 | 0.59 |
| 2:GD:397:TRP:CD2 | 1:GE:256:GLN:O | 2.31 | 0.59 |
| 1:GE:402:ARG:CD | 5:3A:381:ASN:CG | 2.74 | 0.59 |
| 1:HE:292:THR:HG21 | 1:HE:331:SER:HB3 | 1.83 | 0.59 |
| 2:ID:179:VAL:HG21 | 1:IE:258:ASN:C | 2.25 | 0.59 |
| 1:KA:88:HIS:HA | 1:LA:284:GLU:HB2 | 0.60 | 0.59 |
| 1:KC:104:ALA:HB2 | 1:KC:413:MET:HE2 | 1.84 | 0.59 |
| 2:LB:177:ASP:CB | 1:LC:353:VAL:HG12 | 2.32 | 0.59 |
| 2:MB:212:PHE:HZ | 1:MC:326:LYS:HD3 | 0.61 | 0.59 |
| 1:MC:401:LYS:HE3 | 2:MD:344:TRP:CZ3 | 2.37 | 0.59 |
| 6:4A:168:PHE:HD1 | 6:4A:168:PHE:O | 1.85 | 0.59 |
| 6:4C:168:PHE:HD1 | 6:4C:168:PHE:O | 1.85 | 0.59 |
| 7:5B:1543:LEU:O | 7:5B:1573:ARG:CD | 2.51 | 0.59 |
| 1:AA:401:LYS:HE3 | 2:AB:344:TRP:CZ3 | 2.37 | 0.59 |
| 2:AB:179:VAL:CG2 | 1:AC:258:ASN:CA | 2.81 | 0.59 |
| 1:AE:284:GLU:HA | 2:MB:54:ALA:HB1 | 1.83 | 0.59 |
| 2:AF:222:TYR:O | 2:AF:226:ASN:ND2 | 2.28 | 0.59 |
| 2:AF:309:ARG:NH2 | 2:AF:426:GLN:O | 2.32 | 0.59 |
| 1:BE:292:THR:HG21 | 1:BE:331:SER:HB3 | 1.83 | 0.59 |
| 1:DA:404:PHE:HE2 | 2:DB:345:ILE:CD1 | 2.16 | 0.59 |
| 1:EA:224:TYR:HE2 | 2:EB:246:LEU:HD11 | 1.66 | 0.59 |
| 1:EC:104:ALA:HB2 | 1:EC:413:MET:HE2 | 1.84 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:GA:292:THR:HG21 | 1:GA:331:SER:HB3 | 1.83 | 0.59 |
| 2:GB:179:VAL:CG2 | 1:GC:258:ASN:CA | 2.81 | 0.59 |
| 1:GE:409:VAL:CG1 | 5:3A:383:GLU:OE1 | 2.43 | 0.59 |
| 1:JC:88:HIS:CE1 | 1:KC:280:LYS:HB3 | 2.38 | 0.59 |
| 2:JD:212:PHE:CE2 | 1:JE:326:LYS:HD3 | 2.26 | 0.59 |
| 2:KB:177:ASP:OD1 | 1:KC:353:VAL:HG12 | 1.84 | 0.59 |
| 2:LD:221:THR:HG23 | 6:4B:219:ASN:ND2 | 2.17 | 0.59 |
| 1:LE:176:GLN:HE22 | 4:2B:42:PHE:CB | 2.11 | 0.59 |
| 2:LF:228:LEU:HD21 | 6:4D:225:PRO:CG | 2.33 | 0.59 |
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:CG | 2.50 | 0.59 |
| 2:MD:221:THR:CG2 | 6:4B:189:ARG:NH1 | 2.65 | 0.59 |
| 2:MD:390:ARG:CD | 1:ME:439:THR:HG21 | 2.33 | 0.59 |
| 2:MF:79:GLY:C | 6:4D:179:ARG:HD2 | 2.26 | 0.59 |
| 6:4B:168:PHE:HD1 | 6:4B:168:PHE:O | 1.85 | 0.59 |
| 6:4B:195:ASN:HA | 6:4B:198:ASN:HD22 | 1.67 | 0.59 |
| 7:5A:1516:ILE:HD11 | 7:5A:1567:PHE:CG | 2.38 | 0.59 |
| 7:5A:1543:LEU:O | 7:5A:1573:ARG:CD | 2.51 | 0.59 |
| 7:5C:1516:ILE:HD11 | 7:5C:1567:PHE:CG | 2.38 | 0.59 |
| 9:7F:18:VAL:HG11 | 9:7F:42:LEU:CD2 | 2.33 | 0.59 |
| 1:BC:292:THR:HG21 | 1:BC:331:SER:HB3 | 1.83 | 0.59 |
| 2:BD:397:TRP:CD2 | 1:BE:256:GLN:O | 2.30 | 0.59 |
| 2:CD:86:ARG:N | 2:DD:281:TYR:HE1 | 1.94 | 0.59 |
| 1:CE:292:THR:HG21 | 1:CE:331:SER:HB3 | 1.83 | 0.59 |
| 1:DC:292:THR:HG21 | 1:DC:331:SER:HB3 | 1.83 | 0.59 |
| 1:DE:292:THR:HG21 | 1:DE:331:SER:HB3 | 1.83 | 0.59 |
| 1:EA:178:SER:OG | 2:EB:347:ASN:HB3 | 2.03 | 0.59 |
| 1:EC:292:THR:HG21 | 1:EC:331:SER:HB3 | 1.83 | 0.59 |
| 1:IC:393:HIS:NE2 | 5:3C:306:ASP:OD1 | 2.35 | 0.59 |
| 2:LB:274:THR:O | 6:4A:228:LEU:HD21 | 1.99 | 0.59 |
| 2:LF:294:PHE:CD2 | 4:2B:147:PHE:CZ | 2.80 | 0.59 |
| 2:LF:306:ARG:CZ | 4:2B:149:ILE:HG22 | 2.32 | 0.59 |
| 2:LF:306:ARG:CZ | 4:2B:149:ILE:HG21 | 2.31 | 0.59 |
| 2:LF:340:TYR:CB | 4:2B:147:PHE:HB2 | 2.32 | 0.59 |
| 6:4D:195:ASN:HA | 6:4D:198:ASN:HD22 | 1.67 | 0.59 |
| 6:4D:251:TYR:HD2 | 6:4D:288:TYR:CE2 | 2.21 | 0.59 |
| 7:5B:1516:ILE:HD11 | 7:5B:1567:PHE:CG | 2.38 | 0.59 |
| 7:5B:1521:PHE:CE1 | 7:5B:1570:ALA:HB1 | 2.38 | 0.59 |
| 7:5C:1433:GLU:HA | 7:5C:1433:GLU:OE1 | 2.02 | 0.59 |
| 1:AC:105:ARG:NH1 | 2:AD:251:ARG:HD3 | 2.18 | 0.59 |
| 1:AC:394:LYS:NZ | 2:AD:347:ASN:OD1 | 2.36 | 0.59 |
| 2:CB:86:ARG:HB2 | 2:DB:281:TYR:CE1 | 2.28 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:87:PRO:HD3 | 2:DB:281:TYR:CE2 | 2.33 | 0.59 |
| 1:CC:292:THR:HG21 | 1:CC:331:SER:HB3 | 1.83 | 0.59 |
| 2:CD:220:PRO:CD | 1:CE:326:LYS:HG2 | 2.32 | 0.59 |
| 2:DB:397:TRP:CD2 | 1:DC:256:GLN:O | 2.35 | 0.59 |
| 13:EB:501:GDP:C8 | 1:EC:248:LEU:CD1 | 2.85 | 0.59 |
| 2:FB:309:ARG:NH2 | 2:FB:426:GLN:O | 2.32 | 0.59 |
| 1:GE:401:LYS:CE | 2:GF:344:TRP:CZ3 | 2.67 | 0.59 |
| 2:IB:177:ASP:O | 1:IC:352:LYS:HA | 2.02 | 0.59 |
| 2:ID:177:ASP:O | 1:IE:352:LYS:HA | 2.02 | 0.59 |
| 1:KC:394:LYS:NZ | 2:KD:347:ASN:OD1 | 2.36 | 0.59 |
| 2:LD:55:THR:CG2 | 2:MD:283:ALA:C | 2.69 | 0.59 |
| 1:LE:60:LYS:HD3 | 1:ME:283:HIS:HA | 1.84 | 0.59 |
| 4:2C:12:LEU:HD21 | 4:2C:20:LYS:HB2 | 1.79 | 0.59 |
| 6:4A:251:TYR:HD2 | 6:4A:288:TYR:CE2 | 2.21 | 0.59 |
| 6:4B:224:ASN:OD1 | 6:4B:225:PRO:HD2 | 2.02 | 0.59 |
| 6:4B:251:TYR:HD2 | 6:4B:288:TYR:CE2 | 2.21 | 0.59 |
| 7:5A:1521:PHE:CE1 | 7:5A:1570:ALA:HB1 | 2.38 | 0.59 |
| 7:5C:1543:LEU:O | 7:5C:1573:ARG:CD | 2.51 | 0.59 |
| 2:BB:391:ARG:HG3 | 1:BC:346:TRP:CD1 | 2.37 | 0.59 |
| 1:CA:292:THR:HG21 | 1:CA:331:SER:HB3 | 1.83 | 0.59 |
| 2:DD:67:ASP:OD1 | 2:DD:68:LEU:N | 2.36 | 0.59 |
| 2:DD:86:ARG:N | 2:ED:281:TYR:HE1 | 1.99 | 0.59 |
| 1:EA:104:ALA:HB2 | 1:EA:413:MET:HE2 | 1.84 | 0.59 |
| 1:EA:292:THR:HG21 | 1:EA:331:SER:HB3 | 1.83 | 0.59 |
| 1:EE:426:ALA:HB1 | 7:5B:833:PHE:HD1 | 1.67 | 0.59 |
| 1:EE:430:LYS:NZ | 7:5B:834:ASN:HD21 | 1.09 | 0.59 |
| 1:HA:176:GLN:O | 2:HB:347:ASN:ND2 | 2.34 | 0.59 |
| 1:HC:105:ARG:NH1 | 2:HD:251:ARG:HD3 | 2.18 | 0.59 |
| 1:JC:176:GLN:O | 2:JD:347:ASN:ND2 | 2.35 | 0.59 |
| 1:JC:279:GLU:OE1 | 10:8Z:22:UNK:CB | 2.51 | 0.59 |
| 1:KA:104:ALA:HB2 | 1:KA:413:MET:HE2 | 1.84 | 0.59 |
| 2:KB:179:VAL:CG2 | 1:KC:258:ASN:CA | 2.81 | 0.59 |
| 6:4C:251:TYR:HD2 | 6:4C:288:TYR:CE2 | 2.21 | 0.59 |
| 2:AD:67:ASP:OD1 | 2:AD:68:LEU:N | 2.36 | 0.58 |
| 2:AD:224:ASP:OD1 | 6:4C:131:VAL:CA | 2.50 | 0.58 |
| 1:BA:292:THR:HG21 | 1:BA:331:SER:HB3 | 1.83 | 0.58 |
| 1:CA:404:PHE:HE2 | 2:CB:345:ILE:HD12 | 1.68 | 0.58 |
| 2:CB:67:ASP:OD1 | 2:CB:68:LEU:N | 2.36 | 0.58 |
| 2:CD:86:ARG:HB2 | 2:DD:281:TYR:HE1 | 1.67 | 0.58 |
| 2:DB:67:ASP:OD1 | 2:DB:68:LEU:N | 2.36 | 0.58 |
| 13:DB:501:GDP:C8 | 1:DC:248:LEU:CD1 | 2.86 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:DF:67:ASP:OD1 | 2:DF:68:LEU:N | 2.37 | 0.58 |
| 1:EE:426:ALA:HB1 | 7:5B:833:PHE:HB2 | 1.83 | 0.58 |
| 2:FD:179:VAL:CG2 | 1:FE:258:ASN:HA | 2.33 | 0.58 |
| 1:GE:89:PRO:HG3 | 1:HE:280:LYS:HD2 | 1.83 | 0.58 |
| 2:GF:416:ASN:ND2 | 7:5B:1327:LYS:NZ | 2.51 | 0.58 |
| 1:HE:278:ALA:HB2 | 10:8U:21:UNK:CB | 2.33 | 0.58 |
| 1:IA:282:TYR:CG | 10:8V:15:UNK:CB | 2.86 | 0.58 |
| 2:IB:179:VAL:CG2 | 1:IC:258:ASN:CA | 2.81 | 0.58 |
| 2:JB:212:PHE:HZ | 1:JC:326:LYS:CE | 2.14 | 0.58 |
| 1:JC:90:GLU:C | 1:KC:280:LYS:HZ2 | 1.77 | 0.58 |
| 2:KB:212:PHE:HZ | 1:KC:326:LYS:CE | 2.14 | 0.58 |
| 2:LD:228:LEU:HD21 | 6:4B:225:PRO:CB | 2.32 | 0.58 |
| 4:2A:12:LEU:HD21 | 4:2A:20:LYS:HB2 | 1.79 | 0.58 |
| 5:3C:230:ILE:O | 5:3C:332:MET:HG3 | 2.02 | 0.58 |
| 6:4A:108:LYS:O | 6:4A:108:LYS:HD2 | 2.03 | 0.58 |
| 6:4B:108:LYS:O | 6:4B:108:LYS:HD2 | 2.03 | 0.58 |
| 6:4C:108:LYS:O | 6:4C:108:LYS:HD2 | 2.03 | 0.58 |
| 6:4D:108:LYS:O | 6:4D:108:LYS:HD2 | 2.03 | 0.58 |
| 7:5A:1433:GLU:HA | 7:5A:1433:GLU:OE1 | 2.02 | 0.58 |
| 7:5B:1433:GLU:HA | 7:5B:1433:GLU:OE1 | 2.02 | 0.58 |
| 7:5C:836:ARG:HH11 | 7:5C:836:ARG:HG3 | 1.68 | 0.58 |
| 7:5C:836:ARG:HB3 | 7:5C:836:ARG:NH1 | 2.17 | 0.58 |
| 2:AB:67:ASP:OD1 | 2:AB:68:LEU:N | 2.37 | 0.58 |
| 2:AD:309:ARG:NH2 | 2:AD:426:GLN:O | 2.32 | 0.58 |
| 1:BA:401:LYS:HE3 | 2:BB:344:TRP:CZ3 | 2.38 | 0.58 |
| 1:DA:292:THR:HG21 | 1:DA:331:SER:HB3 | 1.83 | 0.58 |
| 2:ED:179:VAL:CG2 | 1:EE:258:ASN:CA | 2.81 | 0.58 |
| 2:FD:428:ALA:HB1 | 7:5A:1080:PHE:HE1 | 0.87 | 0.58 |
| 1:GC:394:LYS:NZ | 2:GD:347:ASN:OD1 | 2.36 | 0.58 |
| 1:HE:313:MET:HE3 | 1:HE:382:THR:HG22 | 1.86 | 0.58 |
| 1:IC:279:GLU:HG2 | 10:8W:22:UNK:HA | 1.85 | 0.58 |
| 1:JE:313:MET:HE3 | 1:JE:382:THR:HG22 | 1.86 | 0.58 |
| 2:KB:276:ARG:CZ | 6:4A:265:TYR:HB2 | 2.33 | 0.58 |
| 2:LB:15:GLN:NE2 | 6:4A:217:ASN:OD1 | 2.35 | 0.58 |
| 2:LD:224:ASP:CA | 6:4B:219:ASN:ND2 | 2.60 | 0.58 |
| 6:4A:224:ASN:OD1 | 6:4A:225:PRO:HD2 | 2.02 | 0.58 |
| 6:4C:224:ASN:OD1 | 6:4C:225:PRO:HD2 | 2.02 | 0.58 |
| 6:4C:244:GLU:HG3 | 6:4C:284:LEU:CD1 | 2.22 | 0.58 |
| 7:5A:827:GLU:CG | 7:5A:849:ARG:HH21 | 2.15 | 0.58 |
| 7:5A:836:ARG:HB3 | 7:5A:836:ARG:NH1 | 2.17 | 0.58 |
| 7:5A:1268:LEU:HD21 | 9:7B:19:LEU:HD13 | 1.84 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1367:LYS:HE3 | 7:5A:1367:LYS:CA | 2.31 | 0.58 |
| 7:5B:907:PHE:CE2 | 7:5B:921:HIS:CD2 | 2.91 | 0.58 |
| 7:5C:827:GLU:CG | 7:5C:849:ARG:HH21 | 2.15 | 0.58 |
| 7:5C:1367:LYS:HE3 | 7:5C:1367:LYS:CA | 2.31 | 0.58 |
| 7:5C:1521:PHE:CE1 | 7:5C:1570:ALA:HB1 | 2.38 | 0.58 |
| 2:AD:212:PHE:CE2 | 1:AE:326:LYS:HD3 | 2.26 | 0.58 |
| 2:AF:55:THR:HG21 | 2:BF:283:ALA:HA | 1.85 | 0.58 |
| 2:AF:67:ASP:OD1 | 2:AF:68:LEU:N | 2.37 | 0.58 |
| 1:BA:404:PHE:HE2 | 2:BB:345:ILE:HD12 | 1.67 | 0.58 |
| 2:BD:222:TYR:CD2 | 1:BE:247:ALA:HB1 | 2.39 | 0.58 |
| 2:CB:222:TYR:CD2 | 1:CC:247:ALA:HB1 | 2.38 | 0.58 |
| 1:CE:101:ASN:ND2 | 2:CF:252:LYS:HG3 | 2.10 | 0.58 |
| 1:EE:426:ALA:HB3 | 7:5B:833:PHE:CB | 2.30 | 0.58 |
| 1:FC:177:VAL:CG2 | 7:5A:915:PHE:CZ | 2.64 | 0.58 |
| 1:FE:402:ARG:HD3 | 7:5B:1259:TYR:HB2 | 1.84 | 0.58 |
| 1:GC:313:MET:HE3 | 1:GC:382:THR:HG22 | 1.86 | 0.58 |
| 1:GE:313:MET:HE3 | 1:GE:382:THR:HG22 | 1.86 | 0.58 |
| 1:HC:282:TYR:CE1 | 10:8T:15:UNK:HA | 2.38 | 0.58 |
| 1:IE:313:MET:HE3 | 1:IE:382:THR:HG22 | 1.86 | 0.58 |
| 1:KC:105:ARG:NH1 | 2:KD:251:ARG:HD3 | 2.18 | 0.58 |
| 1:KE:85:GLN:CA | 1:LE:283:HIS:HD2 | 2.15 | 0.58 |
| 2:LB:179:VAL:HG22 | 1:LC:258:ASN:CB | 2.34 | 0.58 |
| 1:MA:100:ALA:HB1 | 2:MB:252:LYS:CA | 2.33 | 0.58 |
| 2:MB:111:GLU:HA | 3:1A:62:SER:CA | 2.32 | 0.58 |
| 2:MD:221:THR:HB | 6:4B:189:ARG:NH1 | 2.19 | 0.58 |
| 2:MF:67:ASP:OD1 | 2:MF:68:LEU:N | 2.36 | 0.58 |
| 6:4B:179:ARG:HH11 | 6:4B:179:ARG:CG | 2.17 | 0.58 |
| 6:4D:179:ARG:HH11 | 6:4D:179:ARG:CG | 2.17 | 0.58 |
| 7:5A:836:ARG:HH11 | 7:5A:836:ARG:HG3 | 1.68 | 0.58 |
| 7:5A:907:PHE:CE2 | 7:5A:921:HIS:CD2 | 2.91 | 0.58 |
| 7:5A:1438:LEU:O | 7:5A:1438:LEU:HD12 | 2.03 | 0.58 |
| 7:5B:827:GLU:CG | 7:5B:849:ARG:HH21 | 2.15 | 0.58 |
| 7:5B:1367:LYS:HE3 | 7:5B:1367:LYS:CA | 2.31 | 0.58 |
| 7:5B:1548:VAL:HG12 | 7:5B:1566:GLU:N | 2.18 | 0.58 |
| 7:5C:1438:LEU:HD12 | 7:5C:1438:LEU:O | 2.03 | 0.58 |
| 9:7D:18:VAL:HG11 | 9:7D:42:LEU:CD2 | 2.33 | 0.58 |
| 1:AE:313:MET:HE3 | 1:AE:382:THR:HG22 | 1.86 | 0.58 |
| 2:CD:67:ASP:OD1 | 2:CD:68:LEU:N | 2.37 | 0.58 |
| 1:CE:313:MET:HE3 | 1:CE:382:THR:HG22 | 1.86 | 0.58 |
| 2:CF:67:ASP:OD1 | 2:CF:68:LEU:N | 2.37 | 0.58 |
| 1:DC:313:MET:HE3 | 1:DC:382:THR:HG22 | 1.86 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:DE:313:MET:HE3 | 1:DE:382:THR:HG22 | 1.86 | 0.58 |
| 2:EB:83:GLN:O | 2:FB:281:TYR:OH | 2.22 | 0.58 |
| 1:FA:56:THR:O | 1:GA:285:GLN:HB2 | 2.02 | 0.58 |
| 1:FA:282:TYR:CD2 | 10:8M:18:UNK:CB | 2.76 | 0.58 |
| 1:GA:313:MET:HE3 | 1:GA:382:THR:HG22 | 1.86 | 0.58 |
| 1:HC:313:MET:HE3 | 1:HC:382:THR:HG22 | 1.86 | 0.58 |
| 2:IF:67:ASP:OD1 | 2:IF:68:LEU:N | 2.37 | 0.58 |
| 1:JE:279:GLU:OE1 | 10:9A:22:UNK:CB | 2.51 | 0.58 |
| 1:KC:313:MET:HE3 | 1:KC:382:THR:HG22 | 1.86 | 0.58 |
| 1:KE:62:VAL:CG2 | 1:LE:285:GLN:CB | 2.78 | 0.58 |
| 1:KE:313:MET:HE3 | 1:KE:382:THR:HG22 | 1.86 | 0.58 |
| 2:KF:309:ARG:NH2 | 2:KF:426:GLN:O | 2.32 | 0.58 |
| 2:LD:221:THR:HG22 | 6:4B:220:GLY:H | 1.68 | 0.58 |
| 1:LE:60:LYS:HD3 | 1:ME:283:HIS:CB | 2.33 | 0.58 |
| 1:MA:313:MET:HE3 | 1:MA:382:THR:HG22 | 1.86 | 0.58 |
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:SD | 2.42 | 0.58 |
| 7:5B:836:ARG:HB3 | 7:5B:836:ARG:NH1 | 2.17 | 0.58 |
| 7:5B:1119:LEU:HD13 | 7:5B:1135:TYR:CE1 | 2.38 | 0.58 |
| 7:5B:1438:LEU:HD12 | 7:5B:1438:LEU:O | 2.03 | 0.58 |
| 7:5C:907:PHE:CE2 | 7:5C:921:HIS:CD2 | 2.91 | 0.58 |
| 8:6C:146:ILE:HD12 | 8:6C:183:LEU:CB | 2.32 | 0.58 |
| 9:7F:41:PHE:O | 9:7F:45:ARG:HG2 | 2.02 | 0.58 |
| 1:AA:101:ASN:ND2 | 2:AB:252:LYS:HG3 | 2.10 | 0.58 |
| 1:AA:313:MET:HE3 | 1:AA:382:THR:HG22 | 1.86 | 0.58 |
| 1:AC:313:MET:HE3 | 1:AC:382:THR:HG22 | 1.86 | 0.58 |
| 2:AF:322:SER:H | 6:4A:156:PHE:HE2 | 1.50 | 0.58 |
| 2:CB:222:TYR:O | 2:CB:226:ASN:ND2 | 2.28 | 0.58 |
| 2:DF:85:PHE:C | 2:EF:281:TYR:CZ | 2.81 | 0.58 |
| 1:EA:313:MET:HE3 | 1:EA:382:THR:HG22 | 1.86 | 0.58 |
| 2:ED:157:GLU:HA | 7:5A:945:LYS:HZ3 | 1.68 | 0.58 |
| 1:EE:88:HIS:HB3 | 1:EE:91:GLN:HG2 | 1.86 | 0.58 |
| 1:FC:422:ARG:CZ | 7:5A:1170:THR:C | 2.75 | 0.58 |
| 2:FF:331:LEU:HD21 | 7:5B:915:PHE:CZ | 2.39 | 0.58 |
| 1:GA:88:HIS:HB3 | 1:GA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:GC:88:HIS:HB3 | 1:GC:91:GLN:HG2 | 1.86 | 0.58 |
| 2:GF:412:GLU:OE2 | 7:5B:1323:MET:CE | 2.51 | 0.58 |
| 1:HA:313:MET:HE3 | 1:HA:382:THR:HG22 | 1.86 | 0.58 |
| 1:IA:278:ALA:CB | 10:8V:21:UNK:CA | 2.81 | 0.58 |
| 2:ID:67:ASP:OD1 | 2:ID:68:LEU:N | 2.37 | 0.58 |
| 1:JA:313:MET:HE3 | 1:JA:382:THR:HG22 | 1.86 | 0.58 |
| 2:JB:67:ASP:OD1 | 2:JB:68:LEU:N | 2.36 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:JC:90:GLU:CG | 1:KC:280:LYS:HD2 | 2.07 | 0.58 |
| 1:JC:313:MET:HE3 | 1:JC:382:THR:HG22 | 1.86 | 0.58 |
| 1:KA:313:MET:HE3 | 1:KA:382:THR:HG22 | 1.86 | 0.58 |
| 1:LE:313:MET:HE3 | 1:LE:382:THR:HG22 | 1.86 | 0.58 |
| 2:LF:294:PHE:CD2 | 4:2B:147:PHE:HZ | 2.19 | 0.58 |
| 1:MC:313:MET:HE3 | 1:MC:382:THR:HG22 | 1.86 | 0.58 |
| 5:3A:230:ILE:O | 5:3A:332:MET:HG3 | 2.02 | 0.58 |
| 6:4A:179:ARG:HH11 | 6:4A:179:ARG:CG | 2.17 | 0.58 |
| 7:5A:1119:LEU:HD13 | 7:5A:1135:TYR:CE1 | 2.38 | 0.58 |
| 7:5A:1373:PHE:CD1 | 7:5A:1373:PHE:N | 2.72 | 0.58 |
| 7:5A:1487:ASN:CG | 7:5A:1568:LYS:CD | 2.76 | 0.58 |
| 7:5A:1521:PHE:CE2 | 7:5A:1567:PHE:CG | 2.58 | 0.58 |
| 7:5B:827:GLU:HA | 7:5B:841:VAL:CG1 | 2.33 | 0.58 |
| 7:5B:836:ARG:HH11 | 7:5B:836:ARG:HG3 | 1.68 | 0.58 |
| 7:5C:1119:LEU:HD13 | 7:5C:1135:TYR:CE1 | 2.38 | 0.58 |
| 7:5C:1487:ASN:CG | 7:5C:1568:LYS:CD | 2.76 | 0.58 |
| 9:7D:41:PHE:O | 9:7D:45:ARG:HG2 | 2.02 | 0.58 |
| 2:AB:179:VAL:HG21 | 1:AC:258:ASN:C | 2.28 | 0.58 |
| 1:BA:404:PHE:CE2 | 2:BB:345:ILE:CD1 | 2.86 | 0.58 |
| 1:BC:222:PRO:HD2 | 2:BD:324:LYS:HD3 | 1.85 | 0.58 |
| 1:CA:313:MET:HE3 | 1:CA:382:THR:HG22 | 1.86 | 0.58 |
| 1:CC:313:MET:HE3 | 1:CC:382:THR:HG22 | 1.86 | 0.58 |
| 2:CD:179:VAL:HG21 | 1:CE:258:ASN:C | 2.28 | 0.58 |
| 1:DA:313:MET:HE3 | 1:DA:382:THR:HG22 | 1.86 | 0.58 |
| 1:DC:88:HIS:HB3 | 1:DC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:DC:404:PHE:CE2 | 2:DD:345:ILE:CD1 | 2.86 | 0.58 |
| 1:DE:88:HIS:HB3 | 1:DE:91:GLN:HG2 | 1.86 | 0.58 |
| 1:EA:398:MET:SD | 2:EB:345:ILE:CG1 | 2.85 | 0.58 |
| 1:EC:313:MET:HE3 | 1:EC:382:THR:HG22 | 1.86 | 0.58 |
| 2:ED:220:PRO:CD | 1:EE:326:LYS:HG2 | 2.32 | 0.58 |
| 2:EF:67:ASP:OD1 | 2:EF:68:LEU:N | 2.37 | 0.58 |
| 1:FA:422:ARG:HE | 7:5C:1170:THR:CB | 2.15 | 0.58 |
| 2:FD:54:ALA:C | 2:GD:283:ALA:CB | 2.57 | 0.58 |
| 1:FE:313:MET:HE3 | 1:FE:382:THR:HG22 | 1.86 | 0.58 |
| 1:GA:401:LYS:HE3 | 2:GB:344:TRP:CZ3 | 2.38 | 0.58 |
| 1:GE:88:HIS:HB3 | 1:GE:91:GLN:HG2 | 1.86 | 0.58 |
| 1:HA:88:HIS:HB3 | 1:HA:91:GLN:HG2 | 1.86 | 0.58 |
| 2:HB:179:VAL:CG2 | 1:HC:258:ASN:CA | 2.81 | 0.58 |
| 1:HC:394:LYS:NZ | 2:HD:347:ASN:OD1 | 2.36 | 0.58 |
| 1:IC:105:ARG:NH1 | 2:ID:251:ARG:HD3 | 2.18 | 0.58 |
| 1:IC:313:MET:HE3 | 1:IC:382:THR:HG22 | 1.86 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:IC:393:HIS:CB | 5:3C:308:PHE:CE2 | 2.86 | 0.58 |
| 1:IE:88:HIS:HB3 | 1:IE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:JB:179:VAL:CG2 | 1:JC:258:ASN:CA | 2.81 | 0.58 |
| 1:JE:88:HIS:HB3 | 1:JE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:KD:86:ARG:HG2 | 2:LD:288:GLU:CD | 2.28 | 0.58 |
| 1:KE:88:HIS:HB3 | 1:KE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:KF:215:LEU:CD2 | 6:4D:267:ILE:O | 2.41 | 0.58 |
| 2:LB:221:THR:HG22 | 6:4A:220:GLY:H | 1.69 | 0.58 |
| 2:MD:67:ASP:OD1 | 2:MD:68:LEU:N | 2.37 | 0.58 |
| 2:MD:222:TYR:O | 2:MD:226:ASN:ND2 | 2.28 | 0.58 |
| 1:ME:282:TYR:CD1 | 6:4B:98:PRO:HB3 | 2.39 | 0.58 |
| 4:2B:12:LEU:HD21 | 4:2B:20:LYS:HB2 | 1.79 | 0.58 |
| 6:4C:179:ARG:HH11 | 6:4C:179:ARG:CG | 2.17 | 0.58 |
| 7:5A:1275:ILE:HG21 | 9:7B:11:TYR:OH | 2.03 | 0.58 |
| 7:5B:1370:LYS:HD3 | 7:5B:1373:PHE:HZ | 1.68 | 0.58 |
| 7:5B:1419:GLU:HA | 7:5B:1419:GLU:OE1 | 2.04 | 0.58 |
| 7:5B:1487:ASN:CG | 7:5B:1568:LYS:CD | 2.77 | 0.58 |
| 7:5C:1515:GLU:OE1 | 7:5C:1563:SER:OG | 2.20 | 0.58 |
| 2:AB:309:ARG:NH2 | 2:AB:426:GLN:O | 2.32 | 0.58 |
| 1:AE:141:VAL:HG11 | 1:AE:172:TYR:CD1 | 2.38 | 0.58 |
| 2:AF:372:THR:HA | 2:AF:422:TYR:HE2 | 1.69 | 0.58 |
| 1:BC:178:SER:OG | 2:BD:347:ASN:HB3 | 2.03 | 0.58 |
| 1:DA:88:HIS:HB3 | 1:DA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:EA:88:HIS:HB3 | 1:EA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:EC:88:HIS:HB3 | 1:EC:91:GLN:HG2 | 1.86 | 0.58 |
| 2:ED:67:ASP:OD1 | 2:ED:68:LEU:N | 2.37 | 0.58 |
| 1:FA:88:HIS:HB3 | 1:FA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:FA:313:MET:HE3 | 1:FA:382:THR:HG22 | 1.86 | 0.58 |
| 1:FC:313:MET:HE3 | 1:FC:382:THR:HG22 | 1.86 | 0.58 |
| 2:GB:67:ASP:OD1 | 2:GB:68:LEU:N | 2.37 | 0.58 |
| 1:HC:88:HIS:HB3 | 1:HC:91:GLN:HG2 | 1.86 | 0.58 |
| 2:HD:222:TYR:O | 2:HD:226:ASN:ND2 | 2.27 | 0.58 |
| 1:HE:88:HIS:HB3 | 1:HE:91:GLN:HG2 | 1.86 | 0.58 |
| 1:IA:313:MET:HE3 | 1:IA:382:THR:HG22 | 1.86 | 0.58 |
| 2:IB:67:ASP:OD1 | 2:IB:68:LEU:N | 2.37 | 0.58 |
| 1:IC:88:HIS:HB3 | 1:IC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:IC:389:SER:HB2 | 5:3C:307:LYS:CG | 2.32 | 0.58 |
| 1:JA:88:HIS:HB3 | 1:JA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:JC:88:HIS:HB3 | 1:JC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:JC:105:ARG:NH1 | 2:JD:251:ARG:HD3 | 2.18 | 0.58 |
| 2:JD:67:ASP:OD1 | 2:JD:68:LEU:N | 2.37 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:KC:88:HIS:HB3 | 1:KC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:KC:124:LYS:HD3 | 1:LC:290:GLU:HA | 1.84 | 0.58 |
| 2:KD:228:LEU:CD2 | 6:4B:267:ILE:HD12 | 2.33 | 0.58 |
| 1:LA:313:MET:HE3 | 1:LA:382:THR:HG22 | 1.86 | 0.58 |
| 1:LC:313:MET:HE3 | 1:LC:382:THR:HG22 | 1.86 | 0.58 |
| 2:MB:67:ASP:OD1 | 2:MB:68:LEU:N | 2.36 | 0.58 |
| 7:5A:1419:GLU:HA | 7:5A:1419:GLU:OE1 | 2.04 | 0.58 |
| 7:5B:1373:PHE:CD1 | 7:5B:1373:PHE:N | 2.72 | 0.58 |
| 7:5C:1449:LEU:HD22 | 7:5C:1452:HIS:HD2 | 1.68 | 0.58 |
| 9:7B:18:VAL:HG11 | 9:7B:42:LEU:CD2 | 2.33 | 0.58 |
| 9:7C:30:ARG:CZ | 9:7D:3:GLN:HA | 2.23 | 0.58 |
| 9:7E:18:VAL:HG11 | 9:7F:35:ILE:CG2 | 2.34 | 0.58 |
| 2:AB:212:PHE:HZ | 1:AC:326:LYS:HD3 | 0.53 | 0.58 |
| 2:AB:372:THR:HA | 2:AB:422:TYR:HE2 | 1.69 | 0.58 |
| 1:AC:101:ASN:ND2 | 2:AD:252:LYS:HG3 | 2.09 | 0.58 |
| 1:AC:141:VAL:HG11 | 1:AC:172:TYR:CD1 | 2.38 | 0.58 |
| 2:AD:280:GLN:NE2 | 6:4C:139:ASP:OD1 | 2.35 | 0.58 |
| 2:AD:372:THR:HA | 2:AD:422:TYR:HE2 | 1.69 | 0.58 |
| 1:BA:178:SER:OG | 2:BB:347:ASN:HB3 | 2.03 | 0.58 |
| 1:BA:313:MET:HE3 | 1:BA:382:THR:HG22 | 1.86 | 0.58 |
| 1:BC:313:MET:HE3 | 1:BC:382:THR:HG22 | 1.86 | 0.58 |
| 1:CE:88:HIS:HB3 | 1:CE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:DB:177:ASP:C | 1:DC:352:LYS:HA | 2.28 | 0.58 |
| 2:FB:54:ALA:CB | 2:GB:281:TYR:O | 2.52 | 0.58 |
| 1:FC:88:HIS:HB3 | 1:FC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:FE:88:HIS:HB3 | 1:FE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:FF:67:ASP:OD1 | 2:FF:68:LEU:N | 2.37 | 0.58 |
| 1:GE:105:ARG:NH1 | 2:GF:251:ARG:HD3 | 2.19 | 0.58 |
| 1:GE:401:LYS:HE3 | 2:GF:344:TRP:CZ3 | 2.37 | 0.58 |
| 1:HC:176:GLN:O | 2:HD:347:ASN:ND2 | 2.35 | 0.58 |
| 2:HD:212:PHE:CE2 | 1:HE:326:LYS:HD3 | 2.26 | 0.58 |
| 1:HE:410:GLY:CA | 5:3A:329:ARG:NH2 | 2.67 | 0.58 |
| 1:IA:281:ALA:HB3 | 10:8V:18:UNK:CB | 2.34 | 0.58 |
| 1:IE:393:HIS:NE2 | 5:3A:306:ASP:OD1 | 2.37 | 0.58 |
| 2:IF:309:ARG:NH2 | 2:IF:426:GLN:O | 2.32 | 0.58 |
| 1:KA:88:HIS:HB3 | 1:KA:91:GLN:HG2 | 1.86 | 0.58 |
| 2:LB:100:ASN:HB2 | 1:LC:257:THR:HG21 | 1.86 | 0.58 |
| 1:LE:88:HIS:HB3 | 1:LE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:MD:111:GLU:CG | 3:1B:62:SER:HB2 | 2.33 | 0.58 |
| 1:ME:313:MET:HE3 | 1:ME:382:THR:HG22 | 1.86 | 0.58 |
| 6:4B:139:ASP:O | 6:4B:142:SER:OG | 2.20 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:4D:139:ASP:O | 6:4D:142:SER:OG | 2.20 | 0.58 |
| 7:5A:827:GLU:HA | 7:5A:841:VAL:CG1 | 2.33 | 0.58 |
| 7:5A:1515:GLU:OE1 | 7:5A:1563:SER:OG | 2.20 | 0.58 |
| 7:5B:1455:LYS:O | 7:5B:1455:LYS:HE2 | 2.02 | 0.58 |
| 7:5C:827:GLU:HA | 7:5C:841:VAL:CG1 | 2.33 | 0.58 |
| 1:AA:88:HIS:HB3 | 1:AA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:AC:88:HIS:HB3 | 1:AC:91:GLN:HG2 | 1.86 | 0.58 |
| 1:AE:88:HIS:HB3 | 1:AE:91:GLN:HG2 | 1.86 | 0.58 |
| 2:AF:224:ASP:OD1 | 6:4A:131:VAL:N | 2.36 | 0.58 |
| 2:BD:87:PRO:CD | 2:CD:281:TYR:CZ | 2.84 | 0.58 |
| 1:BE:313:MET:HE3 | 1:BE:382:THR:HG22 | 1.86 | 0.58 |
| 1:CA:101:ASN:ND2 | 2:CB:252:LYS:HG3 | 2.11 | 0.58 |
| 2:CB:86:ARG:N | 2:DB:281:TYR:HE1 | 1.95 | 0.58 |
| 2:CD:179:VAL:CG2 | 1:CE:258:ASN:CA | 2.82 | 0.58 |
| 2:CD:179:VAL:CG2 | 1:CE:258:ASN:O | 2.40 | 0.58 |
| 2:DB:222:TYR:CD2 | 1:DC:247:ALA:HB1 | 2.38 | 0.58 |
| 2:DD:60:VAL:HG21 | 2:ED:281:TYR:CE1 | 2.39 | 0.58 |
| 2:EB:67:ASP:OD1 | 2:EB:68:LEU:N | 2.37 | 0.58 |
| 2:FB:84:LEU:O | 2:GB:281:TYR:CE1 | 2.56 | 0.58 |
| 1:FC:56:THR:C | 1:GC:285:GLN:HB3 | 2.29 | 0.58 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:CG | 2.82 | 0.58 |
| 2:FD:67:ASP:OD1 | 2:FD:68:LEU:N | 2.37 | 0.58 |
| 2:FD:390:ARG:HD2 | 1:FE:439:THR:HG21 | 1.86 | 0.58 |
| 1:GA:370:LYS:CG | 10:8P:18:UNK:N | 2.67 | 0.58 |
| 2:IF:87:PRO:CD | 2:JF:281:TYR:CE2 | 2.87 | 0.58 |
| 1:JC:394:LYS:NZ | 2:JD:347:ASN:OD1 | 2.36 | 0.58 |
| 2:KB:118:ASP:OD1 | 4:2C:148:ASN:OD1 | 2.21 | 0.58 |
| 2:KB:177:ASP:HA | 1:KC:353:VAL:HG12 | 1.86 | 0.58 |
| 2:KB:217:LEU:CD1 | 6:4A:263:CYS:SG | 2.91 | 0.58 |
| 2:KD:77:ARG:CG | 2:LD:281:TYR:OH | 2.42 | 0.58 |
| 2:KD:309:ARG:NH2 | 2:KD:426:GLN:O | 2.32 | 0.58 |
| 2:LF:55:THR:CG2 | 2:MF:284:LEU:N | 2.67 | 0.58 |
| 2:MB:391:ARG:O | 1:MC:262:TYR:OH | 2.22 | 0.58 |
| 2:MB:397:TRP:CB | 1:MC:256:GLN:HE22 | 2.13 | 0.58 |
| 2:MD:177:ASP:O | 1:ME:352:LYS:HA | 2.03 | 0.58 |
| 5:3B:230:ILE:O | 5:3B:332:MET:HG3 | 2.02 | 0.58 |
| 6:4C:287:ASP:N | 6:4C:287:ASP:OD2 | 2.30 | 0.58 |
| 7:5A:1077:ASN:CG | 7:5A:1083:THR:HG21 | 2.29 | 0.58 |
| 7:5A:1370:LYS:HD3 | 7:5A:1373:PHE:HZ | 1.68 | 0.58 |
| 7:5A:1449:LEU:HD22 | 7:5A:1452:HIS:HD2 | 1.68 | 0.58 |
| 7:5B:1406:PHE:O | 7:5B:1410:ASN:N | 2.31 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5B:1543:LEU:O | 7:5B:1573:ARG:HD3 | 2.04 | 0.58 |
| 7:5C:1370:LYS:HD3 | 7:5C:1373:PHE:HZ | 1.68 | 0.58 |
| 7:5C:1419:GLU:HA | 7:5C:1419:GLU:OE1 | 2.04 | 0.58 |
| 2:AB:177:ASP:HA | 1:AC:353:VAL:HG12 | 1.86 | 0.58 |
| 2:AD:40:SER:OG | 6:4C:152:PHE:CD2 | 2.43 | 0.58 |
| 2:AD:359:LYS:CA | 6:4C:151:ARG:HH22 | 2.00 | 0.58 |
| 1:BE:88:HIS:HB3 | 1:BE:91:GLN:HG2 | 1.86 | 0.58 |
| 1:CA:88:HIS:HB3 | 1:CA:91:GLN:HG2 | 1.86 | 0.58 |
| 1:CC:88:HIS:HB3 | 1:CC:91:GLN:HG2 | 1.86 | 0.58 |
| 2:EB:212:PHE:CZ | 1:EC:326:LYS:CE | 2.86 | 0.58 |
| 1:EE:313:MET:HE3 | 1:EE:382:THR:HG22 | 1.86 | 0.58 |
| 2:FB:390:ARG:HD2 | 1:FC:439:THR:HG21 | 1.85 | 0.58 |
| 1:FC:222:PRO:HG3 | 2:FD:324:LYS:HD3 | 1.78 | 0.58 |
| 1:FC:423:GLU:HG3 | 7:5A:1256:ARG:NH2 | 2.19 | 0.58 |
| 2:FF:222:TYR:O | 2:FF:226:ASN:ND2 | 2.28 | 0.58 |
| 1:HE:105:ARG:NH1 | 2:HF:251:ARG:HD3 | 2.19 | 0.58 |
| 2:IB:177:ASP:HA | 1:IC:353:VAL:HG12 | 1.86 | 0.58 |
| 1:JE:89:PRO:HG2 | 1:KE:280:LYS:CG | 2.30 | 0.58 |
| 2:JF:67:ASP:OD1 | 2:JF:68:LEU:N | 2.37 | 0.58 |
| 2:KD:54:ALA:HB2 | 2:LD:285:THR:CG2 | 1.99 | 0.58 |
| 2:LB:294:PHE:HD2 | 4:2C:147:PHE:CZ | 2.22 | 0.58 |
| 1:LC:88:HIS:HB3 | 1:LC:91:GLN:HG2 | 1.86 | 0.58 |
| 2:LF:372:THR:HA | 2:LF:422:TYR:HE2 | 1.69 | 0.58 |
| 2:MB:220:PRO:HD2 | 1:MC:326:LYS:HE2 | 1.84 | 0.58 |
| 1:MC:88:HIS:HB3 | 1:MC:91:GLN:HG2 | 1.86 | 0.58 |
| 6:4A:139:ASP:O | 6:4A:142:SER:OG | 2.20 | 0.58 |
| 7:5A:1455:LYS:O | 7:5A:1455:LYS:HE2 | 2.02 | 0.58 |
| 7:5B:1077:ASN:CG | 7:5B:1083:THR:HG21 | 2.29 | 0.58 |
| 7:5C:1077:ASN:CG | 7:5C:1083:THR:HG21 | 2.29 | 0.58 |
| 7:5C:1544:ILE:C | 7:5C:1570:ALA:CB | 2.76 | 0.58 |
| 1:AA:141:VAL:HG11 | 1:AA:172:TYR:CD1 | 2.38 | 0.57 |
| 2:AD:321:MET:HA | 6:4C:156:PHE:CE2 | 2.39 | 0.57 |
| 1:AE:105:ARG:NH1 | 2:AF:251:ARG:HD3 | 2.19 | 0.57 |
| 2:AF:223:GLY:O | 6:4A:131:VAL:CA | 2.52 | 0.57 |
| 1:BA:88:HIS:HB3 | 1:BA:91:GLN:HG2 | 1.86 | 0.57 |
| 2:BB:178:THR:HA | 1:BC:352:LYS:HD3 | 1.85 | 0.57 |
| 2:BB:220:PRO:CD | 1:BC:326:LYS:HE2 | 2.32 | 0.57 |
| 1:BC:88:HIS:HB3 | 1:BC:91:GLN:HG2 | 1.86 | 0.57 |
| 2:BF:372:THR:HA | 2:BF:422:TYR:HE2 | 1.69 | 0.57 |
| 1:CC:401:LYS:CE | 2:CD:344:TRP:CZ3 | 2.71 | 0.57 |
| 1:DE:62:VAL:CG2 | 1:EE:283:HIS:O | 2.47 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DF:25:SER:HG | 2:DF:51:TYR:HH | 1.51 | 0.57 |
| 1:EE:401:LYS:HE3 | 2:EF:344:TRP:CZ3 | 2.39 | 0.57 |
| 1:EE:423:GLU:OE2 | 7:5B:830:VAL:HG11 | 1.96 | 0.57 |
| 2:FB:220:PRO:O | 1:FC:324:VAL:HG13 | 2.04 | 0.57 |
| 1:FE:56:THR:HA | 1:GE:285:GLN:HB3 | 1.86 | 0.57 |
| 1:GA:56:THR:C | 1:HA:285:GLN:HB3 | 2.29 | 0.57 |
| 2:GD:55:THR:CA | 2:HD:283:ALA:CB | 2.65 | 0.57 |
| 2:HB:372:THR:HA | 2:HB:422:TYR:HE2 | 1.69 | 0.57 |
| 2:HD:372:THR:HA | 2:HD:422:TYR:HE2 | 1.69 | 0.57 |
| 1:IA:88:HIS:HB3 | 1:IA:91:GLN:HG2 | 1.86 | 0.57 |
| 2:JB:177:ASP:HA | 1:JC:353:VAL:HG12 | 1.86 | 0.57 |
| 1:JC:88:HIS:O | 1:KC:280:LYS:NZ | 2.37 | 0.57 |
| 1:JC:282:TYR:CZ | 10:8Z:17:UNK:CB | 2.86 | 0.57 |
| 1:JE:88:HIS:O | 1:KE:280:LYS:CE | 2.52 | 0.57 |
| 1:LA:88:HIS:HB3 | 1:LA:91:GLN:HG2 | 1.86 | 0.57 |
| 2:LF:228:LEU:HD23 | 6:4D:225:PRO:HG2 | 1.86 | 0.57 |
| 1:MA:88:HIS:HB3 | 1:MA:91:GLN:HG2 | 1.86 | 0.57 |
| 1:ME:88:HIS:HB3 | 1:ME:91:GLN:HG2 | 1.86 | 0.57 |
| 7:5A:1543:LEU:O | 7:5A:1573:ARG:HD3 | 2.04 | 0.57 |
| 7:5B:1243:ASP:CB | 9:7D:8:ARG:NH1 | 2.67 | 0.57 |
| 7:5B:1515:GLU:OE1 | 7:5B:1563:SER:OG | 2.20 | 0.57 |
| 7:5C:1491:LEU:N | 7:5C:1495:PHE:HB2 | 2.14 | 0.57 |
| 9:7B:41:PHE:O | 9:7B:45:ARG:HG2 | 2.02 | 0.57 |
| 1:CC:101:ASN:ND2 | 2:CD:252:LYS:HG3 | 2.10 | 0.57 |
| 2:EB:391:ARG:HG3 | 1:EC:346:TRP:CD1 | 2.38 | 0.57 |
| 2:FB:67:ASP:OD1 | 2:FB:68:LEU:N | 2.37 | 0.57 |
| 2:FB:106:TYR:CE1 | 7:5C:1295:LYS:N | 2.70 | 0.57 |
| 1:GA:401:LYS:CE | 2:GB:344:TRP:CZ3 | 2.67 | 0.57 |
| 2:GB:177:ASP:HA | 1:GC:353:VAL:HG12 | 1.86 | 0.57 |
| 2:HF:67:ASP:OD1 | 2:HF:68:LEU:N | 2.37 | 0.57 |
| 2:IB:424:GLN:HE21 | 7:5C:1413:GLN:HE21 | 0.61 | 0.57 |
| 1:IC:402:ARG:NH2 | 7:5A:1418:GLN:HA | 2.19 | 0.57 |
| 2:JB:222:TYR:O | 2:JB:226:ASN:ND2 | 2.27 | 0.57 |
| 1:KA:88:HIS:ND1 | 1:LA:284:GLU:OE1 | 2.37 | 0.57 |
| 1:KE:105:ARG:NH1 | 2:KF:251:ARG:HD3 | 2.19 | 0.57 |
| 1:MA:222:PRO:O | 2:MB:322:SER:HB2 | 2.04 | 0.57 |
| 6:4C:223:PHE:N | 6:4C:223:PHE:HD2 | 2.02 | 0.57 |
| 6:4C:282:ASN:OD1 | 6:4C:282:ASN:N | 2.35 | 0.57 |
| 7:5A:1491:LEU:N | 7:5A:1495:PHE:HB2 | 2.14 | 0.57 |
| 7:5B:1449:LEU:HD22 | 7:5B:1452:HIS:HD2 | 1.68 | 0.57 |
| 7:5C:1455:LYS:O | 7:5C:1455:LYS:HE2 | 2.02 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:7E:11:TYR:HD1 | 9:7F:26:LEU:CD2 | 2.01 | 0.57 |
| 1:CA:282:TYR:HE2 | 10:8D:18:UNK:CA | 2.17 | 0.57 |
| 2:CD:222:TYR:O | 2:CD:226:ASN:ND2 | 2.28 | 0.57 |
| 1:DA:141:VAL:HG11 | 1:DA:172:TYR:CD1 | 2.38 | 0.57 |
| 1:EA:404:PHE:CE2 | 2:EB:345:ILE:CD1 | 2.86 | 0.57 |
| 2:GD:416:ASN:CG | 7:5A:1327:LYS:HZ1 | 2.12 | 0.57 |
| 2:HB:177:ASP:HA | 1:HC:353:VAL:HG12 | 1.86 | 0.57 |
| 2:HF:372:THR:HA | 2:HF:422:TYR:HE2 | 1.69 | 0.57 |
| 1:IC:394:LYS:NZ | 2:ID:347:ASN:OD1 | 2.36 | 0.57 |
| 2:ID:309:ARG:NH2 | 2:ID:426:GLN:O | 2.32 | 0.57 |
| 1:JE:91:GLN:H | 1:KE:280:LYS:HZ2 | 0.59 | 0.57 |
| 2:KD:124:ALA:O | 4:2A:37:GLY:C | 2.47 | 0.57 |
| 2:LB:372:THR:HA | 2:LB:422:TYR:HE2 | 1.69 | 0.57 |
| 2:LB:379:LYS:CA | 4:2C:166:ILE:HD12 | 1.83 | 0.57 |
| 2:LD:98:GLY:HA2 | 1:LE:254:GLU:HG3 | 1.84 | 0.57 |
| 2:LD:179:VAL:HG22 | 1:LE:258:ASN:CB | 2.34 | 0.57 |
| 2:LD:372:THR:HA | 2:LD:422:TYR:HE2 | 1.69 | 0.57 |
| 1:LE:60:LYS:CD | 1:ME:283:HIS:CG | 2.86 | 0.57 |
| 2:LF:67:ASP:OD1 | 2:LF:68:LEU:N | 2.36 | 0.57 |
| 1:MA:222:PRO:HG3 | 2:MB:324:LYS:HD3 | 1.83 | 0.57 |
| 2:MD:212:PHE:HZ | 1:ME:326:LYS:HD3 | 0.59 | 0.57 |
| 1:ME:141:VAL:HG11 | 1:ME:172:TYR:CD1 | 2.38 | 0.57 |
| 7:5A:1105:TYR:CB | 7:5A:1165:PRO:HA | 2.34 | 0.57 |
| 7:5A:1408:GLU:HA | 7:5A:1408:GLU:OE1 | 2.03 | 0.57 |
| 7:5A:1487:ASN:CB | 7:5A:1568:LYS:CD | 2.80 | 0.57 |
| 7:5A:1544:ILE:C | 7:5A:1570:ALA:CB | 2.76 | 0.57 |
| 7:5B:1487:ASN:CB | 7:5B:1568:LYS:CD | 2.80 | 0.57 |
| 7:5B:1541:ILE:HG23 | 7:5B:1574:ILE:HD11 | 1.85 | 0.57 |
| 7:5B:1543:LEU:C | 7:5B:1573:ARG:HD3 | 2.29 | 0.57 |
| 7:5C:811:GLN:O | 7:5C:814:LYS:N | 2.38 | 0.57 |
| 7:5C:1105:TYR:CB | 7:5C:1165:PRO:HA | 2.34 | 0.57 |
| 7:5C:1347:LEU:HD13 | 7:5C:1347:LEU:N | 2.19 | 0.57 |
| 7:5C:1408:GLU:HA | 7:5C:1408:GLU:OE1 | 2.03 | 0.57 |
| 7:5C:1543:LEU:O | 7:5C:1573:ARG:HD3 | 2.04 | 0.57 |
| 2:BD:372:THR:HA | 2:BD:422:TYR:HE2 | 1.69 | 0.57 |
| 1:DC:402:ARG:CD | 7:5A:777:ALA:HB2 | 2.32 | 0.57 |
| 1:FC:422:ARG:CZ | 7:5A:1170:THR:CA | 2.81 | 0.57 |
| 2:FF:401:GLU:N | 7:5B:1293:VAL:HG21 | 2.20 | 0.57 |
| 2:HD:67:ASP:OD1 | 2:HD:68:LEU:N | 2.37 | 0.57 |
| 2:HF:222:TYR:O | 2:HF:226:ASN:ND2 | 2.28 | 0.57 |
| 2:IB:397:TRP:CD2 | 1:IC:256:GLN:O | 2.30 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:IB:424:GLN:HE22 | 7:5C:1413:GLN:NE2 | 0.40 | 0.57 |
| 1:JA:404:PHE:HE2 | 2:JB:345:ILE:HD12 | 1.70 | 0.57 |
| 2:JB:179:VAL:HG21 | 1:JC:258:ASN:C | 2.28 | 0.57 |
| 2:KB:179:VAL:HG21 | 1:KC:258:ASN:C | 2.28 | 0.57 |
| 2:KB:309:ARG:NH2 | 2:KB:426:GLN:O | 2.32 | 0.57 |
| 2:KF:54:ALA:CA | 2:LF:285:THR:CG2 | 2.80 | 0.57 |
| 2:KF:55:THR:OG1 | 2:LF:284:LEU:O | 2.23 | 0.57 |
| 1:LA:60:LYS:HD3 | 1:MA:283:HIS:CA | 2.34 | 0.57 |
| 2:LF:221:THR:CG2 | 6:4D:220:GLY:N | 2.68 | 0.57 |
| 1:MC:141:VAL:HG11 | 1:MC:172:TYR:CD1 | 2.38 | 0.57 |
| 2:MD:220:PRO:HD2 | 1:ME:326:LYS:HE2 | 1.86 | 0.57 |
| 6:4A:223:PHE:HD2 | 6:4A:223:PHE:N | 2.02 | 0.57 |
| 6:4B:223:PHE:HD2 | 6:4B:223:PHE:N | 2.02 | 0.57 |
| 6:4C:139:ASP:O | 6:4C:142:SER:OG | 2.20 | 0.57 |
| 7:5A:811:GLN:O | 7:5A:814:LYS:N | 2.38 | 0.57 |
| 7:5A:1262:GLU:O | 7:5A:1266:TYR:CD2 | 2.57 | 0.57 |
| 7:5A:1347:LEU:HD13 | 7:5A:1347:LEU:N | 2.19 | 0.57 |
| 7:5B:811:GLN:O | 7:5B:814:LYS:N | 2.38 | 0.57 |
| 7:5B:1105:TYR:CB | 7:5B:1165:PRO:HA | 2.34 | 0.57 |
| 7:5B:1262:GLU:O | 7:5B:1266:TYR:CD2 | 2.57 | 0.57 |
| 7:5C:1262:GLU:O | 7:5C:1266:TYR:CD2 | 2.58 | 0.57 |
| 7:5C:1487:ASN:CB | 7:5C:1568:LYS:CD | 2.80 | 0.57 |
| 1:BE:404:PHE:HE2 | 2:BF:345:ILE:HD12 | 1.67 | 0.57 |
| 2:BF:67:ASP:OD1 | 2:BF:68:LEU:N | 2.37 | 0.57 |
| 2:CD:100:ASN:HB2 | 1:CE:257:THR:HG21 | 1.86 | 0.57 |
| 2:ED:222:TYR:O | 2:ED:226:ASN:ND2 | 2.28 | 0.57 |
| 1:FC:419:SER:HB2 | 7:5A:1256:ARG:CZ | 2.21 | 0.57 |
| 1:HA:282:TYR:CE1 | 10:8S:15:UNK:HA | 2.39 | 0.57 |
| 2:HB:179:VAL:HG21 | 1:HC:258:ASN:C | 2.28 | 0.57 |
| 1:IE:105:ARG:NH1 | 2:IF:251:ARG:HD3 | 2.19 | 0.57 |
| 2:KB:87:PRO:CG | 2:LB:282:ARG:HG2 | 2.18 | 0.57 |
| 2:KF:273:LEU:N | 6:4D:268:LEU:CD2 | 2.67 | 0.57 |
| 1:LC:221:ARG:NH2 | 2:LD:321:MET:O | 2.35 | 0.57 |
| 2:MD:106:TYR:HE1 | 3:1B:32:ARG:NH1 | 1.92 | 0.57 |
| 2:MD:397:TRP:CD2 | 1:ME:256:GLN:O | 2.28 | 0.57 |
| 2:MF:309:ARG:NH2 | 2:MF:426:GLN:O | 2.32 | 0.57 |
| 6:4D:223:PHE:N | 6:4D:223:PHE:HD2 | 2.02 | 0.57 |
| 6:4D:282:ASN:OD1 | 6:4D:282:ASN:N | 2.34 | 0.57 |
| 7:5A:1541:ILE:HG23 | 7:5A:1574:ILE:HD11 | 1.85 | 0.57 |
| 7:5A:1543:LEU:C | 7:5A:1573:ARG:HD3 | 2.29 | 0.57 |
| 7:5B:1408:GLU:HA | 7:5B:1408:GLU:OE1 | 2.03 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5B:1544:ILE:C | 7:5B:1570:ALA:CB | 2.76 | 0.57 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:HG | 1.87 | 0.57 |
| 2:BB:372:THR:HA | 2:BB:422:TYR:HE2 | 1.69 | 0.57 |
| 2:CF:372:THR:HA | 2:CF:422:TYR:HE2 | 1.69 | 0.57 |
| 2:ED:125:GLU:HA | 7:5A:903:PHE:CE1 | 2.29 | 0.57 |
| 2:FB:222:TYR:O | 2:FB:226:ASN:ND2 | 2.28 | 0.57 |
| 1:HA:278:ALA:HB1 | 10:8S:18:UNK:C | 2.15 | 0.57 |
| 1:HA:404:PHE:HE2 | 2:HB:345:ILE:HD12 | 1.70 | 0.57 |
| 1:IC:402:ARG:CZ | 7:5A:1417:GLN:CB | 2.83 | 0.57 |
| 2:KB:124:ALA:O | 4:2C:37:GLY:O | 2.22 | 0.57 |
| 2:KF:273:LEU:HA | 6:4D:268:LEU:CG | 2.27 | 0.57 |
| 1:LC:60:LYS:NZ | 1:MC:283:HIS:CE1 | 2.73 | 0.57 |
| 2:LF:274:THR:H | 6:4D:228:LEU:HD21 | 1.70 | 0.57 |
| 2:LF:419:VAL:HB | 4:2B:168:LEU:HD11 | 1.87 | 0.57 |
| 1:MA:141:VAL:HG11 | 1:MA:172:TYR:CD1 | 2.38 | 0.57 |
| 2:MB:111:GLU:OE2 | 3:1A:62:SER:HB2 | 2.04 | 0.57 |
| 2:MB:309:ARG:NH2 | 2:MB:426:GLN:O | 2.32 | 0.57 |
| 1:ME:279:GLU:CD | 6:4B:106:ALA:HB3 | 2.30 | 0.57 |
| 4:2A:15:GLU:O | 4:2A:19:MET:N | 2.38 | 0.57 |
| 4:2C:15:GLU:O | 4:2C:19:MET:N | 2.38 | 0.57 |
| 6:4A:287:ASP:N | 6:4A:287:ASP:OD2 | 2.30 | 0.57 |
| 6:4C:132:LYS:HE2 | 6:4C:132:LYS:C | 2.29 | 0.57 |
| 7:5C:1541:ILE:HG23 | 7:5C:1574:ILE:HD11 | 1.85 | 0.57 |
| 9:7A:7:LEU:CD2 | 9:7B:27:GLY:O | 2.37 | 0.57 |
| 1:AA:178:SER:OG | 2:AB:347:ASN:HB3 | 2.05 | 0.57 |
| 2:AF:281:TYR:CE1 | 1:MC:88:HIS:HA | 2.39 | 0.57 |
| 2:BB:87:PRO:CD | 2:CB:281:TYR:CZ | 2.85 | 0.57 |
| 2:CB:139:LEU:HD22 | 2:CB:170:VAL:HG12 | 1.87 | 0.57 |
| 2:DB:139:LEU:HD22 | 2:DB:170:VAL:HG12 | 1.87 | 0.57 |
| 2:DD:139:LEU:HD22 | 2:DD:170:VAL:HG12 | 1.87 | 0.57 |
| 2:DF:139:LEU:HD22 | 2:DF:170:VAL:HG12 | 1.87 | 0.57 |
| 2:ED:55:THR:N | 2:FD:283:ALA:HB2 | 2.19 | 0.57 |
| 1:FA:401:LYS:CE | 2:FB:344:TRP:CZ3 | 2.74 | 0.57 |
| 2:HB:67:ASP:OD1 | 2:HB:68:LEU:N | 2.37 | 0.57 |
| 1:IA:178:SER:OG | 2:IB:347:ASN:HB3 | 2.05 | 0.57 |
| 2:ID:178:THR:HA | 1:IE:352:LYS:HD3 | 1.86 | 0.57 |
| 2:IF:372:THR:HA | 2:IF:422:TYR:HE2 | 1.69 | 0.57 |
| 1:JA:89:PRO:HD2 | 1:KA:283:HIS:CG | 2.40 | 0.57 |
| 1:JA:178:SER:OG | 2:JB:347:ASN:HB3 | 2.05 | 0.57 |
| 1:KA:87:PHE:O | 1:LA:284:GLU:HB3 | 2.05 | 0.57 |
| 2:KF:67:ASP:OD1 | 2:KF:68:LEU:N | 2.37 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KF:77:ARG:HG3 | 2:LF:281:TYR:CE1 | 2.39 | 0.57 |
| 2:KF:372:THR:HA | 2:KF:422:TYR:HE2 | 1.69 | 0.57 |
| 1:LE:221:ARG:NH2 | 2:LF:321:MET:O | 2.35 | 0.57 |
| 2:LF:416:ASN:HA | 4:2B:168:LEU:CD1 | 2.32 | 0.57 |
| 2:MD:309:ARG:NH2 | 2:MD:426:GLN:O | 2.32 | 0.57 |
| 4:2B:15:GLU:O | 4:2B:19:MET:N | 2.38 | 0.57 |
| 4:2C:172:ASP:CB | 4:2C:173:PRO:HD2 | 2.09 | 0.57 |
| 6:4A:132:LYS:HE2 | 6:4A:132:LYS:C | 2.29 | 0.57 |
| 6:4A:248:VAL:HG13 | 6:4A:288:TYR:CD2 | 2.40 | 0.57 |
| 6:4A:282:ASN:N | 6:4A:282:ASN:OD1 | 2.35 | 0.57 |
| 6:4C:248:VAL:HG13 | 6:4C:288:TYR:CD2 | 2.40 | 0.57 |
| 6:4D:99:ARG:CZ | 6:4D:99:ARG:HB2 | 2.35 | 0.57 |
| 6:4D:167:ARG:CZ | 6:4D:167:ARG:HB2 | 2.35 | 0.57 |
| 7:5B:1347:LEU:HD13 | 7:5B:1347:LEU:N | 2.19 | 0.57 |
| 7:5B:1412:LYS:HE2 | 7:5B:1416:LYS:HB2 | 1.85 | 0.57 |
| 7:5B:1487:ASN:CA | 7:5B:1568:LYS:HE2 | 2.24 | 0.57 |
| 7:5B:1521:PHE:CE2 | 7:5B:1567:PHE:CG | 2.58 | 0.57 |
| 9:7A:10:TYR:CE2 | 9:7B:26:LEU:HG | 2.40 | 0.57 |
| 10:8U:36:UNK:O | 10:8U:37:UNK:CB | 2.53 | 0.57 |
| 1:AA:404:PHE:HE2 | 2:AB:345:ILE:HD12 | 1.70 | 0.57 |
| 1:AE:60:LYS:HZ2 | 1:BE:283:HIS:CE1 | 2.23 | 0.57 |
| 2:AF:321:MET:C | 6:4A:156:PHE:HD2 | 2.12 | 0.57 |
| 2:BB:222:TYR:O | 2:BB:226:ASN:ND2 | 2.28 | 0.57 |
| 1:BC:401:LYS:HE3 | 2:BD:344:TRP:CZ3 | 2.39 | 0.57 |
| 2:CD:139:LEU:HD22 | 2:CD:170:VAL:HG12 | 1.87 | 0.57 |
| 1:DC:62:VAL:CG2 | 1:EC:283:HIS:O | 2.49 | 0.57 |
| 2:DF:372:THR:HA | 2:DF:422:TYR:HE2 | 1.69 | 0.57 |
| 2:EB:177:ASP:C | 1:EC:352:LYS:HA | 2.30 | 0.57 |
| 1:EC:224:TYR:HE2 | 2:ED:246:LEU:HD11 | 1.69 | 0.57 |
| 2:EF:139:LEU:HD22 | 2:EF:170:VAL:HG12 | 1.87 | 0.57 |
| 1:GA:404:PHE:HE2 | 2:GB:345:ILE:HD12 | 1.70 | 0.57 |
| 2:IB:424:GLN:HE22 | 7:5C:1413:GLN:HE22 | 0.57 | 0.57 |
| 1:JA:124:LYS:CD | 1:KA:284:GLU:OE1 | 2.53 | 0.57 |
| 2:JB:220:PRO:CD | 1:JC:326:LYS:HE2 | 2.35 | 0.57 |
| 2:JD:85:PHE:HB3 | 2:KD:281:TYR:OH | 2.04 | 0.57 |
| 1:JE:89:PRO:HD2 | 1:KE:280:LYS:HA | 1.85 | 0.57 |
| 1:KA:178:SER:OG | 2:KB:347:ASN:HB3 | 2.05 | 0.57 |
| 1:KC:88:HIS:HA | 1:LC:284:GLU:HA | 1.85 | 0.57 |
| 2:KD:276:ARG:NH2 | 6:4B:265:TYR:HB2 | 2.20 | 0.57 |
| 2:LB:177:ASP:HA | 1:LC:353:VAL:HG12 | 1.87 | 0.57 |
| 2:LD:67:ASP:OD1 | 2:LD:68:LEU:N | 2.37 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1487:ASN:ND2 | 7:5C:1568:LYS:HG2 | 2.18 | 0.57 |
| 7:5C:1543:LEU:C | 7:5C:1573:ARG:HD3 | 2.29 | 0.57 |
| 9:7C:10:TYR:CE2 | 9:7D:26:LEU:HG | 2.40 | 0.57 |
| 1:AE:386:GLU:CD | 3:1A:76:ARG:NH2 | 2.63 | 0.57 |
| 2:BD:67:ASP:OD1 | 2:BD:68:LEU:N | 2.37 | 0.57 |
| 2:BF:139:LEU:HD22 | 2:BF:170:VAL:HG12 | 1.87 | 0.57 |
| 1:CA:60:LYS:HZ3 | 1:DA:283:HIS:CD2 | 2.18 | 0.57 |
| 1:CE:401:LYS:CE | 2:CF:344:TRP:CZ3 | 2.74 | 0.57 |
| 2:CF:139:LEU:HD22 | 2:CF:170:VAL:HG12 | 1.87 | 0.57 |
| 1:EA:404:PHE:HE2 | 2:EB:345:ILE:HD12 | 1.69 | 0.57 |
| 2:EB:222:TYR:O | 2:EB:226:ASN:ND2 | 2.27 | 0.57 |
| 1:EC:62:VAL:CG2 | 1:FC:283:HIS:O | 2.52 | 0.57 |
| 2:ED:139:LEU:HD22 | 2:ED:170:VAL:HG12 | 1.87 | 0.57 |
| 2:FD:222:TYR:O | 2:FD:226:ASN:ND2 | 2.27 | 0.57 |
| 2:FF:139:LEU:HD22 | 2:FF:170:VAL:HG12 | 1.87 | 0.57 |
| 2:GD:178:THR:HA | 1:GE:352:LYS:HD3 | 1.86 | 0.57 |
| 1:GE:56:THR:CA | 1:HE:285:GLN:HB3 | 2.34 | 0.57 |
| 2:IB:309:ARG:NH2 | 2:IB:426:GLN:O | 2.32 | 0.57 |
| 2:KB:228:LEU:HG | 6:4A:267:ILE:HD12 | 1.87 | 0.57 |
| 1:KC:79:ARG:HB3 | 1:LC:280:LYS:NZ | 0.40 | 0.57 |
| 2:KD:372:THR:HA | 2:KD:422:TYR:HE2 | 1.69 | 0.57 |
| 2:LF:139:LEU:HD22 | 2:LF:170:VAL:HG12 | 1.87 | 0.57 |
| 4:2A:172:ASP:CB | 4:2A:173:PRO:HD2 | 2.08 | 0.57 |
| 5:3B:231:THR:CA | 5:3B:332:MET:HA | 2.34 | 0.57 |
| 6:4B:99:ARG:CZ | 6:4B:99:ARG:HB2 | 2.35 | 0.57 |
| 6:4B:248:VAL:HG13 | 6:4B:288:TYR:CD2 | 2.40 | 0.57 |
| 6:4D:248:VAL:HG13 | 6:4D:288:TYR:CD2 | 2.40 | 0.57 |
| 7:5A:1573:ARG:O | 7:5A:1577:LYS:CA | 2.53 | 0.57 |
| 7:5B:1246:LEU:CA | 9:7D:12:GLU:CD | 2.77 | 0.57 |
| 2:AB:139:LEU:HD22 | 2:AB:170:VAL:HG12 | 1.87 | 0.57 |
| 2:AD:177:ASP:HA | 1:AE:353:VAL:HG12 | 1.87 | 0.57 |
| 1:AE:280:LYS:NZ | 2:MB:86:ARG:HH21 | 2.03 | 0.57 |
| 2:BD:176:SER:OG | 1:BE:349:THR:OG1 | 2.23 | 0.57 |
| 2:CD:86:ARG:HB2 | 2:DD:281:TYR:CE1 | 2.31 | 0.57 |
| 2:CD:372:THR:HA | 2:CD:422:TYR:HE2 | 1.69 | 0.57 |
| 2:DB:86:ARG:HA | 2:EB:281:TYR:CD1 | 2.30 | 0.57 |
| 2:ED:180:VAL:HG12 | 1:EE:258:ASN:OD1 | 2.05 | 0.57 |
| 1:FA:141:VAL:HG11 | 1:FA:172:TYR:CD1 | 2.38 | 0.57 |
| 1:FA:401:LYS:HE3 | 2:FB:344:TRP:CZ3 | 2.40 | 0.57 |
| 2:FD:139:LEU:HD22 | 2:FD:170:VAL:HG12 | 1.87 | 0.57 |
| 2:FF:372:THR:HA | 2:FF:422:TYR:HE2 | 1.69 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GA:178:SER:OG | 2:GB:347:ASN:HB3 | 2.05 | 0.57 |
| 2:GB:139:LEU:HD22 | 2:GB:170:VAL:HG12 | 1.87 | 0.57 |
| 2:GB:397:TRP:CD2 | 1:GC:256:GLN:O | 2.30 | 0.57 |
| 2:HB:139:LEU:HD22 | 2:HB:170:VAL:HG12 | 1.87 | 0.57 |
| 2:HD:139:LEU:HD22 | 2:HD:170:VAL:HG12 | 1.87 | 0.57 |
| 2:HF:139:LEU:HD22 | 2:HF:170:VAL:HG12 | 1.87 | 0.57 |
| 1:IA:279:GLU:CA | 10:8V:22:UNK:CB | 2.82 | 0.57 |
| 2:ID:139:LEU:HD22 | 2:ID:170:VAL:HG12 | 1.87 | 0.57 |
| 2:ID:372:THR:HA | 2:ID:422:TYR:HE2 | 1.69 | 0.57 |
| 2:JB:372:THR:HA | 2:JB:422:TYR:HE2 | 1.69 | 0.57 |
| 2:JD:397:TRP:CD2 | 1:JE:256:GLN:O | 2.31 | 0.57 |
| 2:KD:67:ASP:OD1 | 2:KD:68:LEU:N | 2.36 | 0.57 |
| 2:LD:391:ARG:O | 1:LE:262:TYR:OH | 2.23 | 0.57 |
| 6:4B:132:LYS:HE2 | 6:4B:132:LYS:C | 2.29 | 0.57 |
| 6:4B:167:ARG:CZ | 6:4B:167:ARG:HB2 | 2.35 | 0.57 |
| 6:4B:282:ASN:N | 6:4B:282:ASN:OD1 | 2.35 | 0.57 |
| 6:4D:132:LYS:HE2 | 6:4D:132:LYS:C | 2.29 | 0.57 |
| 7:5B:1152:GLU:CD | 8:6B:66:ARG:CZ | 2.78 | 0.57 |
| 7:5C:1436:ARG:HB3 | 7:5C:1436:ARG:NH1 | 2.19 | 0.57 |
| 7:5C:1573:ARG:O | 7:5C:1577:LYS:CA | 2.53 | 0.57 |
| 2:AD:177:ASP:OD1 | 1:AE:353:VAL:HG12 | 1.84 | 0.56 |
| 2:CF:222:TYR:O | 2:CF:226:ASN:ND2 | 2.28 | 0.56 |
| 2:EB:220:PRO:HD2 | 1:EC:326:LYS:CG | 2.31 | 0.56 |
| 1:FA:89:PRO:CG | 1:GA:280:LYS:CG | 2.61 | 0.56 |
| 2:FB:180:VAL:HG12 | 1:FC:258:ASN:OD1 | 2.04 | 0.56 |
| 2:GD:177:ASP:HA | 1:GE:353:VAL:HG12 | 1.87 | 0.56 |
| 2:GF:58:ARG:HD3 | 2:HF:281:TYR:HA | 1.85 | 0.56 |
| 1:HA:278:ALA:HB3 | 10:8S:22:UNK:CA | 2.35 | 0.56 |
| 2:IB:179:VAL:HG21 | 1:IC:258:ASN:C | 2.27 | 0.56 |
| 2:IB:372:THR:HA | 2:IB:422:TYR:HE2 | 1.69 | 0.56 |
| 2:IF:139:LEU:HD22 | 2:IF:170:VAL:HG12 | 1.87 | 0.56 |
| 2:JD:139:LEU:HD22 | 2:JD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:KD:177:ASP:HA | 1:KE:353:VAL:HG12 | 1.87 | 0.56 |
| 2:KF:55:THR:H | 2:LF:285:THR:HG22 | 1.70 | 0.56 |
| 2:KF:276:ARG:NH2 | 6:4D:265:TYR:HB2 | 2.20 | 0.56 |
| 2:LB:397:TRP:CD2 | 1:LC:256:GLN:O | 2.31 | 0.56 |
| 1:LC:141:VAL:HG11 | 1:LC:172:TYR:CD1 | 2.38 | 0.56 |
| 2:LD:139:LEU:HD22 | 2:LD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:LD:309:ARG:NH2 | 2:LD:426:GLN:O | 2.32 | 0.56 |
| 1:LE:141:VAL:HG11 | 1:LE:172:TYR:CD1 | 2.38 | 0.56 |
| 2:MB:372:THR:HA | 2:MB:422:TYR:HE2 | 1.69 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:MF:139:LEU:HD22 | 2:MF:170:VAL:HG12 | 1.87 | 0.56 |
| 5:3A:231:THR:CA | 5:3A:332:MET:HA | 2.34 | 0.56 |
| 6:4A:99:ARG:CZ | 6:4A:99:ARG:HB2 | 2.35 | 0.56 |
| 6:4B:156:PHE:O | 6:4B:156:PHE:HD1 | 1.88 | 0.56 |
| 6:4C:156:PHE:O | 6:4C:156:PHE:HD1 | 1.88 | 0.56 |
| 7:5A:1487:ASN:ND2 | 7:5A:1568:LYS:HG2 | 2.18 | 0.56 |
| 7:5A:1490:LYS:HB3 | 7:5A:1495:PHE:HB2 | 1.87 | 0.56 |
| 7:5B:1490:LYS:HB3 | 7:5B:1495:PHE:HB2 | 1.87 | 0.56 |
| 7:5B:1573:ARG:O | 7:5B:1577:LYS:CA | 2.53 | 0.56 |
| 7:5C:1412:LYS:HE2 | 7:5C:1416:LYS:HB2 | 1.85 | 0.56 |
| 9:7E:14:SER:C | 9:7F:35:ILE:HD11 | 2.30 | 0.56 |
| 10:8I:36:UNK:O | 10:8I:37:UNK:CB | 2.53 | 0.56 |
| 2:AD:223:GLY:O | 6:4C:131:VAL:CA | 2.41 | 0.56 |
| 2:BB:397:TRP:CD2 | 1:BC:256:GLN:O | 2.33 | 0.56 |
| 2:BD:139:LEU:HD22 | 2:BD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:BD:222:TYR:O | 2:BD:226:ASN:ND2 | 2.27 | 0.56 |
| 1:BE:178:SER:OG | 2:BF:347:ASN:HB3 | 2.04 | 0.56 |
| 2:CB:372:THR:HA | 2:CB:422:TYR:HE2 | 1.69 | 0.56 |
| 1:CE:404:PHE:HE2 | 2:CF:345:ILE:HD12 | 1.70 | 0.56 |
| 2:DD:372:THR:HA | 2:DD:422:TYR:HE2 | 1.69 | 0.56 |
| 1:EA:71:GLU:CD | 2:EB:247:ASN:ND2 | 2.63 | 0.56 |
| 2:EF:55:THR:CG2 | 2:FF:284:LEU:N | 2.66 | 0.56 |
| 1:FA:222:PRO:HG2 | 2:FB:324:LYS:CD | 2.34 | 0.56 |
| 2:FB:139:LEU:HD22 | 2:FB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:GB:179:VAL:HG21 | 1:GC:258:ASN:C | 2.28 | 0.56 |
| 2:GD:139:LEU:HD22 | 2:GD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:GF:67:ASP:OD1 | 2:GF:68:LEU:N | 2.37 | 0.56 |
| 2:GF:139:LEU:HD22 | 2:GF:170:VAL:HG12 | 1.87 | 0.56 |
| 2:HD:178:THR:HA | 1:HE:352:LYS:HD3 | 1.86 | 0.56 |
| 1:IA:282:TYR:CB | 10:8V:15:UNK:CB | 2.82 | 0.56 |
| 2:IB:139:LEU:HD22 | 2:IB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:IB:220:PRO:CD | 1:IC:326:LYS:HE2 | 2.35 | 0.56 |
| 1:IE:402:ARG:HH21 | 7:5B:1417:GLN:HG3 | 1.52 | 0.56 |
| 2:JB:139:LEU:HD22 | 2:JB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:JF:139:LEU:HD22 | 2:JF:170:VAL:HG12 | 1.87 | 0.56 |
| 2:KB:372:THR:HA | 2:KB:422:TYR:HE2 | 1.69 | 0.56 |
| 2:KD:125:GLU:HB2 | 2:LD:336:LYS:CE | 2.33 | 0.56 |
| 2:KD:178:THR:HA | 1:KE:352:LYS:HD3 | 1.86 | 0.56 |
| 2:LB:67:ASP:OD1 | 2:LB:68:LEU:N | 2.37 | 0.56 |
| 2:LB:139:LEU:HD22 | 2:LB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:MB:179:VAL:CG2 | 1:MC:258:ASN:CA | 2.83 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:MC:222:PRO:CD | 2:MD:324:LYS:HD3 | 2.35 | 0.56 |
| 2:MD:139:LEU:HD22 | 2:MD:170:VAL:HG12 | 1.87 | 0.56 |
| 1:ME:100:ALA:HB1 | 2:MF:252:LYS:CA | 2.35 | 0.56 |
| 6:4A:156:PHE:HD1 | 6:4A:156:PHE:O | 1.88 | 0.56 |
| 6:4D:156:PHE:O | 6:4D:156:PHE:HD1 | 1.88 | 0.56 |
| 7:5A:1412:LYS:HE2 | 7:5A:1416:LYS:HB2 | 1.85 | 0.56 |
| 7:5A:1436:ARG:HB3 | 7:5A:1436:ARG:NH1 | 2.19 | 0.56 |
| 7:5A:1487:ASN:CA | 7:5A:1568:LYS:HE2 | 2.24 | 0.56 |
| 7:5C:1490:LYS:HB3 | 7:5C:1495:PHE:HB2 | 1.87 | 0.56 |
| 8:6A:4:LYS:HD3 | 8:6A:6:TYR:OH | 2.05 | 0.56 |
| 10:8C:36:UNK:O | 10:8C:37:UNK:CB | 2.53 | 0.56 |
| 10:8K:36:UNK:O | 10:8K:37:UNK:CB | 2.53 | 0.56 |
| 10:8L:36:UNK:O | 10:8L:37:UNK:CB | 2.53 | 0.56 |
| 2:AD:139:LEU:HD22 | 2:AD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:AF:55:THR:CG2 | 2:BF:283:ALA:CB | 2.78 | 0.56 |
| 2:AF:139:LEU:HD22 | 2:AF:170:VAL:HG12 | 1.87 | 0.56 |
| 1:BA:105:ARG:NH1 | 2:BB:251:ARG:HD3 | 2.20 | 0.56 |
| 2:BB:67:ASP:OD1 | 2:BB:68:LEU:N | 2.37 | 0.56 |
| 2:BB:139:LEU:HD22 | 2:BB:170:VAL:HG12 | 1.87 | 0.56 |
| 1:BC:105:ARG:NH1 | 2:BD:251:ARG:HD3 | 2.20 | 0.56 |
| 2:BD:177:ASP:C | 1:BE:352:LYS:HA | 2.30 | 0.56 |
| 1:BE:105:ARG:NH1 | 2:BF:251:ARG:HD3 | 2.20 | 0.56 |
| 1:CC:404:PHE:HE2 | 2:CD:345:ILE:HD12 | 1.70 | 0.56 |
| 1:CE:60:LYS:HD3 | 1:DE:283:HIS:HD2 | 1.70 | 0.56 |
| 2:DB:372:THR:HA | 2:DB:422:TYR:HE2 | 1.69 | 0.56 |
| 2:EB:139:LEU:HD22 | 2:EB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:EB:222:TYR:CD2 | 1:EC:247:ALA:HB1 | 2.40 | 0.56 |
| 1:EC:402:ARG:CD | 7:5A:824:ARG:HH22 | 2.17 | 0.56 |
| 2:ED:83:GLN:O | 2:FD:281:TYR:OH | 2.23 | 0.56 |
| 1:FA:71:GLU:CD | 2:FB:247:ASN:HD22 | 2.12 | 0.56 |
| 1:FA:398:MET:SD | 2:FB:345:ILE:CG1 | 2.80 | 0.56 |
| 2:FD:54:ALA:HB1 | 2:GD:281:TYR:O | 2.06 | 0.56 |
| 2:FD:372:THR:HA | 2:FD:422:TYR:HE2 | 1.69 | 0.56 |
| 1:GC:60:LYS:NZ | 1:HC:283:HIS:CG | 2.64 | 0.56 |
| 1:HA:178:SER:OG | 2:HB:347:ASN:HB3 | 2.05 | 0.56 |
| 2:HB:222:TYR:CD2 | 1:HC:247:ALA:HB1 | 2.40 | 0.56 |
| 2:HB:309:ARG:NH2 | 2:HB:426:GLN:O | 2.32 | 0.56 |
| 2:HD:177:ASP:HA | 1:HE:353:VAL:HG12 | 1.87 | 0.56 |
| 2:ID:177:ASP:HA | 1:IE:353:VAL:HG12 | 1.87 | 0.56 |
| 1:IE:402:ARG:CZ | 7:5B:1417:GLN:CG | 2.71 | 0.56 |
| 2:JD:177:ASP:HA | 1:JE:353:VAL:HG12 | 1.87 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:JD:178:THR:HA | 1:JE:352:LYS:HD3 | 1.86 | 0.56 |
| 2:JD:222:TYR:O | 2:JD:226:ASN:ND2 | 2.28 | 0.56 |
| 2:JD:372:THR:HA | 2:JD:422:TYR:HE2 | 1.69 | 0.56 |
| 1:JE:105:ARG:NH1 | 2:JF:251:ARG:HD3 | 2.19 | 0.56 |
| 2:KB:67:ASP:OD1 | 2:KB:68:LEU:N | 2.37 | 0.56 |
| 2:KB:77:ARG:HG3 | 2:LB:281:TYR:CE1 | 2.38 | 0.56 |
| 2:KB:139:LEU:HD22 | 2:KB:170:VAL:HG12 | 1.87 | 0.56 |
| 1:KC:85:GLN:CG | 1:LC:283:HIS:HD2 | 2.18 | 0.56 |
| 2:KD:139:LEU:HD22 | 2:KD:170:VAL:HG12 | 1.87 | 0.56 |
| 2:KF:139:LEU:HD22 | 2:KF:170:VAL:HG12 | 1.87 | 0.56 |
| 1:LA:141:VAL:HG11 | 1:LA:172:TYR:CD1 | 2.38 | 0.56 |
| 2:LB:179:VAL:HG22 | 1:LC:258:ASN:CG | 2.31 | 0.56 |
| 2:LD:220:PRO:O | 1:LE:324:VAL:CG1 | 2.54 | 0.56 |
| 2:LD:306:ARG:CZ | 4:2A:151:VAL:HG21 | 2.13 | 0.56 |
| 2:LF:309:ARG:NH2 | 2:LF:426:GLN:O | 2.32 | 0.56 |
| 2:MB:78:ALA:HB1 | 6:4A:178:HIS:CD2 | 2.40 | 0.56 |
| 2:MB:139:LEU:HD22 | 2:MB:170:VAL:HG12 | 1.87 | 0.56 |
| 2:MD:177:ASP:OD1 | 1:ME:353:VAL:HG12 | 1.87 | 0.56 |
| 2:MD:177:ASP:OD2 | 1:ME:248:LEU:HD23 | 2.05 | 0.56 |
| 4:2A:149:ILE:HG22 | 4:2A:149:ILE:O | 2.04 | 0.56 |
| 4:2A:164:ARG:HG3 | 4:2A:166:ILE:HG13 | 1.87 | 0.56 |
| 4:2C:149:ILE:HG22 | 4:2C:149:ILE:O | 2.04 | 0.56 |
| 5:3C:231:THR:CA | 5:3C:332:MET:HA | 2.34 | 0.56 |
| 6:4A:167:ARG:CZ | 6:4A:167:ARG:HB2 | 2.35 | 0.56 |
| 6:4C:99:ARG:CZ | 6:4C:99:ARG:HB2 | 2.35 | 0.56 |
| 7:5A:1266:TYR:HB3 | 9:7A:8:ARG:HH22 | 1.70 | 0.56 |
| 7:5B:841:VAL:CG2 | 8:6B:11:PRO:CA | 2.82 | 0.56 |
| 7:5B:1487:ASN:ND2 | 7:5B:1568:LYS:HG2 | 2.18 | 0.56 |
| 8:6B:4:LYS:HD3 | 8:6B:6:TYR:OH | 2.05 | 0.56 |
| 9:7A:42:LEU:CD1 | 9:7B:39:GLY:HA3 | 2.32 | 0.56 |
| 10:8F:36:UNK:O | 10:8F:37:UNK:CB | 2.53 | 0.56 |
| 10:8H:36:UNK:O | 10:8H:37:UNK:CB | 2.53 | 0.56 |
| 10:8J:36:UNK:O | 10:8J:37:UNK:CB | 2.53 | 0.56 |
| 10:8N:36:UNK:O | 10:8N:37:UNK:CB | 2.53 | 0.56 |
| 2:AB:54:ALA:HB1 | 2:BB:281:TYR:O | 2.06 | 0.56 |
| 2:AF:321:MET:HA | 6:4A:156:PHE:CE2 | 2.41 | 0.56 |
| 2:CB:177:ASP:C | 1:CC:352:LYS:HA | 2.31 | 0.56 |
| 2:CD:390:ARG:HD2 | 1:CE:439:THR:HG21 | 1.88 | 0.56 |
| 1:CE:282:TYR:HE2 | 10:8F:18:UNK:HA | 1.67 | 0.56 |
| 1:DE:401:LYS:HE3 | 2:DF:344:TRP:CZ3 | 2.41 | 0.56 |
| 1:EE:222:PRO:CG | 2:EF:324:LYS:CD | 2.82 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:FA:207:GLU:CD | 7:5C:915:PHE:HD2 | 2.14 | 0.56 |
| 1:GA:101:ASN:ND2 | 2:GB:252:LYS:HG3 | 2.10 | 0.56 |
| 2:GB:222:TYR:CD2 | 1:GC:247:ALA:HB1 | 2.40 | 0.56 |
| 2:GD:67:ASP:OD1 | 2:GD:68:LEU:N | 2.37 | 0.56 |
| 2:GF:372:THR:HA | 2:GF:422:TYR:HE2 | 1.69 | 0.56 |
| 2:IB:178:THR:HA | 1:IC:352:LYS:HD3 | 1.87 | 0.56 |
| 2:KD:397:TRP:CD2 | 1:KE:256:GLN:O | 2.31 | 0.56 |
| 1:KE:100:ALA:HB1 | 2:KF:252:LYS:HA | 1.88 | 0.56 |
| 2:LB:208:TYR:OH | 1:LC:325:PRO:HB2 | 2.06 | 0.56 |
| 2:LF:228:LEU:CD2 | 6:4D:225:PRO:HG2 | 2.35 | 0.56 |
| 1:ME:401:LYS:HE3 | 2:MF:344:TRP:CZ3 | 2.40 | 0.56 |
| 2:MF:372:THR:HA | 2:MF:422:TYR:HE2 | 1.69 | 0.56 |
| 4:2C:164:ARG:HG3 | 4:2C:166:ILE:HG13 | 1.88 | 0.56 |
| 5:3A:230:ILE:HG22 | 5:3A:332:MET:HG2 | 1.88 | 0.56 |
| 5:3C:230:ILE:HG22 | 5:3C:332:MET:HG2 | 1.88 | 0.56 |
| 7:5A:1272:ILE:HD11 | 9:7B:11:TYR:HD2 | 1.70 | 0.56 |
| 7:5A:1545:TYR:OH | 7:5A:1560:ILE:O | 2.22 | 0.56 |
| 7:5B:1471:ILE:HD12 | 7:5B:1471:ILE:N | 2.18 | 0.56 |
| 7:5B:1545:TYR:OH | 7:5B:1560:ILE:O | 2.22 | 0.56 |
| 8:6C:57:ARG:NH1 | 8:6C:195:LYS:O | 2.39 | 0.56 |
| 9:7E:10:TYR:OH | 9:7F:31:PRO:O | 2.21 | 0.56 |
| 10:8B:36:UNK:O | 10:8B:37:UNK:CB | 2.53 | 0.56 |
| 10:8G:36:UNK:O | 10:8G:37:UNK:CB | 2.53 | 0.56 |
| 10:8Z:36:UNK:O | 10:8Z:37:UNK:CB | 2.53 | 0.56 |
| 1:DA:101:ASN:ND2 | 2:DB:252:LYS:HG3 | 2.10 | 0.56 |
| 1:DC:100:ALA:HB1 | 2:DD:252:LYS:HA | 1.87 | 0.56 |
| 2:ED:372:THR:HA | 2:ED:422:TYR:HE2 | 1.69 | 0.56 |
| 2:EF:372:THR:HA | 2:EF:422:TYR:HE2 | 1.69 | 0.56 |
| 2:FB:372:THR:HA | 2:FB:422:TYR:HE2 | 1.69 | 0.56 |
| 1:FE:402:ARG:CZ | 7:5B:1259:TYR:HA | 2.36 | 0.56 |
| 1:FE:422:ARG:HE | 7:5B:1170:THR:CB | 2.08 | 0.56 |
| 2:FF:55:THR:H | 2:GF:283:ALA:CA | 2.19 | 0.56 |
| 2:GB:178:THR:HA | 1:GC:352:LYS:HD3 | 1.87 | 0.56 |
| 1:GE:100:ALA:HB1 | 2:GF:252:LYS:HA | 1.88 | 0.56 |
| 2:HB:220:PRO:CD | 1:HC:326:LYS:HE2 | 2.35 | 0.56 |
| 1:IC:278:ALA:CB | 10:8W:22:UNK:N | 2.64 | 0.56 |
| 1:IE:389:SER:HB2 | 5:3A:307:LYS:HB3 | 1.88 | 0.56 |
| 2:JD:220:PRO:CD | 1:JE:326:LYS:HE2 | 2.35 | 0.56 |
| 1:KA:404:PHE:HE2 | 2:KB:345:ILE:HD12 | 1.70 | 0.56 |
| 2:KB:222:TYR:CD2 | 1:KC:247:ALA:HB1 | 2.40 | 0.56 |
| 2:LB:222:TYR:HD2 | 1:LC:247:ALA:HB1 | 1.71 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LB:340:TYR:CD1 | 4:2C:147:PHE:HA | 2.37 | 0.56 |
| 2:LD:228:LEU:HD21 | 6:4B:225:PRO:HB2 | 1.86 | 0.56 |
| 2:LD:274:THR:HG23 | 6:4B:228:LEU:HD22 | 1.87 | 0.56 |
| 2:MB:177:ASP:OD1 | 1:MC:353:VAL:HG12 | 1.90 | 0.56 |
| 2:MD:372:THR:HA | 2:MD:422:TYR:HE2 | 1.69 | 0.56 |
| 4:2B:164:ARG:HG3 | 4:2B:166:ILE:HG13 | 1.88 | 0.56 |
| 5:3B:230:ILE:HG22 | 5:3B:332:MET:HG2 | 1.88 | 0.56 |
| 7:5B:1267:CYS:O | 7:5B:1270:ASP:N | 2.38 | 0.56 |
| 7:5B:1436:ARG:HB3 | 7:5B:1436:ARG:NH1 | 2.19 | 0.56 |
| 7:5B:1560:ILE:HG22 | 7:5B:1566:GLU:OE2 | 2.05 | 0.56 |
| 7:5C:1424:GLN:HE21 | 7:5C:1424:GLN:CA | 2.18 | 0.56 |
| 7:5C:1545:TYR:OH | 7:5C:1560:ILE:O | 2.22 | 0.56 |
| 8:6A:57:ARG:NH1 | 8:6A:195:LYS:O | 2.39 | 0.56 |
| 8:6B:57:ARG:NH1 | 8:6B:195:LYS:O | 2.39 | 0.56 |
| 8:6C:4:LYS:HD3 | 8:6C:6:TYR:OH | 2.05 | 0.56 |
| 9:7E:35:ILE:HG22 | 9:7F:43:LEU:HA | 1.86 | 0.56 |
| 10:8A:36:UNK:O | 10:8A:37:UNK:CB | 2.53 | 0.56 |
| 10:8M:36:UNK:O | 10:8M:37:UNK:CB | 2.53 | 0.56 |
| 2:AF:320:ARG:CD | 6:4A:153:ASP:O | 2.53 | 0.56 |
| 2:DD:394:PHE:CD1 | 1:DE:261:PRO:HA | 2.41 | 0.56 |
| 2:EB:372:THR:HA | 2:EB:422:TYR:HE2 | 1.69 | 0.56 |
| 2:ED:222:TYR:CD2 | 1:EE:247:ALA:HB1 | 2.41 | 0.56 |
| 1:EE:241:SER:OG | 1:EE:250:VAL:O | 2.23 | 0.56 |
| 1:FA:177:VAL:N | 7:5C:915:PHE:CZ | 2.73 | 0.56 |
| 2:HF:25:SER:HG | 2:HF:51:TYR:HH | 1.54 | 0.56 |
| 1:JE:141:VAL:HG11 | 1:JE:172:TYR:CD1 | 2.38 | 0.56 |
| 2:JF:372:THR:HA | 2:JF:422:TYR:HE2 | 1.69 | 0.56 |
| 2:KB:86:ARG:NH1 | 2:LB:283:ALA:HB2 | 2.09 | 0.56 |
| 2:KD:162:ARG:HG3 | 4:2A:36:THR:HB | 1.87 | 0.56 |
| 2:LD:179:VAL:HG22 | 1:LE:258:ASN:CG | 2.31 | 0.56 |
| 2:LD:340:TYR:CG | 4:2A:147:PHE:HB3 | 2.41 | 0.56 |
| 1:MC:222:PRO:HG3 | 2:MD:324:LYS:HD3 | 1.85 | 0.56 |
| 2:MD:111:GLU:OE2 | 3:1B:62:SER:HB2 | 2.06 | 0.56 |
| 4:2B:149:ILE:HG22 | 4:2B:149:ILE:O | 2.04 | 0.56 |
| 7:5A:1267:CYS:O | 7:5A:1270:ASP:N | 2.38 | 0.56 |
| 7:5C:1267:CYS:O | 7:5C:1270:ASP:N | 2.38 | 0.56 |
| 7:5C:1515:GLU:OE1 | 7:5C:1563:SER:HB2 | 2.06 | 0.56 |
| 10:8O:36:UNK:O | 10:8O:37:UNK:CB | 2.53 | 0.56 |
| 10:8Y:36:UNK:O | 10:8Y:37:UNK:CB | 2.53 | 0.56 |
| 2:AF:362:LYS:CG | 6:4A:146:ILE:HB | 2.25 | 0.56 |
| 1:CA:282:TYR:CE2 | 10:8D:18:UNK:CA | 2.86 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DD:176:SER:CB | 1:DE:349:THR:OG1 | 2.53 | 0.56 |
| 1:EC:404:PHE:CE2 | 2:ED:345:ILE:HD11 | 2.41 | 0.56 |
| 2:ED:54:ALA:CB | 2:FD:281:TYR:O | 2.54 | 0.56 |
| 2:EF:55:THR:H | 2:FF:283:ALA:HB2 | 1.71 | 0.56 |
| 1:FC:423:GLU:CG | 7:5A:1256:ARG:NH2 | 2.68 | 0.56 |
| 2:FF:54:ALA:CB | 2:GF:281:TYR:O | 2.53 | 0.56 |
| 2:GB:212:PHE:HZ | 1:GC:326:LYS:CE | 2.14 | 0.56 |
| 2:GB:220:PRO:CD | 1:GC:326:LYS:HE2 | 2.35 | 0.56 |
| 2:GB:372:THR:HA | 2:GB:422:TYR:HE2 | 1.69 | 0.56 |
| 1:IA:404:PHE:HE2 | 2:IB:345:ILE:HD12 | 1.70 | 0.56 |
| 2:IB:222:TYR:CD2 | 1:IC:247:ALA:HB1 | 2.40 | 0.56 |
| 1:JA:101:ASN:ND2 | 2:JB:252:LYS:HG3 | 2.10 | 0.56 |
| 1:JC:141:VAL:HG11 | 1:JC:172:TYR:CD1 | 2.38 | 0.56 |
| 1:KA:87:PHE:O | 1:LA:284:GLU:CA | 2.53 | 0.56 |
| 2:KD:339:SER:HB2 | 7:5A:1504:ARG:NH1 | 2.21 | 0.56 |
| 1:LA:60:LYS:CE | 6:4C:101:ARG:CZ | 2.83 | 0.56 |
| 2:LD:15:GLN:NE2 | 6:4B:217:ASN:OD1 | 2.39 | 0.56 |
| 2:LD:55:THR:HG1 | 2:MD:283:ALA:HA | 1.68 | 0.56 |
| 1:MA:404:PHE:CE2 | 2:MB:345:ILE:HD11 | 2.41 | 0.56 |
| 4:2B:172:ASP:CB | 4:2B:173:PRO:HD2 | 2.08 | 0.56 |
| 6:4C:167:ARG:CZ | 6:4C:167:ARG:HB2 | 2.35 | 0.56 |
| 7:5A:1246:LEU:HG | 9:7B:12:GLU:CG | 2.36 | 0.56 |
| 7:5A:1515:GLU:OE1 | 7:5A:1563:SER:HB2 | 2.06 | 0.56 |
| 7:5B:1530:ILE:HG22 | 7:5B:1574:ILE:HG21 | 1.87 | 0.56 |
| 2:AD:224:ASP:OD1 | 6:4C:132:LYS:CA | 2.52 | 0.56 |
| 2:CD:177:ASP:C | 1:CE:352:LYS:HA | 2.31 | 0.56 |
| 2:DB:60:VAL:HG21 | 2:EB:281:TYR:CE1 | 2.41 | 0.56 |
| 2:FD:222:TYR:CD2 | 1:FE:247:ALA:HB1 | 2.41 | 0.56 |
| 2:FD:402:GLY:O | 7:5A:1296:GLU:OE2 | 2.24 | 0.56 |
| 2:GD:372:THR:HA | 2:GD:422:TYR:HE2 | 1.69 | 0.56 |
| 2:KB:228:LEU:HD23 | 6:4A:267:ILE:HD12 | 1.85 | 0.56 |
| 2:KF:273:LEU:N | 6:4D:268:LEU:HD21 | 2.20 | 0.56 |
| 2:LD:178:THR:HA | 1:LE:352:LYS:HD3 | 1.86 | 0.56 |
| 1:MA:222:PRO:CD | 2:MB:324:LYS:HD3 | 2.36 | 0.56 |
| 1:ME:282:TYR:HD2 | 6:4B:104:ARG:NE | 2.03 | 0.56 |
| 7:5A:1424:GLN:HE21 | 7:5A:1424:GLN:CA | 2.18 | 0.56 |
| 7:5A:1471:ILE:HD12 | 7:5A:1471:ILE:N | 2.18 | 0.56 |
| 7:5A:1560:ILE:HG22 | 7:5A:1566:GLU:OE2 | 2.05 | 0.56 |
| 7:5B:827:GLU:CD | 7:5B:849:ARG:NH2 | 2.42 | 0.56 |
| 7:5B:1491:LEU:HD22 | 7:5B:1495:PHE:CD2 | 2.38 | 0.56 |
| 7:5C:1487:ASN:CA | 7:5C:1568:LYS:HE2 | 2.24 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5C:1533:GLU:CD | 7:5C:1604:ALA:CB | 2.78 | 0.56 |
| 10:8D:36:UNK:O | 10:8D:37:UNK:CB | 2.53 | 0.56 |
| 2:AD:276:ARG:HH12 | 6:4C:137:ASN:HB3 | 1.71 | 0.56 |
| 2:BF:222:TYR:O | 2:BF:226:ASN:ND2 | 2.28 | 0.56 |
| 1:FC:207:GLU:CD | 7:5A:915:PHE:HD2 | 2.14 | 0.56 |
| 1:FC:422:ARG:NE | 7:5A:1170:THR:CB | 2.61 | 0.56 |
| 1:IC:282:TYR:CZ | 10:8W:15:UNK:O | 2.56 | 0.56 |
| 1:JE:88:HIS:O | 1:KE:280:LYS:HE2 | 2.05 | 0.56 |
| 6:4A:239:LEU:C | 6:4A:241:LYS:H | 2.14 | 0.56 |
| 6:4B:239:LEU:C | 6:4B:241:LYS:H | 2.14 | 0.56 |
| 7:5A:827:GLU:CD | 7:5A:849:ARG:NH2 | 2.42 | 0.56 |
| 7:5A:1092:LYS:HA | 7:5A:1095:GLU:HG3 | 1.88 | 0.56 |
| 7:5A:1530:ILE:HG22 | 7:5A:1574:ILE:HG21 | 1.87 | 0.56 |
| 7:5C:1092:LYS:HA | 7:5C:1095:GLU:HG3 | 1.88 | 0.56 |
| 10:9A:36:UNK:O | 10:9A:37:UNK:CB | 2.53 | 0.56 |
| 2:AD:178:THR:HA | 1:AE:352:LYS:HD3 | 1.86 | 0.56 |
| 2:EB:208:TYR:CD2 | 1:EC:326:LYS:HB3 | 2.41 | 0.56 |
| 1:EE:426:ALA:CB | 7:5B:833:PHE:CG | 2.89 | 0.56 |
| 2:FD:177:ASP:C | 1:FE:352:LYS:HA | 2.31 | 0.56 |
| 1:GC:101:ASN:ND2 | 2:GD:252:LYS:HG3 | 2.09 | 0.56 |
| 2:ID:220:PRO:CD | 1:IE:326:LYS:HE2 | 2.35 | 0.56 |
| 1:IE:282:TYR:CD1 | 10:8X:15:UNK:HA | 2.41 | 0.56 |
| 1:JC:101:ASN:ND2 | 2:JD:252:LYS:HG3 | 2.09 | 0.56 |
| 2:JD:86:ARG:HH22 | 2:KD:280:GLN:HB3 | 1.56 | 0.56 |
| 2:KB:178:THR:HA | 1:KC:352:LYS:HD3 | 1.87 | 0.56 |
| 2:KB:228:LEU:CG | 6:4A:267:ILE:HD12 | 2.36 | 0.56 |
| 2:LB:212:PHE:HE2 | 1:LC:326:LYS:HB2 | 1.70 | 0.56 |
| 2:MB:179:VAL:HG21 | 1:MC:258:ASN:C | 2.28 | 0.56 |
| 6:4C:239:LEU:C | 6:4C:241:LYS:H | 2.14 | 0.56 |
| 6:4D:223:PHE:N | 6:4D:223:PHE:CD2 | 2.73 | 0.56 |
| 6:4D:239:LEU:C | 6:4D:241:LYS:H | 2.14 | 0.56 |
| 7:5A:1533:GLU:CD | 7:5A:1604:ALA:CB | 2.78 | 0.56 |
| 7:5B:1092:LYS:HA | 7:5B:1095:GLU:HG3 | 1.88 | 0.56 |
| 7:5B:1401:LYS:H | 7:5B:1401:LYS:CD | 2.03 | 0.56 |
| 7:5C:1560:ILE:HG22 | 7:5C:1566:GLU:OE2 | 2.05 | 0.56 |
| 10:8E:36:UNK:O | 10:8E:37:UNK:CB | 2.53 | 0.56 |
| 2:AB:222:TYR:CD2 | 1:AC:247:ALA:HB1 | 2.40 | 0.55 |
| 2:AD:279:GLN:O | 6:4C:142:SER:HB3 | 2.06 | 0.55 |
| 2:AD:321:MET:C | 6:4C:156:PHE:CE2 | 2.83 | 0.55 |
| 1:AE:100:ALA:HB1 | 2:AF:252:LYS:HA | 1.88 | 0.55 |
| 1:BC:404:PHE:HE2 | 2:BD:345:ILE:HD12 | 1.70 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:BD:177:ASP:OD2 | 1:BE:248:LEU:HD23 | 2.02 | 0.55 |
| 1:BE:404:PHE:CE2 | 2:BF:345:ILE:CD1 | 2.88 | 0.55 |
| 1:DE:100:ALA:HB1 | 2:DF:252:LYS:HA | 1.88 | 0.55 |
| 2:EB:54:ALA:HB1 | 2:FB:281:TYR:O | 2.05 | 0.55 |
| 1:GC:402:ARG:CD | 5:3C:381:ASN:CG | 2.78 | 0.55 |
| 2:GF:416:ASN:ND2 | 7:5B:1327:LYS:CE | 2.68 | 0.55 |
| 1:HE:284:GLU:HG3 | 1:HE:286:LEU:HD22 | 1.88 | 0.55 |
| 2:KB:276:ARG:HE | 6:4A:265:TYR:CB | 1.98 | 0.55 |
| 2:LF:77:ARG:CZ | 6:4D:204:ARG:NH2 | 2.61 | 0.55 |
| 4:2C:147:PHE:CD1 | 4:2C:147:PHE:C | 2.84 | 0.55 |
| 6:4D:242:ARG:O | 6:4D:247:LYS:CE | 2.54 | 0.55 |
| 6:4D:273:ARG:HH21 | 6:4D:273:ARG:CG | 2.20 | 0.55 |
| 7:5B:1424:GLN:HE21 | 7:5B:1424:GLN:CA | 2.18 | 0.55 |
| 7:5B:1544:ILE:CD1 | 7:5B:1574:ILE:CG1 | 2.61 | 0.55 |
| 7:5C:1530:ILE:HG22 | 7:5C:1574:ILE:HG21 | 1.87 | 0.55 |
| 1:AA:176:GLN:O | 2:AB:347:ASN:ND2 | 2.34 | 0.55 |
| 2:AF:280:GLN:NE2 | 6:4A:139:ASP:OD1 | 2.39 | 0.55 |
| 2:CB:177:ASP:OD2 | 1:CC:248:LEU:HD23 | 2.06 | 0.55 |
| 2:DB:25:SER:HG | 2:DB:51:TYR:HH | 1.53 | 0.55 |
| 1:EA:176:GLN:O | 2:EB:347:ASN:ND2 | 2.37 | 0.55 |
| 1:EE:100:ALA:HB1 | 2:EF:252:LYS:CA | 2.36 | 0.55 |
| 2:FB:388:MET:HA | 1:FC:346:TRP:O | 2.07 | 0.55 |
| 1:GA:284:GLU:HG3 | 1:GA:286:LEU:HD22 | 1.88 | 0.55 |
| 1:GC:241:SER:OG | 1:GC:250:VAL:O | 2.23 | 0.55 |
| 1:GE:89:PRO:HD3 | 1:HE:280:LYS:HZ2 | 1.68 | 0.55 |
| 1:GE:284:GLU:HG3 | 1:GE:286:LEU:HD22 | 1.88 | 0.55 |
| 1:HA:284:GLU:HG3 | 1:HA:286:LEU:HD22 | 1.88 | 0.55 |
| 1:HC:284:GLU:HG3 | 1:HC:286:LEU:HD22 | 1.88 | 0.55 |
| 1:HE:100:ALA:HB1 | 2:HF:252:LYS:HA | 1.88 | 0.55 |
| 2:HF:309:ARG:NH2 | 2:HF:426:GLN:O | 2.32 | 0.55 |
| 2:IB:87:PRO:CD | 2:JB:281:TYR:CZ | 2.89 | 0.55 |
| 1:JA:141:VAL:HG11 | 1:JA:172:TYR:CD1 | 2.38 | 0.55 |
| 2:LD:98:GLY:C | 1:LE:254:GLU:HG2 | 2.31 | 0.55 |
| 1:LE:222:PRO:CG | 2:LF:324:LYS:HD2 | 2.26 | 0.55 |
| 2:LF:379:LYS:NZ | 4:2B:166:ILE:N | 2.38 | 0.55 |
| 6:4A:273:ARG:HH21 | 6:4A:273:ARG:CG | 2.20 | 0.55 |
| 6:4B:242:ARG:O | 6:4B:247:LYS:CE | 2.54 | 0.55 |
| 6:4B:273:ARG:HH21 | 6:4B:273:ARG:CG | 2.20 | 0.55 |
| 7:5A:1246:LEU:CA | 9:7B:12:GLU:CD | 2.77 | 0.55 |
| 7:5A:1398:GLU:HB3 | 7:5A:1401:LYS:HE2 | 1.88 | 0.55 |
| 7:5B:1398:GLU:HB3 | 7:5B:1401:LYS:HE2 | 1.89 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5B:1533:GLU:CD | 7:5B:1604:ALA:CB | 2.78 | 0.55 |
| 7:5C:827:GLU:CD | 7:5C:849:ARG:NH2 | 2.42 | 0.55 |
| 2:AB:177:ASP:OD1 | 1:AC:353:VAL:HG12 | 1.84 | 0.55 |
| 2:BD:180:VAL:HG12 | 1:BE:258:ASN:OD1 | 2.06 | 0.55 |
| 2:CB:86:ARG:CA | 2:DB:281:TYR:OH | 2.54 | 0.55 |
| 1:FC:284:GLU:HG3 | 1:FC:286:LEU:HD22 | 1.88 | 0.55 |
| 1:FC:402:ARG:HD3 | 7:5A:1259:TYR:CG | 2.38 | 0.55 |
| 1:FE:284:GLU:HG3 | 1:FE:286:LEU:HD22 | 1.89 | 0.55 |
| 2:GB:222:TYR:O | 2:GB:226:ASN:ND2 | 2.27 | 0.55 |
| 1:GC:284:GLU:HG3 | 1:GC:286:LEU:HD22 | 1.89 | 0.55 |
| 2:JF:222:TYR:O | 2:JF:226:ASN:ND2 | 2.28 | 0.55 |
| 1:KA:100:ALA:HB1 | 2:KB:252:LYS:HA | 1.88 | 0.55 |
| 2:KB:125:GLU:O | 4:2C:39:ALA:N | 2.37 | 0.55 |
| 2:KB:220:PRO:CD | 1:KC:326:LYS:HE2 | 2.35 | 0.55 |
| 2:LB:340:TYR:CD2 | 4:2C:147:PHE:HB3 | 2.41 | 0.55 |
| 1:MA:394:LYS:NZ | 2:MB:347:ASN:OD1 | 2.39 | 0.55 |
| 4:2A:147:PHE:CD1 | 4:2A:147:PHE:C | 2.84 | 0.55 |
| 4:2B:147:PHE:CD1 | 4:2B:147:PHE:C | 2.84 | 0.55 |
| 6:4A:242:ARG:O | 6:4A:247:LYS:CE | 2.54 | 0.55 |
| 6:4C:242:ARG:O | 6:4C:247:LYS:CE | 2.54 | 0.55 |
| 6:4C:273:ARG:CG | 6:4C:273:ARG:HH21 | 2.20 | 0.55 |
| 7:5A:1491:LEU:HD22 | 7:5A:1495:PHE:CD2 | 2.38 | 0.55 |
| 7:5C:1471:ILE:HD12 | 7:5C:1471:ILE:N | 2.18 | 0.55 |
| 2:BD:86:ARG:HA | 2:CD:281:TYR:HH | 1.71 | 0.55 |
| 2:BD:178:THR:HA | 1:BE:352:LYS:HD3 | 1.88 | 0.55 |
| 1:DA:284:GLU:HG3 | 1:DA:286:LEU:HD22 | 1.88 | 0.55 |
| 1:FA:284:GLU:HG3 | 1:FA:286:LEU:HD22 | 1.88 | 0.55 |
| 2:HB:178:THR:HA | 1:HC:352:LYS:HD3 | 1.87 | 0.55 |
| 2:HD:220:PRO:CD | 1:HE:326:LYS:HE2 | 2.35 | 0.55 |
| 1:HE:278:ALA:C | 10:8U:22:UNK:CB | 2.79 | 0.55 |
| 1:IE:284:GLU:HG3 | 1:IE:286:LEU:HD22 | 1.88 | 0.55 |
| 2:JF:25:SER:HG | 2:JF:51:TYR:HH | 1.53 | 0.55 |
| 2:KB:87:PRO:CG | 2:LB:282:ARG:HD2 | 2.35 | 0.55 |
| 1:LA:284:GLU:HG3 | 1:LA:286:LEU:HD22 | 1.89 | 0.55 |
| 1:LC:222:PRO:CG | 2:LD:324:LYS:HD2 | 2.26 | 0.55 |
| 1:LC:284:GLU:HG3 | 1:LC:286:LEU:HD22 | 1.89 | 0.55 |
| 1:LE:60:LYS:HZ2 | 1:ME:283:HIS:CE1 | 2.25 | 0.55 |
| 1:LE:284:GLU:HG3 | 1:LE:286:LEU:HD22 | 1.89 | 0.55 |
| 2:LF:221:THR:HG23 | 6:4D:219:ASN:ND2 | 2.21 | 0.55 |
| 6:4A:223:PHE:CE2 | 6:4A:230:TYR:HB3 | 2.42 | 0.55 |
| 7:5A:1562:LEU:HD13 | 7:5A:1562:LEU:O | 2.07 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5B:1119:LEU:HD13 | 7:5B:1135:TYR:CD1 | 2.41 | 0.55 |
| 7:5B:1152:GLU:CD | 8:6B:66:ARG:NH2 | 2.64 | 0.55 |
| 7:5B:1562:LEU:HD13 | 7:5B:1562:LEU:O | 2.07 | 0.55 |
| 7:5C:1416:LYS:CA | 7:5C:1416:LYS:CE | 2.85 | 0.55 |
| 7:5C:1562:LEU:HD13 | 7:5C:1562:LEU:O | 2.07 | 0.55 |
| 10:8W:36:UNK:O | 10:8W:37:UNK:CB | 2.53 | 0.55 |
| 1:AA:100:ALA:HB1 | 2:AB:252:LYS:HA | 1.88 | 0.55 |
| 1:AA:241:SER:OG | 1:AA:250:VAL:O | 2.23 | 0.55 |
| 2:AF:217:LEU:HD22 | 6:4A:132:LYS:CD | 2.35 | 0.55 |
| 2:CD:42:LEU:HA | 2:CD:45:GLU:HG3 | 1.88 | 0.55 |
| 2:CF:309:ARG:NH2 | 2:CF:426:GLN:O | 2.32 | 0.55 |
| 2:ED:391:ARG:HG3 | 1:EE:346:TRP:CD1 | 2.40 | 0.55 |
| 1:FC:419:SER:HB3 | 7:5A:1256:ARG:CG | 2.34 | 0.55 |
| 1:GA:100:ALA:HB1 | 2:GB:252:LYS:HA | 1.88 | 0.55 |
| 1:GC:89:PRO:HD3 | 1:HC:280:LYS:HZ1 | 1.63 | 0.55 |
| 1:IA:404:PHE:CE2 | 2:IB:345:ILE:CD1 | 2.89 | 0.55 |
| 1:JA:88:HIS:CE1 | 1:KA:280:LYS:C | 2.77 | 0.55 |
| 2:JB:178:THR:HA | 1:JC:352:LYS:HD3 | 1.87 | 0.55 |
| 2:JB:222:TYR:CD2 | 1:JC:247:ALA:HB1 | 2.40 | 0.55 |
| 1:JE:88:HIS:O | 1:KE:280:LYS:NZ | 2.39 | 0.55 |
| 1:JE:284:GLU:HG3 | 1:JE:286:LEU:HD22 | 1.88 | 0.55 |
| 1:KC:85:GLN:CA | 1:LC:283:HIS:CA | 2.51 | 0.55 |
| 1:LC:101:ASN:ND2 | 2:LD:252:LYS:CG | 2.70 | 0.55 |
| 2:LD:379:LYS:HE3 | 4:2A:166:ILE:HG13 | 1.88 | 0.55 |
| 1:LE:178:SER:OG | 2:LF:347:ASN:CB | 2.48 | 0.55 |
| 1:MC:222:PRO:O | 2:MD:322:SER:HB2 | 2.07 | 0.55 |
| 2:MD:221:THR:HG21 | 6:4B:189:ARG:HH22 | 0.52 | 0.55 |
| 6:4A:256:ASN:HD21 | 6:4A:260:ARG:CZ | 2.20 | 0.55 |
| 6:4B:223:PHE:CE2 | 6:4B:230:TYR:HB3 | 2.42 | 0.55 |
| 6:4C:223:PHE:CE2 | 6:4C:230:TYR:HB3 | 2.42 | 0.55 |
| 6:4C:256:ASN:HD21 | 6:4C:260:ARG:CZ | 2.20 | 0.55 |
| 7:5A:1416:LYS:CA | 7:5A:1416:LYS:CE | 2.85 | 0.55 |
| 7:5B:1552:LYS:NZ | 7:5B:1563:SER:H | 2.04 | 0.55 |
| 7:5C:842:LEU:H | 7:5C:842:LEU:CD2 | 2.08 | 0.55 |
| 7:5C:1398:GLU:HB3 | 7:5C:1401:LYS:HE2 | 1.89 | 0.55 |
| 9:7E:38:LEU:HD23 | 9:7F:42:LEU:CD1 | 2.23 | 0.55 |
| 10:8V:36:UNK:O | 10:8V:37:UNK:CB | 2.53 | 0.55 |
| 2:CB:42:LEU:HA | 2:CB:45:GLU:HG3 | 1.88 | 0.55 |
| 1:CC:284:GLU:HG3 | 1:CC:286:LEU:HD22 | 1.88 | 0.55 |
| 1:CE:284:GLU:HG3 | 1:CE:286:LEU:HD22 | 1.89 | 0.55 |
| 2:CF:42:LEU:HA | 2:CF:45:GLU:HG3 | 1.88 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:DC:284:GLU:HG3 | 1:DC:286:LEU:HD22 | 1.89 | 0.55 |
| 2:ED:42:LEU:HA | 2:ED:45:GLU:HG3 | 1.88 | 0.55 |
| 2:ED:176:SER:OG | 1:EE:349:THR:OG1 | 2.19 | 0.55 |
| 2:ED:390:ARG:HD2 | 1:EE:439:THR:HG21 | 1.89 | 0.55 |
| 2:ED:397:TRP:CB | 1:EE:256:GLN:HE22 | 2.13 | 0.55 |
| 2:EF:54:ALA:CB | 2:FF:281:TYR:O | 2.54 | 0.55 |
| 1:FA:404:PHE:CE2 | 2:FB:345:ILE:HD11 | 2.42 | 0.55 |
| 2:FD:106:TYR:CD1 | 7:5A:1295:LYS:N | 2.74 | 0.55 |
| 1:FE:423:GLU:HG3 | 7:5B:1256:ARG:NH2 | 2.21 | 0.55 |
| 2:GD:416:ASN:CG | 7:5A:1327:LYS:NZ | 2.64 | 0.55 |
| 2:IB:424:GLN:HE21 | 7:5C:1413:GLN:CG | 2.19 | 0.55 |
| 1:IC:389:SER:CB | 5:3C:307:LYS:HB3 | 2.36 | 0.55 |
| 1:JE:88:HIS:C | 1:KE:280:LYS:HE2 | 2.26 | 0.55 |
| 1:JE:90:GLU:C | 1:KE:280:LYS:HZ1 | 2.10 | 0.55 |
| 1:KA:284:GLU:HG3 | 1:KA:286:LEU:HD22 | 1.89 | 0.55 |
| 2:KF:125:GLU:CD | 2:LF:332:ASN:HD22 | 2.14 | 0.55 |
| 2:LB:227:HIS:CE1 | 6:4A:226:ILE:CG1 | 2.88 | 0.55 |
| 1:MA:241:SER:OG | 1:MA:250:VAL:O | 2.23 | 0.55 |
| 6:4A:114:GLU:HA | 6:4A:117:ARG:HD2 | 1.89 | 0.55 |
| 6:4B:114:GLU:HA | 6:4B:117:ARG:HD2 | 1.89 | 0.55 |
| 6:4C:114:GLU:HA | 6:4C:117:ARG:HD2 | 1.89 | 0.55 |
| 6:4C:278:TYR:N | 6:4C:278:TYR:HD1 | 2.04 | 0.55 |
| 7:5A:1552:LYS:NZ | 7:5A:1563:SER:H | 2.04 | 0.55 |
| 7:5C:1552:LYS:NZ | 7:5C:1563:SER:H | 2.04 | 0.55 |
| 2:BB:86:ARG:CA | 2:CB:281:TYR:HE1 | 2.20 | 0.55 |
| 1:DE:284:GLU:HG3 | 1:DE:286:LEU:HD22 | 1.89 | 0.55 |
| 2:EB:42:LEU:HA | 2:EB:45:GLU:HG3 | 1.88 | 0.55 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:CG | 2.84 | 0.55 |
| 1:FC:402:ARG:HD2 | 7:5A:1259:TYR:HD2 | 1.69 | 0.55 |
| 1:FE:207:GLU:CD | 7:5B:915:PHE:HD2 | 2.15 | 0.55 |
| 1:FE:419:SER:C | 7:5B:1256:ARG:HH21 | 2.14 | 0.55 |
| 2:GD:86:ARG:NH2 | 2:HD:281:TYR:CZ | 2.61 | 0.55 |
| 2:IB:87:PRO:CD | 2:JB:281:TYR:CE2 | 2.90 | 0.55 |
| 1:IC:284:GLU:HG3 | 1:IC:286:LEU:HD22 | 1.89 | 0.55 |
| 2:KB:79:GLY:HA2 | 6:4A:254:ALA:HB1 | 1.89 | 0.55 |
| 2:KD:54:ALA:CA | 2:LD:285:THR:HG21 | 2.32 | 0.55 |
| 2:LB:58:ARG:NH2 | 2:MB:281:TYR:CZ | 2.74 | 0.55 |
| 2:LD:223:GLY:CA | 6:4B:219:ASN:ND2 | 2.70 | 0.55 |
| 1:ME:284:GLU:HG3 | 1:ME:286:LEU:HD22 | 1.89 | 0.55 |
| 5:3C:230:ILE:HG22 | 5:3C:332:MET:CG | 2.36 | 0.55 |
| 6:4B:256:ASN:HD21 | 6:4B:260:ARG:CZ | 2.20 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4D:114:GLU:HA | 6:4D:117:ARG:HD2 | 1.89 | 0.55 |
| 7:5A:1119:LEU:HD13 | 7:5A:1135:TYR:CD1 | 2.41 | 0.55 |
| 7:5B:1105:TYR:HB3 | 7:5B:1166:LEU:CB | 2.37 | 0.55 |
| 7:5B:1416:LYS:CA | 7:5B:1416:LYS:CE | 2.85 | 0.55 |
| 2:AB:42:LEU:HA | 2:AB:45:GLU:HG3 | 1.88 | 0.55 |
| 2:AB:212:PHE:HZ | 1:AC:326:LYS:CE | 2.14 | 0.55 |
| 1:AE:283:HIS:CB | 2:MB:86:ARG:NH1 | 2.59 | 0.55 |
| 1:BA:222:PRO:HD2 | 2:BB:324:LYS:HD3 | 1.88 | 0.55 |
| 2:BB:42:LEU:HA | 2:BB:45:GLU:HG3 | 1.89 | 0.55 |
| 2:BD:42:LEU:HA | 2:BD:45:GLU:HG3 | 1.89 | 0.55 |
| 2:BF:42:LEU:HA | 2:BF:45:GLU:HG3 | 1.89 | 0.55 |
| 1:CA:284:GLU:HG3 | 1:CA:286:LEU:HD22 | 1.88 | 0.55 |
| 1:CA:404:PHE:CE2 | 2:CB:345:ILE:CD1 | 2.89 | 0.55 |
| 1:CE:141:VAL:HG11 | 1:CE:172:TYR:CD1 | 2.38 | 0.55 |
| 2:DF:114:ASP:OD1 | 2:DF:115:SER:N | 2.40 | 0.55 |
| 2:DF:207:LEU:HB3 | 2:DF:225:LEU:HD22 | 1.89 | 0.55 |
| 1:EE:282:TYR:CD2 | 10:8L:18:UNK:CB | 2.86 | 0.55 |
| 2:EF:83:GLN:O | 2:FF:281:TYR:OH | 2.14 | 0.55 |
| 2:FD:55:THR:H | 2:GD:283:ALA:HB2 | 1.45 | 0.55 |
| 2:GD:220:PRO:CD | 1:GE:326:LYS:HE2 | 2.35 | 0.55 |
| 1:HA:404:PHE:CE2 | 2:HB:345:ILE:CD1 | 2.89 | 0.55 |
| 2:HD:309:ARG:NH2 | 2:HD:426:GLN:O | 2.32 | 0.55 |
| 1:IA:176:GLN:O | 2:IB:347:ASN:ND2 | 2.34 | 0.55 |
| 1:IA:284:GLU:HG3 | 1:IA:286:LEU:HD22 | 1.88 | 0.55 |
| 1:JC:284:GLU:HG3 | 1:JC:286:LEU:HD22 | 1.89 | 0.55 |
| 1:KC:284:GLU:HG3 | 1:KC:286:LEU:HD22 | 1.88 | 0.55 |
| 1:MC:241:SER:OG | 1:MC:250:VAL:O | 2.23 | 0.55 |
| 1:ME:222:PRO:O | 2:MF:322:SER:HB2 | 2.07 | 0.55 |
| 6:4A:278:TYR:N | 6:4A:278:TYR:HD1 | 2.04 | 0.55 |
| 6:4D:223:PHE:CE2 | 6:4D:230:TYR:HB3 | 2.42 | 0.55 |
| 7:5A:1105:TYR:HB3 | 7:5A:1166:LEU:CB | 2.37 | 0.55 |
| 7:5C:1119:LEU:HD13 | 7:5C:1135:TYR:CD1 | 2.41 | 0.55 |
| 7:5C:1491:LEU:HD22 | 7:5C:1495:PHE:CD2 | 2.38 | 0.55 |
| 1:AA:404:PHE:CE2 | 2:AB:345:ILE:CD1 | 2.89 | 0.55 |
| 2:AB:178:THR:HA | 1:AC:352:LYS:HD3 | 1.87 | 0.55 |
| 2:AD:42:LEU:HA | 2:AD:45:GLU:HG3 | 1.89 | 0.55 |
| 2:CB:114:ASP:OD1 | 2:CB:115:SER:N | 2.40 | 0.55 |
| 2:CB:207:LEU:HB3 | 2:CB:225:LEU:HD22 | 1.89 | 0.55 |
| 1:CC:60:LYS:NZ | 1:DC:283:HIS:CE1 | 2.71 | 0.55 |
| 2:CD:114:ASP:OD1 | 2:CD:115:SER:N | 2.40 | 0.55 |
| 2:CD:309:ARG:NH2 | 2:CD:426:GLN:O | 2.32 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CF:114:ASP:OD1 | 2:CF:115:SER:N | 2.40 | 0.55 |
| 2:CF:207:LEU:HB3 | 2:CF:225:LEU:HD22 | 1.89 | 0.55 |
| 2:DB:114:ASP:OD1 | 2:DB:115:SER:N | 2.40 | 0.55 |
| 2:DF:42:LEU:HA | 2:DF:45:GLU:HG3 | 1.89 | 0.55 |
| 1:EA:396:ASP:C | 7:5C:817:LEU:HD21 | 2.32 | 0.55 |
| 1:EC:222:PRO:HD2 | 2:ED:324:LYS:HD3 | 1.87 | 0.55 |
| 1:FE:402:ARG:HH11 | 7:5B:1259:TYR:HD2 | 1.53 | 0.55 |
| 2:FF:332:ASN:CB | 7:5B:909:ASN:HD21 | 2.20 | 0.55 |
| 1:GA:404:PHE:CE2 | 2:GB:345:ILE:CD1 | 2.89 | 0.55 |
| 2:HB:114:ASP:OD1 | 2:HB:115:SER:N | 2.40 | 0.55 |
| 2:HD:114:ASP:OD1 | 2:HD:115:SER:N | 2.40 | 0.55 |
| 2:HF:114:ASP:OD1 | 2:HF:115:SER:N | 2.40 | 0.55 |
| 1:JA:404:PHE:CE2 | 2:JB:345:ILE:CD1 | 2.89 | 0.55 |
| 2:JD:25:SER:HG | 2:JD:51:TYR:HH | 1.54 | 0.55 |
| 2:LB:42:LEU:HA | 2:LB:45:GLU:HG3 | 1.88 | 0.55 |
| 2:LB:306:ARG:HH21 | 4:2C:149:ILE:HG23 | 1.72 | 0.55 |
| 2:LD:379:LYS:HZ1 | 4:2A:166:ILE:CB | 2.20 | 0.55 |
| 1:MC:284:GLU:HG3 | 1:MC:286:LEU:HD22 | 1.88 | 0.55 |
| 6:4D:256:ASN:HD21 | 6:4D:260:ARG:CZ | 2.20 | 0.55 |
| 6:4D:300:SER:O | 6:4D:300:SER:OG | 2.24 | 0.55 |
| 7:5B:818:ARG:HG2 | 7:5B:822:MET:HE3 | 1.89 | 0.55 |
| 7:5B:1548:VAL:HG11 | 7:5B:1566:GLU:N | 2.22 | 0.55 |
| 10:8S:36:UNK:O | 10:8S:37:UNK:CB | 2.53 | 0.55 |
| 1:AC:241:SER:OG | 1:AC:250:VAL:O | 2.23 | 0.55 |
| 1:BA:100:ALA:HB1 | 2:BB:252:LYS:HA | 1.89 | 0.55 |
| 2:BB:280:GLN:NE2 | 10:8B:1:UNK:O | 2.40 | 0.55 |
| 1:CA:100:ALA:HB1 | 2:CB:252:LYS:HA | 1.89 | 0.55 |
| 2:CD:86:ARG:CG | 2:DD:281:TYR:CE1 | 2.41 | 0.55 |
| 2:CD:207:LEU:HB3 | 2:CD:225:LEU:HD22 | 1.89 | 0.55 |
| 1:DA:128:ASN:ND2 | 1:EA:285:GLN:NE2 | 2.54 | 0.55 |
| 2:DD:42:LEU:HA | 2:DD:45:GLU:HG3 | 1.89 | 0.55 |
| 2:DD:114:ASP:OD1 | 2:DD:115:SER:N | 2.40 | 0.55 |
| 2:DD:207:LEU:HB3 | 2:DD:225:LEU:HD22 | 1.89 | 0.55 |
| 2:ED:114:ASP:OD1 | 2:ED:115:SER:N | 2.40 | 0.55 |
| 2:EF:42:LEU:HA | 2:EF:45:GLU:HG3 | 1.88 | 0.55 |
| 2:EF:114:ASP:OD1 | 2:EF:115:SER:N | 2.40 | 0.55 |
| 1:GA:176:GLN:O | 2:GB:347:ASN:ND2 | 2.34 | 0.55 |
| 2:GB:42:LEU:HA | 2:GB:45:GLU:HG3 | 1.88 | 0.55 |
| 1:GC:176:GLN:O | 2:GD:347:ASN:ND2 | 2.35 | 0.55 |
| 2:ID:424:GLN:HE21 | 7:5A:1413:GLN:CG | 2.19 | 0.55 |
| 2:JB:114:ASP:OD1 | 2:JB:115:SER:N | 2.40 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JE:100:ALA:HB1 | 2:JF:252:LYS:HA | 1.88 | 0.55 |
| 2:KD:77:ARG:HG3 | 2:LD:281:TYR:CE1 | 2.38 | 0.55 |
| 1:KE:284:GLU:HG3 | 1:KE:286:LEU:HD22 | 1.88 | 0.55 |
| 2:KF:273:LEU:HG | 6:4D:268:LEU:HD21 | 1.88 | 0.55 |
| 2:LD:42:LEU:HA | 2:LD:45:GLU:HG3 | 1.88 | 0.55 |
| 2:LD:58:ARG:NH2 | 2:MD:281:TYR:CZ | 2.75 | 0.55 |
| 1:ME:241:SER:OG | 1:ME:250:VAL:O | 2.23 | 0.55 |
| 2:MF:218:THR:OG1 | 6:4D:196:GLN:NE2 | 2.37 | 0.55 |
| 5:3A:230:ILE:HG22 | 5:3A:332:MET:CG | 2.36 | 0.55 |
| 5:3B:230:ILE:HG22 | 5:3B:332:MET:CG | 2.36 | 0.55 |
| 7:5A:818:ARG:HG2 | 7:5A:822:MET:HE3 | 1.89 | 0.55 |
| 7:5A:839:GLU:CD | 8:6A:109:ILE:HG13 | 2.32 | 0.55 |
| 7:5A:1401:LYS:H | 7:5A:1401:LYS:CD | 2.03 | 0.55 |
| 7:5C:1105:TYR:HB3 | 7:5C:1166:LEU:CB | 2.37 | 0.55 |
| 10:8X:36:UNK:O | 10:8X:37:UNK:CB | 2.53 | 0.55 |
| 1:AE:101:ASN:ND2 | 2:AF:252:LYS:HG3 | 2.14 | 0.54 |
| 2:AF:42:LEU:HA | 2:AF:45:GLU:HG3 | 1.89 | 0.54 |
| 2:AF:320:ARG:HH12 | 6:4A:152:PHE:C | 2.15 | 0.54 |
| 2:BB:114:ASP:OD1 | 2:BB:115:SER:N | 2.40 | 0.54 |
| 2:BB:127:CYS:SG | 2:BB:130:LEU:HD13 | 2.48 | 0.54 |
| 1:BE:401:LYS:CE | 2:BF:344:TRP:CZ3 | 2.70 | 0.54 |
| 2:CB:100:ASN:HB2 | 1:CC:257:THR:HG21 | 1.89 | 0.54 |
| 2:CD:397:TRP:HE3 | 1:CE:257:THR:CG2 | 2.00 | 0.54 |
| 2:DB:207:LEU:HB3 | 2:DB:225:LEU:HD22 | 1.89 | 0.54 |
| 1:DE:402:ARG:CD | 7:5B:777:ALA:HB2 | 2.33 | 0.54 |
| 2:FF:114:ASP:OD1 | 2:FF:115:SER:N | 2.40 | 0.54 |
| 2:GD:42:LEU:HA | 2:GD:45:GLU:HG3 | 1.89 | 0.54 |
| 2:GF:42:LEU:HA | 2:GF:45:GLU:HG3 | 1.89 | 0.54 |
| 1:IE:100:ALA:HB1 | 2:IF:252:LYS:HA | 1.88 | 0.54 |
| 2:KF:127:CYS:SG | 2:KF:130:LEU:HD13 | 2.48 | 0.54 |
| 1:LA:221:ARG:NH2 | 2:LB:321:MET:O | 2.38 | 0.54 |
| 2:LB:397:TRP:CB | 1:LC:256:GLN:HE22 | 2.16 | 0.54 |
| 2:LD:127:CYS:SG | 2:LD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:LE:89:PRO:N | 1:ME:280:LYS:HZ2 | 2.05 | 0.54 |
| 2:LF:42:LEU:HA | 2:LF:45:GLU:HG3 | 1.88 | 0.54 |
| 2:LF:127:CYS:SG | 2:LF:130:LEU:HD13 | 2.48 | 0.54 |
| 1:MA:279:GLU:O | 6:4C:107:MET:SD | 2.40 | 0.54 |
| 1:MA:284:GLU:HG3 | 1:MA:286:LEU:HD22 | 1.88 | 0.54 |
| 2:MB:114:ASP:OD1 | 2:MB:115:SER:N | 2.40 | 0.54 |
| 2:MD:42:LEU:HA | 2:MD:45:GLU:HG3 | 1.88 | 0.54 |
| 2:MD:114:ASP:OD1 | 2:MD:115:SER:N | 2.40 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4A:167:ARG:HB3 | 6:4A:167:ARG:NH1 | 2.22 | 0.54 |
| 6:4B:167:ARG:NH1 | 6:4B:167:ARG:HB3 | 2.22 | 0.54 |
| 6:4B:278:TYR:N | 6:4B:278:TYR:HD1 | 2.04 | 0.54 |
| 6:4B:300:SER:O | 6:4B:300:SER:OG | 2.24 | 0.54 |
| 6:4D:167:ARG:NH1 | 6:4D:167:ARG:HB3 | 2.22 | 0.54 |
| 7:5A:1548:VAL:HG11 | 7:5A:1566:GLU:N | 2.22 | 0.54 |
| 7:5C:818:ARG:HG2 | 7:5C:822:MET:HE3 | 1.89 | 0.54 |
| 10:8Q:36:UNK:O | 10:8Q:37:UNK:CB | 2.53 | 0.54 |
| 2:AD:127:CYS:SG | 2:AD:130:LEU:HD13 | 2.48 | 0.54 |
| 2:AD:227:HIS:HD1 | 6:4C:135:LEU:HD11 | 1.68 | 0.54 |
| 1:AE:241:SER:OG | 1:AE:250:VAL:O | 2.23 | 0.54 |
| 2:AF:127:CYS:SG | 2:AF:130:LEU:HD13 | 2.48 | 0.54 |
| 2:BB:85:PHE:O | 2:CB:281:TYR:OH | 2.23 | 0.54 |
| 1:CC:141:VAL:HG11 | 1:CC:172:TYR:CD1 | 2.38 | 0.54 |
| 1:CC:401:LYS:HE3 | 2:CD:344:TRP:CZ3 | 2.42 | 0.54 |
| 2:CF:127:CYS:SG | 2:CF:130:LEU:HD13 | 2.48 | 0.54 |
| 2:DD:60:VAL:CG2 | 2:ED:281:TYR:CE1 | 2.89 | 0.54 |
| 1:EA:284:GLU:HG3 | 1:EA:286:LEU:HD22 | 1.88 | 0.54 |
| 2:EB:114:ASP:OD1 | 2:EB:115:SER:N | 2.40 | 0.54 |
| 1:EC:284:GLU:HG3 | 1:EC:286:LEU:HD22 | 1.88 | 0.54 |
| 2:ED:212:PHE:CZ | 1:EE:326:LYS:CE | 2.89 | 0.54 |
| 1:FA:179:THR:O | 2:FB:350:LYS:HA | 2.07 | 0.54 |
| 2:FB:42:LEU:HA | 2:FB:45:GLU:HG3 | 1.88 | 0.54 |
| 2:FB:55:THR:CA | 2:GB:283:ALA:HA | 2.37 | 0.54 |
| 2:FB:179:VAL:HG12 | 1:FC:350:GLY:C | 2.33 | 0.54 |
| 2:FB:332:ASN:HB2 | 7:5C:909:ASN:OD1 | 2.07 | 0.54 |
| 2:FD:114:ASP:OD1 | 2:FD:115:SER:N | 2.40 | 0.54 |
| 1:HA:60:LYS:HD3 | 1:IA:283:HIS:CD2 | 2.42 | 0.54 |
| 1:HC:404:PHE:HE2 | 2:HD:345:ILE:HD12 | 1.73 | 0.54 |
| 1:HC:410:GLY:CA | 5:3C:329:ARG:NH2 | 2.70 | 0.54 |
| 2:HF:207:LEU:HB3 | 2:HF:225:LEU:HD22 | 1.89 | 0.54 |
| 1:JA:284:GLU:HG3 | 1:JA:286:LEU:HD22 | 1.89 | 0.54 |
| 2:KB:158:GLU:CA | 4:2C:34:ASN:HB3 | 1.78 | 0.54 |
| 2:KD:127:CYS:SG | 2:KD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:KE:245:ASP:OD2 | 6:4B:257:LEU:CD1 | 2.56 | 0.54 |
| 2:KF:82:GLY:O | 2:LF:281:TYR:CE1 | 2.59 | 0.54 |
| 2:KF:114:ASP:OD1 | 2:KF:115:SER:N | 2.40 | 0.54 |
| 1:MA:401:LYS:CE | 2:MB:344:TRP:CZ3 | 2.66 | 0.54 |
| 2:MB:42:LEU:HA | 2:MB:45:GLU:HG3 | 1.88 | 0.54 |
| 2:MD:127:CYS:SG | 2:MD:130:LEU:HD13 | 2.48 | 0.54 |
| 2:MF:114:ASP:OD1 | 2:MF:115:SER:N | 2.40 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2C:16:GLN:HA | 4:2C:19:MET:HB2 | 0.58 | 0.54 |
| 6:4A:167:ARG:CZ | 6:4A:167:ARG:CB | 2.85 | 0.54 |
| 6:4B:167:ARG:CZ | 6:4B:167:ARG:CB | 2.85 | 0.54 |
| 6:4C:167:ARG:CZ | 6:4C:167:ARG:CB | 2.85 | 0.54 |
| 6:4C:167:ARG:NH1 | 6:4C:167:ARG:HB3 | 2.22 | 0.54 |
| 6:4C:273:ARG:HG3 | 6:4C:273:ARG:NH2 | 2.22 | 0.54 |
| 6:4D:167:ARG:CZ | 6:4D:167:ARG:CB | 2.85 | 0.54 |
| 7:5A:1544:ILE:CD1 | 7:5A:1574:ILE:CG1 | 2.61 | 0.54 |
| 7:5B:1399:LYS:HZ1 | 7:5B:1399:LYS:HB3 | 1.72 | 0.54 |
| 7:5B:1521:PHE:CA | 7:5B:1567:PHE:HE2 | 2.10 | 0.54 |
| 10:8T:36:UNK:O | 10:8T:37:UNK:CB | 2.53 | 0.54 |
| 2:AB:55:THR:CG2 | 2:BB:283:ALA:CA | 2.66 | 0.54 |
| 1:BA:101:ASN:ND2 | 2:BB:252:LYS:HG3 | 2.14 | 0.54 |
| 2:BD:114:ASP:OD1 | 2:BD:115:SER:N | 2.40 | 0.54 |
| 2:BF:114:ASP:OD1 | 2:BF:115:SER:N | 2.40 | 0.54 |
| 2:CB:309:ARG:NH2 | 2:CB:426:GLN:O | 2.32 | 0.54 |
| 2:DB:42:LEU:HA | 2:DB:45:GLU:HG3 | 1.89 | 0.54 |
| 1:DC:401:LYS:HE3 | 2:DD:344:TRP:CZ3 | 2.43 | 0.54 |
| 2:DD:180:VAL:HG12 | 1:DE:258:ASN:OD1 | 2.07 | 0.54 |
| 2:DD:222:TYR:HD2 | 1:DE:247:ALA:HB1 | 1.72 | 0.54 |
| 1:FC:100:ALA:HB1 | 2:FD:252:LYS:CA | 2.37 | 0.54 |
| 2:FF:55:THR:CB | 2:GF:283:ALA:HA | 2.36 | 0.54 |
| 2:FF:127:CYS:SG | 2:FF:130:LEU:HD13 | 2.48 | 0.54 |
| 2:HD:207:LEU:HB3 | 2:HD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:JD:114:ASP:OD1 | 2:JD:115:SER:N | 2.40 | 0.54 |
| 2:JF:114:ASP:OD1 | 2:JF:115:SER:N | 2.40 | 0.54 |
| 1:KA:404:PHE:CE2 | 2:KB:345:ILE:CD1 | 2.88 | 0.54 |
| 2:KB:114:ASP:OD1 | 2:KB:115:SER:N | 2.40 | 0.54 |
| 2:KD:114:ASP:OD1 | 2:KD:115:SER:N | 2.40 | 0.54 |
| 2:KD:207:LEU:HB3 | 2:KD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:KD:220:PRO:CD | 1:KE:326:LYS:HE2 | 2.35 | 0.54 |
| 2:KF:54:ALA:CA | 2:LF:285:THR:HG21 | 2.36 | 0.54 |
| 2:KF:207:LEU:HB3 | 2:KF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:LB:127:CYS:SG | 2:LB:130:LEU:HD13 | 2.48 | 0.54 |
| 2:LD:77:ARG:CZ | 6:4B:204:ARG:NH2 | 2.59 | 0.54 |
| 2:LF:207:LEU:HB3 | 2:LF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:MD:221:THR:HB | 6:4B:189:ARG:HH12 | 1.72 | 0.54 |
| 2:MF:42:LEU:HA | 2:MF:45:GLU:HG3 | 1.89 | 0.54 |
| 2:MF:127:CYS:SG | 2:MF:130:LEU:HD13 | 2.48 | 0.54 |
| 6:4A:273:ARG:HG3 | 6:4A:273:ARG:NH2 | 2.22 | 0.54 |
| 6:4B:223:PHE:N | 6:4B:223:PHE:CD2 | 2.73 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:4D:278:TYR:CD1 | 6:4D:278:TYR:N | 2.72 | 0.54 |
| 6:4D:278:TYR:N | 6:4D:278:TYR:HD1 | 2.04 | 0.54 |
| 7:5A:1399:LYS:HB3 | 7:5A:1399:LYS:HZ2 | 1.72 | 0.54 |
| 7:5B:842:LEU:HD22 | 7:5B:842:LEU:N | 2.02 | 0.54 |
| 7:5B:1384:GLN:N | 7:5B:1384:GLN:HE21 | 2.05 | 0.54 |
| 7:5C:841:VAL:N | 8:6C:109:ILE:HD11 | 1.62 | 0.54 |
| 10:8P:36:UNK:O | 10:8P:37:UNK:CB | 2.53 | 0.54 |
| 2:AB:127:CYS:SG | 2:AB:130:LEU:HD13 | 2.48 | 0.54 |
| 1:AC:404:PHE:HE2 | 2:AD:345:ILE:HD12 | 1.73 | 0.54 |
| 2:BB:86:ARG:HA | 2:CB:281:TYR:HE1 | 1.66 | 0.54 |
| 2:BB:86:ARG:HA | 2:CB:281:TYR:HH | 1.71 | 0.54 |
| 2:BD:127:CYS:SG | 2:BD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:CA:184:PRO:O | 1:CA:188:ILE:HG12 | 2.08 | 0.54 |
| 2:CB:394:PHE:CD1 | 1:CC:261:PRO:HA | 2.43 | 0.54 |
| 13:CB:501:GDP:C8 | 1:CC:248:LEU:CD1 | 2.90 | 0.54 |
| 1:DC:402:ARG:NE | 7:5A:777:ALA:HB1 | 2.09 | 0.54 |
| 1:EA:396:ASP:HB3 | 7:5C:817:LEU:HD21 | 0.60 | 0.54 |
| 2:EB:127:CYS:SG | 2:EB:130:LEU:HD13 | 2.48 | 0.54 |
| 2:ED:127:CYS:SG | 2:ED:130:LEU:HD13 | 2.48 | 0.54 |
| 2:ED:177:ASP:OD2 | 1:EE:248:LEU:HD23 | 2.07 | 0.54 |
| 2:EF:157:GLU:OE1 | 7:5B:935:LYS:NZ | 2.40 | 0.54 |
| 2:EF:207:LEU:HB3 | 2:EF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:FD:42:LEU:HA | 2:FD:45:GLU:HG3 | 1.89 | 0.54 |
| 2:FD:127:CYS:SG | 2:FD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:FE:419:SER:HB2 | 7:5B:1256:ARG:CZ | 2.24 | 0.54 |
| 2:GB:409:THR:O | 7:5C:1330:ILE:HD13 | 2.07 | 0.54 |
| 2:GD:222:TYR:O | 2:GD:226:ASN:ND2 | 2.27 | 0.54 |
| 1:HA:188:ILE:HD12 | 1:HA:425:LEU:HD11 | 1.90 | 0.54 |
| 2:HB:207:LEU:HB3 | 2:HB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:IB:25:SER:HG | 2:IB:51:TYR:HH | 1.54 | 0.54 |
| 1:IE:241:SER:OG | 1:IE:250:VAL:O | 2.23 | 0.54 |
| 2:JB:207:LEU:HB3 | 2:JB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:JD:207:LEU:HB3 | 2:JD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:JF:207:LEU:HB3 | 2:JF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:KB:207:LEU:HB3 | 2:KB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:KD:42:LEU:HA | 2:KD:45:GLU:HG3 | 1.88 | 0.54 |
| 2:KD:179:VAL:HG22 | 1:KE:258:ASN:CG | 2.33 | 0.54 |
| 2:LF:55:THR:CG2 | 2:MF:284:LEU:H | 2.15 | 0.54 |
| 2:LF:227:HIS:HD1 | 6:4D:226:ILE:HG13 | 1.70 | 0.54 |
| 1:MA:184:PRO:O | 1:MA:188:ILE:HG12 | 2.08 | 0.54 |
| 2:MB:127:CYS:SG | 2:MB:130:LEU:HD13 | 2.48 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:ME:184:PRO:O | 1:ME:188:ILE:HG12 | 2.07 | 0.54 |
| 6:4B:278:TYR:N | 6:4B:278:TYR:CD1 | 2.72 | 0.54 |
| 7:5A:842:LEU:HD22 | 7:5A:842:LEU:N | 2.02 | 0.54 |
| 7:5A:1384:GLN:N | 7:5A:1384:GLN:HE21 | 2.05 | 0.54 |
| 7:5B:1119:LEU:HD23 | 7:5B:1132:LYS:HG3 | 1.87 | 0.54 |
| 1:BE:284:GLU:HG3 | 1:BE:286:LEU:HD22 | 1.88 | 0.54 |
| 1:CA:141:VAL:HG11 | 1:CA:172:TYR:CD1 | 2.38 | 0.54 |
| 2:CD:127:CYS:SG | 2:CD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:CE:222:PRO:CG | 2:CF:324:LYS:CD | 2.84 | 0.54 |
| 1:DA:184:PRO:O | 1:DA:188:ILE:HG12 | 2.08 | 0.54 |
| 2:DD:397:TRP:CB | 1:DE:256:GLN:HE22 | 2.17 | 0.54 |
| 1:EC:393:HIS:HE1 | 7:5A:814:LYS:HG3 | 1.68 | 0.54 |
| 2:ED:207:LEU:HB3 | 2:ED:225:LEU:HD22 | 1.89 | 0.54 |
| 2:EF:127:CYS:SG | 2:EF:130:LEU:HD13 | 2.48 | 0.54 |
| 2:FB:114:ASP:OD1 | 2:FB:115:SER:N | 2.40 | 0.54 |
| 2:FB:127:CYS:SG | 2:FB:130:LEU:HD13 | 2.48 | 0.54 |
| 1:FC:422:ARG:HE | 7:5A:1170:THR:CB | 2.11 | 0.54 |
| 1:GA:184:PRO:O | 1:GA:188:ILE:HG12 | 2.08 | 0.54 |
| 1:HC:188:ILE:HD12 | 1:HC:425:LEU:HD11 | 1.90 | 0.54 |
| 2:HD:42:LEU:HA | 2:HD:45:GLU:HG3 | 1.89 | 0.54 |
| 2:IB:207:LEU:HB3 | 2:IB:225:LEU:HD22 | 1.89 | 0.54 |
| 1:JA:90:GLU:HG2 | 1:KA:280:LYS:CD | 2.35 | 0.54 |
| 1:JA:100:ALA:HB1 | 2:JB:252:LYS:HA | 1.88 | 0.54 |
| 1:KA:85:GLN:O | 1:LA:283:HIS:HA | 2.05 | 0.54 |
| 1:KA:241:SER:OG | 1:KA:250:VAL:O | 2.23 | 0.54 |
| 2:KB:42:LEU:HA | 2:KB:45:GLU:HG3 | 1.89 | 0.54 |
| 2:KB:127:CYS:SG | 2:KB:130:LEU:HD13 | 2.48 | 0.54 |
| 2:KB:159:TYR:CE2 | 4:2C:35:VAL:C | 2.80 | 0.54 |
| 2:KB:222:TYR:O | 2:KB:226:ASN:ND2 | 2.27 | 0.54 |
| 2:KF:125:GLU:CG | 2:LF:336:LYS:HZ3 | 2.05 | 0.54 |
| 2:KF:125:GLU:CB | 2:LF:336:LYS:CE | 2.85 | 0.54 |
| 2:LD:207:LEU:HB3 | 2:LD:225:LEU:HD22 | 1.89 | 0.54 |
| 1:MC:184:PRO:O | 1:MC:188:ILE:HG12 | 2.08 | 0.54 |
| 1:ME:279:GLU:HB2 | 6:4B:110:LYS:CE | 2.35 | 0.54 |
| 4:2A:16:GLN:HA | 4:2A:19:MET:HB2 | 0.58 | 0.54 |
| 6:4A:278:TYR:N | 6:4A:278:TYR:CD1 | 2.72 | 0.54 |
| 6:4A:300:SER:O | 6:4A:300:SER:OG | 2.24 | 0.54 |
| 7:5A:1521:PHE:CA | 7:5A:1567:PHE:HE2 | 2.10 | 0.54 |
| 7:5C:1131:PHE:CE1 | 8:6C:253:PHE:HE1 | 2.25 | 0.54 |
| 1:AC:176:GLN:O | 2:AD:347:ASN:ND2 | 2.35 | 0.54 |
| 2:AD:179:VAL:HG22 | 1:AE:258:ASN:CG | 2.33 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AE:284:GLU:HG3 | 1:AE:286:LEU:HD22 | 1.88 | 0.54 |
| 1:BA:184:PRO:O | 1:BA:188:ILE:HG12 | 2.08 | 0.54 |
| 1:BA:241:SER:OG | 1:BA:250:VAL:O | 2.23 | 0.54 |
| 2:BB:207:LEU:HB3 | 2:BB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:BF:127:CYS:SG | 2:BF:130:LEU:HD13 | 2.48 | 0.54 |
| 1:CC:184:PRO:O | 1:CC:188:ILE:HG12 | 2.08 | 0.54 |
| 2:CD:222:TYR:CD2 | 1:CE:247:ALA:HB1 | 2.42 | 0.54 |
| 1:CE:100:ALA:HB1 | 2:CF:252:LYS:HA | 1.88 | 0.54 |
| 1:CE:184:PRO:O | 1:CE:188:ILE:HG12 | 2.08 | 0.54 |
| 2:CF:86:ARG:HB2 | 2:DF:281:TYR:HE1 | 1.69 | 0.54 |
| 1:DC:184:PRO:O | 1:DC:188:ILE:HG12 | 2.08 | 0.54 |
| 1:DE:184:PRO:O | 1:DE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:EE:284:GLU:HG3 | 1:EE:286:LEU:HD22 | 1.88 | 0.54 |
| 2:FD:55:THR:N | 2:GD:283:ALA:HA | 2.19 | 0.54 |
| 2:GB:55:THR:HG1 | 2:HB:283:ALA:HA | 1.73 | 0.54 |
| 1:GC:184:PRO:O | 1:GC:188:ILE:HG12 | 2.08 | 0.54 |
| 2:HB:42:LEU:HA | 2:HB:45:GLU:HG3 | 1.88 | 0.54 |
| 1:HE:188:ILE:HD12 | 1:HE:425:LEU:HD11 | 1.90 | 0.54 |
| 1:IA:100:ALA:HB1 | 2:IB:252:LYS:HA | 1.88 | 0.54 |
| 1:IA:188:ILE:HD12 | 1:IA:425:LEU:HD11 | 1.90 | 0.54 |
| 2:ID:207:LEU:HB3 | 2:ID:225:LEU:HD22 | 1.89 | 0.54 |
| 1:IE:188:ILE:HD12 | 1:IE:425:LEU:HD11 | 1.90 | 0.54 |
| 2:LB:207:LEU:HB3 | 2:LB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:LB:222:TYR:O | 2:LB:226:ASN:ND2 | 2.28 | 0.54 |
| 2:MB:220:PRO:O | 1:MC:324:VAL:HG11 | 2.08 | 0.54 |
| 4:2B:16:GLN:HA | 4:2B:19:MET:HB2 | 0.58 | 0.54 |
| 6:4A:223:PHE:N | 6:4A:223:PHE:CD2 | 2.73 | 0.54 |
| 6:4B:101:ARG:NH2 | 6:4B:101:ARG:HG3 | 2.15 | 0.54 |
| 6:4B:273:ARG:HG3 | 6:4B:273:ARG:NH2 | 2.22 | 0.54 |
| 7:5A:1119:LEU:HD23 | 7:5A:1132:LYS:HG3 | 1.87 | 0.54 |
| 7:5C:842:LEU:HD22 | 7:5C:842:LEU:N | 2.02 | 0.54 |
| 7:5C:1384:GLN:N | 7:5C:1384:GLN:HE21 | 2.05 | 0.54 |
| 9:7E:7:LEU:HD23 | 9:7F:27:GLY:HA2 | 1.87 | 0.54 |
| 2:AD:212:PHE:HZ | 1:AE:326:LYS:HD3 | 0.53 | 0.54 |
| 2:AF:114:ASP:OD1 | 2:AF:115:SER:N | 2.40 | 0.54 |
| 2:AF:207:LEU:HB3 | 2:AF:225:LEU:HD22 | 1.89 | 0.54 |
| 1:BC:60:LYS:NZ | 1:CC:283:HIS:NE2 | 2.52 | 0.54 |
| 1:BC:101:ASN:ND2 | 2:BD:252:LYS:HG3 | 2.14 | 0.54 |
| 2:CB:127:CYS:SG | 2:CB:130:LEU:HD13 | 2.48 | 0.54 |
| 1:CC:188:ILE:HD12 | 1:CC:425:LEU:HD11 | 1.90 | 0.54 |
| 13:CD:501:GDP:C8 | 1:CE:248:LEU:CD1 | 2.91 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:DC:188:ILE:HD12 | 1:DC:425:LEU:HD11 | 1.90 | 0.54 |
| 2:DD:177:ASP:OD2 | 1:DE:248:LEU:HD23 | 2.08 | 0.54 |
| 2:EB:25:SER:HG | 2:EB:51:TYR:HH | 1.54 | 0.54 |
| 2:EB:207:LEU:HB3 | 2:EB:225:LEU:HD22 | 1.89 | 0.54 |
| 1:EC:184:PRO:O | 1:EC:188:ILE:HG12 | 2.08 | 0.54 |
| 1:FC:60:LYS:HD3 | 1:GC:283:HIS:CD2 | 2.27 | 0.54 |
| 2:FD:207:LEU:HB3 | 2:FD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:FF:42:LEU:HA | 2:FF:45:GLU:HG3 | 1.89 | 0.54 |
| 2:FF:207:LEU:HB3 | 2:FF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:GB:25:SER:HG | 2:GB:51:TYR:HH | 1.55 | 0.54 |
| 2:GB:207:LEU:HB3 | 2:GB:225:LEU:HD22 | 1.89 | 0.54 |
| 1:GC:11:GLN:HG3 | 1:GC:74:VAL:HG11 | 1.90 | 0.54 |
| 2:GD:54:ALA:CB | 2:HD:281:TYR:O | 2.56 | 0.54 |
| 1:GE:184:PRO:O | 1:GE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:HA:184:PRO:O | 1:HA:188:ILE:HG12 | 2.08 | 0.54 |
| 1:IE:141:VAL:HG11 | 1:IE:172:TYR:CD1 | 2.38 | 0.54 |
| 2:JF:127:CYS:SG | 2:JF:130:LEU:HD13 | 2.48 | 0.54 |
| 1:KE:188:ILE:HD12 | 1:KE:425:LEU:HD11 | 1.90 | 0.54 |
| 2:KF:54:ALA:CB | 2:LF:285:THR:HG22 | 2.16 | 0.54 |
| 1:LA:188:ILE:HD12 | 1:LA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:LC:176:GLN:HE22 | 4:2A:42:PHE:HB2 | 1.72 | 0.54 |
| 1:LC:188:ILE:HD12 | 1:LC:425:LEU:HD11 | 1.90 | 0.54 |
| 1:LE:188:ILE:HD12 | 1:LE:425:LEU:HD11 | 1.90 | 0.54 |
| 4:2B:164:ARG:CZ | 4:2B:164:ARG:CB | 2.85 | 0.54 |
| 6:4C:223:PHE:N | 6:4C:223:PHE:CD2 | 2.73 | 0.54 |
| 7:5C:839:GLU:OE2 | 8:6C:11:PRO:CG | 2.56 | 0.54 |
| 7:5C:1119:LEU:HD23 | 7:5C:1132:LYS:HG3 | 1.87 | 0.54 |
| 7:5C:1125:LEU:HD23 | 8:6C:246:TYR:CE2 | 2.43 | 0.54 |
| 1:AC:284:GLU:HG3 | 1:AC:286:LEU:HD22 | 1.88 | 0.54 |
| 2:AD:207:LEU:HB3 | 2:AD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:AD:356:ILE:HD12 | 6:4C:152:PHE:HD1 | 1.63 | 0.54 |
| 1:BA:188:ILE:HD12 | 1:BA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:BA:279:GLU:OE2 | 10:8A:22:UNK:HA | 2.08 | 0.54 |
| 1:BC:184:PRO:O | 1:BC:188:ILE:HG12 | 2.08 | 0.54 |
| 2:BD:207:LEU:HB3 | 2:BD:225:LEU:HD22 | 1.89 | 0.54 |
| 13:BD:501:GDP:C8 | 1:BE:248:LEU:CD1 | 2.90 | 0.54 |
| 2:BF:207:LEU:HB3 | 2:BF:225:LEU:HD22 | 1.89 | 0.54 |
| 1:DA:188:ILE:HD12 | 1:DA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:DA:241:SER:OG | 1:DA:250:VAL:O | 2.23 | 0.54 |
| 2:DB:212:PHE:CZ | 1:DC:326:LYS:CE | 2.90 | 0.54 |
| 1:EA:184:PRO:O | 1:EA:188:ILE:HG12 | 2.08 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:EA:430:LYS:NZ | 7:5C:834:ASN:ND2 | 0.57 | 0.54 |
| 1:EC:188:ILE:HD12 | 1:EC:425:LEU:HD11 | 1.90 | 0.54 |
| 1:FC:423:GLU:HG3 | 7:5A:1256:ARG:HH21 | 1.73 | 0.54 |
| 1:GA:60:LYS:HD3 | 1:HA:283:HIS:CA | 2.38 | 0.54 |
| 1:GC:89:PRO:CD | 1:HC:280:LYS:HD2 | 2.38 | 0.54 |
| 2:GF:114:ASP:OD1 | 2:GF:115:SER:N | 2.40 | 0.54 |
| 1:HA:100:ALA:HB1 | 2:HB:252:LYS:HA | 1.89 | 0.54 |
| 2:HF:42:LEU:HA | 2:HF:45:GLU:HG3 | 1.89 | 0.54 |
| 1:JA:241:SER:OG | 1:JA:250:VAL:O | 2.23 | 0.54 |
| 2:JB:25:SER:HG | 2:JB:51:TYR:HH | 1.55 | 0.54 |
| 2:JD:42:LEU:HA | 2:JD:45:GLU:HG3 | 1.89 | 0.54 |
| 1:KA:188:ILE:HD12 | 1:KA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:KA:394:LYS:NZ | 2:KB:347:ASN:OD1 | 2.41 | 0.54 |
| 2:KD:126:GLY:O | 4:2A:39:ALA:N | 2.41 | 0.54 |
| 2:KF:42:LEU:HA | 2:KF:45:GLU:HG3 | 1.89 | 0.54 |
| 4:2C:164:ARG:CZ | 4:2C:164:ARG:CB | 2.85 | 0.54 |
| 6:4C:300:SER:O | 6:4C:300:SER:OG | 2.24 | 0.54 |
| 7:5A:1096:ASN:OD1 | 7:5A:1097:PRO:HD2 | 2.08 | 0.54 |
| 7:5B:1125:LEU:HD23 | 8:6B:246:TYR:CE2 | 2.43 | 0.54 |
| 7:5C:912:VAL:HG11 | 7:5C:918:ILE:CG1 | 2.37 | 0.54 |
| 7:5C:1096:ASN:OD1 | 7:5C:1097:PRO:HD2 | 2.08 | 0.54 |
| 7:5C:1271:ILE:HB | 9:7E:20:LEU:HD23 | 1.63 | 0.54 |
| 7:5C:1401:LYS:H | 7:5C:1401:LYS:CD | 2.03 | 0.54 |
| 1:AA:284:GLU:HG3 | 1:AA:286:LEU:HD22 | 1.88 | 0.54 |
| 1:AA:394:LYS:NZ | 2:AB:347:ASN:OD1 | 2.41 | 0.54 |
| 1:BC:188:ILE:HD12 | 1:BC:425:LEU:HD11 | 1.90 | 0.54 |
| 1:BC:284:GLU:HG3 | 1:BC:286:LEU:HD22 | 1.89 | 0.54 |
| 1:BC:404:PHE:CE2 | 2:BD:345:ILE:CD1 | 2.89 | 0.54 |
| 2:BD:390:ARG:HD2 | 1:BE:439:THR:HG21 | 1.90 | 0.54 |
| 1:BE:184:PRO:O | 1:BE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:BE:188:ILE:HD12 | 1:BE:425:LEU:HD11 | 1.90 | 0.54 |
| 1:CA:188:ILE:HD12 | 1:CA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:CA:401:LYS:CE | 2:CB:344:TRP:CZ3 | 2.74 | 0.54 |
| 2:DB:397:TRP:CB | 1:DC:256:GLN:HE22 | 2.18 | 0.54 |
| 2:DD:86:ARG:HA | 2:ED:281:TYR:CD1 | 2.33 | 0.54 |
| 1:EA:188:ILE:HD12 | 1:EA:425:LEU:HD11 | 1.90 | 0.54 |
| 1:EC:394:LYS:NZ | 2:ED:347:ASN:OD1 | 2.41 | 0.54 |
| 1:EE:184:PRO:O | 1:EE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:EE:404:PHE:CE2 | 2:EF:345:ILE:HD11 | 2.43 | 0.54 |
| 1:FA:11:GLN:HG3 | 1:FA:74:VAL:HG11 | 1.90 | 0.54 |
| 1:FA:11:GLN:NE2 | 2:FB:247:ASN:OD1 | 2.41 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:184:PRO:O | 1:FA:188:ILE:HG12 | 2.08 | 0.54 |
| 1:FE:184:PRO:O | 1:FE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:FE:222:PRO:HG3 | 2:FF:324:LYS:HD3 | 1.83 | 0.54 |
| 1:GA:11:GLN:HG3 | 1:GA:74:VAL:HG11 | 1.90 | 0.54 |
| 1:GA:188:ILE:HD12 | 1:GA:425:LEU:HD11 | 1.90 | 0.54 |
| 2:GB:58:ARG:NH2 | 2:HB:281:TYR:OH | 2.41 | 0.54 |
| 1:GE:11:GLN:HG3 | 1:GE:74:VAL:HG11 | 1.90 | 0.54 |
| 1:HC:11:GLN:HG3 | 1:HC:74:VAL:HG11 | 1.90 | 0.54 |
| 1:HC:184:PRO:O | 1:HC:188:ILE:HG12 | 2.08 | 0.54 |
| 2:IB:42:LEU:HA | 2:IB:45:GLU:HG3 | 1.89 | 0.54 |
| 2:IB:212:PHE:HZ | 1:IC:326:LYS:CE | 2.14 | 0.54 |
| 1:IC:141:VAL:HG11 | 1:IC:172:TYR:CD1 | 2.38 | 0.54 |
| 1:IC:188:ILE:HD12 | 1:IC:425:LEU:HD11 | 1.90 | 0.54 |
| 1:IC:402:ARG:NH2 | 7:5A:1417:GLN:CA | 2.69 | 0.54 |
| 1:IC:404:PHE:CE2 | 2:ID:345:ILE:CD1 | 2.90 | 0.54 |
| 2:ID:42:LEU:HA | 2:ID:45:GLU:HG3 | 1.89 | 0.54 |
| 1:IE:389:SER:HB2 | 5:3A:307:LYS:CG | 2.37 | 0.54 |
| 2:IF:87:PRO:CD | 2:JF:281:TYR:CZ | 2.91 | 0.54 |
| 2:IF:114:ASP:OD1 | 2:IF:115:SER:N | 2.40 | 0.54 |
| 2:IF:207:LEU:HB3 | 2:IF:225:LEU:HD22 | 1.89 | 0.54 |
| 2:JB:86:ARG:HH21 | 2:KB:280:GLN:HB2 | 1.58 | 0.54 |
| 1:JC:404:PHE:HE2 | 2:JD:345:ILE:HD12 | 1.73 | 0.54 |
| 2:JF:42:LEU:HA | 2:JF:45:GLU:HG3 | 1.89 | 0.54 |
| 1:KC:11:GLN:HG3 | 1:KC:74:VAL:HG11 | 1.90 | 0.54 |
| 1:KC:188:ILE:HD12 | 1:KC:425:LEU:HD11 | 1.90 | 0.54 |
| 2:LD:337:ASN:HD21 | 4:2A:148:ASN:HB2 | 1.73 | 0.54 |
| 2:MB:207:LEU:HB3 | 2:MB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:MD:207:LEU:HB3 | 2:MD:225:LEU:HD22 | 1.89 | 0.54 |
| 2:MD:221:THR:HG21 | 6:4B:189:ARG:NH1 | 2.23 | 0.54 |
| 4:2A:164:ARG:CZ | 4:2A:164:ARG:CB | 2.85 | 0.54 |
| 4:2A:176:ARG:HA | 4:2A:179:VAL:HB | 1.90 | 0.54 |
| 4:2B:176:ARG:HA | 4:2B:179:VAL:HB | 1.90 | 0.54 |
| 4:2C:176:ARG:HA | 4:2C:179:VAL:HB | 1.90 | 0.54 |
| 5:3B:229:PHE:CE1 | 5:3B:331:GLN:OE1 | 2.56 | 0.54 |
| 6:4A:101:ARG:NH2 | 6:4A:101:ARG:HG3 | 2.15 | 0.54 |
| 6:4C:278:TYR:N | 6:4C:278:TYR:CD1 | 2.72 | 0.54 |
| 6:4D:273:ARG:HG3 | 6:4D:273:ARG:NH2 | 2.22 | 0.54 |
| 8:6A:14:ARG:CZ | 8:6A:89:ILE:HG23 | 2.38 | 0.54 |
| 8:6B:14:ARG:CZ | 8:6B:89:ILE:HG23 | 2.38 | 0.54 |
| 9:7C:36:GLN:HA | 9:7D:43:LEU:CD2 | 2.38 | 0.54 |
| 10:8R:36:UNK:O | 10:8R:37:UNK:CB | 2.53 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:207:LEU:HB3 | 2:AB:225:LEU:HD22 | 1.89 | 0.54 |
| 2:AB:220:PRO:CD | 1:AC:326:LYS:HE2 | 2.35 | 0.54 |
| 2:AD:114:ASP:OD1 | 2:AD:115:SER:N | 2.40 | 0.54 |
| 2:AD:220:PRO:CD | 1:AE:326:LYS:HE2 | 2.35 | 0.54 |
| 2:AD:224:ASP:OD1 | 6:4C:131:VAL:N | 2.39 | 0.54 |
| 2:CB:222:TYR:HD2 | 1:CC:247:ALA:HB1 | 1.73 | 0.54 |
| 1:CE:11:GLN:HG3 | 1:CE:74:VAL:HG11 | 1.90 | 0.54 |
| 1:CE:188:ILE:HD12 | 1:CE:425:LEU:HD11 | 1.90 | 0.54 |
| 2:CF:25:SER:HG | 2:CF:51:TYR:HH | 1.55 | 0.54 |
| 2:DB:86:ARG:HB2 | 2:EB:281:TYR:CE1 | 2.43 | 0.54 |
| 1:EA:11:GLN:HG3 | 1:EA:74:VAL:HG11 | 1.90 | 0.54 |
| 1:EA:430:LYS:NZ | 7:5C:834:ASN:HD21 | 1.08 | 0.54 |
| 2:EB:54:ALA:C | 2:FB:283:ALA:HB2 | 2.31 | 0.54 |
| 2:EB:85:PHE:C | 2:FB:281:TYR:OH | 2.51 | 0.54 |
| 2:ED:397:TRP:CD2 | 1:EE:256:GLN:O | 2.29 | 0.54 |
| 1:EE:398:MET:SD | 2:EF:345:ILE:CG1 | 2.84 | 0.54 |
| 1:FC:184:PRO:O | 1:FC:188:ILE:HG12 | 2.08 | 0.54 |
| 2:FD:222:TYR:CE2 | 1:FE:325:PRO:HG2 | 2.42 | 0.54 |
| 1:FE:141:VAL:HG11 | 1:FE:172:TYR:CD1 | 2.38 | 0.54 |
| 2:GB:114:ASP:OD1 | 2:GB:115:SER:N | 2.40 | 0.54 |
| 1:GC:188:ILE:HD12 | 1:GC:425:LEU:HD11 | 1.90 | 0.54 |
| 1:GE:188:ILE:HD12 | 1:GE:425:LEU:HD11 | 1.90 | 0.54 |
| 2:GF:127:CYS:SG | 2:GF:130:LEU:HD13 | 2.48 | 0.54 |
| 1:HE:184:PRO:O | 1:HE:188:ILE:HG12 | 2.08 | 0.54 |
| 1:IC:184:PRO:O | 1:IC:188:ILE:HG12 | 2.08 | 0.54 |
| 1:IE:184:PRO:O | 1:IE:188:ILE:HG12 | 2.08 | 0.54 |
| 2:IF:42:LEU:HA | 2:IF:45:GLU:HG3 | 1.89 | 0.54 |
| 2:JB:42:LEU:HA | 2:JB:45:GLU:HG3 | 1.88 | 0.54 |
| 1:JC:11:GLN:HG3 | 1:JC:74:VAL:HG11 | 1.90 | 0.54 |
| 2:JD:127:CYS:SG | 2:JD:130:LEU:HD13 | 2.48 | 0.54 |
| 1:KA:11:GLN:HG3 | 1:KA:74:VAL:HG11 | 1.90 | 0.54 |
| 1:KA:184:PRO:O | 1:KA:188:ILE:HG12 | 2.08 | 0.54 |
| 2:KB:228:LEU:HD21 | 6:4A:267:ILE:HD12 | 1.87 | 0.54 |
| 2:KD:125:GLU:C | 4:2A:38:VAL:HA | 2.32 | 0.54 |
| 2:LB:114:ASP:OD1 | 2:LB:115:SER:N | 2.40 | 0.54 |
| 1:LC:60:LYS:HZ3 | 1:MC:283:HIS:CE1 | 2.21 | 0.54 |
| 1:LE:222:PRO:CD | 2:LF:324:LYS:CB | 2.86 | 0.54 |
| 6:4C:101:ARG:NH2 | 6:4C:101:ARG:HG3 | 2.15 | 0.54 |
| 7:5A:912:VAL:HG11 | 7:5A:918:ILE:CG1 | 2.37 | 0.54 |
| 7:5B:1096:ASN:OD1 | 7:5B:1097:PRO:HD2 | 2.08 | 0.54 |
| 7:5C:1521:PHE:CA | 7:5C:1567:PHE:HE2 | 2.10 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:6C:14:ARG:CZ | 8:6C:89:ILE:HG23 | 2.38 | 0.54 |
| 9:7A:36:GLN:HA | 9:7B:43:LEU:CD2 | 2.38 | 0.54 |
| 1:AE:184:PRO:O | 1:AE:188:ILE:HG12 | 2.08 | 0.53 |
| 1:BA:284:GLU:HG3 | 1:BA:286:LEU:HD22 | 1.88 | 0.53 |
| 1:BC:241:SER:OG | 1:BC:250:VAL:O | 2.23 | 0.53 |
| 2:DD:25:SER:HG | 2:DD:51:TYR:HH | 1.55 | 0.53 |
| 2:DD:212:PHE:CZ | 1:DE:326:LYS:CE | 2.91 | 0.53 |
| 1:DE:11:GLN:HG3 | 1:DE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:DE:188:ILE:HD12 | 1:DE:425:LEU:HD11 | 1.90 | 0.53 |
| 2:EB:179:VAL:CG2 | 1:EC:258:ASN:CA | 2.86 | 0.53 |
| 1:EE:188:ILE:HD12 | 1:EE:425:LEU:HD11 | 1.90 | 0.53 |
| 1:FA:89:PRO:N | 1:GA:280:LYS:NZ | 2.49 | 0.53 |
| 1:FA:422:ARG:NE | 7:5C:1170:THR:C | 2.66 | 0.53 |
| 1:FC:11:GLN:HG3 | 1:FC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:FC:141:VAL:HG11 | 1:FC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:FD:177:ASP:CG | 1:FE:353:VAL:HG13 | 1.93 | 0.53 |
| 1:GC:141:VAL:HG11 | 1:GC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:GD:25:SER:HG | 2:GD:51:TYR:HH | 1.55 | 0.53 |
| 2:GD:114:ASP:OD1 | 2:GD:115:SER:N | 2.40 | 0.53 |
| 2:GD:207:LEU:HB3 | 2:GD:225:LEU:HD22 | 1.89 | 0.53 |
| 1:GE:141:VAL:HG11 | 1:GE:172:TYR:CD1 | 2.38 | 0.53 |
| 1:GE:178:SER:OG | 2:GF:347:ASN:HB3 | 2.08 | 0.53 |
| 1:HE:11:GLN:HG3 | 1:HE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:IA:11:GLN:HG3 | 1:IA:74:VAL:HG11 | 1.90 | 0.53 |
| 1:IA:141:VAL:HG11 | 1:IA:172:TYR:CD1 | 2.38 | 0.53 |
| 1:IA:184:PRO:O | 1:IA:188:ILE:HG12 | 2.08 | 0.53 |
| 2:IB:127:CYS:SG | 2:IB:130:LEU:HD13 | 2.48 | 0.53 |
| 1:IC:11:GLN:HG3 | 1:IC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:IC:176:GLN:O | 2:ID:347:ASN:ND2 | 2.35 | 0.53 |
| 2:ID:179:VAL:HG22 | 1:IE:258:ASN:CG | 2.33 | 0.53 |
| 1:IE:11:GLN:HG3 | 1:IE:74:VAL:HG11 | 1.90 | 0.53 |
| 2:IF:25:SER:HG | 2:IF:51:TYR:HH | 1.54 | 0.53 |
| 2:JB:397:TRP:CD2 | 1:JC:256:GLN:O | 2.30 | 0.53 |
| 1:KC:241:SER:OG | 1:KC:250:VAL:O | 2.23 | 0.53 |
| 1:KE:178:SER:OG | 2:KF:347:ASN:HB3 | 2.08 | 0.53 |
| 1:LC:47:ASP:OD1 | 6:4A:203:LYS:HE3 | 2.09 | 0.53 |
| 1:LC:56:THR:OG1 | 1:MC:284:GLU:CA | 2.56 | 0.53 |
| 2:MD:25:SER:HG | 2:MD:51:TYR:HH | 1.56 | 0.53 |
| 2:MF:221:THR:HB | 6:4D:189:ARG:HH12 | 1.72 | 0.53 |
| 7:5A:829:GLY:HA2 | 8:6A:109:ILE:HG21 | 1.90 | 0.53 |
| 7:5B:912:VAL:HG11 | 7:5B:918:ILE:CG1 | 2.37 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1398:GLU:OE2 | 7:5C:1398:GLU:HA | 2.05 | 0.53 |
| 1:AA:188:ILE:HD12 | 1:AA:425:LEU:HD11 | 1.90 | 0.53 |
| 2:AB:114:ASP:OD1 | 2:AB:115:SER:N | 2.40 | 0.53 |
| 1:AC:184:PRO:O | 1:AC:188:ILE:HG12 | 2.08 | 0.53 |
| 2:CD:391:ARG:HG3 | 1:CE:346:TRP:CD1 | 2.43 | 0.53 |
| 1:DA:402:ARG:NH2 | 7:5C:777:ALA:CB | 2.42 | 0.53 |
| 2:DB:127:CYS:SG | 2:DB:130:LEU:HD13 | 2.48 | 0.53 |
| 2:EB:125:GLU:CD | 7:5C:903:PHE:HE2 | 2.14 | 0.53 |
| 1:EC:11:GLN:HG3 | 1:EC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:FA:188:ILE:HD12 | 1:FA:425:LEU:HD11 | 1.90 | 0.53 |
| 2:FB:207:LEU:HB3 | 2:FB:225:LEU:HD22 | 1.89 | 0.53 |
| 1:FE:423:GLU:CG | 7:5B:1256:ARG:NH2 | 2.71 | 0.53 |
| 1:GA:141:VAL:HG11 | 1:GA:172:TYR:CD1 | 2.38 | 0.53 |
| 1:GA:394:LYS:NZ | 2:GB:347:ASN:OD1 | 2.41 | 0.53 |
| 1:GC:404:PHE:CE2 | 2:GD:345:ILE:CD1 | 2.90 | 0.53 |
| 1:HA:11:GLN:HG3 | 1:HA:74:VAL:HG11 | 1.90 | 0.53 |
| 2:HB:127:CYS:SG | 2:HB:130:LEU:HD13 | 2.48 | 0.53 |
| 2:IB:114:ASP:OD1 | 2:IB:115:SER:N | 2.40 | 0.53 |
| 2:ID:127:CYS:SG | 2:ID:130:LEU:HD13 | 2.48 | 0.53 |
| 2:JD:86:ARG:NH1 | 2:KD:280:GLN:CB | 2.50 | 0.53 |
| 1:JE:11:GLN:HG3 | 1:JE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:JE:188:ILE:HD12 | 1:JE:425:LEU:HD11 | 1.90 | 0.53 |
| 1:KE:11:GLN:HG3 | 1:KE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:LA:221:ARG:NH1 | 2:LB:324:LYS:H | 2.03 | 0.53 |
| 2:LD:114:ASP:OD1 | 2:LD:115:SER:N | 2.40 | 0.53 |
| 2:LD:294:PHE:O | 4:2A:148:ASN:O | 2.26 | 0.53 |
| 2:MB:221:THR:HB | 6:4A:189:ARG:HH12 | 1.73 | 0.53 |
| 7:5A:1398:GLU:OE2 | 7:5A:1398:GLU:HA | 2.05 | 0.53 |
| 7:5C:1521:PHE:CE2 | 7:5C:1567:PHE:O | 2.61 | 0.53 |
| 1:AC:11:GLN:HG3 | 1:AC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:AC:404:PHE:CE2 | 2:AD:345:ILE:CD1 | 2.90 | 0.53 |
| 1:CA:11:GLN:HG3 | 1:CA:74:VAL:HG11 | 1.90 | 0.53 |
| 1:DC:11:GLN:HG3 | 1:DC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:DC:241:SER:OG | 1:DC:250:VAL:O | 2.23 | 0.53 |
| 1:EE:11:GLN:HG3 | 1:EE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:FC:188:ILE:HD12 | 1:FC:425:LEU:HD11 | 1.90 | 0.53 |
| 1:FE:11:GLN:HG3 | 1:FE:74:VAL:HG11 | 1.90 | 0.53 |
| 2:GD:212:PHE:HZ | 1:GE:326:LYS:HD3 | 0.53 | 0.53 |
| 2:GF:207:LEU:HB3 | 2:GF:225:LEU:HD22 | 1.89 | 0.53 |
| 2:HD:127:CYS:SG | 2:HD:130:LEU:HD13 | 2.48 | 0.53 |
| 2:HD:179:VAL:HG22 | 1:HE:258:ASN:CG | 2.33 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:IC:393:HIS:CB | 5:3C:308:PHE:HE2 | 2.20 | 0.53 |
| 2:ID:114:ASP:OD1 | 2:ID:115:SER:N | 2.40 | 0.53 |
| 2:JB:127:CYS:SG | 2:JB:130:LEU:HD13 | 2.48 | 0.53 |
| 1:JC:90:GLU:C | 1:KC:280:LYS:HZ1 | 2.07 | 0.53 |
| 2:JD:179:VAL:HG22 | 1:JE:258:ASN:CG | 2.33 | 0.53 |
| 1:KC:184:PRO:O | 1:KC:188:ILE:HG12 | 2.08 | 0.53 |
| 1:KE:184:PRO:O | 1:KE:188:ILE:HG12 | 2.08 | 0.53 |
| 1:LC:184:PRO:O | 1:LC:188:ILE:HG12 | 2.08 | 0.53 |
| 1:LE:184:PRO:O | 1:LE:188:ILE:HG12 | 2.08 | 0.53 |
| 2:LF:114:ASP:OD1 | 2:LF:115:SER:N | 2.41 | 0.53 |
| 2:LF:228:LEU:CD2 | 6:4D:225:PRO:CG | 2.87 | 0.53 |
| 1:MA:11:GLN:HG3 | 1:MA:74:VAL:HG11 | 1.90 | 0.53 |
| 2:MF:207:LEU:HB3 | 2:MF:225:LEU:HD22 | 1.89 | 0.53 |
| 7:5A:1405:GLU:O | 7:5A:1409:PHE:N | 2.39 | 0.53 |
| 7:5A:1521:PHE:CE2 | 7:5A:1567:PHE:O | 2.61 | 0.53 |
| 7:5B:1246:LEU:CD2 | 9:7D:12:GLU:HG2 | 2.39 | 0.53 |
| 7:5B:1405:GLU:O | 7:5B:1409:PHE:N | 2.39 | 0.53 |
| 7:5C:1405:GLU:O | 7:5C:1409:PHE:N | 2.39 | 0.53 |
| 9:7E:7:LEU:CD2 | 9:7F:27:GLY:O | 2.43 | 0.53 |
| 1:AA:11:GLN:HG3 | 1:AA:74:VAL:HG11 | 1.90 | 0.53 |
| 1:AA:60:LYS:HZ2 | 1:BA:283:HIS:CE1 | 2.27 | 0.53 |
| 1:AA:184:PRO:O | 1:AA:188:ILE:HG12 | 2.08 | 0.53 |
| 1:BA:11:GLN:HG3 | 1:BA:74:VAL:HG11 | 1.90 | 0.53 |
| 2:BB:25:SER:HG | 2:BB:51:TYR:HH | 1.54 | 0.53 |
| 2:BF:87:PRO:CD | 2:CF:281:TYR:CZ | 2.89 | 0.53 |
| 1:CC:11:GLN:HG3 | 1:CC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:DC:101:ASN:ND2 | 2:DD:252:LYS:HG3 | 2.16 | 0.53 |
| 1:FA:222:PRO:HG3 | 2:FB:324:LYS:CD | 2.37 | 0.53 |
| 13:FD:502:GDP:C8 | 1:FE:248:LEU:CD1 | 2.90 | 0.53 |
| 1:FE:188:ILE:HD12 | 1:FE:425:LEU:HD11 | 1.90 | 0.53 |
| 1:FE:422:ARG:HE | 7:5B:1170:THR:C | 2.16 | 0.53 |
| 1:HC:419:SER:CB | 5:3C:238:ILE:HD12 | 2.33 | 0.53 |
| 2:HF:127:CYS:SG | 2:HF:130:LEU:HD13 | 2.48 | 0.53 |
| 2:ID:212:PHE:CE2 | 1:IE:326:LYS:HD3 | 2.26 | 0.53 |
| 2:IF:127:CYS:SG | 2:IF:130:LEU:HD13 | 2.48 | 0.53 |
| 1:JA:11:GLN:HG3 | 1:JA:74:VAL:HG11 | 1.90 | 0.53 |
| 1:JA:188:ILE:HD12 | 1:JA:425:LEU:HD11 | 1.90 | 0.53 |
| 1:JC:89:PRO:HD3 | 1:KC:283:HIS:NE2 | 2.16 | 0.53 |
| 1:JC:404:PHE:CE2 | 2:JD:345:ILE:CD1 | 2.90 | 0.53 |
| 1:KA:176:GLN:O | 2:KB:347:ASN:ND2 | 2.34 | 0.53 |
| 2:KB:276:ARG:HH22 | 6:4A:266:ASN:H | 1.51 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KF:77:ARG:HD3 | 2:LF:281:TYR:CE2 | 2.43 | 0.53 |
| 2:KF:290:THR:HA | 2:KF:293:MET:HE2 | 1.90 | 0.53 |
| 2:LB:179:VAL:CG2 | 1:LC:258:ASN:O | 2.36 | 0.53 |
| 2:LB:274:THR:HG23 | 6:4A:228:LEU:HD22 | 1.90 | 0.53 |
| 2:LD:227:HIS:CE1 | 6:4B:226:ILE:CG1 | 2.89 | 0.53 |
| 1:LE:11:GLN:HG3 | 1:LE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:MA:96:LYS:HE2 | 2:MB:1:MET:HE3 | 1.90 | 0.53 |
| 1:ME:11:GLN:HG3 | 1:ME:74:VAL:HG11 | 1.90 | 0.53 |
| 2:MF:25:SER:HG | 2:MF:51:TYR:HH | 1.56 | 0.53 |
| 4:2A:112:GLU:OE2 | 4:2A:115:LEU:HD12 | 2.08 | 0.53 |
| 4:2B:112:GLU:OE2 | 4:2B:115:LEU:HD12 | 2.08 | 0.53 |
| 4:2C:112:GLU:OE2 | 4:2C:115:LEU:HD12 | 2.08 | 0.53 |
| 7:5A:1399:LYS:HB3 | 7:5A:1399:LYS:NZ | 2.14 | 0.53 |
| 7:5B:1272:ILE:HG12 | 9:7D:11:TYR:CD2 | 2.44 | 0.53 |
| 7:5B:1398:GLU:OE2 | 7:5B:1398:GLU:HA | 2.05 | 0.53 |
| 7:5B:1416:LYS:NZ | 7:5B:1416:LYS:CA | 2.72 | 0.53 |
| 7:5B:1521:PHE:CE2 | 7:5B:1567:PHE:O | 2.61 | 0.53 |
| 7:5B:1577:LYS:CE | 7:5B:1577:LYS:CA | 2.85 | 0.53 |
| 1:AC:188:ILE:HD12 | 1:AC:425:LEU:HD11 | 1.90 | 0.53 |
| 2:AD:273:LEU:H | 2:AD:292:GLN:HE22 | 1.55 | 0.53 |
| 1:AE:11:GLN:HG3 | 1:AE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:AE:188:ILE:HD12 | 1:AE:425:LEU:HD11 | 1.90 | 0.53 |
| 1:BE:401:LYS:HE3 | 2:BF:344:TRP:CZ3 | 2.42 | 0.53 |
| 1:DA:11:GLN:HG3 | 1:DA:74:VAL:HG11 | 1.90 | 0.53 |
| 2:ED:25:SER:HG | 2:ED:51:TYR:HH | 1.54 | 0.53 |
| 2:ED:54:ALA:C | 2:FD:283:ALA:HB2 | 2.33 | 0.53 |
| 2:EF:55:THR:N | 2:FF:283:ALA:CB | 2.72 | 0.53 |
| 1:FA:419:SER:C | 7:5C:1256:ARG:HH21 | 2.16 | 0.53 |
| 2:FF:55:THR:HG21 | 2:GF:284:LEU:N | 2.08 | 0.53 |
| 2:GB:127:CYS:SG | 2:GB:130:LEU:HD13 | 2.48 | 0.53 |
| 2:GD:127:CYS:SG | 2:GD:130:LEU:HD13 | 2.48 | 0.53 |
| 2:GD:273:LEU:H | 2:GD:292:GLN:HE22 | 1.55 | 0.53 |
| 2:GD:412:GLU:OE2 | 7:5A:1323:MET:HE1 | 2.04 | 0.53 |
| 2:GF:222:TYR:O | 2:GF:226:ASN:ND2 | 2.28 | 0.53 |
| 2:HD:273:LEU:H | 2:HD:292:GLN:HE22 | 1.55 | 0.53 |
| 2:HF:273:LEU:H | 2:HF:292:GLN:HE22 | 1.55 | 0.53 |
| 2:ID:273:LEU:H | 2:ID:292:GLN:HE22 | 1.55 | 0.53 |
| 1:IE:389:SER:HB2 | 5:3A:307:LYS:CB | 2.37 | 0.53 |
| 1:JA:394:LYS:NZ | 2:JB:347:ASN:OD1 | 2.41 | 0.53 |
| 1:JC:90:GLU:HG2 | 1:KC:280:LYS:CD | 2.37 | 0.53 |
| 1:JC:188:ILE:HD12 | 1:JC:425:LEU:HD11 | 1.90 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:JC:241:SER:OG | 1:JC:250:VAL:O | 2.23 | 0.53 |
| 2:KB:290:THR:HA | 2:KB:293:MET:HE2 | 1.90 | 0.53 |
| 2:KD:79:GLY:HA2 | 6:4B:254:ALA:HB1 | 1.90 | 0.53 |
| 1:KE:241:SER:OG | 1:KE:250:VAL:O | 2.23 | 0.53 |
| 1:LA:11:GLN:HG3 | 1:LA:74:VAL:HG11 | 1.90 | 0.53 |
| 1:LA:184:PRO:O | 1:LA:188:ILE:HG12 | 2.08 | 0.53 |
| 1:LC:11:GLN:HG3 | 1:LC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:MC:11:GLN:HG3 | 1:MC:74:VAL:HG11 | 1.90 | 0.53 |
| 2:MD:290:THR:HA | 2:MD:293:MET:HE2 | 1.90 | 0.53 |
| 1:ME:188:ILE:HD12 | 1:ME:425:LEU:HD11 | 1.90 | 0.53 |
| 7:5A:1251:SER:HA | 7:5A:1258:ARG:HH21 | 1.73 | 0.53 |
| 7:5B:1064:LYS:C | 7:5B:1066:GLY:H | 2.17 | 0.53 |
| 7:5B:1312:GLU:HA | 7:5B:1315:ARG:HD2 | 1.91 | 0.53 |
| 7:5B:1548:VAL:HA | 7:5B:1569:GLU:CG | 2.35 | 0.53 |
| 7:5C:1251:SER:HA | 7:5C:1258:ARG:HH21 | 1.73 | 0.53 |
| 7:5C:1399:LYS:NZ | 7:5C:1399:LYS:HB3 | 2.14 | 0.53 |
| 1:BC:11:GLN:HG3 | 1:BC:74:VAL:HG11 | 1.90 | 0.53 |
| 1:BE:11:GLN:HG3 | 1:BE:74:VAL:HG11 | 1.90 | 0.53 |
| 1:CC:60:LYS:HZ3 | 1:DC:283:HIS:CE1 | 2.25 | 0.53 |
| 2:DD:127:CYS:SG | 2:DD:130:LEU:HD13 | 2.48 | 0.53 |
| 2:DF:127:CYS:SG | 2:DF:130:LEU:HD13 | 2.48 | 0.53 |
| 2:EB:222:TYR:CE2 | 1:EC:325:PRO:HG2 | 2.43 | 0.53 |
| 2:EB:273:LEU:H | 2:EB:292:GLN:HE22 | 1.55 | 0.53 |
| 1:EE:141:VAL:HG11 | 1:EE:172:TYR:CD1 | 2.38 | 0.53 |
| 2:EF:273:LEU:H | 2:EF:292:GLN:HE22 | 1.55 | 0.53 |
| 2:FB:273:LEU:H | 2:FB:292:GLN:HE22 | 1.55 | 0.53 |
| 1:FC:179:THR:O | 2:FD:350:LYS:HA | 2.09 | 0.53 |
| 2:FF:332:ASN:HB2 | 7:5B:909:ASN:OD1 | 2.08 | 0.53 |
| 1:GA:398:MET:SD | 2:GB:345:ILE:CG1 | 2.90 | 0.53 |
| 2:GB:273:LEU:H | 2:GB:292:GLN:HE22 | 1.55 | 0.53 |
| 1:GC:404:PHE:HE2 | 2:GD:345:ILE:HD12 | 1.73 | 0.53 |
| 2:GD:179:VAL:HG22 | 1:GE:258:ASN:CB | 2.39 | 0.53 |
| 2:GD:179:VAL:HG22 | 1:GE:258:ASN:CG | 2.33 | 0.53 |
| 2:GD:212:PHE:CE2 | 1:GE:326:LYS:HD3 | 2.26 | 0.53 |
| 1:GE:56:THR:C | 1:HE:285:GLN:CB | 2.51 | 0.53 |
| 2:HB:139:LEU:HD13 | 2:HB:168:SER:HB3 | 1.91 | 0.53 |
| 2:HD:179:VAL:HG22 | 1:HE:258:ASN:CB | 2.39 | 0.53 |
| 2:HF:139:LEU:HD13 | 2:HF:168:SER:HB3 | 1.91 | 0.53 |
| 1:IC:404:PHE:HE2 | 2:ID:345:ILE:HD12 | 1.73 | 0.53 |
| 2:IF:273:LEU:H | 2:IF:292:GLN:HE22 | 1.55 | 0.53 |
| 2:JB:290:THR:HA | 2:JB:293:MET:HE2 | 1.90 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:KA:141:VAL:HG11 | 1:KA:172:TYR:CD1 | 2.38 | 0.53 |
| 2:KD:290:THR:HA | 2:KD:293:MET:HE2 | 1.90 | 0.53 |
| 2:LD:55:THR:H | 2:MD:283:ALA:CA | 2.21 | 0.53 |
| 2:LD:220:PRO:O | 1:LE:324:VAL:HG13 | 2.09 | 0.53 |
| 2:LD:222:TYR:O | 2:LD:226:ASN:ND2 | 2.28 | 0.53 |
| 2:MB:290:THR:HA | 2:MB:293:MET:HE2 | 1.90 | 0.53 |
| 1:MC:188:ILE:HD12 | 1:MC:425:LEU:HD11 | 1.90 | 0.53 |
| 2:MF:290:THR:HA | 2:MF:293:MET:HE2 | 1.90 | 0.53 |
| 7:5A:1243:ASP:HB3 | 9:7B:8:ARG:HH11 | 1.70 | 0.53 |
| 7:5A:1521:PHE:CE2 | 7:5A:1567:PHE:CD1 | 2.96 | 0.53 |
| 7:5A:1577:LYS:CE | 7:5A:1577:LYS:CA | 2.85 | 0.53 |
| 7:5B:1251:SER:HA | 7:5B:1258:ARG:HH21 | 1.73 | 0.53 |
| 7:5B:1399:LYS:HB3 | 7:5B:1399:LYS:NZ | 2.14 | 0.53 |
| 7:5B:1485:LYS:O | 7:5B:1488:GLU:HB3 | 2.09 | 0.53 |
| 7:5B:1503:TYR:CD1 | 7:5B:1508:ARG:CD | 2.86 | 0.53 |
| 2:AD:179:VAL:HG22 | 1:AE:258:ASN:CB | 2.39 | 0.53 |
| 1:AE:178:SER:OG | 2:AF:347:ASN:HB3 | 2.08 | 0.53 |
| 2:AF:273:LEU:H | 2:AF:292:GLN:HE22 | 1.55 | 0.53 |
| 1:BE:100:ALA:HB1 | 2:BF:252:LYS:HA | 1.91 | 0.53 |
| 1:BE:241:SER:OG | 1:BE:250:VAL:O | 2.23 | 0.53 |
| 1:CC:282:TYR:HE2 | 10:8E:18:UNK:HA | 1.73 | 0.53 |
| 2:CD:86:ARG:CA | 2:DD:281:TYR:OH | 2.56 | 0.53 |
| 2:ED:208:TYR:CD2 | 1:EE:326:LYS:HB3 | 2.43 | 0.53 |
| 2:EF:54:ALA:HB1 | 2:FF:281:TYR:O | 2.08 | 0.53 |
| 2:EF:309:ARG:NH2 | 2:EF:426:GLN:O | 2.32 | 0.53 |
| 2:FF:331:LEU:HD21 | 7:5B:915:PHE:CE1 | 2.43 | 0.53 |
| 2:GB:139:LEU:HD13 | 2:GB:168:SER:HB3 | 1.91 | 0.53 |
| 2:GD:409:THR:CB | 7:5A:1330:ILE:HG12 | 2.04 | 0.53 |
| 2:GF:406:MET:CE | 7:5B:1341:LYS:HE3 | 2.39 | 0.53 |
| 1:HA:394:LYS:NZ | 2:HB:347:ASN:OD1 | 2.41 | 0.53 |
| 2:HD:139:LEU:HD13 | 2:HD:168:SER:HB3 | 1.91 | 0.53 |
| 2:IB:273:LEU:H | 2:IB:292:GLN:HE22 | 1.55 | 0.53 |
| 2:IB:290:THR:HA | 2:IB:293:MET:HE2 | 1.90 | 0.53 |
| 2:IB:424:GLN:HE21 | 7:5C:1413:GLN:NE2 | 1.17 | 0.53 |
| 1:IE:178:SER:OG | 2:IF:347:ASN:HB3 | 2.08 | 0.53 |
| 1:JA:184:PRO:O | 1:JA:188:ILE:HG12 | 2.08 | 0.53 |
| 2:JD:290:THR:HA | 2:JD:293:MET:HE2 | 1.90 | 0.53 |
| 1:KC:404:PHE:CE2 | 2:KD:345:ILE:CD1 | 2.90 | 0.53 |
| 2:KD:179:VAL:HG22 | 1:KE:258:ASN:CB | 2.39 | 0.53 |
| 2:KD:222:TYR:O | 2:KD:226:ASN:ND2 | 2.27 | 0.53 |
| 2:KD:273:LEU:H | 2:KD:292:GLN:HE22 | 1.55 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LE:101:ASN:ND2 | 2:LF:252:LYS:CG | 2.72 | 0.53 |
| 2:LF:19:LYS:CE | 6:4D:217:ASN:O | 2.57 | 0.53 |
| 1:MA:188:ILE:HD12 | 1:MA:425:LEU:HD11 | 1.90 | 0.53 |
| 4:2C:112:GLU:OE2 | 4:2C:115:LEU:HD11 | 2.08 | 0.53 |
| 5:3B:224:ASP:HB2 | 5:3B:335:LYS:NZ | 2.24 | 0.53 |
| 7:5A:1064:LYS:C | 7:5A:1066:GLY:H | 2.17 | 0.53 |
| 7:5A:1312:GLU:HA | 7:5A:1315:ARG:HD2 | 1.91 | 0.53 |
| 7:5A:1548:VAL:HA | 7:5A:1569:GLU:CG | 2.35 | 0.53 |
| 7:5B:1475:PHE:CE2 | 7:5B:1565:GLU:OE1 | 2.62 | 0.53 |
| 7:5B:1521:PHE:CE2 | 7:5B:1567:PHE:CD1 | 2.96 | 0.53 |
| 7:5C:839:GLU:OE2 | 8:6C:11:PRO:HG3 | 2.09 | 0.53 |
| 7:5C:1436:ARG:HE | 7:5C:1440:GLU:HG2 | 1.73 | 0.53 |
| 7:5C:1577:LYS:CE | 7:5C:1577:LYS:CA | 2.85 | 0.53 |
| 2:BB:180:VAL:HG12 | 1:BC:258:ASN:OD1 | 2.08 | 0.53 |
| 2:BD:25:SER:HG | 2:BD:51:TYR:HH | 1.54 | 0.53 |
| 2:CB:178:THR:HA | 1:CC:352:LYS:HD3 | 1.90 | 0.53 |
| 1:CC:404:PHE:CE2 | 2:CD:345:ILE:CD1 | 2.90 | 0.53 |
| 1:DC:222:PRO:CG | 2:DD:324:LYS:CD | 2.85 | 0.53 |
| 1:DE:141:VAL:HG11 | 1:DE:172:TYR:CD1 | 2.38 | 0.53 |
| 1:DE:241:SER:OG | 1:DE:250:VAL:O | 2.23 | 0.53 |
| 1:EA:141:VAL:HG11 | 1:EA:172:TYR:CD1 | 2.38 | 0.53 |
| 1:EC:141:VAL:HG11 | 1:EC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:ED:273:LEU:H | 2:ED:292:GLN:HE22 | 1.55 | 0.53 |
| 1:FA:419:SER:HB3 | 7:5C:1256:ARG:CG | 2.37 | 0.53 |
| 2:FD:273:LEU:H | 2:FD:292:GLN:HE22 | 1.55 | 0.53 |
| 1:GA:60:LYS:HD3 | 1:HA:283:HIS:HA | 1.90 | 0.53 |
| 2:GD:139:LEU:HD13 | 2:GD:168:SER:HB3 | 1.91 | 0.53 |
| 2:GF:25:SER:HG | 2:GF:51:TYR:HH | 1.56 | 0.53 |
| 2:ID:139:LEU:HD13 | 2:ID:168:SER:HB3 | 1.90 | 0.53 |
| 2:ID:179:VAL:HG22 | 1:IE:258:ASN:CB | 2.39 | 0.53 |
| 2:ID:290:THR:HA | 2:ID:293:MET:HE2 | 1.90 | 0.53 |
| 1:JE:178:SER:OG | 2:JF:347:ASN:HB3 | 2.08 | 0.53 |
| 2:KB:273:LEU:CB | 6:4A:268:LEU:CG | 2.82 | 0.53 |
| 1:KC:141:VAL:HG11 | 1:KC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:KD:25:SER:HG | 2:KD:51:TYR:HH | 1.55 | 0.53 |
| 2:KD:54:ALA:HA | 2:LD:285:THR:CG2 | 2.39 | 0.53 |
| 2:LB:139:LEU:HD13 | 2:LB:168:SER:HB3 | 1.90 | 0.53 |
| 2:LB:180:VAL:HG12 | 1:LC:258:ASN:OD1 | 2.09 | 0.53 |
| 2:LB:290:THR:HA | 2:LB:293:MET:HE2 | 1.90 | 0.53 |
| 2:LD:212:PHE:CE2 | 1:LE:326:LYS:HB2 | 2.44 | 0.53 |
| 2:LD:290:THR:HA | 2:LD:293:MET:HE2 | 1.90 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:LF:139:LEU:HD13 | 2:LF:168:SER:HB3 | 1.90 | 0.53 |
| 2:LF:290:THR:HA | 2:LF:293:MET:HE2 | 1.90 | 0.53 |
| 2:MB:273:LEU:H | 2:MB:292:GLN:HE22 | 1.55 | 0.53 |
| 5:3A:224:ASP:HB2 | 5:3A:335:LYS:NZ | 2.24 | 0.53 |
| 5:3C:224:ASP:HB2 | 5:3C:335:LYS:NZ | 2.24 | 0.53 |
| 7:5A:1485:LYS:O | 7:5A:1488:GLU:HB3 | 2.09 | 0.53 |
| 7:5C:1064:LYS:C | 7:5C:1066:GLY:H | 2.17 | 0.53 |
| 7:5C:1373:PHE:CD1 | 7:5C:1373:PHE:N | 2.72 | 0.53 |
| 2:AF:290:THR:HA | 2:AF:293:MET:HE2 | 1.90 | 0.53 |
| 1:BC:100:ALA:HB1 | 2:BD:252:LYS:HA | 1.91 | 0.53 |
| 2:DD:273:LEU:H | 2:DD:292:GLN:HE22 | 1.55 | 0.53 |
| 2:DF:273:LEU:H | 2:DF:292:GLN:HE22 | 1.55 | 0.53 |
| 2:EB:85:PHE:C | 2:FB:281:TYR:HH | 2.14 | 0.53 |
| 2:EB:139:LEU:HD13 | 2:EB:168:SER:HB3 | 1.91 | 0.53 |
| 2:ED:139:LEU:HD13 | 2:ED:168:SER:HB3 | 1.90 | 0.53 |
| 2:ED:290:THR:HA | 2:ED:293:MET:HE2 | 1.90 | 0.53 |
| 1:GC:56:THR:O | 1:HC:285:GLN:HA | 2.09 | 0.53 |
| 1:GC:398:MET:SD | 2:GD:345:ILE:CG1 | 2.90 | 0.53 |
| 1:HA:141:VAL:HG11 | 1:HA:172:TYR:CD1 | 2.38 | 0.53 |
| 2:IB:177:ASP:CA | 1:IC:353:VAL:HG12 | 2.39 | 0.53 |
| 2:IF:139:LEU:HD13 | 2:IF:168:SER:HB3 | 1.91 | 0.53 |
| 2:IF:290:THR:HA | 2:IF:293:MET:HE2 | 1.90 | 0.53 |
| 2:JB:177:ASP:CA | 1:JC:353:VAL:HG12 | 2.39 | 0.53 |
| 1:JC:184:PRO:O | 1:JC:188:ILE:HG12 | 2.08 | 0.53 |
| 2:JD:180:VAL:HG12 | 1:JE:258:ASN:OD1 | 2.09 | 0.53 |
| 1:JE:241:SER:OG | 1:JE:250:VAL:O | 2.23 | 0.53 |
| 2:JF:290:THR:HA | 2:JF:293:MET:HE2 | 1.90 | 0.53 |
| 1:KC:404:PHE:HE2 | 2:KD:345:ILE:HD12 | 1.73 | 0.53 |
| 2:KD:180:VAL:HG12 | 1:KE:258:ASN:OD1 | 2.09 | 0.53 |
| 2:LB:55:THR:H | 2:MB:283:ALA:CA | 2.21 | 0.53 |
| 2:LD:139:LEU:HD13 | 2:LD:168:SER:HB3 | 1.91 | 0.53 |
| 2:LD:179:VAL:HG22 | 1:LE:258:ASN:CA | 2.39 | 0.53 |
| 1:LE:222:PRO:CD | 2:LF:324:LYS:HB3 | 2.36 | 0.53 |
| 2:MD:111:GLU:HA | 3:1B:62:SER:CA | 2.39 | 0.53 |
| 4:2A:112:GLU:OE2 | 4:2A:115:LEU:HD11 | 2.08 | 0.53 |
| 5:3A:231:THR:N | 5:3A:335:LYS:HD2 | 1.73 | 0.53 |
| 7:5A:1503:TYR:CD1 | 7:5A:1508:ARG:CD | 2.86 | 0.53 |
| 7:5B:1272:ILE:HD11 | 9:7D:11:TYR:HD2 | 1.74 | 0.53 |
| 2:AD:290:THR:HA | 2:AD:293:MET:HE2 | 1.90 | 0.53 |
| 1:AE:394:LYS:NZ | 2:AF:347:ASN:OD1 | 2.42 | 0.53 |
| 2:BB:179:VAL:HG22 | 1:BC:258:ASN:CB | 2.39 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BF:25:SER:HG | 2:BF:51:TYR:HH | 1.55 | 0.53 |
| 1:CC:100:ALA:HB1 | 2:CD:252:LYS:HA | 1.90 | 0.53 |
| 1:DA:412:GLY:HA2 | 7:5C:792:TYR:CZ | 2.44 | 0.53 |
| 2:DB:273:LEU:H | 2:DB:292:GLN:HE22 | 1.55 | 0.53 |
| 2:DB:290:THR:HA | 2:DB:293:MET:HE2 | 1.90 | 0.53 |
| 1:DC:141:VAL:HG11 | 1:DC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:DD:290:THR:HA | 2:DD:293:MET:HE2 | 1.90 | 0.53 |
| 1:EA:100:ALA:HB1 | 2:EB:252:LYS:CA | 2.39 | 0.53 |
| 2:EB:84:LEU:C | 2:FB:281:TYR:OH | 2.52 | 0.53 |
| 2:EB:290:THR:HA | 2:EB:293:MET:HE2 | 1.90 | 0.53 |
| 2:EF:290:THR:HA | 2:EF:293:MET:HE2 | 1.90 | 0.53 |
| 2:FB:139:LEU:HD13 | 2:FB:168:SER:HB3 | 1.91 | 0.53 |
| 2:GF:139:LEU:HD13 | 2:GF:168:SER:HB3 | 1.91 | 0.53 |
| 2:HB:177:ASP:CA | 1:HC:353:VAL:HG12 | 2.39 | 0.53 |
| 2:HB:273:LEU:H | 2:HB:292:GLN:HE22 | 1.55 | 0.53 |
| 2:HB:290:THR:HA | 2:HB:293:MET:HE2 | 1.90 | 0.53 |
| 1:HC:141:VAL:HG11 | 1:HC:172:TYR:CD1 | 2.38 | 0.53 |
| 2:HD:290:THR:HA | 2:HD:293:MET:HE2 | 1.90 | 0.53 |
| 1:HE:178:SER:OG | 2:HF:347:ASN:HB3 | 2.08 | 0.53 |
| 1:IA:394:LYS:NZ | 2:IB:347:ASN:OD1 | 2.41 | 0.53 |
| 2:JB:273:LEU:H | 2:JB:292:GLN:HE22 | 1.55 | 0.53 |
| 2:JD:273:LEU:H | 2:JD:292:GLN:HE22 | 1.55 | 0.53 |
| 2:KB:25:SER:HG | 2:KB:51:TYR:HH | 1.56 | 0.53 |
| 2:KB:179:VAL:HG22 | 1:KC:258:ASN:CG | 2.34 | 0.53 |
| 2:KB:273:LEU:H | 2:KB:292:GLN:HE22 | 1.55 | 0.53 |
| 1:KE:141:VAL:HG11 | 1:KE:172:TYR:CD1 | 2.38 | 0.53 |
| 1:KE:394:LYS:NZ | 2:KF:347:ASN:OD1 | 2.42 | 0.53 |
| 2:KF:86:ARG:NH2 | 2:LF:281:TYR:O | 2.41 | 0.53 |
| 1:LA:89:PRO:N | 1:MA:280:LYS:HZ2 | 2.07 | 0.53 |
| 1:LC:178:SER:OG | 2:LD:347:ASN:CB | 2.50 | 0.53 |
| 2:LF:340:TYR:CD1 | 4:2B:147:PHE:CA | 2.91 | 0.53 |
| 1:MC:222:PRO:HG2 | 2:MD:324:LYS:HD3 | 1.91 | 0.53 |
| 2:MD:273:LEU:H | 2:MD:292:GLN:HE22 | 1.55 | 0.53 |
| 6:4D:247:LYS:HD3 | 6:4D:247:LYS:N | 2.24 | 0.53 |
| 7:5A:1436:ARG:HE | 7:5A:1440:GLU:HG2 | 1.73 | 0.53 |
| 7:5A:1475:PHE:CE2 | 7:5A:1565:GLU:OE1 | 2.62 | 0.53 |
| 7:5B:1489:PHE:HA | 7:5B:1492:SER:CB | 2.27 | 0.53 |
| 7:5C:1312:GLU:HA | 7:5C:1315:ARG:HD2 | 1.91 | 0.53 |
| 7:5C:1485:LYS:O | 7:5C:1488:GLU:HB3 | 2.09 | 0.53 |
| 2:AB:273:LEU:H | 2:AB:292:GLN:HE22 | 1.55 | 0.52 |
| 2:BD:290:THR:HA | 2:BD:293:MET:HE2 | 1.90 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:176:SER:CB | 1:CC:349:THR:OG1 | 2.57 | 0.52 |
| 2:CB:273:LEU:H | 2:CB:292:GLN:HE22 | 1.55 | 0.52 |
| 2:CD:273:LEU:H | 2:CD:292:GLN:HE22 | 1.55 | 0.52 |
| 2:DF:60:VAL:CG2 | 2:EF:281:TYR:CE1 | 2.92 | 0.52 |
| 2:EF:139:LEU:HD13 | 2:EF:168:SER:HB3 | 1.91 | 0.52 |
| 2:FB:25:SER:HG | 2:FB:51:TYR:HH | 1.56 | 0.52 |
| 2:FD:139:LEU:HD13 | 2:FD:168:SER:HB3 | 1.91 | 0.52 |
| 2:FD:290:THR:HA | 2:FD:293:MET:HE2 | 1.90 | 0.52 |
| 2:FF:273:LEU:H | 2:FF:292:GLN:HE22 | 1.55 | 0.52 |
| 1:GA:222:PRO:HD2 | 2:GB:324:LYS:HD3 | 1.91 | 0.52 |
| 2:GF:273:LEU:H | 2:GF:292:GLN:HE22 | 1.55 | 0.52 |
| 1:HE:401:LYS:CE | 2:HF:344:TRP:CZ3 | 2.67 | 0.52 |
| 2:HF:290:THR:HA | 2:HF:293:MET:HE2 | 1.90 | 0.52 |
| 1:IA:279:GLU:CG | 10:8V:22:UNK:CB | 2.87 | 0.52 |
| 2:IB:139:LEU:HD13 | 2:IB:168:SER:HB3 | 1.91 | 0.52 |
| 1:IC:402:ARG:HH22 | 7:5A:1418:GLN:HA | 1.70 | 0.52 |
| 2:ID:180:VAL:HG12 | 1:IE:258:ASN:OD1 | 2.09 | 0.52 |
| 2:KF:217:LEU:HD13 | 6:4D:263:CYS:SG | 2.49 | 0.52 |
| 2:KF:273:LEU:H | 2:KF:292:GLN:HE22 | 1.55 | 0.52 |
| 2:LB:379:LYS:HB3 | 4:2C:166:ILE:CG1 | 2.32 | 0.52 |
| 1:LC:89:PRO:HG2 | 1:MC:280:LYS:HD2 | 1.80 | 0.52 |
| 2:LD:212:PHE:HE2 | 1:LE:326:LYS:HB2 | 1.75 | 0.52 |
| 2:LD:222:TYR:CD2 | 1:LE:247:ALA:HB1 | 2.45 | 0.52 |
| 2:LF:227:HIS:CE1 | 6:4D:226:ILE:CG1 | 2.88 | 0.52 |
| 2:MF:273:LEU:H | 2:MF:292:GLN:HE22 | 1.55 | 0.52 |
| 6:4B:247:LYS:HD3 | 6:4B:247:LYS:N | 2.24 | 0.52 |
| 7:5A:1120:ASP:CG | 7:5A:1125:LEU:HB2 | 2.34 | 0.52 |
| 7:5B:1436:ARG:HE | 7:5B:1440:GLU:HG2 | 1.73 | 0.52 |
| 7:5C:1120:ASP:CG | 7:5C:1125:LEU:HB2 | 2.34 | 0.52 |
| 7:5C:1503:TYR:CD1 | 7:5C:1508:ARG:CD | 2.86 | 0.52 |
| 7:5C:1548:VAL:HA | 7:5C:1569:GLU:CG | 2.35 | 0.52 |
| 8:6A:108:LYS:HB2 | 8:6A:111:SER:HB2 | 1.91 | 0.52 |
| 8:6B:108:LYS:HB2 | 8:6B:111:SER:HB2 | 1.91 | 0.52 |
| 8:6C:102:ASN:HD21 | 8:6C:134:LYS:C | 2.17 | 0.52 |
| 9:7A:11:TYR:HE1 | 9:7B:26:LEU:CD2 | 1.89 | 0.52 |
| 2:AB:290:THR:HA | 2:AB:293:MET:HE2 | 1.90 | 0.52 |
| 2:BD:318:ARG:HH11 | 2:BD:358:PRO:HG3 | 1.75 | 0.52 |
| 2:CD:212:PHE:CZ | 1:CE:326:LYS:CE | 2.92 | 0.52 |
| 2:CF:273:LEU:H | 2:CF:292:GLN:HE22 | 1.55 | 0.52 |
| 1:DA:400:ALA:HA | 7:5C:775:PRO:HB3 | 1.91 | 0.52 |
| 2:DD:390:ARG:HD2 | 1:DE:439:THR:HG21 | 1.91 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:DF:290:THR:HA | 2:DF:293:MET:HE2 | 1.90 | 0.52 |
| 1:EE:430:LYS:HZ3 | 7:5B:834:ASN:HD21 | 0.89 | 0.52 |
| 2:FB:290:THR:HA | 2:FB:293:MET:HE2 | 1.90 | 0.52 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:CE | 2.81 | 0.52 |
| 1:GC:100:ALA:HB1 | 2:GD:252:LYS:HA | 1.91 | 0.52 |
| 2:HB:177:ASP:CG | 1:HC:353:VAL:HG13 | 1.99 | 0.52 |
| 2:HB:362:LYS:NZ | 10:8S:36:UNK:O | 2.35 | 0.52 |
| 1:HE:141:VAL:HG11 | 1:HE:172:TYR:CD1 | 2.38 | 0.52 |
| 2:JB:86:ARG:HH22 | 2:KB:280:GLN:HB3 | 1.65 | 0.52 |
| 1:JC:398:MET:SD | 2:JD:345:ILE:CG1 | 2.90 | 0.52 |
| 1:JE:184:PRO:O | 1:JE:188:ILE:HG12 | 2.08 | 0.52 |
| 2:KB:139:LEU:HD13 | 2:KB:168:SER:HB3 | 1.91 | 0.52 |
| 1:KC:178:SER:OG | 2:KD:347:ASN:HB3 | 2.09 | 0.52 |
| 2:KD:139:LEU:HD13 | 2:KD:168:SER:HB3 | 1.91 | 0.52 |
| 2:KF:139:LEU:HD13 | 2:KF:168:SER:HB3 | 1.91 | 0.52 |
| 2:LD:224:ASP:CG | 6:4B:219:ASN:ND2 | 2.61 | 0.52 |
| 2:LF:310:TYR:HE2 | 4:2B:147:PHE:CE2 | 2.26 | 0.52 |
| 1:MC:96:LYS:HE2 | 2:MD:1:MET:HE3 | 1.91 | 0.52 |
| 4:2B:112:GLU:OE2 | 4:2B:115:LEU:HD11 | 2.08 | 0.52 |
| 7:5A:1332:GLN:HE21 | 7:5A:1332:GLN:HA | 1.72 | 0.52 |
| 7:5B:1579:LYS:C | 7:5B:1583:ASN:CG | 2.75 | 0.52 |
| 7:5C:1332:GLN:HE21 | 7:5C:1332:GLN:HA | 1.72 | 0.52 |
| 2:AB:177:ASP:CA | 1:AC:353:VAL:HG12 | 2.39 | 0.52 |
| 2:AB:179:VAL:HG22 | 1:AC:258:ASN:CG | 2.34 | 0.52 |
| 1:AC:178:SER:OG | 2:AD:347:ASN:HB3 | 2.09 | 0.52 |
| 2:AD:357:PRO:HG2 | 6:4C:151:ARG:CD | 2.39 | 0.52 |
| 1:BA:60:LYS:NZ | 1:CA:283:HIS:NE2 | 2.54 | 0.52 |
| 2:BB:222:TYR:HD2 | 1:BC:247:ALA:HB1 | 1.74 | 0.52 |
| 1:BE:141:VAL:HG11 | 1:BE:172:TYR:CD1 | 2.38 | 0.52 |
| 2:BF:290:THR:HA | 2:BF:293:MET:HE2 | 1.90 | 0.52 |
| 2:CF:290:THR:HA | 2:CF:293:MET:HE2 | 1.90 | 0.52 |
| 1:DA:404:PHE:HE2 | 2:DB:345:ILE:HD12 | 1.75 | 0.52 |
| 2:DB:180:VAL:HG12 | 1:DC:258:ASN:OD1 | 2.10 | 0.52 |
| 1:EA:430:LYS:HZ1 | 7:5C:834:ASN:HD21 | 0.69 | 0.52 |
| 1:FC:176:GLN:O | 2:FD:347:ASN:ND2 | 2.34 | 0.52 |
| 2:FF:25:SER:HG | 2:FF:51:TYR:HH | 1.56 | 0.52 |
| 2:GB:177:ASP:CA | 1:GC:353:VAL:HG12 | 2.39 | 0.52 |
| 2:HD:318:ARG:HH11 | 2:HD:358:PRO:HG3 | 1.75 | 0.52 |
| 1:HE:196:GLU:HG3 | 5:3A:211:GLN:HE22 | 1.74 | 0.52 |
| 2:LB:305:PRO:HG2 | 4:2C:149:ILE:HD11 | 1.90 | 0.52 |
| 2:LF:318:ARG:HH11 | 2:LF:358:PRO:HG3 | 1.75 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LF:340:TYR:OH | 4:2B:146:PRO:HA | 2.10 | 0.52 |
| 4:2B:105:ALA:HB2 | 4:2B:124:LEU:HD22 | 1.91 | 0.52 |
| 4:2C:105:ALA:HB2 | 4:2C:124:LEU:HD22 | 1.91 | 0.52 |
| 6:4B:164:ARG:NH1 | 6:4B:164:ARG:CB | 2.72 | 0.52 |
| 6:4B:285:ARG:HB3 | 6:4B:285:ARG:CZ | 2.38 | 0.52 |
| 7:5C:1475:PHE:CE2 | 7:5C:1565:GLU:OE1 | 2.62 | 0.52 |
| 2:BB:290:THR:HA | 2:BB:293:MET:HE2 | 1.90 | 0.52 |
| 2:BB:318:ARG:HH11 | 2:BB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:CB:318:ARG:HH11 | 2:CB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:CD:290:THR:HA | 2:CD:293:MET:HE2 | 1.90 | 0.52 |
| 1:CE:404:PHE:CE2 | 2:CF:345:ILE:CD1 | 2.91 | 0.52 |
| 1:DA:401:LYS:HE3 | 2:DB:344:TRP:CZ3 | 2.44 | 0.52 |
| 2:DB:139:LEU:HD13 | 2:DB:168:SER:HB3 | 1.91 | 0.52 |
| 2:DD:178:THR:HA | 1:DE:352:LYS:HD3 | 1.91 | 0.52 |
| 2:DF:60:VAL:HG21 | 2:EF:281:TYR:CE1 | 2.44 | 0.52 |
| 2:ED:178:THR:HA | 1:EE:352:LYS:HD3 | 1.91 | 0.52 |
| 2:FF:139:LEU:HD13 | 2:FF:168:SER:HB3 | 1.91 | 0.52 |
| 2:FF:290:THR:HA | 2:FF:293:MET:HE2 | 1.90 | 0.52 |
| 1:GC:56:THR:OG1 | 1:HC:284:GLU:C | 2.51 | 0.52 |
| 1:GC:178:SER:OG | 2:GD:347:ASN:HB3 | 2.09 | 0.52 |
| 2:GD:290:THR:HA | 2:GD:293:MET:HE2 | 1.90 | 0.52 |
| 2:GF:290:THR:HA | 2:GF:293:MET:HE2 | 1.90 | 0.52 |
| 1:IC:178:SER:OG | 2:ID:347:ASN:HB3 | 2.09 | 0.52 |
| 1:JA:222:PRO:HD2 | 2:JB:324:LYS:HD3 | 1.92 | 0.52 |
| 1:JC:89:PRO:HD2 | 1:KC:283:HIS:CG | 2.40 | 0.52 |
| 1:JC:178:SER:OG | 2:JD:347:ASN:HB3 | 2.09 | 0.52 |
| 2:JD:179:VAL:HG22 | 1:JE:258:ASN:CB | 2.39 | 0.52 |
| 1:JE:101:ASN:ND2 | 2:JF:252:LYS:HG3 | 2.14 | 0.52 |
| 2:JF:273:LEU:H | 2:JF:292:GLN:HE22 | 1.55 | 0.52 |
| 1:KC:100:ALA:HB1 | 2:KD:252:LYS:HA | 1.91 | 0.52 |
| 2:KD:125:GLU:HA | 4:2A:37:GLY:O | 2.09 | 0.52 |
| 2:LD:179:VAL:HG23 | 1:LE:258:ASN:HA | 1.90 | 0.52 |
| 1:LE:35:GLN:HE21 | 6:4B:101:ARG:CB | 2.17 | 0.52 |
| 2:LF:222:TYR:O | 2:LF:226:ASN:ND2 | 2.27 | 0.52 |
| 2:LF:273:LEU:H | 2:LF:292:GLN:HE22 | 1.55 | 0.52 |
| 2:MB:25:SER:HG | 2:MB:51:TYR:HH | 1.56 | 0.52 |
| 4:2A:105:ALA:HB2 | 4:2A:124:LEU:HD22 | 1.91 | 0.52 |
| 6:4A:164:ARG:NH1 | 6:4A:164:ARG:CB | 2.72 | 0.52 |
| 6:4A:247:LYS:HD3 | 6:4A:247:LYS:N | 2.24 | 0.52 |
| 6:4A:285:ARG:HB3 | 6:4A:285:ARG:CZ | 2.38 | 0.52 |
| 6:4D:175:LEU:N | 6:4D:175:LEU:CD2 | 2.73 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:4D:179:ARG:CZ | 6:4D:179:ARG:CB | 2.85 | 0.52 |
| 6:4D:285:ARG:HB3 | 6:4D:285:ARG:CZ | 2.38 | 0.52 |
| 7:5A:1548:VAL:HG12 | 7:5A:1566:GLU:N | 2.19 | 0.52 |
| 7:5B:1120:ASP:CG | 7:5B:1125:LEU:HB2 | 2.34 | 0.52 |
| 7:5B:1312:GLU:HA | 7:5B:1315:ARG:HB3 | 1.90 | 0.52 |
| 7:5B:1332:GLN:HE21 | 7:5B:1332:GLN:HA | 1.72 | 0.52 |
| 7:5B:1548:VAL:CG1 | 7:5B:1566:GLU:C | 2.78 | 0.52 |
| 7:5C:1552:LYS:HZ3 | 7:5C:1563:SER:HB2 | 0.70 | 0.52 |
| 9:7A:42:LEU:HD13 | 9:7B:39:GLY:HA3 | 1.88 | 0.52 |
| 1:AC:342:GLN:HE22 | 3:1C:55:HIS:CE1 | 2.23 | 0.52 |
| 2:BB:273:LEU:H | 2:BB:292:GLN:HE22 | 1.55 | 0.52 |
| 2:BD:273:LEU:H | 2:BD:292:GLN:HE22 | 1.55 | 0.52 |
| 2:BF:273:LEU:H | 2:BF:292:GLN:HE22 | 1.55 | 0.52 |
| 2:BF:318:ARG:HH11 | 2:BF:358:PRO:HG3 | 1.75 | 0.52 |
| 2:CB:25:SER:HG | 2:CB:51:TYR:HH | 1.57 | 0.52 |
| 2:CB:290:THR:HA | 2:CB:293:MET:HE2 | 1.90 | 0.52 |
| 2:CD:318:ARG:HH11 | 2:CD:358:PRO:HG3 | 1.75 | 0.52 |
| 2:CF:318:ARG:HH11 | 2:CF:358:PRO:HG3 | 1.75 | 0.52 |
| 2:DB:318:ARG:HH11 | 2:DB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:DB:390:ARG:HD2 | 1:DC:439:THR:HG21 | 1.92 | 0.52 |
| 2:DD:139:LEU:HD13 | 2:DD:168:SER:HB3 | 1.91 | 0.52 |
| 2:DD:220:PRO:HD2 | 1:DE:326:LYS:CD | 2.39 | 0.52 |
| 2:DD:318:ARG:HH11 | 2:DD:358:PRO:HG3 | 1.75 | 0.52 |
| 1:DE:101:ASN:ND2 | 2:DF:252:LYS:HG3 | 2.16 | 0.52 |
| 2:EB:55:THR:N | 2:FB:283:ALA:HB2 | 2.25 | 0.52 |
| 2:FD:25:SER:HG | 2:FD:51:TYR:HH | 1.56 | 0.52 |
| 2:FD:212:PHE:CZ | 1:FE:326:LYS:CE | 2.87 | 0.52 |
| 2:GD:222:TYR:CD2 | 1:GE:247:ALA:HB1 | 2.44 | 0.52 |
| 1:GE:394:LYS:NZ | 2:GF:347:ASN:OD1 | 2.42 | 0.52 |
| 2:HB:222:TYR:O | 2:HB:226:ASN:ND2 | 2.27 | 0.52 |
| 2:HF:318:ARG:HH11 | 2:HF:358:PRO:HG3 | 1.75 | 0.52 |
| 2:IB:179:VAL:HG22 | 1:IC:258:ASN:CG | 2.34 | 0.52 |
| 2:JD:139:LEU:HD13 | 2:JD:168:SER:HB3 | 1.91 | 0.52 |
| 2:LD:318:ARG:HH11 | 2:LD:358:PRO:HG3 | 1.75 | 0.52 |
| 2:LF:55:THR:CG2 | 2:MF:283:ALA:C | 2.77 | 0.52 |
| 1:MC:282:TYR:HD2 | 6:4A:104:ARG:NE | 2.07 | 0.52 |
| 2:MD:79:GLY:C | 6:4B:179:ARG:HD2 | 2.34 | 0.52 |
| 2:MD:139:LEU:HD13 | 2:MD:168:SER:HB3 | 1.91 | 0.52 |
| 2:MF:139:LEU:HD13 | 2:MF:168:SER:HB3 | 1.91 | 0.52 |
| 6:4A:120:GLN:O | 6:4A:121:ARG:C | 2.52 | 0.52 |
| 6:4B:175:LEU:N | 6:4B:175:LEU:CD2 | 2.73 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:4C:120:GLN:O | 6:4C:121:ARG:C | 2.52 | 0.52 |
| 6:4C:164:ARG:NH1 | 6:4C:164:ARG:CB | 2.72 | 0.52 |
| 7:5A:1272:ILE:HG12 | 9:7B:11:TYR:CE2 | 2.44 | 0.52 |
| 7:5C:1572:LEU:CG | 7:5C:1576:ILE:HD11 | 2.39 | 0.52 |
| 8:6B:102:ASN:HD21 | 8:6B:134:LYS:C | 2.17 | 0.52 |
| 9:7A:15:VAL:CA | 9:7B:35:ILE:HD12 | 2.02 | 0.52 |
| 9:7E:35:ILE:O | 9:7F:43:LEU:CD2 | 2.58 | 0.52 |
| 9:7E:42:LEU:HD13 | 9:7F:39:GLY:CA | 2.40 | 0.52 |
| 1:AA:222:PRO:HD2 | 2:AB:324:LYS:HD3 | 1.92 | 0.52 |
| 1:BA:141:VAL:HG11 | 1:BA:172:TYR:CD1 | 2.38 | 0.52 |
| 1:BC:141:VAL:HG11 | 1:BC:172:TYR:CD1 | 2.38 | 0.52 |
| 2:BD:212:PHE:CZ | 1:BE:326:LYS:CE | 2.91 | 0.52 |
| 2:DB:60:VAL:CG2 | 2:EB:281:TYR:CE1 | 2.92 | 0.52 |
| 2:DF:139:LEU:HD13 | 2:DF:168:SER:HB3 | 1.91 | 0.52 |
| 2:EB:318:ARG:HH11 | 2:EB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:ED:176:SER:CB | 1:EE:349:THR:OG1 | 2.57 | 0.52 |
| 2:ED:318:ARG:HH11 | 2:ED:358:PRO:HG3 | 1.75 | 0.52 |
| 2:FD:54:ALA:CA | 2:GD:283:ALA:CB | 2.52 | 0.52 |
| 1:FE:423:GLU:HG3 | 7:5B:1256:ARG:HH21 | 1.74 | 0.52 |
| 2:GB:290:THR:HA | 2:GB:293:MET:HE2 | 1.90 | 0.52 |
| 2:HB:179:VAL:HG22 | 1:HC:258:ASN:CG | 2.34 | 0.52 |
| 1:HC:100:ALA:HB1 | 2:HD:252:LYS:HA | 1.91 | 0.52 |
| 1:HC:178:SER:OG | 2:HD:347:ASN:HB3 | 2.09 | 0.52 |
| 2:HD:222:TYR:CD2 | 1:HE:247:ALA:HB1 | 2.45 | 0.52 |
| 1:IA:278:ALA:HB3 | 10:8V:21:UNK:CA | 2.39 | 0.52 |
| 2:ID:85:PHE:C | 2:JD:281:TYR:OH | 2.53 | 0.52 |
| 2:IF:85:PHE:C | 2:JF:281:TYR:OH | 2.52 | 0.52 |
| 2:JB:179:VAL:HG22 | 1:JC:258:ASN:CG | 2.35 | 0.52 |
| 2:JF:139:LEU:HD13 | 2:JF:168:SER:HB3 | 1.91 | 0.52 |
| 2:KD:222:TYR:CD2 | 1:KE:247:ALA:HB1 | 2.44 | 0.52 |
| 1:LA:101:ASN:ND2 | 2:LB:252:LYS:CG | 2.73 | 0.52 |
| 2:LB:177:ASP:O | 1:LC:352:LYS:HA | 2.10 | 0.52 |
| 1:LC:101:ASN:ND2 | 2:LD:252:LYS:HG3 | 2.25 | 0.52 |
| 2:LD:273:LEU:H | 2:LD:292:GLN:HE22 | 1.55 | 0.52 |
| 2:MB:139:LEU:HD13 | 2:MB:168:SER:HB3 | 1.91 | 0.52 |
| 6:4A:247:LYS:N | 6:4A:247:LYS:CD | 2.73 | 0.52 |
| 6:4B:120:GLN:O | 6:4B:121:ARG:C | 2.52 | 0.52 |
| 6:4B:247:LYS:N | 6:4B:247:LYS:CD | 2.73 | 0.52 |
| 6:4C:247:LYS:HD3 | 6:4C:247:LYS:N | 2.24 | 0.52 |
| 6:4D:247:LYS:N | 6:4D:247:LYS:CD | 2.73 | 0.52 |
| 7:5A:1285:ARG:HD3 | 7:5A:1285:ARG:N | 2.21 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1312:GLU:HA | 7:5A:1315:ARG:HB3 | 1.90 | 0.52 |
| 7:5A:1343:LYS:CD | 7:5A:1343:LYS:N | 2.73 | 0.52 |
| 7:5A:1579:LYS:C | 7:5A:1583:ASN:CG | 2.75 | 0.52 |
| 7:5B:801:LEU:N | 7:5B:801:LEU:CD2 | 2.73 | 0.52 |
| 7:5B:1343:LYS:CD | 7:5B:1343:LYS:N | 2.73 | 0.52 |
| 7:5C:1312:GLU:HA | 7:5C:1315:ARG:HB3 | 1.90 | 0.52 |
| 7:5C:1399:LYS:HB3 | 7:5C:1399:LYS:HZ1 | 1.74 | 0.52 |
| 2:AB:318:ARG:HH11 | 2:AB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:AD:318:ARG:HH11 | 2:AD:358:PRO:HG3 | 1.75 | 0.52 |
| 2:BB:139:LEU:HD13 | 2:BB:168:SER:HB3 | 1.90 | 0.52 |
| 2:BB:177:ASP:C | 1:BC:352:LYS:HA | 2.34 | 0.52 |
| 1:BC:176:GLN:O | 2:BD:347:ASN:ND2 | 2.35 | 0.52 |
| 2:BD:86:ARG:HA | 2:CD:281:TYR:OH | 2.09 | 0.52 |
| 2:DD:212:PHE:HE2 | 1:DE:326:LYS:HB2 | 1.75 | 0.52 |
| 2:DF:318:ARG:HH11 | 2:DF:358:PRO:HG3 | 1.75 | 0.52 |
| 1:EA:430:LYS:NZ | 7:5C:834:ASN:HD22 | 0.44 | 0.52 |
| 2:EF:318:ARG:HH11 | 2:EF:358:PRO:HG3 | 1.75 | 0.52 |
| 1:FC:222:PRO:HG3 | 2:FD:324:LYS:CD | 2.39 | 0.52 |
| 2:HD:180:VAL:HG12 | 1:HE:258:ASN:OD1 | 2.09 | 0.52 |
| 1:IA:402:ARG:NH2 | 7:5C:1417:GLN:CA | 2.73 | 0.52 |
| 2:JB:139:LEU:HD13 | 2:JB:168:SER:HB3 | 1.91 | 0.52 |
| 1:JE:394:LYS:NZ | 2:JF:347:ASN:OD1 | 2.42 | 0.52 |
| 1:KC:85:GLN:C | 1:LC:283:HIS:CA | 2.77 | 0.52 |
| 1:LA:245:ASP:OD1 | 6:4C:216:ARG:NE | 2.43 | 0.52 |
| 2:LB:318:ARG:HH11 | 2:LB:358:PRO:HG3 | 1.75 | 0.52 |
| 2:LB:394:PHE:CD1 | 1:LC:261:PRO:HA | 2.44 | 0.52 |
| 2:MB:221:THR:HB | 6:4A:189:ARG:NH1 | 2.25 | 0.52 |
| 2:MD:220:PRO:O | 1:ME:324:VAL:HG11 | 2.09 | 0.52 |
| 6:4C:247:LYS:N | 6:4C:247:LYS:CD | 2.73 | 0.52 |
| 6:4C:285:ARG:HB3 | 6:4C:285:ARG:CZ | 2.38 | 0.52 |
| 6:4D:120:GLN:O | 6:4D:121:ARG:C | 2.52 | 0.52 |
| 7:5A:801:LEU:N | 7:5A:801:LEU:CD2 | 2.73 | 0.52 |
| 7:5A:1489:PHE:HA | 7:5A:1492:SER:CB | 2.27 | 0.52 |
| 7:5A:1572:LEU:CG | 7:5A:1576:ILE:HD11 | 2.39 | 0.52 |
| 7:5B:841:VAL:HG23 | 8:6B:11:PRO:HG3 | 1.91 | 0.52 |
| 7:5B:1285:ARG:HD3 | 7:5B:1285:ARG:N | 2.21 | 0.52 |
| 7:5B:1491:LEU:N | 7:5B:1495:PHE:HB2 | 2.13 | 0.52 |
| 7:5C:1285:ARG:HD3 | 7:5C:1285:ARG:N | 2.21 | 0.52 |
| 7:5C:1343:LYS:CD | 7:5C:1343:LYS:N | 2.73 | 0.52 |
| 7:5C:1436:ARG:HH21 | 7:5C:1440:GLU:HB2 | 1.74 | 0.52 |
| 7:5C:1548:VAL:HG12 | 7:5C:1566:GLU:N | 2.18 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:6B:208:LYS:NZ | 8:6B:236:ASP:OD2 | 2.42 | 0.52 |
| 9:7A:7:LEU:CD2 | 9:7B:30:ARG:HE | 2.22 | 0.52 |
| 2:AD:139:LEU:HD13 | 2:AD:168:SER:HB3 | 1.90 | 0.52 |
| 2:AD:222:TYR:CD2 | 1:AE:247:ALA:HB1 | 2.44 | 0.52 |
| 2:AD:406:MET:O | 2:AD:410:GLU:HG3 | 2.10 | 0.52 |
| 2:AF:139:LEU:HD13 | 2:AF:168:SER:HB3 | 1.91 | 0.52 |
| 2:AF:406:MET:O | 2:AF:410:GLU:HG3 | 2.10 | 0.52 |
| 2:CB:139:LEU:HD13 | 2:CB:168:SER:HB3 | 1.91 | 0.52 |
| 2:CB:212:PHE:HE2 | 1:CC:326:LYS:HB2 | 1.75 | 0.52 |
| 2:CD:25:SER:HG | 2:CD:51:TYR:HH | 1.57 | 0.52 |
| 2:CD:397:TRP:CD2 | 1:CE:256:GLN:O | 2.36 | 0.52 |
| 2:CF:139:LEU:HD13 | 2:CF:168:SER:HB3 | 1.91 | 0.52 |
| 2:FD:178:THR:HA | 1:FE:352:LYS:HD3 | 1.90 | 0.52 |
| 1:HC:404:PHE:CE2 | 2:HD:345:ILE:CD1 | 2.90 | 0.52 |
| 2:ID:222:TYR:CD2 | 1:IE:247:ALA:HB1 | 2.44 | 0.52 |
| 2:JD:177:ASP:CA | 1:JE:353:VAL:HG12 | 2.40 | 0.52 |
| 2:KB:86:ARG:HD3 | 2:LB:288:GLU:HG3 | 1.92 | 0.52 |
| 2:KB:98:GLY:CA | 1:KC:254:GLU:CG | 2.48 | 0.52 |
| 1:KC:85:GLN:HA | 1:LC:283:HIS:HD2 | 1.59 | 0.52 |
| 2:KF:222:TYR:O | 2:KF:226:ASN:ND2 | 2.28 | 0.52 |
| 2:LB:273:LEU:H | 2:LB:292:GLN:HE22 | 1.55 | 0.52 |
| 2:LB:379:LYS:HE3 | 4:2C:164:ARG:O | 2.09 | 0.52 |
| 6:4A:175:LEU:N | 6:4A:175:LEU:CD2 | 2.73 | 0.52 |
| 7:5B:1572:LEU:CG | 7:5B:1576:ILE:HD11 | 2.39 | 0.52 |
| 7:5C:801:LEU:N | 7:5C:801:LEU:CD2 | 2.73 | 0.52 |
| 7:5C:1407:GLN:NE2 | 7:5C:1407:GLN:CA | 2.73 | 0.52 |
| 7:5C:1548:VAL:CG1 | 7:5C:1569:GLU:CB | 2.54 | 0.52 |
| 8:6A:102:ASN:HD21 | 8:6A:134:LYS:C | 2.17 | 0.52 |
| 8:6C:177:TYR:HE1 | 8:6C:199:ILE:HD13 | 1.74 | 0.52 |
| 2:AB:406:MET:O | 2:AB:410:GLU:HG3 | 2.10 | 0.52 |
| 1:AC:100:ALA:HB1 | 2:AD:252:LYS:HA | 1.91 | 0.52 |
| 2:AF:318:ARG:HH11 | 2:AF:358:PRO:HG3 | 1.75 | 0.52 |
| 2:DF:84:LEU:C | 2:EF:281:TYR:OH | 2.52 | 0.52 |
| 1:EA:393:HIS:CE1 | 7:5C:814:LYS:CG | 2.92 | 0.52 |
| 2:FB:390:ARG:HD3 | 1:FC:439:THR:HG21 | 1.92 | 0.52 |
| 2:HB:318:ARG:HH11 | 2:HB:358:PRO:HG3 | 1.75 | 0.52 |
| 1:IC:224:TYR:CE2 | 2:ID:246:LEU:HD11 | 2.43 | 0.52 |
| 2:ID:177:ASP:CA | 1:IE:353:VAL:HG12 | 2.40 | 0.52 |
| 2:KB:177:ASP:CA | 1:KC:353:VAL:HG12 | 2.39 | 0.52 |
| 2:KB:180:VAL:HG12 | 1:KC:258:ASN:OD1 | 2.10 | 0.52 |
| 1:KC:176:GLN:O | 2:KD:347:ASN:ND2 | 2.35 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KD:98:GLY:CA | 1:KE:254:GLU:CG | 2.48 | 0.52 |
| 1:LE:222:PRO:CG | 2:LF:324:LYS:HB2 | 2.33 | 0.52 |
| 2:LF:223:GLY:C | 6:4D:219:ASN:CG | 2.73 | 0.52 |
| 2:MB:221:THR:CG2 | 6:4A:189:ARG:NH2 | 2.34 | 0.52 |
| 2:MB:394:PHE:CD1 | 1:MC:261:PRO:HA | 2.44 | 0.52 |
| 1:ME:372:MET:HE1 | 6:4B:96:VAL:O | 1.95 | 0.52 |
| 6:4B:179:ARG:CB | 6:4B:179:ARG:CZ | 2.85 | 0.52 |
| 6:4C:175:LEU:N | 6:4C:175:LEU:CD2 | 2.73 | 0.52 |
| 6:4C:285:ARG:HH11 | 6:4C:285:ARG:CB | 2.22 | 0.52 |
| 6:4D:241:LYS:C | 6:4D:241:LYS:HD3 | 2.32 | 0.52 |
| 7:5A:1436:ARG:HH21 | 7:5A:1440:GLU:HB2 | 1.74 | 0.52 |
| 7:5B:1552:LYS:HZ1 | 7:5B:1563:SER:N | 2.08 | 0.52 |
| 7:5C:1411:LYS:HD3 | 7:5C:1411:LYS:C | 2.34 | 0.52 |
| 7:5C:1484:TYR:HD1 | 7:5C:1568:LYS:CD | 1.93 | 0.52 |
| 7:5C:1521:PHE:CE2 | 7:5C:1567:PHE:CD1 | 2.96 | 0.52 |
| 8:6C:208:LYS:NZ | 8:6C:236:ASP:OD2 | 2.42 | 0.52 |
| 9:7E:35:ILE:HG23 | 9:7F:42:LEU:C | 2.33 | 0.52 |
| 2:AB:25:SER:HG | 2:AB:51:TYR:HH | 1.55 | 0.52 |
| 2:AB:139:LEU:HD13 | 2:AB:168:SER:HB3 | 1.91 | 0.52 |
| 2:BD:139:LEU:HD13 | 2:BD:168:SER:HB3 | 1.91 | 0.52 |
| 1:BE:101:ASN:ND2 | 2:BF:252:LYS:HG3 | 2.17 | 0.52 |
| 2:BF:139:LEU:HD13 | 2:BF:168:SER:HB3 | 1.90 | 0.52 |
| 2:CD:139:LEU:HD13 | 2:CD:168:SER:HB3 | 1.91 | 0.52 |
| 1:EC:118:CYS:O | 1:EC:122:ILE:HG12 | 2.10 | 0.52 |
| 2:HD:177:ASP:CA | 1:HE:353:VAL:HG12 | 2.40 | 0.52 |
| 1:HE:60:LYS:HZ2 | 1:IE:283:HIS:CD2 | 2.27 | 0.52 |
| 1:HE:394:LYS:NZ | 2:HF:347:ASN:OD1 | 2.42 | 0.52 |
| 1:IA:222:PRO:HD2 | 2:IB:324:LYS:HD3 | 1.92 | 0.52 |
| 2:IB:180:VAL:HG12 | 1:IC:258:ASN:OD1 | 2.10 | 0.52 |
| 1:JA:88:HIS:O | 1:KA:280:LYS:CE | 2.58 | 0.52 |
| 1:JE:92:LEU:H | 1:KE:280:LYS:NZ | 2.08 | 0.52 |
| 1:KA:85:GLN:HG2 | 1:LA:283:HIS:CD2 | 2.45 | 0.52 |
| 2:LD:306:ARG:HE | 4:2A:149:ILE:CB | 2.16 | 0.52 |
| 2:MB:221:THR:CG2 | 6:4A:189:ARG:NH1 | 2.73 | 0.52 |
| 5:3B:231:THR:N | 5:3B:335:LYS:HD2 | 1.73 | 0.52 |
| 6:4A:179:ARG:CB | 6:4A:179:ARG:CZ | 2.85 | 0.52 |
| 6:4A:285:ARG:HH11 | 6:4A:285:ARG:CB | 2.22 | 0.52 |
| 6:4C:179:ARG:CB | 6:4C:179:ARG:CZ | 2.85 | 0.52 |
| 6:4C:244:GLU:HG2 | 6:4C:284:LEU:HD13 | 1.80 | 0.52 |
| 6:4D:252:VAL:CG1 | 6:4D:292:VAL:HG22 | 2.40 | 0.52 |
| 7:5A:1152:GLU:OE2 | 8:6A:66:ARG:NH2 | 2.38 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5A:1407:GLN:NE2 | 7:5A:1407:GLN:CA | 2.73 | 0.52 |
| 7:5A:1548:VAL:CG1 | 7:5A:1566:GLU:C | 2.78 | 0.52 |
| 7:5B:1407:GLN:NE2 | 7:5B:1407:GLN:CA | 2.73 | 0.52 |
| 7:5B:1424:GLN:NE2 | 7:5B:1424:GLN:CA | 2.72 | 0.52 |
| 7:5C:841:VAL:HG22 | 8:6C:109:ILE:HG12 | 1.92 | 0.52 |
| 8:6A:208:LYS:NZ | 8:6A:236:ASP:OD2 | 2.42 | 0.52 |
| 9:7A:36:GLN:HA | 9:7B:43:LEU:HD22 | 1.91 | 0.52 |
| 9:7E:7:LEU:HD23 | 9:7F:30:ARG:NE | 2.13 | 0.52 |
| 2:AD:180:VAL:HG12 | 1:AE:258:ASN:OD1 | 2.09 | 0.51 |
| 2:CB:397:TRP:HE3 | 1:CC:257:THR:CG2 | 1.97 | 0.51 |
| 1:CE:208:ALA:O | 1:CE:212:ILE:HG12 | 2.10 | 0.51 |
| 1:DA:118:CYS:O | 1:DA:122:ILE:HG12 | 2.11 | 0.51 |
| 1:EA:118:CYS:O | 1:EA:122:ILE:HG12 | 2.11 | 0.51 |
| 2:EB:220:PRO:CD | 1:EC:326:LYS:HG2 | 2.38 | 0.51 |
| 1:EE:118:CYS:O | 1:EE:122:ILE:HG12 | 2.11 | 0.51 |
| 1:FA:60:LYS:CD | 1:GA:283:HIS:CA | 2.31 | 0.51 |
| 1:FA:241:SER:OG | 1:FA:250:VAL:O | 2.23 | 0.51 |
| 2:FB:406:MET:O | 2:FB:410:GLU:HG3 | 2.10 | 0.51 |
| 1:FC:56:THR:O | 1:GC:285:GLN:CB | 2.58 | 0.51 |
| 1:FC:118:CYS:O | 1:FC:122:ILE:HG12 | 2.11 | 0.51 |
| 1:FC:208:ALA:O | 1:FC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:GD:406:MET:O | 2:GD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:IA:208:ALA:O | 1:IA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:IC:208:ALA:O | 1:IC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:JB:87:PRO:HG2 | 2:KB:277:GLY:C | 2.27 | 0.51 |
| 2:JB:98:GLY:CA | 1:JC:254:GLU:CG | 2.48 | 0.51 |
| 2:JB:180:VAL:HG12 | 1:JC:258:ASN:OD1 | 2.10 | 0.51 |
| 1:JC:88:HIS:O | 1:KC:280:LYS:CE | 2.58 | 0.51 |
| 2:JF:86:ARG:HE | 2:KF:281:TYR:HD2 | 1.57 | 0.51 |
| 2:KB:217:LEU:CB | 6:4A:263:CYS:SG | 2.98 | 0.51 |
| 1:KC:85:GLN:OE1 | 1:LC:283:HIS:N | 2.41 | 0.51 |
| 1:KC:224:TYR:CE2 | 2:KD:246:LEU:HD11 | 2.43 | 0.51 |
| 1:LA:56:THR:OG1 | 1:MA:284:GLU:HA | 2.09 | 0.51 |
| 2:LB:379:LYS:O | 4:2C:166:ILE:CD1 | 2.57 | 0.51 |
| 2:LD:19:LYS:CE | 6:4B:217:ASN:O | 2.58 | 0.51 |
| 1:MA:179:THR:O | 2:MB:350:LYS:HA | 2.09 | 0.51 |
| 2:MB:406:MET:O | 2:MB:410:GLU:HG3 | 2.10 | 0.51 |
| 2:MD:220:PRO:O | 1:ME:324:VAL:HG13 | 2.10 | 0.51 |
| 2:MF:406:MET:O | 2:MF:410:GLU:HG3 | 2.10 | 0.51 |
| 4:2C:10:LYS:HE2 | 4:2C:11:ASN:H | 1.74 | 0.51 |
| 6:4B:252:VAL:CG1 | 6:4B:292:VAL:HG22 | 2.40 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5C:1579:LYS:C | 7:5C:1583:ASN:CG | 2.75 | 0.51 |
| 8:6C:108:LYS:HB2 | 8:6C:111:SER:HB2 | 1.91 | 0.51 |
| 1:AA:208:ALA:O | 1:AA:212:ILE:HG12 | 2.10 | 0.51 |
| 2:AD:177:ASP:CA | 1:AE:353:VAL:HG12 | 2.40 | 0.51 |
| 1:AE:118:CYS:O | 1:AE:122:ILE:HG12 | 2.11 | 0.51 |
| 2:BB:406:MET:O | 2:BB:410:GLU:HG3 | 2.10 | 0.51 |
| 2:BF:406:MET:O | 2:BF:410:GLU:HG3 | 2.10 | 0.51 |
| 1:CA:208:ALA:O | 1:CA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:CC:208:ALA:O | 1:CC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:DC:400:ALA:C | 7:5A:775:PRO:HB3 | 2.34 | 0.51 |
| 2:EB:177:ASP:OD2 | 1:EC:248:LEU:HD23 | 2.06 | 0.51 |
| 1:FA:208:ALA:O | 1:FA:212:ILE:HG12 | 2.10 | 0.51 |
| 2:FB:318:ARG:HH11 | 2:FB:358:PRO:HG3 | 1.75 | 0.51 |
| 1:FC:419:SER:CB | 7:5A:1256:ARG:HG2 | 2.39 | 0.51 |
| 2:FD:318:ARG:HH11 | 2:FD:358:PRO:HG3 | 1.75 | 0.51 |
| 2:FD:406:MET:O | 2:FD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:FE:118:CYS:O | 1:FE:122:ILE:HG12 | 2.11 | 0.51 |
| 2:FF:406:MET:O | 2:FF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:GB:318:ARG:HH11 | 2:GB:358:PRO:HG3 | 1.75 | 0.51 |
| 2:GB:406:MET:O | 2:GB:410:GLU:HG3 | 2.10 | 0.51 |
| 2:GF:406:MET:O | 2:GF:410:GLU:HG3 | 2.10 | 0.51 |
| 1:HE:369:ALA:HA | 10:8U:21:UNK:CB | 2.40 | 0.51 |
| 1:IE:118:CYS:O | 1:IE:122:ILE:HG12 | 2.10 | 0.51 |
| 1:IE:394:LYS:NZ | 2:IF:347:ASN:OD1 | 2.42 | 0.51 |
| 1:JC:88:HIS:HE1 | 1:KC:280:LYS:HB3 | 1.73 | 0.51 |
| 1:LA:60:LYS:CE | 6:4C:101:ARG:NH2 | 2.74 | 0.51 |
| 1:LE:47:ASP:OD1 | 6:4B:203:LYS:CE | 2.58 | 0.51 |
| 2:MD:406:MET:O | 2:MD:410:GLU:HG3 | 2.10 | 0.51 |
| 6:4B:285:ARG:HH11 | 6:4B:285:ARG:CB | 2.22 | 0.51 |
| 7:5A:1411:LYS:HD3 | 7:5A:1411:LYS:C | 2.34 | 0.51 |
| 7:5A:1424:GLN:NE2 | 7:5A:1424:GLN:CA | 2.72 | 0.51 |
| 7:5B:829:GLY:HA2 | 8:6B:109:ILE:CG2 | 2.41 | 0.51 |
| 7:5B:1436:ARG:HH21 | 7:5B:1440:GLU:HB2 | 1.74 | 0.51 |
| 7:5B:1552:LYS:CE | 7:5B:1563:SER:CB | 2.74 | 0.51 |
| 1:AA:118:CYS:O | 1:AA:122:ILE:HG12 | 2.11 | 0.51 |
| 1:AC:118:CYS:O | 1:AC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:BD:394:PHE:CD1 | 1:BE:261:PRO:HA | 2.46 | 0.51 |
| 2:BD:406:MET:O | 2:BD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:CA:222:PRO:CG | 2:CB:324:LYS:CD | 2.87 | 0.51 |
| 2:CD:406:MET:O | 2:CD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:CE:60:LYS:HD3 | 1:DE:283:HIS:CD2 | 2.45 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:DB:176:SER:CB | 1:DC:349:THR:HG1 | 2.22 | 0.51 |
| 2:DB:178:THR:HA | 1:DC:352:LYS:HD3 | 1.92 | 0.51 |
| 1:DC:118:CYS:O | 1:DC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:ED:394:PHE:CD1 | 1:EE:261:PRO:HA | 2.45 | 0.51 |
| 1:EE:208:ALA:O | 1:EE:212:ILE:HG12 | 2.10 | 0.51 |
| 1:FA:118:CYS:O | 1:FA:122:ILE:HG12 | 2.11 | 0.51 |
| 1:FC:401:LYS:HE3 | 2:FD:344:TRP:CZ3 | 2.46 | 0.51 |
| 1:FE:208:ALA:O | 1:FE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:GB:179:VAL:HG22 | 1:GC:258:ASN:CG | 2.34 | 0.51 |
| 2:GD:318:ARG:HH11 | 2:GD:358:PRO:HG3 | 1.75 | 0.51 |
| 2:GF:58:ARG:CZ | 2:HF:281:TYR:CE1 | 2.93 | 0.51 |
| 2:GF:58:ARG:CZ | 2:HF:281:TYR:CE2 | 2.93 | 0.51 |
| 1:HA:208:ALA:O | 1:HA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:HA:222:PRO:HD2 | 2:HB:324:LYS:HD3 | 1.92 | 0.51 |
| 1:HC:208:ALA:O | 1:HC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:IE:208:ALA:O | 1:IE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:JD:98:GLY:CA | 1:JE:254:GLU:CG | 2.48 | 0.51 |
| 1:KA:208:ALA:O | 1:KA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:KA:398:MET:SD | 2:KB:345:ILE:CG1 | 2.90 | 0.51 |
| 2:KB:130:LEU:CB | 4:2C:37:GLY:HA2 | 2.37 | 0.51 |
| 2:LF:221:THR:HG22 | 6:4D:220:GLY:H | 1.74 | 0.51 |
| 1:MA:279:GLU:HB2 | 6:4C:110:LYS:CE | 2.40 | 0.51 |
| 1:MC:394:LYS:NZ | 2:MD:347:ASN:OD1 | 2.43 | 0.51 |
| 2:MD:176:SER:OG | 1:ME:349:THR:OG1 | 2.26 | 0.51 |
| 2:MD:178:THR:HA | 1:ME:352:LYS:HD3 | 1.91 | 0.51 |
| 4:2A:10:LYS:HE2 | 4:2A:11:ASN:H | 1.74 | 0.51 |
| 5:3A:170:PHE:CE1 | 5:3A:198:MET:HE2 | 2.46 | 0.51 |
| 5:3C:170:PHE:CE1 | 5:3C:198:MET:HE2 | 2.46 | 0.51 |
| 7:5A:1272:ILE:CD1 | 9:7B:11:TYR:HD2 | 2.23 | 0.51 |
| 7:5C:1424:GLN:NE2 | 7:5C:1424:GLN:CA | 2.72 | 0.51 |
| 7:5C:1474:LEU:HD22 | 7:5C:1576:ILE:HD11 | 1.92 | 0.51 |
| 7:5C:1489:PHE:HA | 7:5C:1492:SER:CB | 2.27 | 0.51 |
| 8:6B:195:LYS:HG3 | 8:6B:201:ASP:OD1 | 2.11 | 0.51 |
| 9:7C:36:GLN:HA | 9:7D:43:LEU:HD22 | 1.91 | 0.51 |
| 2:BB:10:GLY:O | 2:BB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:BF:10:GLY:O | 2:BF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:DA:208:ALA:O | 1:DA:212:ILE:HG12 | 2.10 | 0.51 |
| 2:DB:176:SER:CB | 1:DC:349:THR:OG1 | 2.58 | 0.51 |
| 1:DC:208:ALA:O | 1:DC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:DD:406:MET:O | 2:DD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:DE:118:CYS:O | 1:DE:122:ILE:HG12 | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:EB:180:VAL:HG12 | 1:EC:258:ASN:OD1 | 2.10 | 0.51 |
| 2:EB:397:TRP:CB | 1:EC:256:GLN:HE22 | 2.17 | 0.51 |
| 2:EF:86:ARG:CA | 2:FF:281:TYR:CE1 | 2.91 | 0.51 |
| 2:EF:406:MET:O | 2:EF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:GB:55:THR:CG2 | 2:HB:284:LEU:H | 2.14 | 0.51 |
| 1:GE:118:CYS:O | 1:GE:122:ILE:HG12 | 2.11 | 0.51 |
| 1:HE:208:ALA:O | 1:HE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:IB:405:GLU:OE2 | 5:3C:36:LYS:HB3 | 2.10 | 0.51 |
| 1:IC:118:CYS:O | 1:IC:122:ILE:HG12 | 2.11 | 0.51 |
| 1:IE:279:GLU:CG | 10:8X:22:UNK:HA | 2.40 | 0.51 |
| 2:JB:318:ARG:HH11 | 2:JB:358:PRO:HG3 | 1.75 | 0.51 |
| 1:KC:398:MET:SD | 2:KD:345:ILE:CG1 | 2.90 | 0.51 |
| 2:KD:10:GLY:O | 2:KD:14:ASN:ND2 | 2.44 | 0.51 |
| 2:KD:55:THR:CG2 | 2:LD:363:MET:CE | 2.63 | 0.51 |
| 2:KD:77:ARG:CD | 2:LD:281:TYR:CZ | 2.93 | 0.51 |
| 1:KE:88:HIS:CA | 1:LE:284:GLU:HB3 | 2.25 | 0.51 |
| 1:KE:208:ALA:O | 1:KE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:KF:318:ARG:HH11 | 2:KF:358:PRO:HG3 | 1.75 | 0.51 |
| 1:LA:35:GLN:HE21 | 6:4C:101:ARG:CB | 2.19 | 0.51 |
| 1:LC:208:ALA:O | 1:LC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:LE:118:CYS:O | 1:LE:122:ILE:HG12 | 2.11 | 0.51 |
| 1:LE:208:ALA:O | 1:LE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:LF:10:GLY:O | 2:LF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:MA:208:ALA:O | 1:MA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:MC:208:ALA:O | 1:MC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:ME:208:ALA:O | 1:ME:212:ILE:HG12 | 2.10 | 0.51 |
| 4:2B:10:LYS:HE2 | 4:2B:11:ASN:H | 1.74 | 0.51 |
| 5:3B:170:PHE:CE1 | 5:3B:198:MET:HE2 | 2.46 | 0.51 |
| 6:4A:244:GLU:HG2 | 6:4A:284:LEU:HD13 | 1.80 | 0.51 |
| 6:4A:252:VAL:CG1 | 6:4A:292:VAL:HG22 | 2.41 | 0.51 |
| 8:6A:195:LYS:HG3 | 8:6A:201:ASP:OD1 | 2.11 | 0.51 |
| 9:7C:7:LEU:CD2 | 9:7D:30:ARG:HE | 2.22 | 0.51 |
| 1:AA:398:MET:SD | 2:AB:345:ILE:CG1 | 2.90 | 0.51 |
| 1:AC:208:ALA:O | 1:AC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:AE:208:ALA:O | 1:AE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:BD:10:GLY:O | 2:BD:14:ASN:ND2 | 2.44 | 0.51 |
| 2:CF:406:MET:O | 2:CF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:DB:391:ARG:HG3 | 1:DC:346:TRP:CD1 | 2.46 | 0.51 |
| 2:DB:406:MET:O | 2:DB:410:GLU:HG3 | 2.10 | 0.51 |
| 2:DD:86:ARG:N | 2:ED:281:TYR:CZ | 2.78 | 0.51 |
| 1:DE:208:ALA:O | 1:DE:212:ILE:HG12 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:EA:208:ALA:O | 1:EA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:EC:208:ALA:O | 1:EC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:ED:55:THR:CG2 | 2:FD:284:LEU:N | 2.73 | 0.51 |
| 2:ED:406:MET:O | 2:ED:410:GLU:HG3 | 2.10 | 0.51 |
| 1:GA:118:CYS:O | 1:GA:122:ILE:HG12 | 2.11 | 0.51 |
| 2:GB:135:ILE:HB | 2:GB:166:THR:HG22 | 1.93 | 0.51 |
| 1:GC:118:CYS:O | 1:GC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:GD:177:ASP:CA | 1:GE:353:VAL:HG12 | 2.40 | 0.51 |
| 2:GD:180:VAL:HG12 | 1:GE:258:ASN:OD1 | 2.09 | 0.51 |
| 2:GF:135:ILE:HB | 2:GF:166:THR:HG22 | 1.93 | 0.51 |
| 2:GF:416:ASN:CG | 7:5B:1327:LYS:CE | 2.84 | 0.51 |
| 1:HC:60:LYS:HZ2 | 1:IC:283:HIS:CD2 | 2.28 | 0.51 |
| 2:HD:10:GLY:O | 2:HD:14:ASN:ND2 | 2.44 | 0.51 |
| 2:HD:135:ILE:HB | 2:HD:166:THR:HG22 | 1.93 | 0.51 |
| 2:HD:406:MET:O | 2:HD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:IA:118:CYS:O | 1:IA:122:ILE:HG12 | 2.11 | 0.51 |
| 1:IA:398:MET:SD | 2:IB:345:ILE:CG1 | 2.90 | 0.51 |
| 1:IC:398:MET:SD | 2:ID:345:ILE:CG1 | 2.90 | 0.51 |
| 2:JB:406:MET:O | 2:JB:410:GLU:HG3 | 2.10 | 0.51 |
| 2:JD:318:ARG:HH11 | 2:JD:358:PRO:HG3 | 1.75 | 0.51 |
| 2:JD:406:MET:O | 2:JD:410:GLU:HG3 | 2.10 | 0.51 |
| 2:JF:88:ASP:CB | 2:KF:278:SER:CB | 2.79 | 0.51 |
| 1:KC:208:ALA:O | 1:KC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:KD:318:ARG:HH11 | 2:KD:358:PRO:HG3 | 1.75 | 0.51 |
| 1:KE:118:CYS:O | 1:KE:122:ILE:HG12 | 2.11 | 0.51 |
| 2:KF:10:GLY:O | 2:KF:14:ASN:ND2 | 2.44 | 0.51 |
| 2:LB:10:GLY:O | 2:LB:14:ASN:ND2 | 2.44 | 0.51 |
| 1:LC:118:CYS:O | 1:LC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:LD:10:GLY:O | 2:LD:14:ASN:ND2 | 2.44 | 0.51 |
| 6:4C:273:ARG:HH21 | 6:4C:273:ARG:HG3 | 1.75 | 0.51 |
| 6:4D:244:GLU:HG2 | 6:4D:284:LEU:HD13 | 1.80 | 0.51 |
| 6:4D:285:ARG:HH11 | 6:4D:285:ARG:CB | 2.22 | 0.51 |
| 7:5A:1474:LEU:HD22 | 7:5A:1576:ILE:HD11 | 1.91 | 0.51 |
| 7:5A:1552:LYS:HZ1 | 7:5A:1563:SER:N | 2.09 | 0.51 |
| 7:5B:1565:GLU:CB | 7:5B:1568:LYS:HD2 | 2.38 | 0.51 |
| 7:5C:1548:VAL:CG1 | 7:5C:1566:GLU:C | 2.78 | 0.51 |
| 8:6C:190:PRO:HD3 | 8:6C:256:TYR:OH | 2.11 | 0.51 |
| 2:BB:220:PRO:HD2 | 1:BC:326:LYS:CG | 2.36 | 0.51 |
| 1:BC:208:ALA:O | 1:BC:212:ILE:HG12 | 2.10 | 0.51 |
| 1:CA:118:CYS:O | 1:CA:122:ILE:HG12 | 2.11 | 0.51 |
| 2:CB:406:MET:O | 2:CB:410:GLU:HG3 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CD:135:ILE:HB | 2:CD:166:THR:HG22 | 1.93 | 0.51 |
| 1:CE:401:LYS:HE3 | 2:CF:344:TRP:CZ3 | 2.46 | 0.51 |
| 2:DF:406:MET:O | 2:DF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:EB:10:GLY:O | 2:EB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:EB:135:ILE:HB | 2:EB:166:THR:HG22 | 1.93 | 0.51 |
| 2:EB:390:ARG:HD2 | 1:EC:439:THR:HG21 | 1.93 | 0.51 |
| 2:EB:406:MET:O | 2:EB:410:GLU:HG3 | 2.10 | 0.51 |
| 1:EE:430:LYS:HZ1 | 7:5B:834:ASN:ND2 | 0.70 | 0.51 |
| 2:FB:394:PHE:HE2 | 1:FC:258:ASN:C | 2.18 | 0.51 |
| 2:FF:55:THR:HG23 | 2:GF:283:ALA:HB1 | 1.84 | 0.51 |
| 1:GC:208:ALA:O | 1:GC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:GD:10:GLY:O | 2:GD:14:ASN:ND2 | 2.44 | 0.51 |
| 2:GD:212:PHE:HZ | 1:GE:326:LYS:CE | 2.19 | 0.51 |
| 1:GE:208:ALA:O | 1:GE:212:ILE:HG12 | 2.10 | 0.51 |
| 2:HB:10:GLY:O | 2:HB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:HF:135:ILE:HB | 2:HF:166:THR:HG22 | 1.93 | 0.51 |
| 2:HF:406:MET:O | 2:HF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:IF:135:ILE:HB | 2:IF:166:THR:HG22 | 1.93 | 0.51 |
| 1:JA:208:ALA:O | 1:JA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:JE:88:HIS:C | 1:KE:280:LYS:HD3 | 2.32 | 0.51 |
| 2:JF:406:MET:O | 2:JF:410:GLU:HG3 | 2.10 | 0.51 |
| 2:KB:10:GLY:O | 2:KB:14:ASN:ND2 | 2.44 | 0.51 |
| 1:KC:118:CYS:O | 1:KC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:KD:276:ARG:CZ | 6:4B:265:TYR:HB2 | 2.40 | 0.51 |
| 1:LA:118:CYS:O | 1:LA:122:ILE:HG12 | 2.11 | 0.51 |
| 1:LE:47:ASP:OD1 | 6:4B:203:LYS:NZ | 2.41 | 0.51 |
| 1:MA:118:CYS:O | 1:MA:122:ILE:HG12 | 2.11 | 0.51 |
| 6:4B:244:GLU:HG2 | 6:4B:284:LEU:HD13 | 1.80 | 0.51 |
| 7:5A:1484:TYR:HD1 | 7:5A:1568:LYS:CD | 1.92 | 0.51 |
| 7:5A:1565:GLU:CB | 7:5A:1568:LYS:HD2 | 2.38 | 0.51 |
| 7:5B:1411:LYS:HD3 | 7:5B:1411:LYS:C | 2.34 | 0.51 |
| 7:5C:1384:GLN:H | 7:5C:1384:GLN:NE2 | 2.08 | 0.51 |
| 2:BF:86:ARG:HA | 2:CF:281:TYR:HH | 1.75 | 0.51 |
| 2:BF:86:ARG:CA | 2:CF:281:TYR:HE1 | 2.18 | 0.51 |
| 1:CC:118:CYS:O | 1:CC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:CF:135:ILE:HB | 2:CF:166:THR:HG22 | 1.93 | 0.51 |
| 1:DC:402:ARG:CZ | 7:5A:777:ALA:HB1 | 2.30 | 0.51 |
| 2:DD:135:ILE:HB | 2:DD:166:THR:HG22 | 1.93 | 0.51 |
| 2:DF:135:ILE:HB | 2:DF:166:THR:HG22 | 1.93 | 0.51 |
| 2:FB:10:GLY:O | 2:FB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:FB:135:ILE:HB | 2:FB:166:THR:HG22 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:FF:318:ARG:HH11 | 2:FF:358:PRO:HG3 | 1.75 | 0.51 |
| 2:GD:135:ILE:HB | 2:GD:166:THR:HG22 | 1.93 | 0.51 |
| 2:GF:10:GLY:O | 2:GF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:HA:118:CYS:O | 1:HA:122:ILE:HG12 | 2.11 | 0.51 |
| 2:HF:10:GLY:O | 2:HF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:JC:208:ALA:O | 1:JC:212:ILE:HG12 | 2.10 | 0.51 |
| 2:JD:135:ILE:HB | 2:JD:166:THR:HG22 | 1.93 | 0.51 |
| 2:JF:135:ILE:HB | 2:JF:166:THR:HG22 | 1.93 | 0.51 |
| 1:KA:357:TYR:OH | 6:4C:257:LEU:CD2 | 2.59 | 0.51 |
| 1:LA:60:LYS:HE3 | 6:4C:101:ARG:CZ | 2.41 | 0.51 |
| 1:LA:208:ALA:O | 1:LA:212:ILE:HG12 | 2.10 | 0.51 |
| 1:LC:101:ASN:HD22 | 2:LD:252:LYS:HG3 | 1.75 | 0.51 |
| 2:MB:10:GLY:O | 2:MB:14:ASN:ND2 | 2.44 | 0.51 |
| 1:MC:279:GLU:CD | 6:4A:106:ALA:HB3 | 2.36 | 0.51 |
| 2:MD:180:VAL:HG12 | 1:ME:258:ASN:OD1 | 2.10 | 0.51 |
| 2:MD:394:PHE:CD1 | 1:ME:261:PRO:HA | 2.45 | 0.51 |
| 6:4A:273:ARG:HH21 | 6:4A:273:ARG:HG3 | 1.75 | 0.51 |
| 6:4B:256:ASN:HD21 | 6:4B:260:ARG:HE | 1.57 | 0.51 |
| 6:4C:247:LYS:CD | 6:4C:247:LYS:H | 2.12 | 0.51 |
| 7:5C:841:VAL:H | 8:6C:109:ILE:HD11 | 1.67 | 0.51 |
| 7:5C:1347:LEU:N | 7:5C:1347:LEU:CD1 | 2.73 | 0.51 |
| 8:6C:195:LYS:HG3 | 8:6C:201:ASP:OD1 | 2.11 | 0.51 |
| 1:AE:71:GLU:CD | 2:AF:247:ASN:ND2 | 2.69 | 0.51 |
| 1:BA:208:ALA:O | 1:BA:212:ILE:HG12 | 2.10 | 0.51 |
| 2:BB:179:VAL:HG22 | 1:BC:258:ASN:CG | 2.36 | 0.51 |
| 1:BE:208:ALA:O | 1:BE:212:ILE:HG12 | 2.10 | 0.51 |
| 1:CA:401:LYS:HE3 | 2:CB:344:TRP:CZ3 | 2.45 | 0.51 |
| 2:CB:135:ILE:HB | 2:CB:166:THR:HG22 | 1.93 | 0.51 |
| 1:CE:118:CYS:O | 1:CE:122:ILE:HG12 | 2.11 | 0.51 |
| 2:CF:10:GLY:O | 2:CF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:DC:71:GLU:CD | 2:DD:247:ASN:ND2 | 2.69 | 0.51 |
| 2:ED:10:GLY:O | 2:ED:14:ASN:ND2 | 2.44 | 0.51 |
| 2:ED:220:PRO:HD2 | 1:EE:326:LYS:CD | 2.40 | 0.51 |
| 2:EF:10:GLY:O | 2:EF:14:ASN:ND2 | 2.44 | 0.51 |
| 1:FC:402:ARG:HD3 | 7:5A:1259:TYR:CB | 2.41 | 0.51 |
| 2:FD:10:GLY:O | 2:FD:14:ASN:ND2 | 2.44 | 0.51 |
| 1:GA:208:ALA:O | 1:GA:212:ILE:HG12 | 2.10 | 0.51 |
| 2:GF:318:ARG:HH11 | 2:GF:358:PRO:HG3 | 1.75 | 0.51 |
| 2:HB:135:ILE:HB | 2:HB:166:THR:HG22 | 1.93 | 0.51 |
| 2:HB:180:VAL:HG12 | 1:HC:258:ASN:OD1 | 2.10 | 0.51 |
| 2:HB:406:MET:O | 2:HB:410:GLU:HG3 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:IB:135:ILE:HB | 2:IB:166:THR:HG22 | 1.93 | 0.51 |
| 1:IC:100:ALA:HB1 | 2:ID:252:LYS:HA | 1.91 | 0.51 |
| 2:ID:318:ARG:HH11 | 2:ID:358:PRO:HG3 | 1.75 | 0.51 |
| 1:JC:224:TYR:CE2 | 2:JD:246:LEU:HD11 | 2.43 | 0.51 |
| 2:JD:222:TYR:CD2 | 1:JE:247:ALA:HB1 | 2.44 | 0.51 |
| 1:JE:88:HIS:C | 1:KE:280:LYS:CE | 2.83 | 0.51 |
| 2:JF:10:GLY:O | 2:JF:14:ASN:ND2 | 2.44 | 0.51 |
| 2:JF:318:ARG:HH11 | 2:JF:358:PRO:HG3 | 1.75 | 0.51 |
| 2:KF:54:ALA:CA | 2:LF:285:THR:HG22 | 2.41 | 0.51 |
| 1:LE:101:ASN:ND2 | 2:LF:252:LYS:HG3 | 2.26 | 0.51 |
| 1:MC:118:CYS:O | 1:MC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:MD:10:GLY:O | 2:MD:14:ASN:ND2 | 2.44 | 0.51 |
| 6:4B:179:ARG:CG | 6:4B:179:ARG:NH1 | 2.72 | 0.51 |
| 6:4B:266:ASN:HB2 | 6:4B:273:ARG:HE | 1.76 | 0.51 |
| 6:4B:273:ARG:HH21 | 6:4B:273:ARG:HG3 | 1.75 | 0.51 |
| 6:4C:252:VAL:CG1 | 6:4C:292:VAL:HG22 | 2.41 | 0.51 |
| 6:4D:179:ARG:CG | 6:4D:179:ARG:NH1 | 2.72 | 0.51 |
| 6:4D:273:ARG:HH21 | 6:4D:273:ARG:HG3 | 1.74 | 0.51 |
| 7:5A:1384:GLN:H | 7:5A:1384:GLN:NE2 | 2.08 | 0.51 |
| 7:5A:1552:LYS:HZ3 | 7:5A:1563:SER:HB2 | 0.68 | 0.51 |
| 7:5B:1474:LEU:HD22 | 7:5B:1576:ILE:HD11 | 1.91 | 0.51 |
| 7:5B:1487:ASN:OD1 | 7:5B:1568:LYS:CD | 2.58 | 0.51 |
| 7:5C:1434:LYS:CE | 7:5C:1434:LYS:CA | 2.86 | 0.51 |
| 7:5C:1565:GLU:CB | 7:5C:1568:LYS:HD2 | 2.38 | 0.51 |
| 1:AE:283:HIS:CB | 2:MB:86:ARG:HH12 | 2.18 | 0.51 |
| 2:DB:87:PRO:HD2 | 2:EB:281:TYR:CE2 | 2.46 | 0.51 |
| 2:DB:135:ILE:HB | 2:DB:166:THR:HG22 | 1.93 | 0.51 |
| 2:DB:394:PHE:CD1 | 1:DC:261:PRO:HA | 2.46 | 0.51 |
| 2:ED:135:ILE:HB | 2:ED:166:THR:HG22 | 1.93 | 0.51 |
| 1:FE:402:ARG:HD2 | 7:5B:1259:TYR:HD2 | 1.74 | 0.51 |
| 2:FF:10:GLY:O | 2:FF:14:ASN:ND2 | 2.44 | 0.51 |
| 2:FF:135:ILE:HB | 2:FF:166:THR:HG22 | 1.93 | 0.51 |
| 2:GB:10:GLY:O | 2:GB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:GB:179:VAL:HG22 | 1:GC:258:ASN:CB | 2.41 | 0.51 |
| 2:GF:54:ALA:HB1 | 2:HF:281:TYR:O | 2.11 | 0.51 |
| 2:ID:135:ILE:HB | 2:ID:166:THR:HG22 | 1.93 | 0.51 |
| 2:IF:318:ARG:HH11 | 2:IF:358:PRO:HG3 | 1.75 | 0.51 |
| 2:IF:424:GLN:CG | 7:5B:1413:GLN:HE21 | 2.23 | 0.51 |
| 1:JA:282:TYR:CZ | 10:8Y:17:UNK:CB | 2.93 | 0.51 |
| 2:JB:135:ILE:HB | 2:JB:166:THR:HG22 | 1.93 | 0.51 |
| 2:JD:10:GLY:O | 2:JD:14:ASN:ND2 | 2.44 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JE:208:ALA:O | 1:JE:212:ILE:HG12 | 2.10 | 0.51 |
| 1:KA:118:CYS:O | 1:KA:122:ILE:HG12 | 2.11 | 0.51 |
| 2:KD:406:MET:O | 2:KD:410:GLU:HG3 | 2.10 | 0.51 |
| 1:KE:71:GLU:CD | 2:KF:247:ASN:ND2 | 2.69 | 0.51 |
| 2:LD:379:LYS:HE3 | 4:2A:164:ARG:O | 2.11 | 0.51 |
| 2:MB:222:TYR:O | 2:MB:226:ASN:ND2 | 2.28 | 0.51 |
| 6:4A:179:ARG:CG | 6:4A:179:ARG:NH1 | 2.72 | 0.51 |
| 6:4A:266:ASN:HB2 | 6:4A:273:ARG:HE | 1.76 | 0.51 |
| 6:4B:241:LYS:C | 6:4B:241:LYS:HD3 | 2.32 | 0.51 |
| 6:4C:266:ASN:HB2 | 6:4C:273:ARG:HE | 1.76 | 0.51 |
| 6:4D:266:ASN:HB2 | 6:4D:273:ARG:HE | 1.76 | 0.51 |
| 7:5A:1347:LEU:N | 7:5A:1347:LEU:CD1 | 2.73 | 0.51 |
| 7:5A:1487:ASN:OD1 | 7:5A:1568:LYS:CD | 2.58 | 0.51 |
| 7:5B:1484:TYR:C | 7:5B:1487:ASN:HB2 | 2.36 | 0.51 |
| 7:5C:1552:LYS:HZ1 | 7:5C:1563:SER:N | 2.09 | 0.51 |
| 2:AB:135:ILE:HB | 2:AB:166:THR:HG22 | 1.93 | 0.51 |
| 1:AC:224:TYR:CE2 | 2:AD:246:LEU:HD11 | 2.43 | 0.51 |
| 1:AC:398:MET:SD | 2:AD:345:ILE:CG1 | 2.90 | 0.51 |
| 2:AD:25:SER:HG | 2:AD:51:TYR:HH | 1.56 | 0.51 |
| 2:AF:25:SER:HG | 2:AF:51:TYR:HH | 1.55 | 0.51 |
| 2:DB:222:TYR:HD2 | 1:DC:247:ALA:HB1 | 1.75 | 0.51 |
| 1:EC:178:SER:OG | 2:ED:347:ASN:HB3 | 2.11 | 0.51 |
| 2:ED:55:THR:HG23 | 2:FD:283:ALA:CB | 2.40 | 0.51 |
| 1:FA:11:GLN:HE22 | 2:FB:246:LEU:HA | 1.75 | 0.51 |
| 1:FC:241:SER:OG | 1:FC:250:VAL:O | 2.23 | 0.51 |
| 2:FD:135:ILE:HB | 2:FD:166:THR:HG22 | 1.93 | 0.51 |
| 2:FD:179:VAL:CG2 | 1:FE:258:ASN:CA | 2.89 | 0.51 |
| 1:HC:118:CYS:O | 1:HC:122:ILE:HG12 | 2.11 | 0.51 |
| 2:IB:10:GLY:O | 2:IB:14:ASN:ND2 | 2.44 | 0.51 |
| 2:ID:10:GLY:O | 2:ID:14:ASN:ND2 | 2.44 | 0.51 |
| 1:IE:71:GLU:CD | 2:IF:247:ASN:ND2 | 2.69 | 0.51 |
| 1:JA:224:TYR:CE2 | 2:JB:246:LEU:HD11 | 2.44 | 0.51 |
| 1:KA:222:PRO:HD2 | 2:KB:324:LYS:HD3 | 1.92 | 0.51 |
| 2:KB:135:ILE:HB | 2:KB:166:THR:HG22 | 1.93 | 0.51 |
| 1:KC:359:PRO:HB3 | 6:4A:299:TYR:CZ | 2.40 | 0.51 |
| 2:KD:135:ILE:HB | 2:KD:166:THR:HG22 | 1.93 | 0.51 |
| 2:KD:177:ASP:CA | 1:KE:353:VAL:HG12 | 2.40 | 0.51 |
| 2:LB:406:MET:O | 2:LB:410:GLU:HG3 | 2.10 | 0.51 |
| 1:LE:245:ASP:OD1 | 6:4B:216:ARG:NE | 2.44 | 0.51 |
| 1:ME:118:CYS:O | 1:ME:122:ILE:HG12 | 2.11 | 0.51 |
| 2:MF:10:GLY:O | 2:MF:14:ASN:ND2 | 2.44 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:MF:318:ARG:HH11 | 2:MF:358:PRO:HG3 | 1.75 | 0.51 |
| 6:4A:247:LYS:CD | 6:4A:247:LYS:H | 2.12 | 0.51 |
| 6:4C:251:TYR:HB2 | 6:4C:288:TYR:HE2 | 1.74 | 0.51 |
| 6:4D:106:ALA:HB3 | 6:4D:107:MET:HE3 | 1.93 | 0.51 |
| 6:4D:139:ASP:CG | 6:4D:140:PRO:HD2 | 2.34 | 0.51 |
| 7:5A:1548:VAL:CG1 | 7:5A:1569:GLU:CB | 2.54 | 0.51 |
| 7:5B:1272:ILE:HG12 | 9:7D:11:TYR:CE2 | 2.46 | 0.51 |
| 7:5B:1384:GLN:H | 7:5B:1384:GLN:NE2 | 2.08 | 0.51 |
| 7:5C:841:VAL:O | 8:6C:9:LEU:O | 2.29 | 0.51 |
| 7:5C:1487:ASN:OD1 | 7:5C:1568:LYS:CD | 2.58 | 0.51 |
| 9:7A:10:TYR:OH | 9:7B:31:PRO:O | 2.21 | 0.51 |
| 9:7A:15:VAL:HG12 | 9:7B:35:ILE:CB | 2.41 | 0.51 |
| 9:7A:39:GLY:N | 9:7B:43:LEU:HD21 | 2.26 | 0.51 |
| 9:7C:15:VAL:HG13 | 9:7D:35:ILE:CD1 | 1.92 | 0.51 |
| 1:AA:224:TYR:CE2 | 2:AB:246:LEU:HD11 | 2.44 | 0.50 |
| 2:AB:179:VAL:HG22 | 1:AC:258:ASN:CB | 2.41 | 0.50 |
| 2:AD:135:ILE:HB | 2:AD:166:THR:HG22 | 1.93 | 0.50 |
| 1:AE:176:GLN:O | 2:AF:347:ASN:ND2 | 2.40 | 0.50 |
| 2:AF:135:ILE:HB | 2:AF:166:THR:HG22 | 1.93 | 0.50 |
| 2:BB:135:ILE:HB | 2:BB:166:THR:HG22 | 1.93 | 0.50 |
| 2:BF:86:ARG:HA | 2:CF:281:TYR:OH | 2.10 | 0.50 |
| 2:CD:10:GLY:O | 2:CD:14:ASN:ND2 | 2.44 | 0.50 |
| 1:DA:222:PRO:CG | 2:DB:324:LYS:CD | 2.88 | 0.50 |
| 2:DB:177:ASP:OD2 | 1:DC:248:LEU:HD23 | 2.07 | 0.50 |
| 2:EB:157:GLU:HA | 7:5C:945:LYS:NZ | 2.25 | 0.50 |
| 2:EB:177:ASP:CA | 1:EC:353:VAL:HG12 | 2.41 | 0.50 |
| 1:EC:393:HIS:CE1 | 7:5A:814:LYS:CG | 2.90 | 0.50 |
| 2:ED:222:TYR:CE2 | 1:EE:325:PRO:HG2 | 2.45 | 0.50 |
| 1:EE:401:LYS:CE | 2:EF:344:TRP:CZ3 | 2.74 | 0.50 |
| 2:EF:135:ILE:HB | 2:EF:166:THR:HG22 | 1.93 | 0.50 |
| 2:FB:222:TYR:CD2 | 1:FC:247:ALA:HB1 | 2.46 | 0.50 |
| 2:GB:55:THR:H | 2:HB:283:ALA:CA | 2.24 | 0.50 |
| 2:HB:179:VAL:HG22 | 1:HC:258:ASN:CB | 2.41 | 0.50 |
| 1:HE:118:CYS:O | 1:HE:122:ILE:HG12 | 2.11 | 0.50 |
| 2:IB:318:ARG:HH11 | 2:IB:358:PRO:HG3 | 1.75 | 0.50 |
| 1:JC:100:ALA:HB1 | 2:JD:252:LYS:HA | 1.92 | 0.50 |
| 2:KB:406:MET:O | 2:KB:410:GLU:HG3 | 2.10 | 0.50 |
| 2:KF:135:ILE:HB | 2:KF:166:THR:HG22 | 1.93 | 0.50 |
| 2:LB:135:ILE:HB | 2:LB:166:THR:HG22 | 1.93 | 0.50 |
| 2:LD:406:MET:O | 2:LD:410:GLU:HG3 | 2.10 | 0.50 |
| 2:LF:58:ARG:NH2 | 2:MF:281:TYR:CZ | 2.79 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:HA | 2.10 | 0.50 |
| 2:MD:318:ARG:HH11 | 2:MD:358:PRO:HG3 | 1.75 | 0.50 |
| 1:ME:96:LYS:HE2 | 2:MF:1:MET:HE3 | 1.93 | 0.50 |
| 6:4D:256:ASN:HD21 | 6:4D:260:ARG:HE | 1.58 | 0.50 |
| 7:5A:1404:LYS:HZ1 | 7:5A:1408:GLU:HB2 | 1.75 | 0.50 |
| 7:5A:1484:TYR:C | 7:5A:1487:ASN:HB2 | 2.36 | 0.50 |
| 7:5A:1552:LYS:CE | 7:5A:1563:SER:CB | 2.73 | 0.50 |
| 7:5B:1416:LYS:HA | 7:5B:1416:LYS:CE | 2.41 | 0.50 |
| 8:6A:177:TYR:HE1 | 8:6A:199:ILE:HD13 | 1.74 | 0.50 |
| 8:6B:177:TYR:HE1 | 8:6B:199:ILE:HD13 | 1.74 | 0.50 |
| 2:AF:356:ILE:HG23 | 6:4A:152:PHE:CE1 | 2.45 | 0.50 |
| 2:AF:357:PRO:O | 6:4A:151:ARG:CZ | 2.59 | 0.50 |
| 1:BA:176:GLN:O | 2:BB:347:ASN:ND2 | 2.36 | 0.50 |
| 2:BD:135:ILE:HB | 2:BD:166:THR:HG22 | 1.93 | 0.50 |
| 2:BF:135:ILE:HB | 2:BF:166:THR:HG22 | 1.93 | 0.50 |
| 1:FA:56:THR:C | 1:GA:285:GLN:HB2 | 2.35 | 0.50 |
| 2:FD:397:TRP:CH2 | 1:FE:255:PHE:O | 2.57 | 0.50 |
| 2:HD:177:ASP:CG | 1:HE:353:VAL:HG13 | 2.00 | 0.50 |
| 2:JB:10:GLY:O | 2:JB:14:ASN:ND2 | 2.44 | 0.50 |
| 1:JC:279:GLU:CD | 10:8Z:22:UNK:CB | 2.84 | 0.50 |
| 2:KB:318:ARG:HH11 | 2:KB:358:PRO:HG3 | 1.75 | 0.50 |
| 2:KF:406:MET:O | 2:KF:410:GLU:HG3 | 2.10 | 0.50 |
| 2:LD:135:ILE:HB | 2:LD:166:THR:HG22 | 1.93 | 0.50 |
| 2:LF:406:MET:O | 2:LF:410:GLU:HG3 | 2.10 | 0.50 |
| 1:ME:372:MET:CE | 6:4B:96:VAL:CB | 2.89 | 0.50 |
| 6:4A:106:ALA:HB3 | 6:4A:107:MET:HE3 | 1.94 | 0.50 |
| 6:4A:282:ASN:HA | 6:4A:285:ARG:HB2 | 1.93 | 0.50 |
| 6:4B:139:ASP:CG | 6:4B:140:PRO:HD2 | 2.34 | 0.50 |
| 6:4B:248:VAL:HA | 6:4B:251:TYR:CD2 | 2.46 | 0.50 |
| 6:4B:282:ASN:HA | 6:4B:285:ARG:HB2 | 1.93 | 0.50 |
| 6:4C:179:ARG:CG | 6:4C:179:ARG:NH1 | 2.72 | 0.50 |
| 6:4C:282:ASN:HA | 6:4C:285:ARG:HB2 | 1.93 | 0.50 |
| 6:4D:248:VAL:HA | 6:4D:251:TYR:CD2 | 2.47 | 0.50 |
| 6:4D:282:ASN:HA | 6:4D:285:ARG:HB2 | 1.93 | 0.50 |
| 7:5A:1267:CYS:SG | 9:7A:12:GLU:OE2 | 2.56 | 0.50 |
| 7:5A:1416:LYS:HA | 7:5A:1416:LYS:CE | 2.41 | 0.50 |
| 7:5B:943:LEU:HD22 | 7:5B:1030:PHE:CE2 | 2.46 | 0.50 |
| 7:5B:1347:LEU:N | 7:5B:1347:LEU:CD1 | 2.73 | 0.50 |
| 7:5B:1399:LYS:NZ | 7:5B:1399:LYS:CB | 2.73 | 0.50 |
| 2:CD:176:SER:CB | 1:CE:349:THR:OG1 | 2.58 | 0.50 |
| 1:FA:181:VAL:HG12 | 2:FB:348:ASN:HA | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FA:402:ARG:HD3 | 7:5C:1259:TYR:HB2 | 1.91 | 0.50 |
| 1:FC:419:SER:C | 7:5A:1256:ARG:HH21 | 2.18 | 0.50 |
| 1:FE:241:SER:OG | 1:FE:250:VAL:O | 2.23 | 0.50 |
| 2:GB:212:PHE:CZ | 1:GC:326:LYS:CE | 2.93 | 0.50 |
| 2:KB:179:VAL:HG22 | 1:KC:258:ASN:CB | 2.41 | 0.50 |
| 2:KD:32:PRO:HG2 | 6:4B:279:LEU:HD21 | 1.92 | 0.50 |
| 2:LB:19:LYS:CE | 6:4A:217:ASN:O | 2.60 | 0.50 |
| 1:LE:60:LYS:CE | 6:4B:101:ARG:CZ | 2.89 | 0.50 |
| 2:LF:135:ILE:HB | 2:LF:166:THR:HG22 | 1.93 | 0.50 |
| 2:MB:135:ILE:HB | 2:MB:166:THR:HG22 | 1.93 | 0.50 |
| 2:MD:135:ILE:HB | 2:MD:166:THR:HG22 | 1.93 | 0.50 |
| 1:ME:222:PRO:CD | 2:MF:324:LYS:HD3 | 2.41 | 0.50 |
| 7:5A:1399:LYS:NZ | 7:5A:1399:LYS:CB | 2.73 | 0.50 |
| 7:5B:1484:TYR:HD1 | 7:5B:1568:LYS:CD | 1.92 | 0.50 |
| 7:5C:1416:LYS:HA | 7:5C:1416:LYS:CE | 2.41 | 0.50 |
| 7:5C:1436:ARG:CZ | 7:5C:1436:ARG:C | 2.85 | 0.50 |
| 7:5C:1484:TYR:C | 7:5C:1487:ASN:HB2 | 2.36 | 0.50 |
| 8:6A:190:PRO:HD3 | 8:6A:256:TYR:OH | 2.11 | 0.50 |
| 9:7C:15:VAL:HG12 | 9:7D:35:ILE:CB | 2.41 | 0.50 |
| 2:BD:179:VAL:CG2 | 1:BE:258:ASN:O | 2.36 | 0.50 |
| 2:CB:10:GLY:O | 2:CB:14:ASN:ND2 | 2.44 | 0.50 |
| 2:DB:10:GLY:O | 2:DB:14:ASN:ND2 | 2.44 | 0.50 |
| 2:FB:55:THR:CG2 | 2:GB:283:ALA:CA | 2.58 | 0.50 |
| 1:HE:71:GLU:CD | 2:HF:247:ASN:ND2 | 2.69 | 0.50 |
| 2:IB:98:GLY:CA | 1:IC:254:GLU:CG | 2.48 | 0.50 |
| 2:IB:179:VAL:HG22 | 1:IC:258:ASN:CB | 2.41 | 0.50 |
| 2:IB:406:MET:O | 2:IB:410:GLU:HG3 | 2.10 | 0.50 |
| 2:ID:406:MET:O | 2:ID:410:GLU:HG3 | 2.10 | 0.50 |
| 2:IF:10:GLY:O | 2:IF:14:ASN:ND2 | 2.44 | 0.50 |
| 2:JB:179:VAL:HG22 | 1:JC:258:ASN:CB | 2.41 | 0.50 |
| 1:JE:118:CYS:O | 1:JE:122:ILE:HG12 | 2.11 | 0.50 |
| 2:LB:223:GLY:CA | 6:4A:219:ASN:HD22 | 2.24 | 0.50 |
| 2:LD:221:THR:CG2 | 6:4B:219:ASN:ND2 | 2.75 | 0.50 |
| 6:4A:248:VAL:HA | 6:4A:251:TYR:CD2 | 2.47 | 0.50 |
| 6:4A:251:TYR:HB2 | 6:4A:288:TYR:HE2 | 1.74 | 0.50 |
| 6:4C:248:VAL:HA | 6:4C:251:TYR:CD2 | 2.47 | 0.50 |
| 7:5A:1030:PHE:CZ | 7:5A:1034:ILE:CD1 | 2.95 | 0.50 |
| 7:5A:1271:ILE:CA | 9:7A:20:LEU:CD2 | 2.48 | 0.50 |
| 7:5A:1275:ILE:HG21 | 9:7B:11:TYR:HH | 1.76 | 0.50 |
| 7:5A:1370:LYS:CA | 7:5A:1370:LYS:CE | 2.85 | 0.50 |
| 7:5A:1436:ARG:CZ | 7:5A:1436:ARG:C | 2.85 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:872:GLU:OE1 | 8:6B:90:ARG:NH1 | 2.44 | 0.50 |
| 7:5B:1030:PHE:CZ | 7:5B:1034:ILE:CD1 | 2.95 | 0.50 |
| 7:5B:1370:LYS:CA | 7:5B:1370:LYS:CE | 2.85 | 0.50 |
| 7:5B:1471:ILE:O | 7:5B:1473:GLU:N | 2.39 | 0.50 |
| 9:7A:15:VAL:HG13 | 9:7B:35:ILE:CD1 | 1.92 | 0.50 |
| 2:AB:10:GLY:O | 2:AB:14:ASN:ND2 | 2.44 | 0.50 |
| 1:AC:221:ARG:HE | 6:4C:156:PHE:HE2 | 1.49 | 0.50 |
| 2:AF:10:GLY:O | 2:AF:14:ASN:ND2 | 2.44 | 0.50 |
| 2:BB:86:ARG:HA | 2:CB:281:TYR:OH | 2.12 | 0.50 |
| 1:FE:100:ALA:HB1 | 2:FF:252:LYS:CA | 2.41 | 0.50 |
| 1:GE:71:GLU:CD | 2:GF:247:ASN:ND2 | 2.69 | 0.50 |
| 1:HE:282:TYR:HE2 | 10:8U:19:UNK:CA | 2.12 | 0.50 |
| 1:IE:176:GLN:O | 2:IF:347:ASN:ND2 | 2.40 | 0.50 |
| 2:JB:212:PHE:CZ | 1:JC:326:LYS:CE | 2.93 | 0.50 |
| 2:KB:273:LEU:CA | 6:4A:268:LEU:HG | 2.37 | 0.50 |
| 2:LD:294:PHE:HD2 | 4:2A:147:PHE:HZ | 1.59 | 0.50 |
| 2:LD:379:LYS:O | 4:2A:166:ILE:HD13 | 2.08 | 0.50 |
| 6:4A:139:ASP:CG | 6:4A:140:PRO:HD2 | 2.34 | 0.50 |
| 6:4A:251:TYR:CE2 | 6:4A:280:VAL:HG12 | 2.46 | 0.50 |
| 6:4C:139:ASP:CG | 6:4C:140:PRO:HD2 | 2.34 | 0.50 |
| 7:5A:943:LEU:HD22 | 7:5A:1030:PHE:CE2 | 2.46 | 0.50 |
| 7:5A:1434:LYS:CE | 7:5A:1434:LYS:CA | 2.86 | 0.50 |
| 7:5B:1436:ARG:CZ | 7:5B:1436:ARG:C | 2.85 | 0.50 |
| 7:5B:1515:GLU:OE1 | 7:5B:1563:SER:HB2 | 2.06 | 0.50 |
| 7:5B:1552:LYS:NZ | 7:5B:1563:SER:N | 2.59 | 0.50 |
| 7:5C:1030:PHE:CZ | 7:5C:1034:ILE:CD1 | 2.95 | 0.50 |
| 7:5C:1246:LEU:CA | 9:7F:12:GLU:CD | 2.80 | 0.50 |
| 7:5C:1370:LYS:CA | 7:5C:1370:LYS:CE | 2.85 | 0.50 |
| 7:5C:1399:LYS:NZ | 7:5C:1399:LYS:CB | 2.73 | 0.50 |
| 7:5C:1552:LYS:NZ | 7:5C:1563:SER:N | 2.59 | 0.50 |
| 8:6B:190:PRO:HD3 | 8:6B:256:TYR:OH | 2.11 | 0.50 |
| 9:7C:39:GLY:N | 9:7D:43:LEU:HD21 | 2.27 | 0.50 |
| 2:AB:180:VAL:HG12 | 1:AC:258:ASN:OD1 | 2.10 | 0.50 |
| 2:AD:10:GLY:O | 2:AD:14:ASN:ND2 | 2.44 | 0.50 |
| 1:BA:118:CYS:O | 1:BA:122:ILE:HG12 | 2.11 | 0.50 |
| 2:BB:177:ASP:HA | 1:BC:353:VAL:HG12 | 1.94 | 0.50 |
| 1:BC:118:CYS:O | 1:BC:122:ILE:HG12 | 2.11 | 0.50 |
| 1:CA:60:LYS:NZ | 1:DA:283:HIS:CE1 | 2.76 | 0.50 |
| 2:CF:86:ARG:CG | 2:DF:281:TYR:CE1 | 2.47 | 0.50 |
| 1:DA:62:VAL:CG2 | 1:EA:283:HIS:O | 2.50 | 0.50 |
| 1:FC:222:PRO:HG2 | 2:FD:324:LYS:CD | 2.40 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:FD:332:ASN:HB2 | 7:5A:909:ASN:OD1 | 2.11 | 0.50 |
| 2:GF:416:ASN:HB3 | 7:5B:1327:LYS:HE2 | 1.92 | 0.50 |
| 2:HB:212:PHE:CZ | 1:HC:326:LYS:CE | 2.93 | 0.50 |
| 2:IF:406:MET:O | 2:IF:410:GLU:HG3 | 2.10 | 0.50 |
| 1:JC:118:CYS:O | 1:JC:122:ILE:HG12 | 2.11 | 0.50 |
| 1:KA:359:PRO:HG3 | 6:4C:299:TYR:CD2 | 2.47 | 0.50 |
| 2:LB:413:SER:HB2 | 4:2C:171:VAL:HG22 | 1.92 | 0.50 |
| 2:LD:179:VAL:HG22 | 1:LE:258:ASN:HA | 1.92 | 0.50 |
| 2:LF:19:LYS:NZ | 6:4D:217:ASN:O | 2.43 | 0.50 |
| 2:MB:318:ARG:HH11 | 2:MB:358:PRO:HG3 | 1.75 | 0.50 |
| 2:MF:135:ILE:HB | 2:MF:166:THR:HG22 | 1.93 | 0.50 |
| 4:2A:144:ASN:O | 4:2A:144:ASN:ND2 | 2.43 | 0.50 |
| 4:2B:144:ASN:O | 4:2B:144:ASN:ND2 | 2.43 | 0.50 |
| 6:4B:251:TYR:HB2 | 6:4B:288:TYR:HE2 | 1.74 | 0.50 |
| 7:5C:890:ILE:CD1 | 7:5C:1072:PHE:CE1 | 2.95 | 0.50 |
| 8:6A:62:ALA:HB2 | 8:6A:87:TYR:CE1 | 2.47 | 0.50 |
| 8:6B:62:ALA:HB2 | 8:6B:87:TYR:CE1 | 2.47 | 0.50 |
| 8:6C:62:ALA:HB2 | 8:6C:87:TYR:CE1 | 2.47 | 0.50 |
| 8:6C:136:LEU:HD23 | 8:6C:140:GLN:CB | 2.42 | 0.50 |
| 2:DD:10:GLY:O | 2:DD:14:ASN:ND2 | 2.44 | 0.50 |
| 2:DF:10:GLY:O | 2:DF:14:ASN:ND2 | 2.44 | 0.50 |
| 2:FD:220:PRO:HD2 | 1:FE:326:LYS:CE | 2.35 | 0.50 |
| 1:FE:422:ARG:CZ | 7:5B:1170:THR:HA | 2.35 | 0.50 |
| 1:GC:409:VAL:CB | 5:3C:383:GLU:OE1 | 2.60 | 0.50 |
| 2:GD:409:THR:CG2 | 7:5A:1330:ILE:HD13 | 2.40 | 0.50 |
| 1:GE:176:GLN:O | 2:GF:347:ASN:ND2 | 2.40 | 0.50 |
| 2:GF:409:THR:O | 7:5B:1330:ILE:HD13 | 2.12 | 0.50 |
| 1:HC:369:ALA:HB1 | 10:8T:18:UNK:HA | 1.93 | 0.50 |
| 1:HC:398:MET:SD | 2:HD:345:ILE:CG1 | 2.90 | 0.50 |
| 1:JE:71:GLU:CD | 2:JF:247:ASN:ND2 | 2.69 | 0.50 |
| 1:KA:357:TYR:OH | 6:4C:257:LEU:HD23 | 2.12 | 0.50 |
| 2:LB:379:LYS:HZ1 | 4:2C:166:ILE:CB | 2.25 | 0.50 |
| 2:LD:179:VAL:HG21 | 1:LE:258:ASN:CA | 2.41 | 0.50 |
| 2:LD:179:VAL:CG2 | 1:LE:258:ASN:O | 2.37 | 0.50 |
| 2:LF:221:THR:CG2 | 6:4D:219:ASN:ND2 | 2.75 | 0.50 |
| 2:MD:179:VAL:HG22 | 1:ME:258:ASN:CB | 2.42 | 0.50 |
| 1:ME:357:TYR:CE2 | 6:4B:185:ARG:NH2 | 2.71 | 0.50 |
| 4:2C:144:ASN:O | 4:2C:144:ASN:ND2 | 2.43 | 0.50 |
| 6:4B:251:TYR:CE2 | 6:4B:280:VAL:HG12 | 2.46 | 0.50 |
| 6:4C:251:TYR:CE2 | 6:4C:280:VAL:HG12 | 2.46 | 0.50 |
| 7:5A:890:ILE:CD1 | 7:5A:1072:PHE:CE1 | 2.95 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5A:1552:LYS:NZ | 7:5A:1563:SER:N | 2.59 | 0.50 |
| 7:5C:836:ARG:CG | 7:5C:836:ARG:NH1 | 2.71 | 0.50 |
| 9:7C:18:VAL:HG21 | 9:7D:35:ILE:CG2 | 2.30 | 0.50 |
| 1:BA:71:GLU:CD | 2:BB:247:ASN:ND2 | 2.69 | 0.50 |
| 2:GB:180:VAL:HG12 | 1:GC:258:ASN:OD1 | 2.10 | 0.50 |
| 2:KB:87:PRO:HD2 | 2:LB:282:ARG:CG | 2.39 | 0.50 |
| 2:KD:221:THR:HB | 6:4B:261:SER:O | 2.12 | 0.50 |
| 1:KE:237:SER:HA | 1:KE:320:ARG:HH11 | 1.77 | 0.50 |
| 2:MD:221:THR:CB | 6:4B:189:ARG:HH12 | 2.24 | 0.50 |
| 6:4A:241:LYS:C | 6:4A:241:LYS:HD3 | 2.32 | 0.50 |
| 6:4D:251:TYR:HB2 | 6:4D:288:TYR:HE2 | 1.74 | 0.50 |
| 7:5B:890:ILE:CD1 | 7:5B:1072:PHE:CE1 | 2.95 | 0.50 |
| 7:5C:943:LEU:HD22 | 7:5C:1030:PHE:CE2 | 2.46 | 0.50 |
| 7:5C:1113:ILE:HG12 | 7:5C:1157:THR:CG2 | 2.41 | 0.50 |
| 9:7E:11:TYR:CZ | 9:7F:26:LEU:HB3 | 2.43 | 0.50 |
| 1:AC:221:ARG:HG3 | 6:4C:156:PHE:CZ | 2.47 | 0.50 |
| 2:AD:356:ILE:CD1 | 6:4C:152:PHE:CD1 | 2.82 | 0.50 |
| 2:BB:212:PHE:CZ | 1:BC:326:LYS:CE | 2.91 | 0.50 |
| 1:BE:71:GLU:CD | 2:BF:247:ASN:ND2 | 2.69 | 0.50 |
| 1:BE:118:CYS:O | 1:BE:122:ILE:HG12 | 2.11 | 0.50 |
| 1:DE:412:GLY:HA2 | 7:5B:792:TYR:CZ | 2.47 | 0.50 |
| 1:EA:222:PRO:CG | 2:EB:324:LYS:CD | 2.87 | 0.50 |
| 1:EA:430:LYS:HZ1 | 7:5C:834:ASN:ND2 | 0.51 | 0.50 |
| 2:FD:208:TYR:CD2 | 1:FE:326:LYS:HB3 | 2.46 | 0.50 |
| 2:GD:409:THR:CG2 | 7:5A:1330:ILE:CD1 | 2.64 | 0.50 |
| 1:JA:89:PRO:HD2 | 1:KA:283:HIS:CE1 | 2.27 | 0.50 |
| 1:JA:118:CYS:O | 1:JA:122:ILE:HG12 | 2.11 | 0.50 |
| 2:KF:25:SER:HG | 2:KF:51:TYR:HH | 1.54 | 0.50 |
| 2:LB:212:PHE:CZ | 1:LC:326:LYS:CG | 2.91 | 0.50 |
| 1:LC:47:ASP:OD1 | 6:4A:203:LYS:CE | 2.59 | 0.50 |
| 1:LC:56:THR:O | 1:MC:285:GLN:HB3 | 2.10 | 0.50 |
| 2:LF:337:ASN:ND2 | 4:2B:148:ASN:H | 2.10 | 0.50 |
| 2:MB:221:THR:HG21 | 6:4A:189:ARG:NH1 | 2.26 | 0.50 |
| 1:MC:71:GLU:CD | 2:MD:247:ASN:HD22 | 2.19 | 0.50 |
| 1:MC:179:THR:O | 2:MD:350:LYS:HA | 2.11 | 0.50 |
| 1:MC:401:LYS:CE | 2:MD:344:TRP:CZ3 | 2.69 | 0.50 |
| 6:4B:247:LYS:CD | 6:4B:247:LYS:H | 2.12 | 0.50 |
| 6:4D:247:LYS:CD | 6:4D:247:LYS:H | 2.12 | 0.50 |
| 7:5A:1386:LYS:NZ | 7:5A:1386:LYS:N | 2.60 | 0.50 |
| 7:5A:1418:GLN:HA | 7:5A:1418:GLN:OE1 | 2.12 | 0.50 |
| 7:5B:1272:ILE:CD1 | 9:7D:11:TYR:CD2 | 2.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5B:1386:LYS:NZ | 7:5B:1386:LYS:N | 2.60 | 0.50 |
| 7:5B:1418:GLN:HA | 7:5B:1418:GLN:OE1 | 2.12 | 0.50 |
| 7:5C:1418:GLN:OE1 | 7:5C:1418:GLN:HA | 2.12 | 0.50 |
| 7:5C:1552:LYS:CE | 7:5C:1563:SER:CB | 2.73 | 0.50 |
| 9:7C:42:LEU:HD13 | 9:7D:39:GLY:HA3 | 1.88 | 0.50 |
| 1:AA:237:SER:HA | 1:AA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:AC:237:SER:HA | 1:AC:320:ARG:HH11 | 1.77 | 0.49 |
| 2:BD:179:VAL:HG22 | 1:BE:258:ASN:CB | 2.42 | 0.49 |
| 1:DC:176:GLN:O | 2:DD:347:ASN:ND2 | 2.35 | 0.49 |
| 1:FE:402:ARG:HD3 | 7:5B:1259:TYR:CG | 2.44 | 0.49 |
| 2:IB:212:PHE:CZ | 1:IC:326:LYS:CE | 2.93 | 0.49 |
| 1:IE:278:ALA:CB | 10:8X:18:UNK:O | 2.41 | 0.49 |
| 1:JA:90:GLU:HG2 | 1:KA:280:LYS:HB3 | 1.93 | 0.49 |
| 1:KA:237:SER:HA | 1:KA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:KC:237:SER:HA | 1:KC:320:ARG:HH11 | 1.77 | 0.49 |
| 2:KF:159:TYR:CE2 | 4:2B:36:THR:N | 2.53 | 0.49 |
| 2:KF:221:THR:HB | 6:4D:261:SER:O | 2.10 | 0.49 |
| 1:LA:222:PRO:HG2 | 2:LB:324:LYS:CB | 2.36 | 0.49 |
| 2:LB:54:ALA:CA | 2:MB:283:ALA:HB2 | 2.42 | 0.49 |
| 6:4D:251:TYR:CE2 | 6:4D:280:VAL:HG12 | 2.46 | 0.49 |
| 7:5A:1113:ILE:HG12 | 7:5A:1157:THR:CG2 | 2.41 | 0.49 |
| 7:5A:1471:ILE:O | 7:5A:1473:GLU:N | 2.39 | 0.49 |
| 7:5C:1548:VAL:CB | 7:5C:1566:GLU:O | 2.60 | 0.49 |
| 8:6A:136:LEU:HD23 | 8:6A:140:GLN:CB | 2.42 | 0.49 |
| 2:AD:281:TYR:CZ | 1:MA:60:LYS:NZ | 2.80 | 0.49 |
| 1:AE:237:SER:HA | 1:AE:320:ARG:HH11 | 1.77 | 0.49 |
| 2:BB:179:VAL:CG2 | 1:BC:258:ASN:O | 2.38 | 0.49 |
| 2:BB:394:PHE:CD1 | 1:BC:261:PRO:HA | 2.47 | 0.49 |
| 1:BC:237:SER:HA | 1:BC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:BE:237:SER:HA | 1:BE:320:ARG:HH11 | 1.77 | 0.49 |
| 2:CB:179:VAL:HG22 | 1:CC:258:ASN:CB | 2.42 | 0.49 |
| 2:FB:54:ALA:CB | 2:GB:283:ALA:HB2 | 2.25 | 0.49 |
| 2:FB:372:THR:HA | 2:FB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:FC:56:THR:O | 1:GC:285:GLN:CA | 2.60 | 0.49 |
| 2:FF:372:THR:HA | 2:FF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:GA:60:LYS:HZ3 | 1:HA:283:HIS:CE1 | 2.27 | 0.49 |
| 1:GA:89:PRO:CD | 1:HA:280:LYS:CD | 2.89 | 0.49 |
| 1:GA:179:THR:O | 2:GB:350:LYS:HA | 2.12 | 0.49 |
| 2:GD:58:ARG:CZ | 2:HD:281:TYR:CZ | 2.95 | 0.49 |
| 2:HB:372:THR:HA | 2:HB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:HC:141:VAL:HG12 | 1:HC:171:ILE:O | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HE:141:VAL:HG12 | 1:HE:171:ILE:O | 2.13 | 0.49 |
| 1:JC:237:SER:HA | 1:JC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:JE:141:VAL:HG12 | 1:JE:171:ILE:O | 2.12 | 0.49 |
| 2:LB:221:THR:CG2 | 6:4A:219:ASN:ND2 | 2.75 | 0.49 |
| 2:MB:180:VAL:HG12 | 1:MC:258:ASN:OD1 | 2.11 | 0.49 |
| 1:MC:178:SER:OG | 2:MD:347:ASN:HB3 | 2.11 | 0.49 |
| 2:MD:218:THR:OG1 | 6:4B:196:GLN:NE2 | 2.40 | 0.49 |
| 7:5A:847:GLY:HA3 | 8:6A:17:LYS:NZ | 2.27 | 0.49 |
| 7:5A:1548:VAL:CB | 7:5A:1566:GLU:O | 2.60 | 0.49 |
| 7:5B:1434:LYS:CE | 7:5B:1434:LYS:CA | 2.86 | 0.49 |
| 7:5B:1548:VAL:CG1 | 7:5B:1569:GLU:CB | 2.54 | 0.49 |
| 7:5C:1386:LYS:N | 7:5C:1386:LYS:NZ | 2.60 | 0.49 |
| 7:5C:1404:LYS:C | 7:5C:1404:LYS:CE | 2.85 | 0.49 |
| 8:6B:136:LEU:HD23 | 8:6B:140:GLN:CB | 2.42 | 0.49 |
| 1:AA:222:PRO:HG3 | 2:AB:324:LYS:HD3 | 1.94 | 0.49 |
| 2:AB:98:GLY:CA | 1:AC:254:GLU:CG | 2.48 | 0.49 |
| 2:AD:98:GLY:CA | 1:AE:254:GLU:CG | 2.48 | 0.49 |
| 1:CA:60:LYS:HZ3 | 1:DA:283:HIS:CE1 | 2.29 | 0.49 |
| 1:GA:60:LYS:NZ | 1:HA:283:HIS:CG | 2.70 | 0.49 |
| 1:GE:89:PRO:CG | 1:HE:280:LYS:HD2 | 2.41 | 0.49 |
| 1:HA:179:THR:O | 2:HB:350:LYS:HA | 2.12 | 0.49 |
| 2:HD:372:THR:HA | 2:HD:422:TYR:CE2 | 2.48 | 0.49 |
| 2:IB:372:THR:HA | 2:IB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:IE:141:VAL:HG12 | 1:IE:171:ILE:O | 2.13 | 0.49 |
| 2:IF:372:THR:HA | 2:IF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:JA:237:SER:HA | 1:JA:320:ARG:HH11 | 1.77 | 0.49 |
| 2:JB:372:THR:HA | 2:JB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:JC:90:GLU:CG | 1:KC:280:LYS:HB3 | 2.41 | 0.49 |
| 2:JD:372:THR:HA | 2:JD:422:TYR:CE2 | 2.48 | 0.49 |
| 2:LB:372:THR:HA | 2:LB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:LC:141:VAL:HG12 | 1:LC:171:ILE:O | 2.13 | 0.49 |
| 2:LD:379:LYS:NZ | 4:2A:166:ILE:HB | 2.27 | 0.49 |
| 1:LE:60:LYS:HD3 | 1:ME:283:HIS:CA | 2.42 | 0.49 |
| 2:MF:221:THR:CG2 | 6:4D:189:ARG:CZ | 2.73 | 0.49 |
| 2:MF:372:THR:HA | 2:MF:422:TYR:CE2 | 2.48 | 0.49 |
| 4:2B:164:ARG:C | 4:2B:164:ARG:HD3 | 2.38 | 0.49 |
| 7:5B:947:GLU:OE1 | 7:5B:1037:LYS:NZ | 2.43 | 0.49 |
| 7:5B:1481:GLN:O | 7:5B:1485:LYS:HB2 | 2.12 | 0.49 |
| 7:5B:1548:VAL:CB | 7:5B:1566:GLU:O | 2.60 | 0.49 |
| 7:5B:1552:LYS:HZ3 | 7:5B:1563:SER:HB2 | 0.67 | 0.49 |
| 7:5C:1416:LYS:CD | 7:5C:1416:LYS:C | 2.85 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:BA:222:PRO:HG3 | 2:BB:324:LYS:HD3 | 1.94 | 0.49 |
| 1:BA:237:SER:HA | 1:BA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:CA:141:VAL:HG12 | 1:CA:171:ILE:O | 2.13 | 0.49 |
| 2:CB:180:VAL:HG12 | 1:CC:258:ASN:OD1 | 2.12 | 0.49 |
| 1:CC:141:VAL:HG12 | 1:CC:171:ILE:O | 2.13 | 0.49 |
| 1:CE:141:VAL:HG12 | 1:CE:171:ILE:O | 2.13 | 0.49 |
| 1:FA:141:VAL:HG12 | 1:FA:171:ILE:O | 2.13 | 0.49 |
| 2:FB:332:ASN:CG | 7:5C:909:ASN:ND2 | 2.67 | 0.49 |
| 1:FC:141:VAL:HG12 | 1:FC:171:ILE:O | 2.13 | 0.49 |
| 2:FD:372:THR:HA | 2:FD:422:TYR:CE2 | 2.48 | 0.49 |
| 1:FE:60:LYS:CE | 1:GE:283:HIS:CG | 2.92 | 0.49 |
| 1:FE:141:VAL:HG12 | 1:FE:171:ILE:O | 2.13 | 0.49 |
| 1:GC:141:VAL:HG12 | 1:GC:171:ILE:O | 2.13 | 0.49 |
| 1:HA:141:VAL:HG12 | 1:HA:171:ILE:O | 2.13 | 0.49 |
| 1:IC:141:VAL:HG12 | 1:IC:171:ILE:O | 2.13 | 0.49 |
| 2:ID:372:THR:HA | 2:ID:422:TYR:CE2 | 2.48 | 0.49 |
| 1:JC:141:VAL:HG12 | 1:JC:171:ILE:O | 2.13 | 0.49 |
| 1:JE:88:HIS:HE1 | 1:KE:280:LYS:HB3 | 1.74 | 0.49 |
| 1:JE:237:SER:HA | 1:JE:320:ARG:HH11 | 1.77 | 0.49 |
| 2:JF:372:THR:HA | 2:JF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:LA:141:VAL:HG12 | 1:LA:171:ILE:O | 2.13 | 0.49 |
| 1:LA:178:SER:OG | 2:LB:347:ASN:CB | 2.52 | 0.49 |
| 2:LB:223:GLY:HA3 | 6:4A:219:ASN:CA | 2.40 | 0.49 |
| 1:LC:237:SER:HA | 1:LC:320:ARG:HH11 | 1.77 | 0.49 |
| 2:LF:372:THR:HA | 2:LF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:MA:282:TYR:HD2 | 6:4C:104:ARG:NE | 2.09 | 0.49 |
| 2:MB:372:THR:HA | 2:MB:422:TYR:CE2 | 2.48 | 0.49 |
| 2:MD:179:VAL:HG22 | 1:ME:258:ASN:CG | 2.37 | 0.49 |
| 1:ME:141:VAL:HG12 | 1:ME:171:ILE:O | 2.13 | 0.49 |
| 4:2A:164:ARG:HD3 | 4:2A:164:ARG:C | 2.38 | 0.49 |
| 4:2C:164:ARG:HD3 | 4:2C:164:ARG:C | 2.38 | 0.49 |
| 6:4B:106:ALA:HB3 | 6:4B:107:MET:HE3 | 1.93 | 0.49 |
| 6:4B:175:LEU:N | 6:4B:175:LEU:HD22 | 2.26 | 0.49 |
| 6:4D:175:LEU:N | 6:4D:175:LEU:HD22 | 2.26 | 0.49 |
| 7:5A:1404:LYS:C | 7:5A:1404:LYS:CE | 2.85 | 0.49 |
| 7:5A:1416:LYS:CD | 7:5A:1416:LYS:C | 2.85 | 0.49 |
| 7:5A:1521:PHE:HE1 | 7:5A:1570:ALA:HB1 | 1.78 | 0.49 |
| 7:5B:1484:TYR:CG | 7:5B:1568:LYS:HD3 | 2.47 | 0.49 |
| 7:5B:1521:PHE:HE1 | 7:5B:1570:ALA:HB1 | 1.78 | 0.49 |
| 7:5C:1125:LEU:HD23 | 8:6C:246:TYR:HE2 | 1.76 | 0.49 |
| 1:AE:141:VAL:HG12 | 1:AE:171:ILE:O | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:BB:501:GDP:C8 | 1:BC:248:LEU:CD1 | 2.95 | 0.49 |
| 1:BC:141:VAL:HG12 | 1:BC:171:ILE:O | 2.13 | 0.49 |
| 1:BC:394:LYS:NZ | 2:BD:347:ASN:OD1 | 2.46 | 0.49 |
| 1:BE:141:VAL:HG12 | 1:BE:171:ILE:O | 2.13 | 0.49 |
| 1:CA:237:SER:HA | 1:CA:320:ARG:HH11 | 1.77 | 0.49 |
| 2:CB:212:PHE:CE2 | 1:CC:326:LYS:HB2 | 2.48 | 0.49 |
| 2:CB:372:THR:HA | 2:CB:422:TYR:CE2 | 2.48 | 0.49 |
| 2:CB:397:TRP:CB | 1:CC:256:GLN:HE22 | 2.16 | 0.49 |
| 1:CC:237:SER:HA | 1:CC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:CE:237:SER:HA | 1:CE:320:ARG:HH11 | 1.77 | 0.49 |
| 2:CF:372:THR:HA | 2:CF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:DC:237:SER:HA | 1:DC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:DE:237:SER:HA | 1:DE:320:ARG:HH11 | 1.77 | 0.49 |
| 1:EA:393:HIS:HE1 | 7:5C:814:LYS:HG3 | 1.71 | 0.49 |
| 1:FC:88:HIS:C | 1:GC:280:LYS:HZ2 | 2.19 | 0.49 |
| 1:GA:56:THR:O | 1:HA:285:GLN:CB | 2.59 | 0.49 |
| 1:HC:179:THR:O | 2:HD:350:LYS:HA | 2.13 | 0.49 |
| 2:HF:372:THR:HA | 2:HF:422:TYR:CE2 | 2.48 | 0.49 |
| 2:LD:372:THR:HA | 2:LD:422:TYR:CE2 | 2.48 | 0.49 |
| 1:LE:141:VAL:HG12 | 1:LE:171:ILE:O | 2.13 | 0.49 |
| 2:LF:379:LYS:O | 4:2B:166:ILE:HD13 | 2.02 | 0.49 |
| 1:MC:141:VAL:HG12 | 1:MC:171:ILE:O | 2.13 | 0.49 |
| 2:MD:110:ALA:C | 3:1B:61:HIS:HB3 | 2.33 | 0.49 |
| 2:MD:372:THR:HA | 2:MD:422:TYR:CE2 | 2.48 | 0.49 |
| 6:4A:175:LEU:N | 6:4A:175:LEU:HD22 | 2.26 | 0.49 |
| 7:5A:826:LEU:CD2 | 7:5A:840:GLY:CA | 2.75 | 0.49 |
| 7:5A:1481:GLN:O | 7:5A:1485:LYS:HB2 | 2.12 | 0.49 |
| 7:5B:1416:LYS:CD | 7:5B:1416:LYS:C | 2.85 | 0.49 |
| 7:5C:1443:LYS:C | 7:5C:1443:LYS:CD | 2.85 | 0.49 |
| 7:5C:1481:GLN:O | 7:5C:1485:LYS:HB2 | 2.13 | 0.49 |
| 1:AC:141:VAL:HG12 | 1:AC:171:ILE:O | 2.13 | 0.49 |
| 1:AE:283:HIS:O | 2:MB:54:ALA:HB2 | 2.07 | 0.49 |
| 2:CD:180:VAL:HG12 | 1:CE:258:ASN:OD1 | 2.13 | 0.49 |
| 2:CD:372:THR:HA | 2:CD:422:TYR:CE2 | 2.48 | 0.49 |
| 1:DA:237:SER:HA | 1:DA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:EC:237:SER:HA | 1:EC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:EE:88:HIS:CE1 | 1:EE:90:GLU:HG2 | 2.48 | 0.49 |
| 1:FA:56:THR:OG1 | 1:GA:285:GLN:HA | 2.13 | 0.49 |
| 2:FB:208:TYR:CD2 | 1:FC:326:LYS:HB3 | 2.47 | 0.49 |
| 2:FB:220:PRO:HD2 | 1:FC:326:LYS:HG2 | 1.93 | 0.49 |
| 1:GA:141:VAL:HG12 | 1:GA:171:ILE:O | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:IA:141:VAL:HG12 | 1:IA:171:ILE:O | 2.13 | 0.49 |
| 1:KC:127:ASP:OD2 | 1:LC:334:THR:CG2 | 2.61 | 0.49 |
| 1:LE:237:SER:HA | 1:LE:320:ARG:HH11 | 1.77 | 0.49 |
| 2:LF:15:GLN:NE2 | 6:4D:217:ASN:OD1 | 2.46 | 0.49 |
| 2:LF:340:TYR:HB2 | 4:2B:147:PHE:HB2 | 1.94 | 0.49 |
| 1:MA:141:VAL:HG12 | 1:MA:171:ILE:O | 2.13 | 0.49 |
| 4:2B:16:GLN:CA | 4:2B:19:MET:H | 2.25 | 0.49 |
| 6:4A:99:ARG:HH21 | 6:4A:103:GLU:HG3 | 1.78 | 0.49 |
| 6:4C:99:ARG:HH21 | 6:4C:103:GLU:HG3 | 1.78 | 0.49 |
| 6:4C:168:PHE:C | 6:4C:168:PHE:CD1 | 2.90 | 0.49 |
| 7:5A:947:GLU:OE1 | 7:5A:1037:LYS:NZ | 2.43 | 0.49 |
| 7:5B:773:ARG:C | 7:5B:773:ARG:CD | 2.85 | 0.49 |
| 7:5C:1521:PHE:HE1 | 7:5C:1570:ALA:HB1 | 1.78 | 0.49 |
| 9:7E:30:ARG:HH11 | 9:7F:3:GLN:HG2 | 1.77 | 0.49 |
| 1:AE:283:HIS:O | 2:MB:54:ALA:HB3 | 2.03 | 0.49 |
| 2:AF:223:GLY:C | 6:4A:131:VAL:CA | 2.65 | 0.49 |
| 1:BA:278:ALA:CB | 10:8A:21:UNK:CB | 2.91 | 0.49 |
| 1:CA:241:SER:OG | 1:CA:250:VAL:O | 2.23 | 0.49 |
| 1:DA:141:VAL:HG12 | 1:DA:171:ILE:O | 2.13 | 0.49 |
| 2:DB:212:PHE:HE2 | 1:DC:326:LYS:HB2 | 1.78 | 0.49 |
| 1:DC:141:VAL:HG12 | 1:DC:171:ILE:O | 2.13 | 0.49 |
| 1:DE:71:GLU:CD | 2:DF:247:ASN:ND2 | 2.71 | 0.49 |
| 2:DF:86:ARG:HA | 2:EF:281:TYR:CD1 | 2.39 | 0.49 |
| 1:EA:237:SER:HA | 1:EA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:EE:141:VAL:HG12 | 1:EE:171:ILE:O | 2.13 | 0.49 |
| 2:FF:106:TYR:CD1 | 7:5B:1295:LYS:N | 2.80 | 0.49 |
| 2:GB:372:THR:HA | 2:GB:422:TYR:CE2 | 2.48 | 0.49 |
| 1:GC:179:THR:O | 2:GD:350:LYS:HA | 2.13 | 0.49 |
| 1:GC:237:SER:HA | 1:GC:320:ARG:HH11 | 1.77 | 0.49 |
| 2:GD:372:THR:HA | 2:GD:422:TYR:CE2 | 2.48 | 0.49 |
| 1:GE:141:VAL:HG12 | 1:GE:171:ILE:O | 2.13 | 0.49 |
| 1:HE:237:SER:HA | 1:HE:320:ARG:HH11 | 1.77 | 0.49 |
| 1:HE:404:PHE:CE2 | 2:HF:345:ILE:HD11 | 2.48 | 0.49 |
| 1:IA:237:SER:HA | 1:IA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:IE:404:PHE:CE2 | 2:IF:345:ILE:HD11 | 2.48 | 0.49 |
| 1:JA:141:VAL:HG12 | 1:JA:171:ILE:O | 2.13 | 0.49 |
| 1:KA:222:PRO:HG3 | 2:KB:324:LYS:HD3 | 1.94 | 0.49 |
| 2:KB:276:ARG:NH2 | 6:4A:265:TYR:HB2 | 2.27 | 0.49 |
| 1:KE:245:ASP:OD2 | 6:4B:257:LEU:HD12 | 2.12 | 0.49 |
| 1:LA:237:SER:HA | 1:LA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:LC:56:THR:C | 1:MC:285:GLN:HB3 | 2.38 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:ME:279:GLU:OE1 | 6:4B:107:MET:CG | 2.60 | 0.49 |
| 4:2A:16:GLN:CA | 4:2A:19:MET:H | 2.25 | 0.49 |
| 4:2C:16:GLN:CA | 4:2C:19:MET:H | 2.25 | 0.49 |
| 6:4C:241:LYS:C | 6:4C:241:LYS:HD3 | 2.32 | 0.49 |
| 6:4C:248:VAL:HA | 6:4C:251:TYR:CE2 | 2.48 | 0.49 |
| 7:5A:773:ARG:C | 7:5A:773:ARG:CD | 2.85 | 0.49 |
| 7:5A:1484:TYR:CG | 7:5A:1568:LYS:HD3 | 2.47 | 0.49 |
| 7:5B:1404:LYS:C | 7:5B:1404:LYS:CE | 2.85 | 0.49 |
| 1:AA:71:GLU:CD | 2:AB:247:ASN:ND2 | 2.71 | 0.49 |
| 2:AF:217:LEU:HD22 | 6:4A:132:LYS:HD3 | 1.95 | 0.49 |
| 1:BA:141:VAL:HG12 | 1:BA:171:ILE:O | 2.13 | 0.49 |
| 2:BD:222:TYR:HD2 | 1:BE:247:ALA:HB1 | 1.76 | 0.49 |
| 2:CF:86:ARG:CA | 2:DF:281:TYR:OH | 2.60 | 0.49 |
| 2:DD:84:LEU:C | 2:ED:281:TYR:OH | 2.56 | 0.49 |
| 1:DE:141:VAL:HG12 | 1:DE:171:ILE:O | 2.13 | 0.49 |
| 1:EC:60:LYS:HD3 | 1:FC:283:HIS:HA | 1.95 | 0.49 |
| 1:EC:88:HIS:CE1 | 1:EC:90:GLU:HG2 | 2.48 | 0.49 |
| 1:FA:237:SER:HA | 1:FA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:GA:237:SER:HA | 1:GA:320:ARG:HH11 | 1.77 | 0.49 |
| 1:GA:370:LYS:HG2 | 10:8P:18:UNK:N | 2.28 | 0.49 |
| 1:IC:237:SER:HA | 1:IC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:IE:279:GLU:HG2 | 10:8X:22:UNK:HA | 1.94 | 0.49 |
| 2:LB:296:ALA:H | 4:2C:149:ILE:HA | 1.77 | 0.49 |
| 1:LC:88:HIS:CE1 | 1:LC:90:GLU:HG2 | 2.48 | 0.49 |
| 1:MA:178:SER:OG | 2:MB:347:ASN:HB3 | 2.11 | 0.49 |
| 2:MF:221:THR:CB | 6:4D:189:ARG:HH12 | 2.26 | 0.49 |
| 6:4A:248:VAL:HA | 6:4A:251:TYR:CE2 | 2.48 | 0.49 |
| 6:4B:248:VAL:HA | 6:4B:251:TYR:CE2 | 2.48 | 0.49 |
| 7:5B:1250:VAL:HG11 | 7:5B:1262:GLU:HG3 | 1.95 | 0.49 |
| 7:5C:1250:VAL:HG11 | 7:5C:1262:GLU:HG3 | 1.95 | 0.49 |
| 7:5C:1471:ILE:O | 7:5C:1473:GLU:N | 2.39 | 0.49 |
| 9:7E:15:VAL:HG12 | 9:7F:35:ILE:HA | 1.95 | 0.49 |
| 1:AA:88:HIS:CE1 | 1:AA:90:GLU:HG2 | 2.48 | 0.49 |
| 1:AC:88:HIS:CE1 | 1:AC:90:GLU:HG2 | 2.48 | 0.49 |
| 1:BE:176:GLN:O | 2:BF:347:ASN:ND2 | 2.39 | 0.49 |
| 1:CA:88:HIS:CE1 | 1:CA:90:GLU:HG2 | 2.48 | 0.49 |
| 1:CC:88:HIS:CE1 | 1:CC:90:GLU:HG2 | 2.48 | 0.49 |
| 1:DA:100:ALA:HB1 | 2:DB:252:LYS:HA | 1.94 | 0.49 |
| 1:DC:412:GLY:HA2 | 7:5A:792:TYR:CZ | 2.47 | 0.49 |
| 2:DD:86:ARG:HB2 | 2:ED:281:TYR:CE1 | 2.47 | 0.49 |
| 1:EA:88:HIS:CE1 | 1:EA:90:GLU:HG2 | 2.48 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:EB:178:THR:HA | 1:EC:352:LYS:HD3 | 1.94 | 0.49 |
| 1:EE:237:SER:HA | 1:EE:320:ARG:HH11 | 1.77 | 0.49 |
| 1:FA:62:VAL:CG2 | 1:GA:283:HIS:O | 2.61 | 0.49 |
| 1:FE:237:SER:HA | 1:FE:320:ARG:HH11 | 1.77 | 0.49 |
| 1:GE:237:SER:HA | 1:GE:320:ARG:HH11 | 1.77 | 0.49 |
| 1:GE:404:PHE:CE2 | 2:GF:345:ILE:HD11 | 2.48 | 0.49 |
| 2:GF:372:THR:HA | 2:GF:422:TYR:CE2 | 2.48 | 0.49 |
| 1:HC:237:SER:HA | 1:HC:320:ARG:HH11 | 1.77 | 0.49 |
| 2:ID:212:PHE:HZ | 1:IE:326:LYS:CE | 2.19 | 0.49 |
| 1:JA:89:PRO:CD | 1:KA:280:LYS:HA | 2.41 | 0.49 |
| 2:JB:88:ASP:HB2 | 2:KB:278:SER:CB | 2.40 | 0.49 |
| 1:KA:124:LYS:CD | 1:LA:293:ASN:HB2 | 2.40 | 0.49 |
| 2:KB:32:PRO:CG | 6:4A:279:LEU:HD21 | 2.39 | 0.49 |
| 2:KF:130:LEU:HB3 | 2:KF:162:ARG:HD2 | 1.95 | 0.49 |
| 1:LA:88:HIS:CE1 | 1:LA:90:GLU:HG2 | 2.48 | 0.49 |
| 2:LB:212:PHE:CE2 | 1:LC:326:LYS:HB2 | 2.47 | 0.49 |
| 1:LC:222:PRO:CD | 2:LD:324:LYS:CB | 2.89 | 0.49 |
| 1:LE:71:GLU:OE1 | 2:LF:247:ASN:ND2 | 2.46 | 0.49 |
| 1:LE:88:HIS:CE1 | 1:LE:90:GLU:HG2 | 2.48 | 0.49 |
| 2:LF:228:LEU:HD21 | 6:4D:225:PRO:CB | 2.42 | 0.49 |
| 2:LF:310:TYR:HE2 | 4:2B:147:PHE:CZ | 2.31 | 0.49 |
| 2:LF:379:LYS:CE | 4:2B:164:ARG:O | 2.61 | 0.49 |
| 2:MB:221:THR:CB | 6:4A:189:ARG:HH12 | 2.26 | 0.49 |
| 4:2A:30:CYS:SG | 4:2A:52:ILE:HG13 | 2.53 | 0.49 |
| 4:2A:164:ARG:C | 4:2A:164:ARG:CD | 2.85 | 0.49 |
| 4:2B:30:CYS:SG | 4:2B:52:ILE:HG13 | 2.52 | 0.49 |
| 4:2C:30:CYS:SG | 4:2C:52:ILE:HG13 | 2.53 | 0.49 |
| 6:4A:168:PHE:C | 6:4A:168:PHE:CD1 | 2.90 | 0.49 |
| 6:4B:99:ARG:HH21 | 6:4B:103:GLU:HG3 | 1.78 | 0.49 |
| 6:4C:175:LEU:N | 6:4C:175:LEU:HD22 | 2.26 | 0.49 |
| 6:4D:248:VAL:HA | 6:4D:251:TYR:CE2 | 2.48 | 0.49 |
| 7:5A:1250:VAL:HG11 | 7:5A:1262:GLU:HG3 | 1.95 | 0.49 |
| 7:5C:1332:GLN:CA | 7:5C:1332:GLN:NE2 | 2.75 | 0.49 |
| 7:5C:1484:TYR:CG | 7:5C:1568:LYS:HD3 | 2.47 | 0.49 |
| 9:7C:11:TYR:OH | 9:7D:26:LEU:HB3 | 2.13 | 0.49 |
| 9:7C:11:TYR:CG | 9:7D:23:LEU:CD2 | 2.96 | 0.49 |
| 1:AA:60:LYS:NZ | 1:BA:283:HIS:CE1 | 2.81 | 0.49 |
| 1:AA:141:VAL:HG12 | 1:AA:171:ILE:O | 2.13 | 0.49 |
| 1:AE:88:HIS:CE1 | 1:AE:90:GLU:HG2 | 2.48 | 0.49 |
| 2:AF:130:LEU:HB3 | 2:AF:162:ARG:HD2 | 1.95 | 0.49 |
| 2:DB:372:THR:HA | 2:DB:422:TYR:CE2 | 2.48 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:EB:177:ASP:HA | 1:EC:353:VAL:HG12 | 1.95 | 0.49 |
| 1:EC:141:VAL:HG12 | 1:EC:171:ILE:O | 2.13 | 0.49 |
| 1:FC:237:SER:HA | 1:FC:320:ARG:HH11 | 1.77 | 0.49 |
| 1:FC:402:ARG:HH12 | 7:5A:1262:GLU:HB2 | 1.78 | 0.49 |
| 1:FE:135:PHE:HB2 | 1:FE:166:LYS:HG2 | 1.95 | 0.49 |
| 1:HE:410:GLY:HA2 | 5:3A:329:ARG:NH2 | 2.19 | 0.49 |
| 1:IA:71:GLU:CD | 2:IB:247:ASN:ND2 | 2.71 | 0.49 |
| 1:IA:278:ALA:HB3 | 10:8V:21:UNK:CB | 2.34 | 0.49 |
| 1:JE:404:PHE:CE2 | 2:JF:345:ILE:HD11 | 2.48 | 0.49 |
| 1:KA:88:HIS:CE1 | 1:KA:90:GLU:HG2 | 2.48 | 0.49 |
| 1:KE:404:PHE:CE2 | 2:KF:345:ILE:HD11 | 2.48 | 0.49 |
| 2:KF:272:PRO:C | 6:4D:268:LEU:HD23 | 2.34 | 0.49 |
| 2:LB:331:LEU:HD22 | 4:2C:42:PHE:HZ | 0.69 | 0.49 |
| 2:LD:306:ARG:HH21 | 4:2A:149:ILE:HG23 | 1.75 | 0.49 |
| 2:MF:130:LEU:HB3 | 2:MF:162:ARG:HD2 | 1.95 | 0.49 |
| 5:3C:229:PHE:CZ | 5:3C:331:GLN:CD | 2.65 | 0.49 |
| 6:4D:99:ARG:HH21 | 6:4D:103:GLU:HG3 | 1.78 | 0.49 |
| 6:4D:251:TYR:CD2 | 6:4D:280:VAL:HG11 | 2.48 | 0.49 |
| 6:4D:289:LYS:CA | 6:4D:289:LYS:CE | 2.85 | 0.49 |
| 7:5A:1332:GLN:CA | 7:5A:1332:GLN:NE2 | 2.75 | 0.49 |
| 7:5B:841:VAL:N | 8:6B:109:ILE:CD1 | 2.63 | 0.49 |
| 7:5B:1113:ILE:HG12 | 7:5B:1157:THR:CG2 | 2.41 | 0.49 |
| 7:5B:1552:LYS:HZ1 | 7:5B:1563:SER:H | 1.59 | 0.49 |
| 7:5C:1332:GLN:N | 7:5C:1332:GLN:NE2 | 2.60 | 0.49 |
| 2:AD:130:LEU:HB3 | 2:AD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:BA:384:ILE:O | 1:BA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:BC:384:ILE:O | 1:BC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:BE:88:HIS:CE1 | 1:BE:90:GLU:HG2 | 2.48 | 0.48 |
| 1:BE:384:ILE:O | 1:BE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:BF:130:LEU:HB3 | 2:BF:162:ARG:HD2 | 1.95 | 0.48 |
| 2:CB:397:TRP:CD2 | 1:CC:256:GLN:O | 2.41 | 0.48 |
| 1:CE:88:HIS:CE1 | 1:CE:90:GLU:HG2 | 2.48 | 0.48 |
| 2:DD:372:THR:HA | 2:DD:422:TYR:CE2 | 2.48 | 0.48 |
| 1:EA:141:VAL:HG12 | 1:EA:171:ILE:O | 2.13 | 0.48 |
| 2:EB:55:THR:CG2 | 2:FB:284:LEU:N | 2.71 | 0.48 |
| 1:EC:396:ASP:O | 7:5A:817:LEU:HD11 | 2.13 | 0.48 |
| 2:ED:177:ASP:OD2 | 1:EE:353:VAL:HG11 | 2.01 | 0.48 |
| 1:FA:60:LYS:CE | 1:GA:283:HIS:CA | 2.88 | 0.48 |
| 1:FA:88:HIS:CE1 | 1:FA:90:GLU:HG2 | 2.48 | 0.48 |
| 2:FB:212:PHE:CZ | 1:FC:326:LYS:CE | 2.87 | 0.48 |
| 1:FE:176:GLN:O | 2:FF:347:ASN:ND2 | 2.37 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:FE:222:PRO:HG3 | 2:FF:324:LYS:CD | 2.41 | 0.48 |
| 1:GA:71:GLU:CD | 2:GB:247:ASN:ND2 | 2.71 | 0.48 |
| 1:HE:384:ILE:O | 1:HE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:IB:424:GLN:NE2 | 7:5C:1413:GLN:HE22 | 1.20 | 0.48 |
| 1:IC:179:THR:O | 2:ID:350:LYS:HA | 2.13 | 0.48 |
| 1:IE:384:ILE:O | 1:IE:387:VAL:HG22 | 2.13 | 0.48 |
| 1:IE:393:HIS:CB | 5:3A:308:PHE:CD2 | 2.96 | 0.48 |
| 1:KA:71:GLU:CD | 2:KB:247:ASN:ND2 | 2.71 | 0.48 |
| 1:KA:141:VAL:HG12 | 1:KA:171:ILE:O | 2.13 | 0.48 |
| 1:KC:88:HIS:CE1 | 1:KC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:KC:141:VAL:HG12 | 1:KC:171:ILE:O | 2.13 | 0.48 |
| 2:KD:54:ALA:CB | 2:LD:285:THR:HG23 | 2.09 | 0.48 |
| 1:KE:88:HIS:CE1 | 1:KE:90:GLU:HG2 | 2.48 | 0.48 |
| 1:KE:141:VAL:HG12 | 1:KE:171:ILE:O | 2.13 | 0.48 |
| 1:KE:176:GLN:O | 2:KF:347:ASN:ND2 | 2.40 | 0.48 |
| 2:LB:55:THR:HG1 | 2:MB:283:ALA:HA | 1.75 | 0.48 |
| 2:LB:130:LEU:HB3 | 2:LB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:LD:130:LEU:HB3 | 2:LD:162:ARG:HD2 | 1.95 | 0.48 |
| 2:MB:130:LEU:HB3 | 2:MB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:MD:130:LEU:HB3 | 2:MD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:ME:88:HIS:CE1 | 1:ME:90:GLU:HG2 | 2.48 | 0.48 |
| 5:3A:229:PHE:CZ | 5:3A:331:GLN:CD | 2.65 | 0.48 |
| 6:4A:251:TYR:CD2 | 6:4A:280:VAL:HG11 | 2.48 | 0.48 |
| 6:4B:168:PHE:C | 6:4B:168:PHE:CD1 | 2.90 | 0.48 |
| 6:4B:251:TYR:CD2 | 6:4B:280:VAL:HG11 | 2.48 | 0.48 |
| 7:5B:826:LEU:CD2 | 7:5B:840:GLY:CA | 2.75 | 0.48 |
| 7:5C:947:GLU:OE1 | 7:5C:1037:LYS:NZ | 2.43 | 0.48 |
| 7:5C:1131:PHE:CE1 | 8:6C:253:PHE:CE1 | 3.00 | 0.48 |
| 8:6A:169:VAL:HG13 | 8:6A:194:CYS:SG | 2.53 | 0.48 |
| 8:6B:169:VAL:HG13 | 8:6B:194:CYS:SG | 2.53 | 0.48 |
| 9:7A:11:TYR:CG | 9:7B:23:LEU:CD2 | 2.96 | 0.48 |
| 1:AA:179:THR:O | 2:AB:350:LYS:HA | 2.12 | 0.48 |
| 1:AE:224:TYR:CE2 | 2:AF:246:LEU:HD11 | 2.46 | 0.48 |
| 2:AF:321:MET:C | 6:4A:156:PHE:CE2 | 2.90 | 0.48 |
| 1:BA:88:HIS:CE1 | 1:BA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:BC:71:GLU:CD | 2:BD:247:ASN:ND2 | 2.70 | 0.48 |
| 1:BC:88:HIS:CE1 | 1:BC:90:GLU:HG2 | 2.48 | 0.48 |
| 2:CB:212:PHE:CZ | 1:CC:326:LYS:CE | 2.92 | 0.48 |
| 2:CD:394:PHE:CD1 | 1:CE:261:PRO:HA | 2.49 | 0.48 |
| 1:DC:231:ILE:O | 1:DC:235:ILE:HG12 | 2.14 | 0.48 |
| 2:DF:372:THR:HA | 2:DF:422:TYR:CE2 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:EA:394:LYS:NZ | 2:EB:347:ASN:OD1 | 2.46 | 0.48 |
| 1:EA:430:LYS:HZ2 | 7:5C:834:ASN:HB2 | 1.76 | 0.48 |
| 2:ED:85:PHE:C | 2:FD:281:TYR:OH | 2.54 | 0.48 |
| 2:ED:86:ARG:HA | 2:FD:281:TYR:CZ | 2.48 | 0.48 |
| 1:FA:135:PHE:HB2 | 1:FA:166:LYS:HG2 | 1.95 | 0.48 |
| 13:FB:502:GDP:C8 | 1:FC:248:LEU:CD1 | 2.96 | 0.48 |
| 1:FC:135:PHE:HB2 | 1:FC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:FE:207:GLU:OE1 | 7:5B:915:PHE:CG | 2.66 | 0.48 |
| 1:GA:231:ILE:O | 1:GA:235:ILE:HG12 | 2.13 | 0.48 |
| 1:GC:89:PRO:CG | 1:HC:280:LYS:NZ | 2.76 | 0.48 |
| 1:GE:60:LYS:CD | 1:HE:283:HIS:HA | 2.41 | 0.48 |
| 1:GE:231:ILE:O | 1:GE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:HA:237:SER:HA | 1:HA:320:ARG:HH11 | 1.77 | 0.48 |
| 1:IA:179:THR:O | 2:IB:350:LYS:HA | 2.12 | 0.48 |
| 1:IA:384:ILE:O | 1:IA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:IC:317:MET:HA | 1:IC:377:MET:HA | 1.96 | 0.48 |
| 1:IC:384:ILE:O | 1:IC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:IE:237:SER:HA | 1:IE:320:ARG:HH11 | 1.77 | 0.48 |
| 1:JA:179:THR:O | 2:JB:350:LYS:HA | 2.12 | 0.48 |
| 1:JA:231:ILE:O | 1:JA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:JE:231:ILE:O | 1:JE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:KA:231:ILE:O | 1:KA:235:ILE:HG12 | 2.14 | 0.48 |
| 2:KB:130:LEU:HB3 | 2:KB:162:ARG:HD2 | 1.95 | 0.48 |
| 1:KC:317:MET:HA | 1:KC:377:MET:HA | 1.96 | 0.48 |
| 2:KD:130:LEU:HB3 | 2:KD:162:ARG:HD2 | 1.95 | 0.48 |
| 2:LD:55:THR:HG22 | 2:MD:283:ALA:HB1 | 1.90 | 0.48 |
| 2:LF:130:LEU:HB3 | 2:LF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:MC:88:HIS:CE1 | 1:MC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:MC:384:ILE:O | 1:MC:387:VAL:HG22 | 2.13 | 0.48 |
| 2:MD:177:ASP:HA | 1:ME:353:VAL:HG12 | 1.95 | 0.48 |
| 1:ME:384:ILE:O | 1:ME:387:VAL:HG22 | 2.13 | 0.48 |
| 3:1A:70:TRP:CZ2 | 3:1A:93:ILE:HG21 | 2.48 | 0.48 |
| 3:1B:70:TRP:CZ2 | 3:1B:93:ILE:HG21 | 2.48 | 0.48 |
| 4:2B:164:ARG:C | 4:2B:164:ARG:CD | 2.85 | 0.48 |
| 5:3B:229:PHE:CZ | 5:3B:331:GLN:CD | 2.65 | 0.48 |
| 6:4B:110:LYS:HD2 | 6:4B:110:LYS:H | 1.77 | 0.48 |
| 6:4B:289:LYS:CA | 6:4B:289:LYS:CE | 2.85 | 0.48 |
| 6:4C:251:TYR:CD2 | 6:4C:280:VAL:HG11 | 2.48 | 0.48 |
| 6:4C:289:LYS:CA | 6:4C:289:LYS:CE | 2.85 | 0.48 |
| 6:4D:110:LYS:HD2 | 6:4D:110:LYS:H | 1.77 | 0.48 |
| 6:4D:168:PHE:HD1 | 6:4D:168:PHE:C | 2.20 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:4D:168:PHE:C | 6:4D:168:PHE:CD1 | 2.90 | 0.48 |
| 7:5A:839:GLU:CD | 8:6A:107:PRO:C | 2.79 | 0.48 |
| 7:5A:1332:GLN:N | 7:5A:1332:GLN:NE2 | 2.60 | 0.48 |
| 7:5B:872:GLU:OE2 | 8:6B:90:ARG:NH1 | 2.41 | 0.48 |
| 7:5B:1332:GLN:CA | 7:5B:1332:GLN:NE2 | 2.75 | 0.48 |
| 7:5C:839:GLU:OE2 | 8:6C:109:ILE:N | 2.45 | 0.48 |
| 7:5C:1406:PHE:O | 7:5C:1410:ASN:N | 2.31 | 0.48 |
| 2:AB:130:LEU:HB3 | 2:AB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:AF:223:GLY:HA3 | 6:4A:131:VAL:CB | 2.27 | 0.48 |
| 2:AF:224:ASP:OD1 | 6:4A:131:VAL:CA | 2.60 | 0.48 |
| 2:BB:130:LEU:HB3 | 2:BB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:BD:130:LEU:HB3 | 2:BD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:BE:60:LYS:HD3 | 1:CE:283:HIS:CD2 | 2.47 | 0.48 |
| 1:CC:241:SER:OG | 1:CC:250:VAL:O | 2.23 | 0.48 |
| 1:CC:384:ILE:O | 1:CC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:DA:231:ILE:O | 1:DA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:DE:135:PHE:HB2 | 1:DE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:DE:231:ILE:O | 1:DE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:EC:135:PHE:HB2 | 1:EC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:EC:384:ILE:O | 1:EC:387:VAL:HG22 | 2.13 | 0.48 |
| 2:ED:98:GLY:CA | 1:EE:254:GLU:CG | 2.51 | 0.48 |
| 1:EE:135:PHE:HB2 | 1:EE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:EE:384:ILE:O | 1:EE:387:VAL:HG22 | 2.13 | 0.48 |
| 1:FC:88:HIS:CE1 | 1:FC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:FC:207:GLU:OE1 | 7:5A:915:PHE:CG | 2.66 | 0.48 |
| 1:GA:222:PRO:HG3 | 2:GB:324:LYS:HD3 | 1.94 | 0.48 |
| 1:GC:231:ILE:O | 1:GC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:GE:88:HIS:CE1 | 1:GE:90:GLU:HG2 | 2.48 | 0.48 |
| 1:HA:135:PHE:HB2 | 1:HA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:HA:222:PRO:HG3 | 2:HB:324:LYS:HD3 | 1.94 | 0.48 |
| 1:HA:384:ILE:O | 1:HA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:HC:384:ILE:O | 1:HC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:IA:88:HIS:CE1 | 1:IA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:IA:317:MET:HA | 1:IA:377:MET:HA | 1.96 | 0.48 |
| 1:JC:231:ILE:O | 1:JC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:KA:85:GLN:HG2 | 1:LA:283:HIS:HD2 | 1.78 | 0.48 |
| 1:KA:317:MET:HA | 1:KA:377:MET:HA | 1.96 | 0.48 |
| 1:KC:88:HIS:ND1 | 1:LC:284:GLU:OE1 | 2.47 | 0.48 |
| 1:KE:317:MET:HA | 1:KE:377:MET:HA | 1.96 | 0.48 |
| 2:LB:55:THR:HG22 | 2:MB:283:ALA:HB1 | 1.96 | 0.48 |
| 1:LC:71:GLU:OE1 | 2:LD:247:ASN:ND2 | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LC:317:MET:HA | 1:LC:377:MET:HA | 1.96 | 0.48 |
| 1:LE:101:ASN:HD22 | 2:LF:252:LYS:HG3 | 1.77 | 0.48 |
| 1:MA:88:HIS:CE1 | 1:MA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:MA:384:ILE:O | 1:MA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:ME:237:SER:HA | 1:ME:320:ARG:HH11 | 1.77 | 0.48 |
| 1:ME:317:MET:HA | 1:ME:377:MET:HA | 1.96 | 0.48 |
| 3:1C:70:TRP:CZ2 | 3:1C:93:ILE:HG21 | 2.48 | 0.48 |
| 4:2A:176:ARG:O | 4:2A:179:VAL:N | 2.47 | 0.48 |
| 4:2C:176:ARG:O | 4:2C:179:VAL:N | 2.47 | 0.48 |
| 6:4A:110:LYS:HD2 | 6:4A:110:LYS:H | 1.77 | 0.48 |
| 6:4C:110:LYS:HD2 | 6:4C:110:LYS:H | 1.77 | 0.48 |
| 7:5A:874:GLN:CB | 8:6A:59:LYS:HZ2 | 2.12 | 0.48 |
| 7:5A:1366:TRP:CE3 | 7:5A:1366:TRP:CA | 2.96 | 0.48 |
| 7:5B:1404:LYS:HZ1 | 7:5B:1408:GLU:HB2 | 1.76 | 0.48 |
| 7:5B:1524:PHE:CE1 | 7:5B:1571:MET:SD | 3.05 | 0.48 |
| 7:5C:1366:TRP:CA | 7:5C:1366:TRP:CE3 | 2.96 | 0.48 |
| 1:AE:284:GLU:HA | 2:MB:54:ALA:CB | 2.43 | 0.48 |
| 1:BE:135:PHE:HB2 | 1:BE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:CA:384:ILE:O | 1:CA:387:VAL:HG22 | 2.13 | 0.48 |
| 2:CD:178:THR:HA | 1:CE:352:LYS:HD3 | 1.95 | 0.48 |
| 1:DA:88:HIS:CE1 | 1:DA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:DA:135:PHE:HB2 | 1:DA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:DA:398:MET:SD | 2:DB:345:ILE:CG1 | 2.94 | 0.48 |
| 1:DC:88:HIS:CE1 | 1:DC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:DC:135:PHE:HB2 | 1:DC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:DE:88:HIS:CE1 | 1:DE:90:GLU:HG2 | 2.48 | 0.48 |
| 1:EA:135:PHE:HB2 | 1:EA:166:LYS:HG2 | 1.95 | 0.48 |
| 2:EB:289:LEU:HD13 | 2:EB:365:VAL:HG23 | 1.96 | 0.48 |
| 2:EF:289:LEU:HD13 | 2:EF:365:VAL:HG23 | 1.96 | 0.48 |
| 1:GC:88:HIS:CE1 | 1:GC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:GE:135:PHE:HB2 | 1:GE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:GE:384:ILE:O | 1:GE:387:VAL:HG22 | 2.13 | 0.48 |
| 1:HC:135:PHE:HB2 | 1:HC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:IA:135:PHE:HB2 | 1:IA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:IA:222:PRO:HG3 | 2:IB:324:LYS:HD3 | 1.94 | 0.48 |
| 1:IC:135:PHE:HB2 | 1:IC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:IE:135:PHE:HB2 | 1:IE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:JA:384:ILE:O | 1:JA:387:VAL:HG22 | 2.13 | 0.48 |
| 2:JB:130:LEU:HB3 | 2:JB:162:ARG:HD2 | 1.95 | 0.48 |
| 1:JC:317:MET:HA | 1:JC:377:MET:HA | 1.96 | 0.48 |
| 1:JC:384:ILE:O | 1:JC:387:VAL:HG22 | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:JE:317:MET:HA | 1:JE:377:MET:HA | 1.96 | 0.48 |
| 2:KB:125:GLU:O | 4:2C:38:VAL:HA | 2.13 | 0.48 |
| 2:KB:212:PHE:CZ | 1:KC:326:LYS:CE | 2.93 | 0.48 |
| 1:KC:179:THR:O | 2:KD:350:LYS:HA | 2.13 | 0.48 |
| 2:KF:124:ALA:O | 4:2B:37:GLY:C | 2.56 | 0.48 |
| 1:LA:101:ASN:ND2 | 2:LB:252:LYS:HG3 | 2.29 | 0.48 |
| 2:LD:289:LEU:HD13 | 2:LD:365:VAL:HG23 | 1.96 | 0.48 |
| 4:2B:176:ARG:O | 4:2B:179:VAL:N | 2.47 | 0.48 |
| 4:2C:144:ASN:ND2 | 4:2C:144:ASN:N | 2.60 | 0.48 |
| 6:4A:289:LYS:CA | 6:4A:289:LYS:CE | 2.85 | 0.48 |
| 6:4C:278:TYR:HD1 | 6:4C:278:TYR:H | 1.61 | 0.48 |
| 7:5A:1105:TYR:HB2 | 7:5A:1165:PRO:HA | 1.96 | 0.48 |
| 7:5A:1244:LEU:HD12 | 7:5A:1244:LEU:HA | 1.61 | 0.48 |
| 7:5A:1524:PHE:CE1 | 7:5A:1571:MET:SD | 3.05 | 0.48 |
| 7:5B:1366:TRP:CE3 | 7:5B:1366:TRP:CA | 2.96 | 0.48 |
| 7:5C:1524:PHE:CE1 | 7:5C:1571:MET:SD | 3.05 | 0.48 |
| 1:AA:384:ILE:O | 1:AA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:AC:179:THR:O | 2:AD:350:LYS:HA | 2.13 | 0.48 |
| 1:AE:282:TYR:O | 2:MB:55:THR:OG1 | 2.28 | 0.48 |
| 1:BA:394:LYS:NZ | 2:BB:347:ASN:OD1 | 2.44 | 0.48 |
| 2:BB:212:PHE:HE2 | 1:BC:326:LYS:HB2 | 1.79 | 0.48 |
| 2:BD:289:LEU:HD13 | 2:BD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:BE:231:ILE:O | 1:BE:235:ILE:HG12 | 2.14 | 0.48 |
| 2:BF:289:LEU:HD13 | 2:BF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:CB:390:ARG:HD2 | 1:CC:439:THR:HG21 | 1.95 | 0.48 |
| 2:CD:130:LEU:HB3 | 2:CD:162:ARG:HD2 | 1.95 | 0.48 |
| 2:CD:222:TYR:HD2 | 1:CE:247:ALA:HB1 | 1.78 | 0.48 |
| 1:CE:183:GLU:N | 1:CE:184:PRO:HD2 | 2.29 | 0.48 |
| 1:CE:384:ILE:O | 1:CE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:CF:130:LEU:HB3 | 2:CF:162:ARG:HD2 | 1.95 | 0.48 |
| 2:DB:130:LEU:HB3 | 2:DB:162:ARG:HD2 | 1.95 | 0.48 |
| 1:DC:221:ARG:NH1 | 2:DD:324:LYS:N | 2.61 | 0.48 |
| 2:DD:212:PHE:CE2 | 1:DE:326:LYS:HB2 | 2.48 | 0.48 |
| 1:EA:231:ILE:O | 1:EA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:EA:384:ILE:O | 1:EA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:EC:231:ILE:O | 1:EC:235:ILE:HG12 | 2.14 | 0.48 |
| 2:ED:54:ALA:HB1 | 2:FD:281:TYR:O | 2.13 | 0.48 |
| 2:ED:289:LEU:HD13 | 2:ED:365:VAL:HG23 | 1.96 | 0.48 |
| 1:EE:231:ILE:O | 1:EE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:FA:419:SER:CB | 7:5C:1256:ARG:HG2 | 2.40 | 0.48 |
| 1:FC:231:ILE:O | 1:FC:235:ILE:HG12 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:FD:130:LEU:HB3 | 2:FD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:FE:88:HIS:CE1 | 1:FE:90:GLU:HG2 | 2.48 | 0.48 |
| 1:FE:222:PRO:HG2 | 2:FF:324:LYS:CD | 2.41 | 0.48 |
| 1:FE:231:ILE:O | 1:FE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:GA:135:PHE:HB2 | 1:GA:166:LYS:HG2 | 1.95 | 0.48 |
| 2:IB:130:LEU:HB3 | 2:IB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:ID:130:LEU:HB3 | 2:ID:162:ARG:HD2 | 1.95 | 0.48 |
| 1:IE:317:MET:HA | 1:IE:377:MET:HA | 1.96 | 0.48 |
| 2:IF:130:LEU:HB3 | 2:IF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:JA:135:PHE:HB2 | 1:JA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:JA:317:MET:HA | 1:JA:377:MET:HA | 1.96 | 0.48 |
| 1:JE:384:ILE:O | 1:JE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:KB:215:LEU:CD1 | 6:4A:267:ILE:CB | 2.87 | 0.48 |
| 2:KB:289:LEU:HD13 | 2:KB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:KC:183:GLU:N | 1:KC:184:PRO:HD2 | 2.29 | 0.48 |
| 1:KC:231:ILE:O | 1:KC:235:ILE:HG12 | 2.14 | 0.48 |
| 2:KD:77:ARG:HD3 | 2:LD:281:TYR:CE2 | 2.49 | 0.48 |
| 1:KE:231:ILE:O | 1:KE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:KE:384:ILE:O | 1:KE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:KF:289:LEU:HD13 | 2:KF:365:VAL:HG23 | 1.96 | 0.48 |
| 1:LA:56:THR:OG1 | 1:MA:284:GLU:CA | 2.61 | 0.48 |
| 1:LA:135:PHE:HB2 | 1:LA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:LA:317:MET:HA | 1:LA:377:MET:HA | 1.96 | 0.48 |
| 1:LC:135:PHE:HB2 | 1:LC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:LE:135:PHE:HB2 | 1:LE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:LE:221:ARG:HH11 | 2:LF:325:GLU:H | 1.61 | 0.48 |
| 1:LE:231:ILE:O | 1:LE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:LE:317:MET:HA | 1:LE:377:MET:HA | 1.96 | 0.48 |
| 2:LF:310:TYR:CE2 | 4:2B:147:PHE:CE2 | 3.02 | 0.48 |
| 1:MA:237:SER:HA | 1:MA:320:ARG:HH11 | 1.77 | 0.48 |
| 1:MA:317:MET:HA | 1:MA:377:MET:HA | 1.96 | 0.48 |
| 1:MC:237:SER:HA | 1:MC:320:ARG:HH11 | 1.77 | 0.48 |
| 1:MC:317:MET:HA | 1:MC:377:MET:HA | 1.96 | 0.48 |
| 4:2B:144:ASN:O | 4:2B:145:GLN:CG | 2.56 | 0.48 |
| 4:2B:164:ARG:NH1 | 4:2B:164:ARG:CB | 2.75 | 0.48 |
| 6:4B:168:PHE:HD1 | 6:4B:168:PHE:C | 2.20 | 0.48 |
| 7:5A:1484:TYR:CB | 7:5A:1568:LYS:HD3 | 2.43 | 0.48 |
| 7:5B:1105:TYR:HB2 | 7:5B:1165:PRO:HA | 1.96 | 0.48 |
| 7:5B:1332:GLN:N | 7:5B:1332:GLN:NE2 | 2.60 | 0.48 |
| 7:5B:1484:TYR:CB | 7:5B:1568:LYS:HD3 | 2.43 | 0.48 |
| 7:5C:1105:TYR:HB2 | 7:5C:1165:PRO:HA | 1.96 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1247:LYS:HE2 | 7:5C:1248:LEU:CG | 2.43 | 0.48 |
| 8:6C:169:VAL:HG13 | 8:6C:194:CYS:SG | 2.53 | 0.48 |
| 9:7E:15:VAL:HG12 | 9:7F:35:ILE:CA | 2.43 | 0.48 |
| 2:AF:289:LEU:HD13 | 2:AF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:BD:177:ASP:HA | 1:BE:353:VAL:HG12 | 1.96 | 0.48 |
| 1:CC:60:LYS:HD3 | 1:DC:283:HIS:HD2 | 1.79 | 0.48 |
| 2:CD:177:ASP:OD2 | 1:CE:248:LEU:HD23 | 2.08 | 0.48 |
| 1:DA:404:PHE:CE2 | 2:DB:345:ILE:CD1 | 2.95 | 0.48 |
| 2:EB:130:LEU:HB3 | 2:EB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:ED:130:LEU:HB3 | 2:ED:162:ARG:HD2 | 1.95 | 0.48 |
| 1:FA:89:PRO:HA | 1:GA:280:LYS:HZ2 | 1.73 | 0.48 |
| 2:FB:130:LEU:HB3 | 2:FB:162:ARG:HD2 | 1.95 | 0.48 |
| 2:FD:289:LEU:HD13 | 2:FD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:FE:422:ARG:NE | 7:5B:1170:THR:C | 2.72 | 0.48 |
| 2:FF:289:LEU:HD13 | 2:FF:365:VAL:HG23 | 1.96 | 0.48 |
| 1:GC:135:PHE:HB2 | 1:GC:166:LYS:HG2 | 1.95 | 0.48 |
| 2:GF:130:LEU:HB3 | 2:GF:162:ARG:HD2 | 1.95 | 0.48 |
| 2:GF:289:LEU:HD13 | 2:GF:365:VAL:HG23 | 1.96 | 0.48 |
| 1:HA:60:LYS:NZ | 1:IA:283:HIS:CE1 | 2.82 | 0.48 |
| 1:HA:88:HIS:CE1 | 1:HA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:HA:224:TYR:CE2 | 2:HB:246:LEU:HD11 | 2.44 | 0.48 |
| 1:HC:88:HIS:CE1 | 1:HC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:HC:196:GLU:HG3 | 5:3C:211:GLN:HE22 | 1.79 | 0.48 |
| 1:HE:135:PHE:HB2 | 1:HE:166:LYS:HG2 | 1.95 | 0.48 |
| 2:IB:289:LEU:HD13 | 2:IB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:IC:88:HIS:CE1 | 1:IC:90:GLU:HG2 | 2.48 | 0.48 |
| 1:IE:231:ILE:O | 1:IE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:JA:88:HIS:CE1 | 1:JA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:JC:135:PHE:HB2 | 1:JC:166:LYS:HG2 | 1.95 | 0.48 |
| 2:JD:130:LEU:HB3 | 2:JD:162:ARG:HD2 | 1.95 | 0.48 |
| 2:KD:289:LEU:HD13 | 2:KD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:LA:231:ILE:O | 1:LA:235:ILE:HG12 | 2.14 | 0.48 |
| 2:LB:289:LEU:HD13 | 2:LB:365:VAL:HG23 | 1.96 | 0.48 |
| 2:LD:222:TYR:HD2 | 1:LE:247:ALA:HB1 | 1.77 | 0.48 |
| 2:LF:289:LEU:HD13 | 2:LF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:MB:106:TYR:HE1 | 3:1A:32:ARG:NH1 | 2.01 | 0.48 |
| 2:MB:289:LEU:HD13 | 2:MB:365:VAL:HG23 | 1.96 | 0.48 |
| 2:MD:289:LEU:HD13 | 2:MD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:ME:279:GLU:OE1 | 6:4B:107:MET:HA | 2.10 | 0.48 |
| 4:2A:65:ASN:O | 4:2A:69:LYS:HE3 | 2.14 | 0.48 |
| 4:2A:144:ASN:ND2 | 4:2A:144:ASN:N | 2.60 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2A:164:ARG:NH1 | 4:2A:164:ARG:CB | 2.75 | 0.48 |
| 4:2B:65:ASN:O | 4:2B:69:LYS:HE3 | 2.14 | 0.48 |
| 6:4C:256:ASN:HD21 | 6:4C:260:ARG:HE | 1.57 | 0.48 |
| 7:5A:1247:LYS:HE2 | 7:5A:1248:LEU:CG | 2.43 | 0.48 |
| 7:5A:1377:LYS:HE3 | 7:5A:1377:LYS:HB2 | 1.44 | 0.48 |
| 7:5A:1412:LYS:C | 7:5A:1412:LYS:CD | 2.85 | 0.48 |
| 7:5B:1125:LEU:CD1 | 8:6B:245:GLN:OE1 | 2.53 | 0.48 |
| 7:5B:1247:LYS:HE2 | 7:5B:1248:LEU:CG | 2.43 | 0.48 |
| 7:5B:1412:LYS:C | 7:5B:1412:LYS:CD | 2.85 | 0.48 |
| 7:5C:1484:TYR:CB | 7:5C:1568:LYS:HD3 | 2.43 | 0.48 |
| 2:AB:289:LEU:HD13 | 2:AB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:AC:60:LYS:HZ2 | 1:BC:283:HIS:CE1 | 2.32 | 0.48 |
| 1:AC:384:ILE:O | 1:AC:387:VAL:HG22 | 2.13 | 0.48 |
| 2:AF:281:TYR:CZ | 1:MC:60:LYS:NZ | 2.80 | 0.48 |
| 1:BA:231:ILE:O | 1:BA:235:ILE:HG12 | 2.14 | 0.48 |
| 2:BB:289:LEU:HD13 | 2:BB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:BC:135:PHE:HB2 | 1:BC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:BC:231:ILE:O | 1:BC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:CA:135:PHE:HB2 | 1:CA:166:LYS:HG2 | 1.95 | 0.48 |
| 2:CB:130:LEU:HB3 | 2:CB:162:ARG:HD2 | 1.95 | 0.48 |
| 1:CC:135:PHE:HB2 | 1:CC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:CC:183:GLU:N | 1:CC:184:PRO:HD2 | 2.29 | 0.48 |
| 2:CD:289:LEU:HD13 | 2:CD:365:VAL:HG23 | 1.96 | 0.48 |
| 2:CF:289:LEU:HD13 | 2:CF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:DB:289:LEU:HD13 | 2:DB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:EA:241:SER:OG | 1:EA:250:VAL:O | 2.23 | 0.48 |
| 2:EF:130:LEU:HB3 | 2:EF:162:ARG:HD2 | 1.95 | 0.48 |
| 2:FB:177:ASP:C | 1:FC:352:LYS:HA | 2.38 | 0.48 |
| 2:FB:289:LEU:HD13 | 2:FB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:FC:56:THR:OG1 | 1:GC:285:GLN:N | 2.46 | 0.48 |
| 2:FD:177:ASP:O | 1:FE:352:LYS:CD | 2.43 | 0.48 |
| 2:FD:332:ASN:CB | 7:5A:909:ASN:HD21 | 2.27 | 0.48 |
| 1:GA:88:HIS:CE1 | 1:GA:90:GLU:HG2 | 2.48 | 0.48 |
| 1:GA:384:ILE:O | 1:GA:387:VAL:HG22 | 2.13 | 0.48 |
| 1:GC:384:ILE:O | 1:GC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:HA:398:MET:SD | 2:HB:345:ILE:CG1 | 2.90 | 0.48 |
| 2:HB:130:LEU:HB3 | 2:HB:162:ARG:HD2 | 1.95 | 0.48 |
| 1:HE:88:HIS:CE1 | 1:HE:90:GLU:HG2 | 2.48 | 0.48 |
| 2:HF:130:LEU:HB3 | 2:HF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:IC:231:ILE:O | 1:IC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:IE:88:HIS:CE1 | 1:IE:90:GLU:HG2 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:JE:90:GLU:HG2 | 1:KE:280:LYS:CD | 2.41 | 0.48 |
| 1:JE:282:TYR:OH | 10:9A:17:UNK:C | 2.53 | 0.48 |
| 2:JF:130:LEU:HB3 | 2:JF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:KA:183:GLU:N | 1:KA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:KA:384:ILE:O | 1:KA:387:VAL:HG22 | 2.13 | 0.48 |
| 2:KD:177:ASP:C | 1:KE:352:LYS:HA | 2.39 | 0.48 |
| 1:KE:135:PHE:HB2 | 1:KE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:KE:183:GLU:N | 1:KE:184:PRO:HD2 | 2.29 | 0.48 |
| 2:LB:305:PRO:HG2 | 4:2C:149:ILE:CD1 | 2.44 | 0.48 |
| 1:LC:231:ILE:O | 1:LC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:LE:56:THR:OG1 | 1:ME:284:GLU:HA | 2.14 | 0.48 |
| 2:LF:410:GLU:OE1 | 4:2B:182:PHE:CE1 | 2.67 | 0.48 |
| 1:MC:11:GLN:HE22 | 2:MD:246:LEU:HA | 1.79 | 0.48 |
| 1:ME:135:PHE:HB2 | 1:ME:166:LYS:HG2 | 1.95 | 0.48 |
| 2:MF:289:LEU:HD13 | 2:MF:365:VAL:HG23 | 1.96 | 0.48 |
| 4:2C:65:ASN:O | 4:2C:69:LYS:HE3 | 2.14 | 0.48 |
| 4:2C:164:ARG:NH1 | 4:2C:164:ARG:CB | 2.75 | 0.48 |
| 6:4A:256:ASN:HD21 | 6:4A:260:ARG:HE | 1.57 | 0.48 |
| 6:4C:230:TYR:O | 6:4C:230:TYR:HD2 | 1.95 | 0.48 |
| 7:5A:844:PHE:CG | 7:5A:849:ARG:HD2 | 2.48 | 0.48 |
| 7:5A:1404:LYS:HE3 | 7:5A:1404:LYS:HB3 | 1.49 | 0.48 |
| 7:5C:844:PHE:CG | 7:5C:849:ARG:HD2 | 2.48 | 0.48 |
| 10:8T:33:UNK:C | 10:8T:35:UNK:N | 2.76 | 0.48 |
| 10:8X:33:UNK:C | 10:8X:35:UNK:N | 2.76 | 0.48 |
| 1:AA:231:ILE:O | 1:AA:235:ILE:HG12 | 2.14 | 0.48 |
| 2:AD:289:LEU:HD13 | 2:AD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:AE:222:PRO:HG3 | 2:AF:324:LYS:HD3 | 1.95 | 0.48 |
| 1:AE:384:ILE:O | 1:AE:387:VAL:HG22 | 2.13 | 0.48 |
| 1:BA:183:GLU:N | 1:BA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:CA:183:GLU:N | 1:CA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:CE:135:PHE:HB2 | 1:CE:166:LYS:HG2 | 1.95 | 0.48 |
| 2:DB:220:PRO:HD2 | 1:DC:326:LYS:CD | 2.44 | 0.48 |
| 1:DC:128:ASN:ND2 | 1:EC:285:GLN:NE2 | 2.61 | 0.48 |
| 2:DD:130:LEU:HB3 | 2:DD:162:ARG:HD2 | 1.95 | 0.48 |
| 2:DD:289:LEU:HD13 | 2:DD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:DE:384:ILE:O | 1:DE:387:VAL:HG22 | 2.13 | 0.48 |
| 2:EF:55:THR:H | 2:FF:283:ALA:CB | 2.25 | 0.48 |
| 1:FA:183:GLU:N | 1:FA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:FA:231:ILE:O | 1:FA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:FA:384:ILE:O | 1:FA:387:VAL:HG22 | 2.13 | 0.48 |
| 2:FB:133:PHE:HB2 | 2:FB:164:MET:SD | 2.54 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:FC:422:ARG:HE | 7:5A:1170:THR:C | 2.22 | 0.48 |
| 2:FF:130:LEU:HB3 | 2:FF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:GA:224:TYR:CE2 | 2:GB:246:LEU:HD11 | 2.44 | 0.48 |
| 2:GD:289:LEU:HD13 | 2:GD:365:VAL:HG23 | 1.96 | 0.48 |
| 1:GE:409:VAL:HG13 | 5:3A:383:GLU:OE2 | 1.93 | 0.48 |
| 1:HA:60:LYS:HZ2 | 1:IA:283:HIS:CE1 | 2.32 | 0.48 |
| 1:HA:317:MET:HA | 1:HA:377:MET:HA | 1.96 | 0.48 |
| 2:HB:289:LEU:HD13 | 2:HB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:HC:317:MET:HA | 1:HC:377:MET:HA | 1.96 | 0.48 |
| 1:HE:231:ILE:O | 1:HE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:IA:183:GLU:N | 1:IA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:IC:183:GLU:N | 1:IC:184:PRO:HD2 | 2.29 | 0.48 |
| 2:JB:289:LEU:HD13 | 2:JB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:JE:135:PHE:HB2 | 1:JE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:KA:179:THR:O | 2:KB:350:LYS:HA | 2.12 | 0.48 |
| 2:KB:54:ALA:CA | 2:LB:285:THR:HG21 | 2.30 | 0.48 |
| 1:KC:135:PHE:HB2 | 1:KC:166:LYS:HG2 | 1.95 | 0.48 |
| 1:KC:384:ILE:O | 1:KC:387:VAL:HG22 | 2.13 | 0.48 |
| 1:LA:222:PRO:CD | 2:LB:324:LYS:CB | 2.91 | 0.48 |
| 1:LA:384:ILE:O | 1:LA:387:VAL:HG22 | 2.13 | 0.48 |
| 2:LB:25:SER:HG | 2:LB:51:TYR:HH | 1.56 | 0.48 |
| 2:LB:295:ASP:OD1 | 4:2C:150:GLN:OE1 | 2.32 | 0.48 |
| 1:LC:221:ARG:NH1 | 2:LD:324:LYS:H | 2.09 | 0.48 |
| 2:LF:410:GLU:OE1 | 4:2B:182:PHE:HE1 | 1.97 | 0.48 |
| 1:ME:222:PRO:HG3 | 2:MF:324:LYS:HD3 | 1.93 | 0.48 |
| 4:2A:144:ASN:O | 4:2A:145:GLN:CG | 2.56 | 0.48 |
| 4:2B:144:ASN:ND2 | 4:2B:144:ASN:N | 2.60 | 0.48 |
| 6:4A:168:PHE:HD1 | 6:4A:168:PHE:C | 2.20 | 0.48 |
| 6:4A:278:TYR:HD1 | 6:4A:278:TYR:H | 1.61 | 0.48 |
| 6:4D:230:TYR:O | 6:4D:230:TYR:HD2 | 1.95 | 0.48 |
| 6:4D:239:LEU:C | 6:4D:241:LYS:N | 2.71 | 0.48 |
| 7:5A:1474:LEU:CD2 | 7:5A:1576:ILE:HD11 | 2.43 | 0.48 |
| 7:5B:844:PHE:CG | 7:5B:849:ARG:HD2 | 2.48 | 0.48 |
| 7:5B:1474:LEU:CD2 | 7:5B:1576:ILE:HD11 | 2.43 | 0.48 |
| 7:5B:1499:LYS:HG2 | 7:5B:1503:TYR:CE2 | 2.49 | 0.48 |
| 7:5C:924:LEU:HB3 | 7:5C:1017:SER:HB2 | 1.95 | 0.48 |
| 7:5C:1125:LEU:HD11 | 8:6C:245:GLN:CD | 2.13 | 0.48 |
| 7:5C:1412:LYS:C | 7:5C:1412:LYS:CD | 2.85 | 0.48 |
| 9:7A:18:VAL:HG21 | 9:7B:35:ILE:CG2 | 2.30 | 0.48 |
| 10:8R:33:UNK:C | 10:8R:35:UNK:N | 2.76 | 0.48 |
| 2:AB:212:PHE:CZ | 1:AC:326:LYS:CE | 2.93 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AE:135:PHE:HB2 | 1:AE:166:LYS:HG2 | 1.95 | 0.48 |
| 1:BA:135:PHE:HB2 | 1:BA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:BC:183:GLU:N | 1:BC:184:PRO:HD2 | 2.29 | 0.48 |
| 2:BD:133:PHE:HB2 | 2:BD:164:MET:SD | 2.54 | 0.48 |
| 2:BD:390:ARG:CD | 1:BE:439:THR:HG21 | 2.44 | 0.48 |
| 1:BE:222:PRO:CG | 2:BF:324:LYS:CD | 2.90 | 0.48 |
| 2:CB:289:LEU:HD13 | 2:CB:365:VAL:HG23 | 1.96 | 0.48 |
| 1:CE:71:GLU:CD | 2:CF:247:ASN:ND2 | 2.72 | 0.48 |
| 1:CE:231:ILE:O | 1:CE:235:ILE:HG12 | 2.14 | 0.48 |
| 1:DA:183:GLU:N | 1:DA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:DC:183:GLU:N | 1:DC:184:PRO:HD2 | 2.29 | 0.48 |
| 2:DF:130:LEU:HB3 | 2:DF:162:ARG:HD2 | 1.95 | 0.48 |
| 1:FC:183:GLU:N | 1:FC:184:PRO:HD2 | 2.29 | 0.48 |
| 1:FE:60:LYS:HD2 | 1:GE:283:HIS:HD2 | 1.77 | 0.48 |
| 1:FE:183:GLU:N | 1:FE:184:PRO:HD2 | 2.29 | 0.48 |
| 2:GB:289:LEU:HD13 | 2:GB:365:VAL:HG23 | 1.96 | 0.48 |
| 2:GB:405:GLU:OE2 | 7:5C:1337:ASP:OD2 | 2.30 | 0.48 |
| 2:GD:130:LEU:HB3 | 2:GD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:HC:231:ILE:O | 1:HC:235:ILE:HG12 | 2.14 | 0.48 |
| 1:IA:231:ILE:O | 1:IA:235:ILE:HG12 | 2.14 | 0.48 |
| 2:IB:424:GLN:CD | 7:5C:1413:GLN:HE22 | 1.98 | 0.48 |
| 2:IB:424:GLN:HE21 | 7:5C:1413:GLN:HG3 | 1.78 | 0.48 |
| 2:ID:177:ASP:C | 1:IE:352:LYS:HA | 2.39 | 0.48 |
| 2:ID:289:LEU:HD13 | 2:ID:365:VAL:HG23 | 1.96 | 0.48 |
| 1:JA:183:GLU:N | 1:JA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:JC:91:GLN:H | 1:KC:280:LYS:HZ3 | 1.48 | 0.48 |
| 1:JC:183:GLU:N | 1:JC:184:PRO:HD2 | 2.29 | 0.48 |
| 1:JE:89:PRO:HD2 | 1:KE:283:HIS:CG | 2.48 | 0.48 |
| 2:JF:85:PHE:CB | 2:KF:281:TYR:OH | 2.61 | 0.48 |
| 1:KA:87:PHE:C | 1:LA:284:GLU:HA | 2.39 | 0.48 |
| 1:KA:135:PHE:HB2 | 1:KA:166:LYS:HG2 | 1.95 | 0.48 |
| 2:KD:133:PHE:HB2 | 2:KD:164:MET:SD | 2.54 | 0.48 |
| 2:LD:133:PHE:HB2 | 2:LD:164:MET:SD | 2.54 | 0.48 |
| 2:LD:212:PHE:CZ | 1:LE:326:LYS:CG | 2.90 | 0.48 |
| 1:MA:135:PHE:HB2 | 1:MA:166:LYS:HG2 | 1.95 | 0.48 |
| 1:MA:183:GLU:N | 1:MA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:MA:231:ILE:O | 1:MA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:MA:398:MET:SD | 2:MB:345:ILE:CG1 | 2.92 | 0.48 |
| 2:MB:111:GLU:CA | 3:1A:62:SER:HA | 2.39 | 0.48 |
| 2:MB:177:ASP:OD2 | 1:MC:248:LEU:HD23 | 2.13 | 0.48 |
| 1:MC:135:PHE:HB2 | 1:MC:166:LYS:HG2 | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:MC:183:GLU:N | 1:MC:184:PRO:HD2 | 2.29 | 0.48 |
| 2:MD:133:PHE:HB2 | 2:MD:164:MET:SD | 2.54 | 0.48 |
| 1:ME:183:GLU:N | 1:ME:184:PRO:HD2 | 2.29 | 0.48 |
| 2:MF:133:PHE:HB2 | 2:MF:164:MET:SD | 2.54 | 0.48 |
| 4:2C:144:ASN:O | 4:2C:145:GLN:CG | 2.56 | 0.48 |
| 7:5A:924:LEU:HB3 | 7:5A:1017:SER:HB2 | 1.95 | 0.48 |
| 7:5A:1499:LYS:HG2 | 7:5A:1503:TYR:CE2 | 2.49 | 0.48 |
| 7:5C:1142:PHE:CD1 | 7:5C:1146:LEU:HD12 | 2.45 | 0.48 |
| 7:5C:1474:LEU:CD2 | 7:5C:1576:ILE:HD11 | 2.43 | 0.48 |
| 8:6C:102:ASN:ND2 | 8:6C:134:LYS:O | 2.47 | 0.48 |
| 10:8I:33:UNK:C | 10:8I:35:UNK:N | 2.76 | 0.48 |
| 10:8S:33:UNK:C | 10:8S:35:UNK:N | 2.76 | 0.48 |
| 1:AC:135:PHE:HB2 | 1:AC:166:LYS:HG2 | 1.95 | 0.48 |
| 2:BB:133:PHE:HB2 | 2:BB:164:MET:SD | 2.54 | 0.48 |
| 2:BF:133:PHE:HB2 | 2:BF:164:MET:SD | 2.54 | 0.48 |
| 1:CC:231:ILE:O | 1:CC:235:ILE:HG12 | 2.14 | 0.48 |
| 2:CD:133:PHE:HB2 | 2:CD:164:MET:SD | 2.54 | 0.48 |
| 2:DB:208:TYR:CD2 | 1:DC:326:LYS:HB3 | 2.49 | 0.48 |
| 2:DF:257:LEU:HA | 2:DF:312:THR:HG21 | 1.96 | 0.48 |
| 2:FB:332:ASN:CB | 7:5C:909:ASN:HD21 | 2.26 | 0.48 |
| 1:FC:384:ILE:O | 1:FC:387:VAL:HG22 | 2.13 | 0.48 |
| 2:FD:133:PHE:HB2 | 2:FD:164:MET:SD | 2.54 | 0.48 |
| 2:FF:402:GLY:O | 7:5B:1296:GLU:OE2 | 2.32 | 0.48 |
| 1:HA:183:GLU:N | 1:HA:184:PRO:HD2 | 2.29 | 0.48 |
| 1:HA:231:ILE:O | 1:HA:235:ILE:HG12 | 2.14 | 0.48 |
| 1:HC:183:GLU:N | 1:HC:184:PRO:HD2 | 2.29 | 0.48 |
| 1:HC:224:TYR:CE2 | 2:HD:246:LEU:HD11 | 2.43 | 0.48 |
| 2:HD:130:LEU:HB3 | 2:HD:162:ARG:HD2 | 1.95 | 0.48 |
| 1:HE:317:MET:HA | 1:HE:377:MET:HA | 1.96 | 0.48 |
| 2:HF:289:LEU:HD13 | 2:HF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:IB:133:PHE:HB2 | 2:IB:164:MET:SD | 2.54 | 0.48 |
| 2:ID:133:PHE:HB2 | 2:ID:164:MET:SD | 2.54 | 0.48 |
| 2:ID:424:GLN:NE2 | 7:5A:1413:GLN:NE2 | 0.61 | 0.48 |
| 2:IF:289:LEU:HD13 | 2:IF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:JB:133:PHE:HB2 | 2:JB:164:MET:SD | 2.54 | 0.48 |
| 1:JC:88:HIS:CE1 | 1:JC:90:GLU:HG2 | 2.48 | 0.48 |
| 2:JF:87:PRO:CD | 2:KF:281:TYR:CE2 | 2.53 | 0.48 |
| 2:JF:289:LEU:HD13 | 2:JF:365:VAL:HG23 | 1.96 | 0.48 |
| 2:KB:372:THR:HA | 2:KB:422:TYR:CE2 | 2.48 | 0.48 |
| 1:LA:71:GLU:OE1 | 2:LB:247:ASN:ND2 | 2.46 | 0.48 |
| 1:LA:101:ASN:HD22 | 2:LB:252:LYS:HG3 | 1.79 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LB:179:VAL:HG23 | 1:LC:258:ASN:HA | 1.92 | 0.48 |
| 2:LF:55:THR:H | 2:MF:283:ALA:CA | 2.26 | 0.48 |
| 4:2C:164:ARG:C | 4:2C:164:ARG:CD | 2.85 | 0.48 |
| 6:4A:230:TYR:O | 6:4A:230:TYR:HD2 | 1.95 | 0.48 |
| 6:4B:278:TYR:HD1 | 6:4B:278:TYR:H | 1.61 | 0.48 |
| 7:5A:1552:LYS:HZ1 | 7:5A:1563:SER:H | 1.60 | 0.48 |
| 7:5C:1490:LYS:CB | 7:5C:1495:PHE:HB2 | 2.43 | 0.48 |
| 9:7A:11:TYR:OH | 9:7B:26:LEU:HB3 | 2.13 | 0.48 |
| 2:AD:133:PHE:HB2 | 2:AD:164:MET:SD | 2.54 | 0.47 |
| 2:AD:212:PHE:HZ | 1:AE:326:LYS:CE | 2.19 | 0.47 |
| 2:AD:280:GLN:O | 6:4C:141:LYS:NZ | 2.34 | 0.47 |
| 1:AE:317:MET:HA | 1:AE:377:MET:HA | 1.96 | 0.47 |
| 2:AF:133:PHE:HB2 | 2:AF:164:MET:SD | 2.54 | 0.47 |
| 1:BE:183:GLU:N | 1:BE:184:PRO:HD2 | 2.29 | 0.47 |
| 1:CE:224:TYR:CE2 | 2:CF:246:LEU:HD11 | 2.46 | 0.47 |
| 2:CF:133:PHE:HB2 | 2:CF:164:MET:SD | 2.54 | 0.47 |
| 2:DB:133:PHE:HB2 | 2:DB:164:MET:SD | 2.54 | 0.47 |
| 2:DB:257:LEU:HA | 2:DB:312:THR:HG21 | 1.96 | 0.47 |
| 1:DC:384:ILE:O | 1:DC:387:VAL:HG22 | 2.13 | 0.47 |
| 1:DE:183:GLU:N | 1:DE:184:PRO:HD2 | 2.29 | 0.47 |
| 2:DF:289:LEU:HD13 | 2:DF:365:VAL:HG23 | 1.96 | 0.47 |
| 2:EB:86:ARG:HD3 | 2:FB:281:TYR:HB3 | 1.52 | 0.47 |
| 2:EB:372:THR:HA | 2:EB:422:TYR:CE2 | 2.48 | 0.47 |
| 1:FE:221:ARG:NH1 | 2:FF:324:LYS:N | 2.62 | 0.47 |
| 1:FE:384:ILE:O | 1:FE:387:VAL:HG22 | 2.13 | 0.47 |
| 1:FE:402:ARG:HH12 | 7:5B:1262:GLU:HB2 | 1.78 | 0.47 |
| 2:GB:130:LEU:HB3 | 2:GB:162:ARG:HD2 | 1.95 | 0.47 |
| 1:GC:224:TYR:CE2 | 2:GD:246:LEU:HD11 | 2.43 | 0.47 |
| 1:GE:60:LYS:HZ2 | 1:HE:283:HIS:CE1 | 2.30 | 0.47 |
| 2:HB:133:PHE:HB2 | 2:HB:164:MET:SD | 2.54 | 0.47 |
| 2:HD:133:PHE:HB2 | 2:HD:164:MET:SD | 2.54 | 0.47 |
| 2:HD:289:LEU:HD13 | 2:HD:365:VAL:HG23 | 1.96 | 0.47 |
| 1:JC:179:THR:O | 2:JD:350:LYS:HA | 2.13 | 0.47 |
| 2:JD:133:PHE:HB2 | 2:JD:164:MET:SD | 2.54 | 0.47 |
| 2:JD:289:LEU:HD13 | 2:JD:365:VAL:HG23 | 1.96 | 0.47 |
| 2:JF:133:PHE:HB2 | 2:JF:164:MET:SD | 2.54 | 0.47 |
| 2:KB:133:PHE:HB2 | 2:KB:164:MET:SD | 2.54 | 0.47 |
| 2:KB:177:ASP:C | 1:KC:352:LYS:HA | 2.39 | 0.47 |
| 2:KB:228:LEU:HG | 6:4A:267:ILE:CD1 | 2.44 | 0.47 |
| 2:KD:257:LEU:HA | 2:KD:312:THR:HG21 | 1.96 | 0.47 |
| 2:KF:133:PHE:HB2 | 2:KF:164:MET:SD | 2.54 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LB:133:PHE:HB2 | 2:LB:164:MET:SD | 2.54 | 0.47 |
| 2:LB:224:ASP:CG | 6:4A:219:ASN:ND2 | 2.65 | 0.47 |
| 2:LD:54:ALA:CA | 2:MD:283:ALA:HB2 | 2.44 | 0.47 |
| 1:LE:183:GLU:N | 1:LE:184:PRO:HD2 | 2.29 | 0.47 |
| 2:LF:416:ASN:HA | 4:2B:168:LEU:HD11 | 1.96 | 0.47 |
| 1:MA:71:GLU:CD | 2:MB:247:ASN:HD22 | 2.21 | 0.47 |
| 2:MB:133:PHE:HB2 | 2:MB:164:MET:SD | 2.54 | 0.47 |
| 1:MC:231:ILE:O | 1:MC:235:ILE:HG12 | 2.14 | 0.47 |
| 6:4B:178:HIS:ND1 | 6:4B:178:HIS:C | 2.72 | 0.47 |
| 6:4B:230:TYR:O | 6:4B:230:TYR:HD2 | 1.95 | 0.47 |
| 6:4D:164:ARG:NH1 | 6:4D:164:ARG:CB | 2.72 | 0.47 |
| 7:5A:1285:ARG:N | 7:5A:1285:ARG:CD | 2.73 | 0.47 |
| 7:5A:1406:PHE:O | 7:5A:1410:ASN:N | 2.31 | 0.47 |
| 7:5B:924:LEU:HB3 | 7:5B:1017:SER:HB2 | 1.95 | 0.47 |
| 7:5C:1285:ARG:N | 7:5C:1285:ARG:CD | 2.73 | 0.47 |
| 7:5C:1416:LYS:NZ | 7:5C:1416:LYS:CA | 2.72 | 0.47 |
| 7:5C:1499:LYS:HG2 | 7:5C:1503:TYR:CE2 | 2.49 | 0.47 |
| 1:AA:135:PHE:HB2 | 1:AA:166:LYS:HG2 | 1.95 | 0.47 |
| 1:AA:317:MET:HA | 1:AA:377:MET:HA | 1.96 | 0.47 |
| 1:AC:231:ILE:O | 1:AC:235:ILE:HG12 | 2.14 | 0.47 |
| 1:AC:317:MET:HA | 1:AC:377:MET:HA | 1.96 | 0.47 |
| 1:AE:284:GLU:CA | 2:MB:54:ALA:HB1 | 2.43 | 0.47 |
| 1:AE:404:PHE:CE2 | 2:AF:345:ILE:HD11 | 2.48 | 0.47 |
| 2:CB:133:PHE:HB2 | 2:CB:164:MET:SD | 2.54 | 0.47 |
| 1:DA:384:ILE:O | 1:DA:387:VAL:HG22 | 2.13 | 0.47 |
| 2:DD:257:LEU:HA | 2:DD:312:THR:HG21 | 1.96 | 0.47 |
| 2:ED:177:ASP:CA | 1:EE:353:VAL:HG12 | 2.44 | 0.47 |
| 2:ED:257:LEU:HA | 2:ED:312:THR:HG21 | 1.96 | 0.47 |
| 1:FC:181:VAL:HG12 | 2:FD:348:ASN:HA | 1.95 | 0.47 |
| 2:FF:133:PHE:HB2 | 2:FF:164:MET:SD | 2.55 | 0.47 |
| 2:FF:332:ASN:CG | 7:5B:909:ASN:ND2 | 2.71 | 0.47 |
| 2:GD:55:THR:H | 2:HD:283:ALA:N | 2.11 | 0.47 |
| 2:GD:226:ASN:ND2 | 13:GD:501:GDP:HN1 | 2.12 | 0.47 |
| 1:GE:222:PRO:HD2 | 2:GF:324:LYS:HD3 | 1.96 | 0.47 |
| 1:HA:71:GLU:CD | 2:HB:247:ASN:ND2 | 2.71 | 0.47 |
| 2:IB:177:ASP:C | 1:IC:352:LYS:HA | 2.39 | 0.47 |
| 1:IE:183:GLU:N | 1:IE:184:PRO:HD2 | 2.29 | 0.47 |
| 1:JA:71:GLU:CD | 2:JB:247:ASN:ND2 | 2.71 | 0.47 |
| 2:JD:177:ASP:C | 1:JE:352:LYS:HA | 2.39 | 0.47 |
| 1:JE:88:HIS:CE1 | 1:JE:90:GLU:HG2 | 2.48 | 0.47 |
| 1:JE:183:GLU:N | 1:JE:184:PRO:HD2 | 2.29 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:KF:257:LEU:HA | 2:KF:312:THR:HG21 | 1.96 | 0.47 |
| 1:LC:384:ILE:O | 1:LC:387:VAL:HG22 | 2.13 | 0.47 |
| 1:LE:384:ILE:O | 1:LE:387:VAL:HG22 | 2.13 | 0.47 |
| 2:LF:133:PHE:HB2 | 2:LF:164:MET:SD | 2.54 | 0.47 |
| 6:4A:97:GLN:HA | 6:4A:98:PRO:HD3 | 1.58 | 0.47 |
| 6:4A:178:HIS:ND1 | 6:4A:178:HIS:C | 2.72 | 0.47 |
| 6:4B:239:LEU:C | 6:4B:241:LYS:N | 2.71 | 0.47 |
| 6:4C:168:PHE:HD1 | 6:4C:168:PHE:C | 2.20 | 0.47 |
| 6:4D:215:LYS:HB2 | 6:4D:215:LYS:HE3 | 1.47 | 0.47 |
| 7:5A:836:ARG:CB | 7:5A:836:ARG:NH1 | 2.73 | 0.47 |
| 7:5A:1490:LYS:CB | 7:5A:1495:PHE:HB2 | 2.43 | 0.47 |
| 7:5C:836:ARG:CB | 7:5C:836:ARG:NH1 | 2.73 | 0.47 |
| 1:AA:183:GLU:N | 1:AA:184:PRO:HD2 | 2.29 | 0.47 |
| 2:AB:257:LEU:HA | 2:AB:312:THR:HG21 | 1.96 | 0.47 |
| 1:AE:231:ILE:O | 1:AE:235:ILE:HG12 | 2.14 | 0.47 |
| 2:BB:248:SER:HA | 2:BB:252:LYS:HE2 | 1.97 | 0.47 |
| 1:CA:231:ILE:O | 1:CA:235:ILE:HG12 | 2.14 | 0.47 |
| 1:CE:241:SER:OG | 1:CE:250:VAL:O | 2.23 | 0.47 |
| 2:CF:257:LEU:HA | 2:CF:312:THR:HG21 | 1.96 | 0.47 |
| 2:DD:133:PHE:HB2 | 2:DD:164:MET:SD | 2.54 | 0.47 |
| 1:EA:183:GLU:N | 1:EA:184:PRO:HD2 | 2.29 | 0.47 |
| 2:EB:257:LEU:HA | 2:EB:312:THR:HG21 | 1.96 | 0.47 |
| 1:EC:241:SER:OG | 1:EC:250:VAL:O | 2.23 | 0.47 |
| 2:ED:372:THR:HA | 2:ED:422:TYR:CE2 | 2.48 | 0.47 |
| 1:FA:402:ARG:CZ | 7:5C:1259:TYR:HA | 2.44 | 0.47 |
| 1:FE:179:THR:O | 2:FF:350:LYS:HA | 2.15 | 0.47 |
| 1:FE:317:MET:HA | 1:FE:377:MET:HA | 1.96 | 0.47 |
| 2:GB:226:ASN:ND2 | 13:GB:501:GDP:HN1 | 2.12 | 0.47 |
| 2:GB:248:SER:HA | 2:GB:252:LYS:HE2 | 1.97 | 0.47 |
| 2:GD:248:SER:HA | 2:GD:252:LYS:HE2 | 1.97 | 0.47 |
| 2:GD:257:LEU:HA | 2:GD:312:THR:HG21 | 1.96 | 0.47 |
| 2:GF:86:ARG:NH2 | 2:HF:281:TYR:CE1 | 2.65 | 0.47 |
| 2:GF:257:LEU:HA | 2:GF:312:THR:HG21 | 1.96 | 0.47 |
| 1:HE:183:GLU:N | 1:HE:184:PRO:HD2 | 2.29 | 0.47 |
| 2:IB:248:SER:HA | 2:IB:252:LYS:HE2 | 1.97 | 0.47 |
| 2:IF:133:PHE:HB2 | 2:IF:164:MET:SD | 2.54 | 0.47 |
| 2:IF:248:SER:HA | 2:IF:252:LYS:HE2 | 1.97 | 0.47 |
| 1:JA:222:PRO:HG3 | 2:JB:324:LYS:HD3 | 1.94 | 0.47 |
| 2:JB:86:ARG:CZ | 2:KB:280:GLN:CA | 2.92 | 0.47 |
| 1:KA:357:TYR:CE1 | 6:4C:257:LEU:HG | 2.49 | 0.47 |
| 2:KB:257:LEU:HA | 2:KB:312:THR:HG21 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:KD:372:THR:HA | 2:KD:422:TYR:CE2 | 2.48 | 0.47 |
| 2:LF:295:ASP:OD1 | 4:2B:150:GLN:HB2 | 2.14 | 0.47 |
| 2:MD:179:VAL:CG2 | 1:ME:258:ASN:O | 2.40 | 0.47 |
| 1:ME:231:ILE:O | 1:ME:235:ILE:HG12 | 2.14 | 0.47 |
| 6:4A:251:TYR:CZ | 6:4A:280:VAL:CG1 | 2.97 | 0.47 |
| 6:4C:178:HIS:ND1 | 6:4C:178:HIS:C | 2.72 | 0.47 |
| 6:4D:278:TYR:HD1 | 6:4D:278:TYR:H | 1.61 | 0.47 |
| 7:5A:1142:PHE:CD1 | 7:5A:1146:LEU:HD12 | 2.45 | 0.47 |
| 7:5B:844:PHE:CD2 | 7:5B:849:ARG:CD | 2.96 | 0.47 |
| 7:5C:773:ARG:C | 7:5C:773:ARG:CD | 2.85 | 0.47 |
| 7:5C:1436:ARG:CG | 7:5C:1436:ARG:NH1 | 2.71 | 0.47 |
| 10:8U:33:UNK:C | 10:8U:35:UNK:N | 2.76 | 0.47 |
| 10:8V:33:UNK:C | 10:8V:35:UNK:N | 2.76 | 0.47 |
| 2:AB:133:PHE:HB2 | 2:AB:164:MET:SD | 2.54 | 0.47 |
| 1:AE:60:LYS:NZ | 1:BE:283:HIS:CE1 | 2.83 | 0.47 |
| 2:BB:257:LEU:HA | 2:BB:312:THR:HG21 | 1.96 | 0.47 |
| 2:BD:248:SER:HA | 2:BD:252:LYS:HE2 | 1.97 | 0.47 |
| 2:BF:248:SER:HA | 2:BF:252:LYS:HE2 | 1.97 | 0.47 |
| 2:CD:212:PHE:HE2 | 1:CE:326:LYS:HB2 | 1.80 | 0.47 |
| 2:CF:100:ASN:HD22 | 2:CF:103:LYS:HB2 | 1.79 | 0.47 |
| 2:DB:100:ASN:HD22 | 2:DB:103:LYS:HB2 | 1.79 | 0.47 |
| 1:DC:400:ALA:CA | 7:5A:775:PRO:HB3 | 2.44 | 0.47 |
| 1:DE:317:MET:HA | 1:DE:377:MET:HA | 1.96 | 0.47 |
| 2:DF:133:PHE:HB2 | 2:DF:164:MET:SD | 2.55 | 0.47 |
| 2:DF:226:ASN:ND2 | 13:DF:501:GDP:HN1 | 2.12 | 0.47 |
| 1:EC:183:GLU:N | 1:EC:184:PRO:HD2 | 2.29 | 0.47 |
| 2:EF:257:LEU:HA | 2:EF:312:THR:HG21 | 1.96 | 0.47 |
| 1:FA:317:MET:HA | 1:FA:377:MET:HA | 1.96 | 0.47 |
| 1:FC:317:MET:HA | 1:FC:377:MET:HA | 1.96 | 0.47 |
| 2:FD:106:TYR:O | 7:5A:1298:LYS:CD | 2.61 | 0.47 |
| 1:GA:183:GLU:N | 1:GA:184:PRO:HD2 | 2.29 | 0.47 |
| 1:GC:89:PRO:CD | 1:HC:280:LYS:HZ1 | 2.21 | 0.47 |
| 2:GD:133:PHE:HB2 | 2:GD:164:MET:SD | 2.54 | 0.47 |
| 2:HD:177:ASP:C | 1:HE:352:LYS:HA | 2.39 | 0.47 |
| 2:HF:133:PHE:HB2 | 2:HF:164:MET:SD | 2.54 | 0.47 |
| 2:ID:248:SER:HA | 2:ID:252:LYS:HE2 | 1.97 | 0.47 |
| 2:ID:424:GLN:NE2 | 7:5A:1413:GLN:HE21 | 0.55 | 0.47 |
| 2:KB:276:ARG:NH2 | 6:4A:265:TYR:CB | 2.75 | 0.47 |
| 2:KD:215:LEU:HD13 | 6:4B:267:ILE:CB | 2.41 | 0.47 |
| 1:LC:183:GLU:N | 1:LC:184:PRO:HD2 | 2.29 | 0.47 |
| 2:LF:100:ASN:HD22 | 2:LF:103:LYS:HB2 | 1.79 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:MB:110:ALA:C | 3:1A:61:HIS:HB3 | 2.36 | 0.47 |
| 1:MC:279:GLU:HB2 | 6:4A:110:LYS:CE | 2.43 | 0.47 |
| 5:3C:71:LYS:HE2 | 5:3C:87:LEU:HD22 | 1.96 | 0.47 |
| 6:4B:251:TYR:CZ | 6:4B:280:VAL:CG1 | 2.97 | 0.47 |
| 7:5A:841:VAL:HG23 | 8:6A:11:PRO:CA | 2.41 | 0.47 |
| 7:5A:844:PHE:CD2 | 7:5A:849:ARG:CD | 2.96 | 0.47 |
| 7:5B:836:ARG:CB | 7:5B:836:ARG:NH1 | 2.73 | 0.47 |
| 7:5B:1285:ARG:N | 7:5B:1285:ARG:CD | 2.73 | 0.47 |
| 7:5B:1490:LYS:CB | 7:5B:1495:PHE:HB2 | 2.44 | 0.47 |
| 7:5C:844:PHE:CD2 | 7:5C:849:ARG:CD | 2.96 | 0.47 |
| 7:5C:1244:LEU:HD12 | 7:5C:1244:LEU:HA | 1.61 | 0.47 |
| 7:5C:1377:LYS:HB2 | 7:5C:1377:LYS:HE3 | 1.44 | 0.47 |
| 7:5C:1404:LYS:HE3 | 7:5C:1404:LYS:HB3 | 1.49 | 0.47 |
| 8:6A:4:LYS:HD3 | 8:6A:6:TYR:HH | 1.79 | 0.47 |
| 8:6B:102:ASN:ND2 | 8:6B:134:LYS:O | 2.47 | 0.47 |
| 10:8W:33:UNK:C | 10:8W:35:UNK:N | 2.76 | 0.47 |
| 1:AC:183:GLU:N | 1:AC:184:PRO:HD2 | 2.29 | 0.47 |
| 2:AD:177:ASP:C | 1:AE:352:LYS:HA | 2.39 | 0.47 |
| 2:AD:257:LEU:HA | 2:AD:312:THR:HG21 | 1.96 | 0.47 |
| 2:AD:356:ILE:CG2 | 6:4C:152:PHE:HE1 | 2.27 | 0.47 |
| 1:BE:317:MET:HA | 1:BE:377:MET:HA | 1.96 | 0.47 |
| 1:CC:222:PRO:CG | 2:CD:324:LYS:CD | 2.91 | 0.47 |
| 1:CE:317:MET:HA | 1:CE:377:MET:HA | 1.96 | 0.47 |
| 1:DA:221:ARG:NH1 | 2:DB:324:LYS:N | 2.62 | 0.47 |
| 1:DA:402:ARG:CD | 7:5C:777:ALA:HB2 | 2.44 | 0.47 |
| 2:DB:226:ASN:ND2 | 13:DB:501:GDP:HN1 | 2.12 | 0.47 |
| 2:DD:55:THR:HG23 | 2:ED:283:ALA:HA | 1.96 | 0.47 |
| 2:DD:226:ASN:ND2 | 13:DD:501:GDP:HN1 | 2.12 | 0.47 |
| 1:DE:258:ASN:ND2 | 1:DE:352:LYS:HD3 | 2.30 | 0.47 |
| 2:DF:100:ASN:HD22 | 2:DF:103:LYS:HB2 | 1.79 | 0.47 |
| 1:EE:183:GLU:N | 1:EE:184:PRO:HD2 | 2.29 | 0.47 |
| 1:FC:87:PHE:O | 1:GC:280:LYS:NZ | 2.47 | 0.47 |
| 1:FC:404:PHE:CE2 | 2:FD:345:ILE:HD11 | 2.50 | 0.47 |
| 2:GB:133:PHE:HB2 | 2:GB:164:MET:SD | 2.54 | 0.47 |
| 2:GB:257:LEU:HA | 2:GB:312:THR:HG21 | 1.96 | 0.47 |
| 1:GC:183:GLU:N | 1:GC:184:PRO:HD2 | 2.29 | 0.47 |
| 2:GF:133:PHE:HB2 | 2:GF:164:MET:SD | 2.54 | 0.47 |
| 2:GF:248:SER:HA | 2:GF:252:LYS:HE2 | 1.97 | 0.47 |
| 1:HC:278:ALA:HB2 | 10:8T:18:UNK:O | 2.05 | 0.47 |
| 1:HE:222:PRO:HD2 | 2:HF:324:LYS:HD3 | 1.96 | 0.47 |
| 2:JF:11:GLN:O | 2:JF:15:GLN:HG2 | 2.15 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:KD:55:THR:OG1 | 2:LD:284:LEU:O | 2.30 | 0.47 |
| 2:KF:91:VAL:HG21 | 2:KF:116:VAL:HB | 1.96 | 0.47 |
| 1:LA:183:GLU:N | 1:LA:184:PRO:HD2 | 2.29 | 0.47 |
| 2:LF:224:ASP:CB | 6:4D:219:ASN:HD21 | 2.27 | 0.47 |
| 2:MB:11:GLN:O | 2:MB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:MB:176:SER:OG | 1:MC:349:THR:OG1 | 2.19 | 0.47 |
| 2:MF:248:SER:HA | 2:MF:252:LYS:HE2 | 1.97 | 0.47 |
| 4:2A:143:LEU:HB3 | 4:2A:144:ASN:H | 1.60 | 0.47 |
| 4:2C:143:LEU:HB3 | 4:2C:144:ASN:H | 1.60 | 0.47 |
| 6:4B:97:GLN:HA | 6:4B:98:PRO:HD3 | 1.58 | 0.47 |
| 6:4C:251:TYR:CZ | 6:4C:280:VAL:CG1 | 2.97 | 0.47 |
| 7:5A:840:GLY:HA3 | 8:6A:109:ILE:HG21 | 1.96 | 0.47 |
| 7:5A:1436:ARG:CG | 7:5A:1436:ARG:NH1 | 2.71 | 0.47 |
| 7:5B:1480:VAL:HG22 | 7:5B:1572:LEU:HD13 | 1.97 | 0.47 |
| 7:5C:1131:PHE:HE1 | 8:6C:253:PHE:CE1 | 2.32 | 0.47 |
| 8:6A:102:ASN:ND2 | 8:6A:134:LYS:O | 2.47 | 0.47 |
| 2:AB:91:VAL:HG21 | 2:AB:116:VAL:HB | 1.96 | 0.47 |
| 2:AD:11:GLN:O | 2:AD:15:GLN:HG2 | 2.15 | 0.47 |
| 1:AE:222:PRO:HD2 | 2:AF:324:LYS:HD3 | 1.96 | 0.47 |
| 2:AF:11:GLN:O | 2:AF:15:GLN:HG2 | 2.15 | 0.47 |
| 1:BC:317:MET:HA | 1:BC:377:MET:HA | 1.96 | 0.47 |
| 2:BD:177:ASP:CA | 1:BE:353:VAL:HG12 | 2.44 | 0.47 |
| 2:CB:179:VAL:HG22 | 1:CC:258:ASN:CA | 2.45 | 0.47 |
| 2:CD:390:ARG:CD | 1:CE:439:THR:HG21 | 2.45 | 0.47 |
| 1:DA:258:ASN:ND2 | 1:DA:352:LYS:HD3 | 2.30 | 0.47 |
| 1:DC:258:ASN:ND2 | 1:DC:352:LYS:HD3 | 2.30 | 0.47 |
| 1:DC:317:MET:HA | 1:DC:377:MET:HA | 1.96 | 0.47 |
| 1:DC:402:ARG:HE | 7:5A:777:ALA:HB3 | 1.49 | 0.47 |
| 2:DD:100:ASN:HD22 | 2:DD:103:LYS:HB2 | 1.80 | 0.47 |
| 1:EC:423:GLU:CD | 7:5A:830:VAL:CG1 | 2.60 | 0.47 |
| 13:ED:502:GDP:H8 | 1:EE:248:LEU:CD1 | 2.28 | 0.47 |
| 1:EE:317:MET:HA | 1:EE:377:MET:HA | 1.96 | 0.47 |
| 2:EF:25:SER:OG | 2:EF:51:TYR:OH | 2.32 | 0.47 |
| 1:FE:177:VAL:N | 7:5B:915:PHE:CZ | 2.82 | 0.47 |
| 1:FE:404:PHE:CE2 | 2:FF:345:ILE:HD11 | 2.50 | 0.47 |
| 1:GC:258:ASN:ND2 | 1:GC:352:LYS:HD3 | 2.30 | 0.47 |
| 1:GC:317:MET:HA | 1:GC:377:MET:HA | 1.96 | 0.47 |
| 1:GE:258:ASN:ND2 | 1:GE:352:LYS:HD3 | 2.30 | 0.47 |
| 1:GE:317:MET:HA | 1:GE:377:MET:HA | 1.96 | 0.47 |
| 2:HD:55:THR:HG23 | 2:ID:283:ALA:HA | 1.97 | 0.47 |
| 1:HE:60:LYS:HD3 | 1:IE:283:HIS:CD2 | 2.49 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HF:11:GLN:O | 2:HF:15:GLN:HG2 | 2.15 | 0.47 |
| 1:JE:222:PRO:HD2 | 2:JF:324:LYS:HD3 | 1.96 | 0.47 |
| 1:KA:258:ASN:ND2 | 1:KA:352:LYS:HD3 | 2.30 | 0.47 |
| 2:KD:124:ALA:O | 4:2A:38:VAL:CG1 | 2.60 | 0.47 |
| 1:KE:222:PRO:HG3 | 2:KF:324:LYS:HD3 | 1.95 | 0.47 |
| 2:KF:162:ARG:HG3 | 4:2B:36:THR:HB | 1.96 | 0.47 |
| 1:LE:222:PRO:CG | 2:LF:324:LYS:CB | 2.91 | 0.47 |
| 1:LE:222:PRO:HG3 | 2:LF:324:LYS:HD3 | 1.72 | 0.47 |
| 2:LF:257:LEU:HA | 2:LF:312:THR:HG21 | 1.96 | 0.47 |
| 1:MA:357:TYR:CE2 | 6:4C:185:ARG:NH2 | 2.71 | 0.47 |
| 2:MB:248:SER:HA | 2:MB:252:LYS:HE2 | 1.97 | 0.47 |
| 5:3A:71:LYS:HE2 | 5:3A:87:LEU:HD22 | 1.96 | 0.47 |
| 6:4A:239:LEU:C | 6:4A:241:LYS:N | 2.71 | 0.47 |
| 6:4D:108:LYS:HE2 | 6:4D:108:LYS:HB3 | 1.36 | 0.47 |
| 6:4D:251:TYR:CZ | 6:4D:280:VAL:CG1 | 2.98 | 0.47 |
| 7:5A:1122:LYS:HB2 | 7:5A:1124:ILE:HG12 | 1.97 | 0.47 |
| 7:5A:1416:LYS:NZ | 7:5A:1416:LYS:CA | 2.72 | 0.47 |
| 7:5A:1480:VAL:HG22 | 7:5A:1572:LEU:HD13 | 1.97 | 0.47 |
| 7:5B:1407:GLN:NE2 | 7:5B:1407:GLN:C | 2.71 | 0.47 |
| 7:5C:1122:LYS:HB2 | 7:5C:1124:ILE:HG12 | 1.97 | 0.47 |
| 7:5C:1480:VAL:HG22 | 7:5C:1572:LEU:HD13 | 1.97 | 0.47 |
| 7:5C:1552:LYS:HZ1 | 7:5C:1563:SER:H | 1.60 | 0.47 |
| 10:8K:33:UNK:C | 10:8K:35:UNK:N | 2.76 | 0.47 |
| 2:AB:11:GLN:O | 2:AB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:AB:177:ASP:C | 1:AC:352:LYS:HA | 2.39 | 0.47 |
| 2:AB:372:THR:HA | 2:AB:422:TYR:CE2 | 2.48 | 0.47 |
| 1:AC:222:PRO:HG3 | 2:AD:324:LYS:HD3 | 1.95 | 0.47 |
| 2:AD:91:VAL:HG21 | 2:AD:116:VAL:HB | 1.96 | 0.47 |
| 2:AD:356:ILE:CG2 | 6:4C:152:PHE:CE1 | 2.97 | 0.47 |
| 2:AD:357:PRO:O | 6:4C:151:ARG:NE | 2.48 | 0.47 |
| 2:AF:91:VAL:HG21 | 2:AF:116:VAL:HB | 1.96 | 0.47 |
| 2:AF:257:LEU:HA | 2:AF:312:THR:HG21 | 1.96 | 0.47 |
| 2:BB:11:GLN:O | 2:BB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:BB:100:ASN:HD22 | 2:BB:103:LYS:HB2 | 1.79 | 0.47 |
| 2:BD:257:LEU:HA | 2:BD:312:THR:HG21 | 1.96 | 0.47 |
| 1:CA:224:TYR:CE2 | 2:CB:246:LEU:HD11 | 2.46 | 0.47 |
| 1:CA:317:MET:HA | 1:CA:377:MET:HA | 1.96 | 0.47 |
| 2:CB:100:ASN:HD22 | 2:CB:103:LYS:HB2 | 1.79 | 0.47 |
| 1:CC:317:MET:HA | 1:CC:377:MET:HA | 1.96 | 0.47 |
| 2:CD:100:ASN:HD22 | 2:CD:103:LYS:HB2 | 1.79 | 0.47 |
| 2:CD:248:SER:HA | 2:CD:252:LYS:HE2 | 1.97 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CD:257:LEU:HA | 2:CD:312:THR:HG21 | 1.96 | 0.47 |
| 1:CE:258:ASN:ND2 | 1:CE:352:LYS:HD3 | 2.30 | 0.47 |
| 2:CF:248:SER:HA | 2:CF:252:LYS:HE2 | 1.97 | 0.47 |
| 1:DE:147:SER:HB2 | 1:DE:190:SER:HB3 | 1.97 | 0.47 |
| 1:DE:176:GLN:O | 2:DF:347:ASN:ND2 | 2.38 | 0.47 |
| 1:EA:317:MET:HA | 1:EA:377:MET:HA | 1.96 | 0.47 |
| 1:EA:396:ASP:OD2 | 7:5C:817:LEU:HD23 | 2.15 | 0.47 |
| 2:EF:133:PHE:HB2 | 2:EF:164:MET:SD | 2.54 | 0.47 |
| 2:EF:372:THR:HA | 2:EF:422:TYR:CE2 | 2.48 | 0.47 |
| 2:FB:248:SER:HA | 2:FB:252:LYS:HE2 | 1.97 | 0.47 |
| 1:FE:258:ASN:ND2 | 1:FE:352:LYS:HD3 | 2.30 | 0.47 |
| 1:FE:402:ARG:HD3 | 7:5B:1259:TYR:CB | 2.44 | 0.47 |
| 1:GA:258:ASN:ND2 | 1:GA:352:LYS:HD3 | 2.30 | 0.47 |
| 1:GA:317:MET:HA | 1:GA:377:MET:HA | 1.96 | 0.47 |
| 2:GD:100:ASN:HD22 | 2:GD:103:LYS:HB2 | 1.79 | 0.47 |
| 2:GD:177:ASP:C | 1:GE:352:LYS:HA | 2.39 | 0.47 |
| 2:GF:11:GLN:O | 2:GF:15:GLN:HG2 | 2.15 | 0.47 |
| 2:GF:100:ASN:HD22 | 2:GF:103:LYS:HB2 | 1.80 | 0.47 |
| 2:HB:177:ASP:C | 1:HC:352:LYS:HA | 2.39 | 0.47 |
| 2:HD:11:GLN:O | 2:HD:15:GLN:HG2 | 2.15 | 0.47 |
| 1:HE:147:SER:HB2 | 1:HE:190:SER:HB3 | 1.97 | 0.47 |
| 1:HE:398:MET:SD | 2:HF:345:ILE:CG1 | 2.92 | 0.47 |
| 2:HF:257:LEU:HA | 2:HF:312:THR:HG21 | 1.96 | 0.47 |
| 2:ID:226:ASN:ND2 | 13:ID:501:GDP:HN1 | 2.12 | 0.47 |
| 2:IF:11:GLN:O | 2:IF:15:GLN:HG2 | 2.15 | 0.47 |
| 2:IF:226:ASN:ND2 | 13:IF:501:GDP:HN1 | 2.12 | 0.47 |
| 1:JA:279:GLU:HA | 10:8Y:22:UNK:CB | 2.44 | 0.47 |
| 2:JB:85:PHE:HB3 | 2:KB:281:TYR:OH | 2.15 | 0.47 |
| 2:JB:177:ASP:C | 1:JC:352:LYS:HA | 2.39 | 0.47 |
| 2:JD:11:GLN:O | 2:JD:15:GLN:HG2 | 2.15 | 0.47 |
| 2:KB:91:VAL:HG21 | 2:KB:116:VAL:HB | 1.96 | 0.47 |
| 2:KB:217:LEU:CA | 6:4A:265:TYR:OH | 2.57 | 0.47 |
| 1:KC:79:ARG:C | 1:LC:280:LYS:NZ | 2.69 | 0.47 |
| 1:KC:258:ASN:ND2 | 1:KC:352:LYS:HD3 | 2.30 | 0.47 |
| 2:KD:11:GLN:O | 2:KD:15:GLN:HG2 | 2.15 | 0.47 |
| 2:KD:91:VAL:HG21 | 2:KD:116:VAL:HB | 1.97 | 0.47 |
| 2:KF:372:THR:HA | 2:KF:422:TYR:CE2 | 2.48 | 0.47 |
| 2:LB:11:GLN:O | 2:LB:15:GLN:HG2 | 2.15 | 0.47 |
| 1:LC:258:ASN:ND2 | 1:LC:352:LYS:HD3 | 2.30 | 0.47 |
| 2:LD:100:ASN:HD22 | 2:LD:103:LYS:HB2 | 1.79 | 0.47 |
| 1:LE:258:ASN:ND2 | 1:LE:352:LYS:HD3 | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:LF:54:ALA:CA | 2:MF:283:ALA:HB2 | 2.45 | 0.47 |
| 2:MB:91:VAL:HG21 | 2:MB:116:VAL:HB | 1.97 | 0.47 |
| 2:MD:11:GLN:O | 2:MD:15:GLN:HG2 | 2.15 | 0.47 |
| 2:MD:248:SER:HA | 2:MD:252:LYS:HE2 | 1.97 | 0.47 |
| 2:MF:11:GLN:O | 2:MF:15:GLN:HG2 | 2.15 | 0.47 |
| 2:MF:221:THR:CB | 6:4D:189:ARG:NH1 | 2.78 | 0.47 |
| 5:3B:71:LYS:HE2 | 5:3B:87:LEU:HD22 | 1.96 | 0.47 |
| 6:4A:113:ILE:HB | 6:4A:117:ARG:HH21 | 1.79 | 0.47 |
| 6:4C:113:ILE:HB | 6:4C:117:ARG:HH21 | 1.79 | 0.47 |
| 7:5A:806:GLN:HE21 | 7:5A:806:GLN:C | 2.22 | 0.47 |
| 7:5A:843:LEU:N | 7:5A:843:LEU:CD2 | 2.78 | 0.47 |
| 7:5A:1407:GLN:NE2 | 7:5A:1407:GLN:C | 2.71 | 0.47 |
| 7:5A:1424:GLN:NE2 | 7:5A:1424:GLN:HA | 2.29 | 0.47 |
| 7:5A:1534:ILE:HA | 7:5A:1581:ILE:HB | 1.97 | 0.47 |
| 7:5B:806:GLN:C | 7:5B:806:GLN:HE21 | 2.22 | 0.47 |
| 7:5B:843:LEU:N | 7:5B:843:LEU:CD2 | 2.78 | 0.47 |
| 7:5B:1122:LYS:HB2 | 7:5B:1124:ILE:HG12 | 1.97 | 0.47 |
| 7:5B:1142:PHE:CD1 | 7:5B:1146:LEU:HD12 | 2.45 | 0.47 |
| 7:5B:1436:ARG:NE | 7:5B:1436:ARG:C | 2.72 | 0.47 |
| 7:5B:1534:ILE:HA | 7:5B:1581:ILE:HB | 1.97 | 0.47 |
| 7:5C:843:LEU:CD2 | 7:5C:843:LEU:N | 2.78 | 0.47 |
| 7:5C:1342:GLU:HA | 7:5C:1342:GLU:OE2 | 2.15 | 0.47 |
| 7:5C:1407:GLN:NE2 | 7:5C:1407:GLN:C | 2.71 | 0.47 |
| 7:5C:1424:GLN:NE2 | 7:5C:1424:GLN:HA | 2.29 | 0.47 |
| 7:5C:1534:ILE:HA | 7:5C:1581:ILE:HB | 1.97 | 0.47 |
| 8:6C:46:ILE:HG21 | 8:6C:149:ILE:HG23 | 1.96 | 0.47 |
| 9:7C:10:TYR:OH | 9:7D:31:PRO:O | 2.21 | 0.47 |
| 1:AE:183:GLU:N | 1:AE:184:PRO:HD2 | 2.29 | 0.47 |
| 1:BA:317:MET:HA | 1:BA:377:MET:HA | 1.96 | 0.47 |
| 2:BD:11:GLN:O | 2:BD:15:GLN:HG2 | 2.15 | 0.47 |
| 2:BD:100:ASN:HD22 | 2:BD:103:LYS:HB2 | 1.79 | 0.47 |
| 2:BF:11:GLN:O | 2:BF:15:GLN:HG2 | 2.15 | 0.47 |
| 2:BF:257:LEU:HA | 2:BF:312:THR:HG21 | 1.96 | 0.47 |
| 1:CA:71:GLU:CD | 2:CB:247:ASN:ND2 | 2.73 | 0.47 |
| 2:CB:176:SER:CB | 1:CC:349:THR:HG1 | 2.27 | 0.47 |
| 2:CB:248:SER:HA | 2:CB:252:LYS:HE2 | 1.97 | 0.47 |
| 2:CB:257:LEU:HA | 2:CB:312:THR:HG21 | 1.96 | 0.47 |
| 1:CC:2:ARG:HD2 | 1:CC:242:LEU:O | 2.15 | 0.47 |
| 1:DA:317:MET:HA | 1:DA:377:MET:HA | 1.96 | 0.47 |
| 1:DA:414:GLU:OE2 | 7:5C:789:LYS:NZ | 2.47 | 0.47 |
| 2:EB:248:SER:HA | 2:EB:252:LYS:HE2 | 1.97 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:56:THR:OG1 | 1:GA:284:GLU:CA | 2.62 | 0.47 |
| 2:FB:55:THR:OG1 | 2:GB:283:ALA:HA | 2.13 | 0.47 |
| 1:GC:188:ILE:HD12 | 1:GC:425:LEU:CD1 | 2.45 | 0.47 |
| 2:GD:11:GLN:O | 2:GD:15:GLN:HG2 | 2.15 | 0.47 |
| 1:GE:183:GLU:N | 1:GE:184:PRO:HD2 | 2.29 | 0.47 |
| 1:GE:188:ILE:HD12 | 1:GE:425:LEU:CD1 | 2.45 | 0.47 |
| 1:HA:147:SER:HB2 | 1:HA:190:SER:HB3 | 1.97 | 0.47 |
| 1:HC:258:ASN:ND2 | 1:HC:352:LYS:HD3 | 2.30 | 0.47 |
| 1:IA:369:ALA:HB1 | 10:8V:18:UNK:HA | 1.96 | 0.47 |
| 2:ID:11:GLN:O | 2:ID:15:GLN:HG2 | 2.15 | 0.47 |
| 2:JB:11:GLN:O | 2:JB:15:GLN:HG2 | 2.15 | 0.47 |
| 1:JC:89:PRO:HD2 | 1:KC:280:LYS:HA | 1.96 | 0.47 |
| 2:KB:11:GLN:O | 2:KB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:KF:11:GLN:O | 2:KF:15:GLN:HG2 | 2.15 | 0.47 |
| 1:LA:258:ASN:ND2 | 1:LA:352:LYS:HD3 | 2.30 | 0.47 |
| 2:LD:11:GLN:O | 2:LD:15:GLN:HG2 | 2.15 | 0.47 |
| 1:LE:147:SER:HB2 | 1:LE:190:SER:HB3 | 1.97 | 0.47 |
| 2:MD:208:TYR:OH | 1:ME:325:PRO:HB2 | 2.15 | 0.47 |
| 2:MF:100:ASN:HD22 | 2:MF:103:LYS:HB2 | 1.79 | 0.47 |
| 6:4D:161:LYS:HE2 | 6:4D:164:ARG:HH22 | 1.80 | 0.47 |
| 6:4D:241:LYS:HD3 | 6:4D:241:LYS:HA | 1.51 | 0.47 |
| 7:5A:1436:ARG:NE | 7:5A:1436:ARG:C | 2.72 | 0.47 |
| 7:5A:1440:GLU:HA | 7:5A:1440:GLU:OE1 | 2.15 | 0.47 |
| 7:5B:800:LYS:HE2 | 7:5B:800:LYS:HB2 | 1.82 | 0.47 |
| 7:5B:1370:LYS:HD3 | 7:5B:1373:PHE:CZ | 2.49 | 0.47 |
| 7:5C:1436:ARG:NE | 7:5C:1436:ARG:C | 2.72 | 0.47 |
| 7:5C:1440:GLU:OE1 | 7:5C:1440:GLU:HA | 2.15 | 0.47 |
| 8:6B:46:ILE:HG21 | 8:6B:149:ILE:HG23 | 1.96 | 0.47 |
| 10:8J:33:UNK:C | 10:8J:35:UNK:N | 2.76 | 0.47 |
| 1:AC:2:ARG:HD2 | 1:AC:242:LEU:O | 2.15 | 0.47 |
| 2:BB:91:VAL:HG21 | 2:BB:116:VAL:HB | 1.97 | 0.47 |
| 2:BB:390:ARG:HD2 | 1:BC:439:THR:HG21 | 1.97 | 0.47 |
| 2:BF:91:VAL:HG21 | 2:BF:116:VAL:HB | 1.96 | 0.47 |
| 2:BF:100:ASN:HD22 | 2:BF:103:LYS:HB2 | 1.79 | 0.47 |
| 2:BF:372:THR:HA | 2:BF:422:TYR:CE2 | 2.48 | 0.47 |
| 2:CB:220:PRO:HD2 | 1:CC:326:LYS:CD | 2.45 | 0.47 |
| 1:DA:147:SER:HB2 | 1:DA:190:SER:HB3 | 1.97 | 0.47 |
| 1:DC:2:ARG:HD2 | 1:DC:242:LEU:O | 2.15 | 0.47 |
| 1:DC:147:SER:HB2 | 1:DC:190:SER:HB3 | 1.97 | 0.47 |
| 1:DE:402:ARG:HD2 | 7:5B:777:ALA:CB | 2.43 | 0.47 |
| 1:EA:258:ASN:ND2 | 1:EA:352:LYS:HD3 | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EC:317:MET:HA | 1:EC:377:MET:HA | 1.96 | 0.47 |
| 2:ED:248:SER:HA | 2:ED:252:LYS:HE2 | 1.97 | 0.47 |
| 1:FC:258:ASN:ND2 | 1:FC:352:LYS:HD3 | 2.30 | 0.47 |
| 1:FC:398:MET:SD | 2:FD:345:ILE:CG1 | 2.88 | 0.47 |
| 2:FD:248:SER:HA | 2:FD:252:LYS:HE2 | 1.97 | 0.47 |
| 2:FF:100:ASN:HD22 | 2:FF:103:LYS:HB2 | 1.79 | 0.47 |
| 2:FF:248:SER:HA | 2:FF:252:LYS:HE2 | 1.97 | 0.47 |
| 1:GA:188:ILE:HD12 | 1:GA:425:LEU:CD1 | 2.45 | 0.47 |
| 2:GB:11:GLN:O | 2:GB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:GB:100:ASN:HD22 | 2:GB:103:LYS:HB2 | 1.80 | 0.47 |
| 2:HB:11:GLN:O | 2:HB:15:GLN:HG2 | 2.15 | 0.47 |
| 1:HC:188:ILE:HD12 | 1:HC:425:LEU:CD1 | 2.45 | 0.47 |
| 2:ID:25:SER:HG | 2:ID:51:TYR:HH | 1.56 | 0.47 |
| 1:JE:92:LEU:H | 1:KE:280:LYS:HZ1 | 1.61 | 0.47 |
| 2:KB:100:ASN:HD22 | 2:KB:103:LYS:HB2 | 1.79 | 0.47 |
| 2:KD:217:LEU:CG | 6:4B:263:CYS:SG | 3.02 | 0.47 |
| 1:KE:258:ASN:ND2 | 1:KE:352:LYS:HD3 | 2.30 | 0.47 |
| 1:LA:147:SER:HB2 | 1:LA:190:SER:HB3 | 1.97 | 0.47 |
| 2:LB:384:GLN:HB3 | 1:LC:348:PRO:HG2 | 1.97 | 0.47 |
| 1:LC:221:ARG:HH11 | 2:LD:325:GLU:H | 1.63 | 0.47 |
| 2:LD:257:LEU:HA | 2:LD:312:THR:HG21 | 1.96 | 0.47 |
| 2:MB:257:LEU:HA | 2:MB:312:THR:HG21 | 1.96 | 0.47 |
| 2:MD:91:VAL:HG21 | 2:MD:116:VAL:HB | 1.97 | 0.47 |
| 1:ME:394:LYS:NZ | 2:MF:347:ASN:OD1 | 2.47 | 0.47 |
| 2:MF:91:VAL:HG21 | 2:MF:116:VAL:HB | 1.96 | 0.47 |
| 4:2A:12:LEU:HB3 | 4:2A:17:ILE:CG1 | 2.45 | 0.47 |
| 4:2B:12:LEU:HB3 | 4:2B:17:ILE:CG1 | 2.45 | 0.47 |
| 4:2B:29:TYR:CE2 | 4:2B:60:PHE:HD2 | 2.31 | 0.47 |
| 4:2B:143:LEU:HB3 | 4:2B:144:ASN:H | 1.60 | 0.47 |
| 4:2C:29:TYR:CE2 | 4:2C:60:PHE:HD2 | 2.31 | 0.47 |
| 6:4B:161:LYS:HE2 | 6:4B:164:ARG:HH22 | 1.80 | 0.47 |
| 6:4C:161:LYS:HE2 | 6:4C:164:ARG:HH22 | 1.80 | 0.47 |
| 6:4C:244:GLU:HG2 | 6:4C:284:LEU:CD2 | 2.45 | 0.47 |
| 6:4D:97:GLN:HA | 6:4D:98:PRO:HD3 | 1.58 | 0.47 |
| 6:4D:110:LYS:CE | 6:4D:113:ILE:HD11 | 2.44 | 0.47 |
| 6:4D:132:LYS:CE | 6:4D:132:LYS:CA | 2.84 | 0.47 |
| 6:4D:244:GLU:HG2 | 6:4D:284:LEU:CD2 | 2.44 | 0.47 |
| 6:4D:251:TYR:CZ | 6:4D:280:VAL:HG12 | 2.50 | 0.47 |
| 7:5A:1342:GLU:OE2 | 7:5A:1342:GLU:HA | 2.15 | 0.47 |
| 7:5A:1370:LYS:HD3 | 7:5A:1373:PHE:CZ | 2.49 | 0.47 |
| 7:5B:826:LEU:O | 7:5B:840:GLY:O | 2.33 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1366:TRP:CE3 | 7:5B:1366:TRP:HA | 2.50 | 0.47 |
| 7:5B:1440:GLU:OE1 | 7:5B:1440:GLU:HA | 2.15 | 0.47 |
| 10:8E:33:UNK:C | 10:8E:35:UNK:N | 2.76 | 0.47 |
| 10:8L:33:UNK:C | 10:8L:35:UNK:N | 2.76 | 0.47 |
| 1:AA:2:ARG:HD2 | 1:AA:242:LEU:O | 2.15 | 0.47 |
| 1:AE:2:ARG:HD2 | 1:AE:242:LEU:O | 2.15 | 0.47 |
| 2:BD:91:VAL:HG21 | 2:BD:116:VAL:HB | 1.97 | 0.47 |
| 1:CA:2:ARG:HD2 | 1:CA:242:LEU:O | 2.15 | 0.47 |
| 1:CC:258:ASN:ND2 | 1:CC:352:LYS:HD3 | 2.30 | 0.47 |
| 1:CE:2:ARG:HD2 | 1:CE:242:LEU:O | 2.15 | 0.47 |
| 1:DA:2:ARG:HD2 | 1:DA:242:LEU:O | 2.15 | 0.47 |
| 1:DA:181:VAL:HG21 | 2:DB:256:ASN:O | 2.15 | 0.47 |
| 2:DD:208:TYR:CD2 | 1:DE:326:LYS:HB3 | 2.50 | 0.47 |
| 1:DE:2:ARG:HD2 | 1:DE:242:LEU:O | 2.15 | 0.47 |
| 2:EB:133:PHE:HB2 | 2:EB:164:MET:SD | 2.54 | 0.47 |
| 1:EC:258:ASN:ND2 | 1:EC:352:LYS:HD3 | 2.30 | 0.47 |
| 2:ED:133:PHE:HB2 | 2:ED:164:MET:SD | 2.54 | 0.47 |
| 2:ED:390:ARG:CD | 1:EE:439:THR:HG21 | 2.45 | 0.47 |
| 1:EE:147:SER:HB2 | 1:EE:190:SER:HB3 | 1.97 | 0.47 |
| 1:EE:188:ILE:HD12 | 1:EE:425:LEU:CD1 | 2.45 | 0.47 |
| 1:FA:88:HIS:NE2 | 1:GA:284:GLU:OE1 | 2.47 | 0.47 |
| 1:FE:147:SER:HB2 | 1:FE:190:SER:HB3 | 1.97 | 0.47 |
| 2:FF:257:LEU:HA | 2:FF:312:THR:HG21 | 1.96 | 0.47 |
| 2:GB:177:ASP:C | 1:GC:352:LYS:HA | 2.39 | 0.47 |
| 1:HA:188:ILE:HD12 | 1:HA:425:LEU:CD1 | 2.45 | 0.47 |
| 1:HA:258:ASN:ND2 | 1:HA:352:LYS:HD3 | 2.30 | 0.47 |
| 2:HB:25:SER:HG | 2:HB:51:TYR:HH | 1.56 | 0.47 |
| 1:HC:147:SER:HB2 | 1:HC:190:SER:HB3 | 1.97 | 0.47 |
| 1:HE:179:THR:O | 2:HF:350:LYS:HA | 2.15 | 0.47 |
| 1:HE:258:ASN:ND2 | 1:HE:352:LYS:HD3 | 2.30 | 0.47 |
| 2:HF:100:ASN:HD22 | 2:HF:103:LYS:HB2 | 1.79 | 0.47 |
| 1:IA:402:ARG:CZ | 7:5C:1417:GLN:CA | 2.93 | 0.47 |
| 2:IB:11:GLN:O | 2:IB:15:GLN:HG2 | 2.15 | 0.47 |
| 2:IB:91:VAL:HG21 | 2:IB:116:VAL:HB | 1.96 | 0.47 |
| 2:IB:226:ASN:ND2 | 13:IB:501:GDP:HN1 | 2.12 | 0.47 |
| 1:JA:147:SER:HB2 | 1:JA:190:SER:HB3 | 1.97 | 0.47 |
| 2:JB:91:VAL:HG21 | 2:JB:116:VAL:HB | 1.97 | 0.47 |
| 1:JE:147:SER:HB2 | 1:JE:190:SER:HB3 | 1.97 | 0.47 |
| 2:KB:87:PRO:HD2 | 2:LB:282:ARG:HG2 | 1.97 | 0.47 |
| 2:KD:100:ASN:HD22 | 2:KD:103:LYS:HB2 | 1.79 | 0.47 |
| 2:KD:221:THR:HB | 6:4B:261:SER:HA | 1.38 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:KF:248:SER:HA | 2:KF:252:LYS:HE2 | 1.97 | 0.47 |
| 2:LB:91:VAL:HG21 | 2:LB:116:VAL:HB | 1.96 | 0.47 |
| 2:LB:100:ASN:HD22 | 2:LB:103:LYS:HB2 | 1.79 | 0.47 |
| 1:LC:147:SER:HB2 | 1:LC:190:SER:HB3 | 1.97 | 0.47 |
| 1:LE:241:SER:OG | 1:LE:250:VAL:O | 2.23 | 0.47 |
| 2:LF:11:GLN:O | 2:LF:15:GLN:HG2 | 2.15 | 0.47 |
| 1:ME:2:ARG:HD2 | 1:ME:242:LEU:O | 2.15 | 0.47 |
| 6:4A:161:LYS:HE2 | 6:4A:164:ARG:HH22 | 1.80 | 0.47 |
| 6:4A:244:GLU:HG2 | 6:4A:284:LEU:CD2 | 2.45 | 0.47 |
| 6:4B:251:TYR:CZ | 6:4B:280:VAL:HG12 | 2.50 | 0.47 |
| 6:4C:239:LEU:C | 6:4C:241:LYS:N | 2.71 | 0.47 |
| 6:4C:241:LYS:HD3 | 6:4C:241:LYS:O | 2.15 | 0.47 |
| 7:5A:826:LEU:O | 7:5A:840:GLY:O | 2.33 | 0.47 |
| 7:5A:1399:LYS:NZ | 7:5A:1399:LYS:C | 2.73 | 0.47 |
| 7:5B:1120:ASP:CG | 7:5B:1125:LEU:H | 2.22 | 0.47 |
| 7:5B:1399:LYS:NZ | 7:5B:1399:LYS:C | 2.73 | 0.47 |
| 7:5B:1424:GLN:NE2 | 7:5B:1424:GLN:HA | 2.29 | 0.47 |
| 7:5C:806:GLN:C | 7:5C:806:GLN:HE21 | 2.23 | 0.47 |
| 7:5C:826:LEU:O | 7:5C:840:GLY:O | 2.33 | 0.47 |
| 7:5C:1370:LYS:HD3 | 7:5C:1373:PHE:CZ | 2.49 | 0.47 |
| 8:6A:46:ILE:HG21 | 8:6A:149:ILE:HG23 | 1.96 | 0.47 |
| 9:7E:42:LEU:HD12 | 9:7F:39:GLY:HA3 | 1.95 | 0.47 |
| 10:8P:33:UNK:C | 10:8P:35:UNK:N | 2.76 | 0.47 |
| 10:8Q:33:UNK:C | 10:8Q:35:UNK:N | 2.76 | 0.47 |
| 2:BD:212:PHE:HE2 | 1:BE:326:LYS:HB2 | 1.80 | 0.46 |
| 1:CA:147:SER:HB2 | 1:CA:190:SER:HB3 | 1.97 | 0.46 |
| 1:CC:147:SER:HB2 | 1:CC:190:SER:HB3 | 1.97 | 0.46 |
| 2:DD:391:ARG:HG3 | 1:DE:346:TRP:CD1 | 2.50 | 0.46 |
| 2:DF:11:GLN:O | 2:DF:15:GLN:HG2 | 2.15 | 0.46 |
| 1:EA:188:ILE:HD12 | 1:EA:425:LEU:CD1 | 2.45 | 0.46 |
| 2:EB:11:GLN:O | 2:EB:15:GLN:HG2 | 2.15 | 0.46 |
| 2:EB:100:ASN:HD22 | 2:EB:103:LYS:HB2 | 1.79 | 0.46 |
| 1:EC:2:ARG:HD2 | 1:EC:242:LEU:O | 2.15 | 0.46 |
| 1:EC:147:SER:HB2 | 1:EC:190:SER:HB3 | 1.97 | 0.46 |
| 1:EC:188:ILE:HD12 | 1:EC:425:LEU:CD1 | 2.45 | 0.46 |
| 2:ED:100:ASN:HD22 | 2:ED:103:LYS:HB2 | 1.79 | 0.46 |
| 1:EE:2:ARG:HD2 | 1:EE:242:LEU:O | 2.15 | 0.46 |
| 2:EF:248:SER:HA | 2:EF:252:LYS:HE2 | 1.97 | 0.46 |
| 2:FB:402:GLY:O | 7:5C:1296:GLU:OE2 | 2.33 | 0.46 |
| 2:FD:100:ASN:HD22 | 2:FD:103:LYS:HB2 | 1.79 | 0.46 |
| 1:GA:60:LYS:NZ | 1:HA:283:HIS:CE1 | 2.82 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:HA:241:SER:OG | 1:HA:250:VAL:O | 2.23 | 0.46 |
| 2:HD:100:ASN:HD22 | 2:HD:103:LYS:HB2 | 1.79 | 0.46 |
| 2:HD:212:PHE:HZ | 1:HE:326:LYS:CE | 2.19 | 0.46 |
| 2:HD:257:LEU:HA | 2:HD:312:THR:HG21 | 1.96 | 0.46 |
| 1:HE:188:ILE:HD12 | 1:HE:425:LEU:CD1 | 2.45 | 0.46 |
| 1:HE:196:GLU:HG3 | 5:3A:211:GLN:NE2 | 2.30 | 0.46 |
| 1:IC:2:ARG:HD2 | 1:IC:242:LEU:O | 2.15 | 0.46 |
| 1:IE:2:ARG:HD2 | 1:IE:242:LEU:O | 2.15 | 0.46 |
| 1:JC:147:SER:HB2 | 1:JC:190:SER:HB3 | 1.97 | 0.46 |
| 2:JD:91:VAL:HG21 | 2:JD:116:VAL:HB | 1.97 | 0.46 |
| 1:KA:2:ARG:HD2 | 1:KA:242:LEU:O | 2.15 | 0.46 |
| 1:KA:147:SER:HB2 | 1:KA:190:SER:HB3 | 1.97 | 0.46 |
| 2:KB:273:LEU:HB3 | 6:4A:268:LEU:HG | 1.97 | 0.46 |
| 2:KB:339:SER:HB2 | 7:5C:1504:ARG:NH1 | 2.30 | 0.46 |
| 1:KC:147:SER:HB2 | 1:KC:190:SER:HB3 | 1.97 | 0.46 |
| 2:LB:177:ASP:C | 1:LC:352:LYS:HA | 2.41 | 0.46 |
| 1:LE:2:ARG:HD2 | 1:LE:242:LEU:O | 2.15 | 0.46 |
| 1:MA:222:PRO:HG2 | 2:MB:324:LYS:HD3 | 1.92 | 0.46 |
| 2:MB:220:PRO:O | 1:MC:324:VAL:HG13 | 2.13 | 0.46 |
| 1:MC:2:ARG:HD2 | 1:MC:242:LEU:O | 2.15 | 0.46 |
| 2:MD:100:ASN:HD22 | 2:MD:103:LYS:HB2 | 1.79 | 0.46 |
| 1:ME:401:LYS:CE | 2:MF:344:TRP:CZ3 | 2.71 | 0.46 |
| 4:2A:29:TYR:CE2 | 4:2A:60:PHE:HD2 | 2.31 | 0.46 |
| 4:2C:12:LEU:HB3 | 4:2C:17:ILE:CG1 | 2.45 | 0.46 |
| 6:4A:251:TYR:CZ | 6:4A:280:VAL:HG12 | 2.50 | 0.46 |
| 6:4B:110:LYS:CE | 6:4B:113:ILE:HD11 | 2.44 | 0.46 |
| 6:4B:113:ILE:HB | 6:4B:117:ARG:HH21 | 1.79 | 0.46 |
| 6:4B:244:GLU:HG2 | 6:4B:284:LEU:CD2 | 2.44 | 0.46 |
| 6:4D:164:ARG:CB | 6:4D:164:ARG:CZ | 2.92 | 0.46 |
| 7:5A:1120:ASP:CG | 7:5A:1125:LEU:H | 2.22 | 0.46 |
| 7:5A:1366:TRP:CE3 | 7:5A:1366:TRP:HA | 2.50 | 0.46 |
| 7:5B:1342:GLU:HA | 7:5B:1342:GLU:OE2 | 2.15 | 0.46 |
| 7:5C:1366:TRP:CE3 | 7:5C:1366:TRP:HA | 2.50 | 0.46 |
| 7:5C:1413:GLN:OE1 | 7:5C:1413:GLN:HA | 2.15 | 0.46 |
| 1:BC:188:ILE:HD12 | 1:BC:425:LEU:CD1 | 2.45 | 0.46 |
| 2:BD:372:THR:HA | 2:BD:422:TYR:CE2 | 2.48 | 0.46 |
| 1:BE:60:LYS:HZ2 | 1:CE:283:HIS:CD2 | 2.34 | 0.46 |
| 1:BE:188:ILE:HD12 | 1:BE:425:LEU:CD1 | 2.45 | 0.46 |
| 1:CA:258:ASN:ND2 | 1:CA:352:LYS:HD3 | 2.30 | 0.46 |
| 1:CE:147:SER:HB2 | 1:CE:190:SER:HB3 | 1.97 | 0.46 |
| 1:CE:221:ARG:NH1 | 2:CF:324:LYS:N | 2.63 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:DD:11:GLN:O | 2:DD:15:GLN:HG2 | 2.15 | 0.46 |
| 2:DD:179:VAL:HG22 | 1:DE:258:ASN:CB | 2.44 | 0.46 |
| 1:EC:426:ALA:HB1 | 7:5A:833:PHE:HB2 | 1.93 | 0.46 |
| 2:ED:11:GLN:O | 2:ED:15:GLN:HG2 | 2.15 | 0.46 |
| 1:EE:179:THR:O | 2:EF:350:LYS:HA | 2.15 | 0.46 |
| 1:EE:258:ASN:ND2 | 1:EE:352:LYS:HD3 | 2.30 | 0.46 |
| 2:EF:11:GLN:O | 2:EF:15:GLN:HG2 | 2.15 | 0.46 |
| 2:EF:91:VAL:HG21 | 2:EF:116:VAL:HB | 1.96 | 0.46 |
| 2:EF:100:ASN:HD22 | 2:EF:103:LYS:HB2 | 1.79 | 0.46 |
| 1:FA:2:ARG:HD2 | 1:FA:242:LEU:O | 2.15 | 0.46 |
| 1:FA:258:ASN:ND2 | 1:FA:352:LYS:HD3 | 2.30 | 0.46 |
| 2:FD:257:LEU:HA | 2:FD:312:THR:HG21 | 1.96 | 0.46 |
| 1:FE:2:ARG:HD2 | 1:FE:242:LEU:O | 2.15 | 0.46 |
| 1:FE:419:SER:CB | 7:5B:1256:ARG:HG2 | 2.34 | 0.46 |
| 2:FF:11:GLN:O | 2:FF:15:GLN:HG2 | 2.15 | 0.46 |
| 1:GE:222:PRO:HG3 | 2:GF:324:LYS:HD3 | 1.95 | 0.46 |
| 1:IA:188:ILE:HD12 | 1:IA:425:LEU:CD1 | 2.45 | 0.46 |
| 1:IA:409:VAL:HG21 | 7:5C:1421:PHE:HZ | 1.80 | 0.46 |
| 2:ID:91:VAL:HG21 | 2:ID:116:VAL:HB | 1.96 | 0.46 |
| 2:JB:257:LEU:HA | 2:JB:312:THR:HG21 | 1.96 | 0.46 |
| 2:JF:91:VAL:HG21 | 2:JF:116:VAL:HB | 1.96 | 0.46 |
| 1:KA:188:ILE:HD12 | 1:KA:425:LEU:CD1 | 2.45 | 0.46 |
| 1:KC:2:ARG:HD2 | 1:KC:242:LEU:O | 2.15 | 0.46 |
| 1:KE:147:SER:HB2 | 1:KE:190:SER:HB3 | 1.97 | 0.46 |
| 2:KF:79:GLY:HA2 | 6:4D:254:ALA:HB1 | 1.96 | 0.46 |
| 2:KF:124:ALA:O | 4:2B:38:VAL:HG13 | 2.15 | 0.46 |
| 2:KF:127:CYS:HB2 | 4:2B:38:VAL:HG21 | 1.42 | 0.46 |
| 1:LA:221:ARG:HH11 | 2:LB:325:GLU:H | 1.63 | 0.46 |
| 2:LB:18:ALA:CB | 6:4A:217:ASN:ND2 | 2.71 | 0.46 |
| 2:LB:257:LEU:HA | 2:LB:312:THR:HG21 | 1.96 | 0.46 |
| 2:LD:223:GLY:CA | 6:4B:219:ASN:HD22 | 2.28 | 0.46 |
| 2:MD:257:LEU:HA | 2:MD:312:THR:HG21 | 1.96 | 0.46 |
| 1:ME:258:ASN:ND2 | 1:ME:352:LYS:HD3 | 2.30 | 0.46 |
| 2:MF:226:ASN:ND2 | 13:MF:502:GDP:HN1 | 2.12 | 0.46 |
| 2:MF:257:LEU:HA | 2:MF:312:THR:HG21 | 1.96 | 0.46 |
| 6:4A:110:LYS:CE | 6:4A:113:ILE:HD11 | 2.44 | 0.46 |
| 7:5A:848:SER:C | 7:5A:850:GLU:N | 2.73 | 0.46 |
| 7:5A:1413:GLN:HA | 7:5A:1413:GLN:OE1 | 2.15 | 0.46 |
| 7:5B:773:ARG:C | 7:5B:773:ARG:NE | 2.73 | 0.46 |
| 7:5B:1404:LYS:HE3 | 7:5B:1404:LYS:HB3 | 1.49 | 0.46 |
| 7:5B:1413:GLN:OE1 | 7:5B:1413:GLN:HA | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1515:GLU:OE1 | 7:5B:1563:SER:CA | 2.62 | 0.46 |
| 7:5C:773:ARG:C | 7:5C:773:ARG:NE | 2.73 | 0.46 |
| 7:5C:1105:TYR:CD1 | 7:5C:1165:PRO:CA | 2.81 | 0.46 |
| 7:5C:1399:LYS:NZ | 7:5C:1399:LYS:C | 2.73 | 0.46 |
| 7:5C:1515:GLU:OE1 | 7:5C:1563:SER:CA | 2.62 | 0.46 |
| 10:8Y:33:UNK:C | 10:8Y:35:UNK:N | 2.76 | 0.46 |
| 10:8Z:33:UNK:C | 10:8Z:35:UNK:N | 2.76 | 0.46 |
| 2:AB:248:SER:HA | 2:AB:252:LYS:HE2 | 1.97 | 0.46 |
| 1:BA:188:ILE:HD12 | 1:BA:425:LEU:CD1 | 2.45 | 0.46 |
| 2:BB:177:ASP:CA | 1:BC:353:VAL:HG12 | 2.45 | 0.46 |
| 1:BC:60:LYS:HD3 | 1:CC:283:HIS:CD2 | 2.50 | 0.46 |
| 1:BE:2:ARG:HD2 | 1:BE:242:LEU:O | 2.15 | 0.46 |
| 1:CC:188:ILE:HD12 | 1:CC:425:LEU:CD1 | 2.45 | 0.46 |
| 1:CE:179:THR:O | 2:CF:350:LYS:HA | 2.14 | 0.46 |
| 2:DB:11:GLN:O | 2:DB:15:GLN:HG2 | 2.15 | 0.46 |
| 2:DB:87:PRO:HD2 | 2:EB:281:TYR:CD2 | 2.50 | 0.46 |
| 1:DE:221:ARG:NH1 | 2:DF:324:LYS:N | 2.63 | 0.46 |
| 2:DF:86:ARG:NH2 | 2:EF:281:TYR:CE2 | 1.78 | 0.46 |
| 2:DF:248:SER:HA | 2:DF:252:LYS:HE2 | 1.97 | 0.46 |
| 1:EA:147:SER:HB2 | 1:EA:190:SER:HB3 | 1.97 | 0.46 |
| 2:EB:179:VAL:CG2 | 1:EC:258:ASN:O | 2.42 | 0.46 |
| 2:ED:91:VAL:HG21 | 2:ED:116:VAL:HB | 1.96 | 0.46 |
| 1:FA:56:THR:HG1 | 1:GA:284:GLU:C | 2.15 | 0.46 |
| 1:FC:2:ARG:HD2 | 1:FC:242:LEU:O | 2.15 | 0.46 |
| 1:FC:147:SER:HB2 | 1:FC:190:SER:HB3 | 1.97 | 0.46 |
| 2:FD:11:GLN:O | 2:FD:15:GLN:HG2 | 2.15 | 0.46 |
| 1:GE:241:SER:OG | 1:GE:250:VAL:O | 2.23 | 0.46 |
| 2:GF:406:MET:HE3 | 7:5B:1341:LYS:HE3 | 1.98 | 0.46 |
| 1:HC:60:LYS:HD3 | 1:IC:283:HIS:CD2 | 2.50 | 0.46 |
| 1:IA:2:ARG:HD2 | 1:IA:242:LEU:O | 2.15 | 0.46 |
| 1:IE:258:ASN:ND2 | 1:IE:352:LYS:HD3 | 2.30 | 0.46 |
| 1:JA:2:ARG:HD2 | 1:JA:242:LEU:O | 2.15 | 0.46 |
| 1:JE:258:ASN:ND2 | 1:JE:352:LYS:HD3 | 2.30 | 0.46 |
| 1:KC:188:ILE:HD12 | 1:KC:425:LEU:CD1 | 2.45 | 0.46 |
| 2:KD:88:ASP:OD2 | 4:2A:150:GLN:NE2 | 2.38 | 0.46 |
| 2:KD:248:SER:HA | 2:KD:252:LYS:HE2 | 1.97 | 0.46 |
| 1:KE:2:ARG:HD2 | 1:KE:242:LEU:O | 2.15 | 0.46 |
| 1:KE:188:ILE:HD12 | 1:KE:425:LEU:CD1 | 2.45 | 0.46 |
| 1:LA:222:PRO:HD2 | 2:LB:324:LYS:CG | 2.45 | 0.46 |
| 2:LB:177:ASP:CA | 1:LC:353:VAL:HG12 | 2.45 | 0.46 |
| 1:LC:2:ARG:HD2 | 1:LC:242:LEU:O | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LD:223:GLY:HA3 | 6:4B:219:ASN:CA | 2.43 | 0.46 |
| 2:LF:223:GLY:CA | 6:4D:219:ASN:ND2 | 2.79 | 0.46 |
| 2:LF:379:LYS:CE | 4:2B:166:ILE:HG13 | 2.39 | 0.46 |
| 1:MA:372:MET:CE | 6:4C:96:VAL:CB | 2.93 | 0.46 |
| 2:MB:100:ASN:HD22 | 2:MB:103:LYS:HB2 | 1.79 | 0.46 |
| 2:MD:111:GLU:CA | 3:1B:62:SER:HA | 2.45 | 0.46 |
| 4:2B:164:ARG:NE | 4:2B:164:ARG:CA | 2.73 | 0.46 |
| 6:4A:164:ARG:CB | 6:4A:164:ARG:CZ | 2.92 | 0.46 |
| 6:4A:241:LYS:HD3 | 6:4A:241:LYS:O | 2.15 | 0.46 |
| 6:4B:164:ARG:CB | 6:4B:164:ARG:CZ | 2.92 | 0.46 |
| 6:4B:266:ASN:HD22 | 6:4B:273:ARG:HH11 | 1.63 | 0.46 |
| 6:4C:251:TYR:CZ | 6:4C:280:VAL:HG12 | 2.50 | 0.46 |
| 6:4D:113:ILE:HB | 6:4D:117:ARG:HH21 | 1.79 | 0.46 |
| 6:4D:241:LYS:HD3 | 6:4D:241:LYS:O | 2.15 | 0.46 |
| 6:4D:266:ASN:HD22 | 6:4D:273:ARG:HH11 | 1.63 | 0.46 |
| 7:5A:872:GLU:CD | 8:6A:90:ARG:NH1 | 2.74 | 0.46 |
| 7:5A:1407:GLN:C | 7:5A:1407:GLN:CD | 2.83 | 0.46 |
| 7:5B:835:GLN:HE21 | 7:5B:835:GLN:HA | 1.80 | 0.46 |
| 7:5B:866:TYR:CD1 | 7:5B:958:GLU:HG3 | 2.50 | 0.46 |
| 7:5B:1407:GLN:C | 7:5B:1407:GLN:CD | 2.83 | 0.46 |
| 7:5C:912:VAL:CG1 | 7:5C:918:ILE:HG13 | 2.45 | 0.46 |
| 7:5C:1120:ASP:CG | 7:5C:1125:LEU:H | 2.22 | 0.46 |
| 7:5C:1407:GLN:C | 7:5C:1407:GLN:CD | 2.83 | 0.46 |
| 7:5C:1490:LYS:HD3 | 7:5C:1490:LYS:HA | 1.40 | 0.46 |
| 10:8A:33:UNK:C | 10:8A:35:UNK:N | 2.76 | 0.46 |
| 10:8M:33:UNK:C | 10:8M:35:UNK:N | 2.76 | 0.46 |
| 1:AA:258:ASN:ND2 | 1:AA:352:LYS:HD3 | 2.30 | 0.46 |
| 1:AC:71:GLU:CD | 2:AD:247:ASN:ND2 | 2.74 | 0.46 |
| 2:BB:372:THR:HA | 2:BB:422:TYR:CE2 | 2.48 | 0.46 |
| 2:CB:91:VAL:HG21 | 2:CB:116:VAL:HB | 1.96 | 0.46 |
| 1:DC:188:ILE:HD12 | 1:DC:425:LEU:CD1 | 2.45 | 0.46 |
| 1:DC:401:LYS:HE3 | 1:DC:401:LYS:HB2 | 1.74 | 0.46 |
| 2:DD:248:SER:HA | 2:DD:252:LYS:HE2 | 1.97 | 0.46 |
| 1:EE:396:ASP:C | 7:5B:817:LEU:HD11 | 2.40 | 0.46 |
| 1:FA:176:GLN:NE2 | 7:5C:915:PHE:HA | 2.30 | 0.46 |
| 2:FB:100:ASN:HD22 | 2:FB:103:LYS:HB2 | 1.79 | 0.46 |
| 2:FB:220:PRO:CD | 1:FC:326:LYS:HE2 | 2.37 | 0.46 |
| 2:FB:257:LEU:HA | 2:FB:312:THR:HG21 | 1.96 | 0.46 |
| 1:GA:241:SER:OG | 1:GA:250:VAL:O | 2.23 | 0.46 |
| 1:GE:401:LYS:HE3 | 1:GE:401:LYS:HB2 | 1.74 | 0.46 |
| 2:HB:100:ASN:HD22 | 2:HB:103:LYS:HB2 | 1.80 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:HB:257:LEU:HA | 2:HB:312:THR:HG21 | 1.96 | 0.46 |
| 1:HE:222:PRO:HG3 | 2:HF:324:LYS:HD3 | 1.95 | 0.46 |
| 1:IA:147:SER:HB2 | 1:IA:190:SER:HB3 | 1.97 | 0.46 |
| 2:IB:424:GLN:HE21 | 7:5C:1413:GLN:CD | 1.86 | 0.46 |
| 1:IC:188:ILE:HD12 | 1:IC:425:LEU:CD1 | 2.45 | 0.46 |
| 1:IC:258:ASN:ND2 | 1:IC:352:LYS:HD3 | 2.30 | 0.46 |
| 1:IC:434:GLU:HG3 | 5:3C:61:SER:HA | 1.97 | 0.46 |
| 2:IF:91:VAL:HG21 | 2:IF:116:VAL:HB | 1.96 | 0.46 |
| 2:IF:100:ASN:HD22 | 2:IF:103:LYS:HB2 | 1.79 | 0.46 |
| 1:JC:2:ARG:HD2 | 1:JC:242:LEU:O | 2.15 | 0.46 |
| 2:KB:118:ASP:OD1 | 4:2C:148:ASN:CG | 2.54 | 0.46 |
| 2:KF:100:ASN:HD22 | 2:KF:103:LYS:HB2 | 1.79 | 0.46 |
| 2:KF:159:TYR:HE2 | 4:2B:35:VAL:O | 1.94 | 0.46 |
| 1:LA:2:ARG:HD2 | 1:LA:242:LEU:O | 2.15 | 0.46 |
| 1:LA:241:SER:OG | 1:LA:250:VAL:O | 2.23 | 0.46 |
| 1:LC:245:ASP:CG | 6:4A:216:ARG:NE | 2.62 | 0.46 |
| 2:LD:91:VAL:HG21 | 2:LD:116:VAL:HB | 1.96 | 0.46 |
| 2:MB:177:ASP:C | 1:MC:352:LYS:HA | 2.40 | 0.46 |
| 4:2B:33:GLN:HG2 | 4:2B:56:CYS:SG | 2.56 | 0.46 |
| 4:2C:33:GLN:HG2 | 4:2C:56:CYS:SG | 2.56 | 0.46 |
| 6:4C:164:ARG:CB | 6:4C:164:ARG:CZ | 2.92 | 0.46 |
| 6:4C:265:TYR:CD2 | 6:4C:265:TYR:C | 2.94 | 0.46 |
| 7:5A:866:TYR:CD1 | 7:5A:958:GLU:HG3 | 2.50 | 0.46 |
| 7:5A:1515:GLU:OE1 | 7:5A:1563:SER:CA | 2.62 | 0.46 |
| 7:5B:847:GLY:HA3 | 8:6B:17:LYS:NZ | 2.30 | 0.46 |
| 7:5B:848:SER:C | 7:5B:850:GLU:N | 2.73 | 0.46 |
| 8:6C:84:LEU:HG | 8:6C:88:VAL:HG23 | 1.98 | 0.46 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:HD21 | 1.97 | 0.46 |
| 10:8B:33:UNK:C | 10:8B:35:UNK:N | 2.76 | 0.46 |
| 10:8G:33:UNK:C | 10:8G:35:UNK:N | 2.76 | 0.46 |
| 1:AE:258:ASN:ND2 | 1:AE:352:LYS:HD3 | 2.30 | 0.46 |
| 1:BA:258:ASN:ND2 | 1:BA:352:LYS:HD3 | 2.30 | 0.46 |
| 2:BB:179:VAL:HG23 | 1:BC:258:ASN:HA | 1.96 | 0.46 |
| 2:BD:98:GLY:CA | 1:BE:254:GLU:CG | 2.54 | 0.46 |
| 1:CA:188:ILE:HD12 | 1:CA:425:LEU:CD1 | 2.45 | 0.46 |
| 2:CB:179:VAL:HG22 | 1:CC:258:ASN:CG | 2.40 | 0.46 |
| 2:CD:11:GLN:O | 2:CD:15:GLN:HG2 | 2.15 | 0.46 |
| 2:DD:179:VAL:HG22 | 1:DE:258:ASN:CA | 2.46 | 0.46 |
| 1:DE:188:ILE:HD12 | 1:DE:425:LEU:CD1 | 2.45 | 0.46 |
| 2:DF:287:PRO:HA | 2:DF:290:THR:HG22 | 1.98 | 0.46 |
| 1:EA:2:ARG:HD2 | 1:EA:242:LEU:O | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:EB:91:VAL:HG21 | 2:EB:116:VAL:HB | 1.96 | 0.46 |
| 2:EB:98:GLY:CA | 1:EC:254:GLU:CG | 2.49 | 0.46 |
| 2:EF:125:GLU:CG | 7:5B:903:PHE:HD2 | 2.15 | 0.46 |
| 1:FA:147:SER:HB2 | 1:FA:190:SER:HB3 | 1.97 | 0.46 |
| 2:FB:178:THR:HA | 1:FC:352:LYS:HD3 | 1.96 | 0.46 |
| 1:FC:177:VAL:N | 7:5A:915:PHE:CZ | 2.83 | 0.46 |
| 2:GD:179:VAL:HG23 | 1:GE:258:ASN:HA | 1.97 | 0.46 |
| 1:GE:179:THR:O | 2:GF:350:LYS:HA | 2.15 | 0.46 |
| 2:HD:25:SER:HG | 2:HD:51:TYR:HH | 1.57 | 0.46 |
| 1:IA:241:SER:OG | 1:IA:250:VAL:O | 2.23 | 0.46 |
| 2:IB:100:ASN:HD22 | 2:IB:103:LYS:HB2 | 1.79 | 0.46 |
| 1:IC:389:SER:CB | 5:3C:307:LYS:CD | 2.54 | 0.46 |
| 1:IC:389:SER:O | 5:3C:308:PHE:CE2 | 2.69 | 0.46 |
| 1:IE:179:THR:O | 2:IF:350:LYS:HA | 2.15 | 0.46 |
| 1:IE:188:ILE:HD12 | 1:IE:425:LEU:CD1 | 2.45 | 0.46 |
| 2:IF:257:LEU:HA | 2:IF:312:THR:HG21 | 1.96 | 0.46 |
| 1:JE:176:GLN:O | 2:JF:347:ASN:ND2 | 2.40 | 0.46 |
| 2:JF:100:ASN:HD22 | 2:JF:103:LYS:HB2 | 1.79 | 0.46 |
| 2:JF:257:LEU:HA | 2:JF:312:THR:HG21 | 1.95 | 0.46 |
| 1:LC:241:SER:OG | 1:LC:250:VAL:O | 2.23 | 0.46 |
| 2:LF:224:ASP:CA | 6:4D:219:ASN:HD21 | 2.24 | 0.46 |
| 2:LF:248:SER:HA | 2:LF:252:LYS:HE2 | 1.97 | 0.46 |
| 1:MA:2:ARG:HD2 | 1:MA:242:LEU:O | 2.15 | 0.46 |
| 1:MA:11:GLN:HE22 | 2:MB:246:LEU:HA | 1.81 | 0.46 |
| 1:MA:224:TYR:CE2 | 2:MB:246:LEU:HD11 | 2.42 | 0.46 |
| 1:MC:258:ASN:ND2 | 1:MC:352:LYS:HD3 | 2.30 | 0.46 |
| 2:MD:176:SER:HG | 1:ME:349:THR:HG1 | 1.58 | 0.46 |
| 4:2A:18:ARG:HH12 | 4:2A:122:GLU:CD | 2.23 | 0.46 |
| 4:2A:33:GLN:HG2 | 4:2A:56:CYS:SG | 2.56 | 0.46 |
| 4:2B:12:LEU:HD12 | 4:2B:13:THR:H | 1.80 | 0.46 |
| 4:2C:18:ARG:HH12 | 4:2C:122:GLU:CD | 2.23 | 0.46 |
| 6:4A:265:TYR:CD2 | 6:4A:265:TYR:C | 2.94 | 0.46 |
| 6:4A:266:ASN:HD22 | 6:4A:273:ARG:HH11 | 1.63 | 0.46 |
| 6:4B:241:LYS:HD3 | 6:4B:241:LYS:HA | 1.52 | 0.46 |
| 6:4C:110:LYS:CE | 6:4C:113:ILE:HD11 | 2.44 | 0.46 |
| 7:5A:773:ARG:C | 7:5A:773:ARG:NE | 2.73 | 0.46 |
| 7:5A:1105:TYR:CD1 | 7:5A:1165:PRO:CA | 2.81 | 0.46 |
| 7:5A:1271:ILE:HA | 9:7A:20:LEU:CD2 | 2.13 | 0.46 |
| 7:5B:1105:TYR:CD1 | 7:5B:1165:PRO:CA | 2.81 | 0.46 |
| 7:5B:1443:LYS:C | 7:5B:1443:LYS:CD | 2.85 | 0.46 |
| 7:5C:866:TYR:CD1 | 7:5C:958:GLU:HG3 | 2.50 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:874:GLN:HB3 | 8:6C:59:LYS:HZ3 | 1.79 | 0.46 |
| 7:5C:1404:LYS:HZ1 | 7:5C:1408:GLU:HB2 | 1.78 | 0.46 |
| 7:5C:1521:PHE:CE2 | 7:5C:1567:PHE:CE1 | 2.96 | 0.46 |
| 10:8H:33:UNK:C | 10:8H:35:UNK:N | 2.76 | 0.46 |
| 10:8N:33:UNK:C | 10:8N:35:UNK:N | 2.76 | 0.46 |
| 10:8O:33:UNK:C | 10:8O:35:UNK:N | 2.76 | 0.46 |
| 1:AA:147:SER:HB2 | 1:AA:190:SER:HB3 | 1.97 | 0.46 |
| 1:AC:147:SER:HB2 | 1:AC:190:SER:HB3 | 1.97 | 0.46 |
| 1:AC:181:VAL:HG21 | 2:AD:256:ASN:O | 2.16 | 0.46 |
| 1:AC:258:ASN:ND2 | 1:AC:352:LYS:HD3 | 2.30 | 0.46 |
| 2:AD:248:SER:HA | 2:AD:252:LYS:HE2 | 1.97 | 0.46 |
| 1:AE:147:SER:HB2 | 1:AE:190:SER:HB3 | 1.97 | 0.46 |
| 1:BA:60:LYS:HZ2 | 1:CA:283:HIS:CD2 | 2.34 | 0.46 |
| 1:BA:179:THR:O | 2:BB:350:LYS:HA | 2.15 | 0.46 |
| 2:CD:91:VAL:HG21 | 2:CD:116:VAL:HB | 1.96 | 0.46 |
| 1:CE:188:ILE:HD12 | 1:CE:425:LEU:CD1 | 2.45 | 0.46 |
| 2:CF:11:GLN:O | 2:CF:15:GLN:HG2 | 2.15 | 0.46 |
| 1:DA:188:ILE:HD12 | 1:DA:425:LEU:CD1 | 2.45 | 0.46 |
| 2:ED:287:PRO:HA | 2:ED:290:THR:HG22 | 1.98 | 0.46 |
| 2:EF:287:PRO:HA | 2:EF:290:THR:HG22 | 1.98 | 0.46 |
| 2:FB:11:GLN:O | 2:FB:15:GLN:HG2 | 2.15 | 0.46 |
| 2:FB:91:VAL:HG21 | 2:FB:116:VAL:HB | 1.96 | 0.46 |
| 2:FB:287:PRO:HA | 2:FB:290:THR:HG22 | 1.98 | 0.46 |
| 1:GA:2:ARG:HD2 | 1:GA:242:LEU:O | 2.15 | 0.46 |
| 1:GA:147:SER:HB2 | 1:GA:190:SER:HB3 | 1.97 | 0.46 |
| 2:GB:287:PRO:HA | 2:GB:290:THR:HG22 | 1.98 | 0.46 |
| 1:HC:241:SER:OG | 1:HC:250:VAL:O | 2.23 | 0.46 |
| 2:HF:55:THR:HG23 | 2:IF:283:ALA:HA | 1.98 | 0.46 |
| 2:HF:248:SER:HA | 2:HF:252:LYS:HE2 | 1.97 | 0.46 |
| 1:IC:71:GLU:CD | 2:ID:247:ASN:ND2 | 2.74 | 0.46 |
| 1:IC:147:SER:HB2 | 1:IC:190:SER:HB3 | 1.97 | 0.46 |
| 2:ID:100:ASN:HD22 | 2:ID:103:LYS:HB2 | 1.79 | 0.46 |
| 2:ID:179:VAL:HG23 | 1:IE:258:ASN:HA | 1.97 | 0.46 |
| 1:IE:222:PRO:HD2 | 2:IF:324:LYS:HD3 | 1.96 | 0.46 |
| 1:JC:258:ASN:ND2 | 1:JC:352:LYS:HD3 | 2.30 | 0.46 |
| 2:JD:100:ASN:HD22 | 2:JD:103:LYS:HB2 | 1.79 | 0.46 |
| 1:JE:2:ARG:HD2 | 1:JE:242:LEU:O | 2.15 | 0.46 |
| 2:JF:248:SER:HA | 2:JF:252:LYS:HE2 | 1.97 | 0.46 |
| 2:KB:248:SER:HA | 2:KB:252:LYS:HE2 | 1.97 | 0.46 |
| 1:KC:71:GLU:CD | 2:KD:247:ASN:ND2 | 2.74 | 0.46 |
| 1:KC:222:PRO:HG3 | 2:KD:324:LYS:HD3 | 1.95 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:KE:222:PRO:HD2 | 2:KF:324:LYS:HD3 | 1.96 | 0.46 |
| 2:LD:379:LYS:O | 4:2A:166:ILE:CD1 | 2.54 | 0.46 |
| 2:LF:91:VAL:HG21 | 2:LF:116:VAL:HB | 1.96 | 0.46 |
| 2:LF:337:ASN:HD21 | 4:2B:148:ASN:HB2 | 1.81 | 0.46 |
| 1:MA:258:ASN:ND2 | 1:MA:352:LYS:HD3 | 2.30 | 0.46 |
| 2:MB:176:SER:CB | 1:MC:349:THR:OG1 | 2.63 | 0.46 |
| 1:ME:279:GLU:HB2 | 6:4B:110:LYS:NZ | 2.30 | 0.46 |
| 6:4A:264:GLY:O | 6:4A:273:ARG:HD2 | 2.16 | 0.46 |
| 6:4B:264:GLY:O | 6:4B:273:ARG:HD2 | 2.16 | 0.46 |
| 6:4B:265:TYR:CD2 | 6:4B:265:TYR:C | 2.94 | 0.46 |
| 6:4C:243:ASP:HB3 | 6:4C:247:LYS:HD2 | 1.68 | 0.46 |
| 6:4C:266:ASN:HD22 | 6:4C:273:ARG:HH11 | 1.63 | 0.46 |
| 6:4D:264:GLY:O | 6:4D:273:ARG:HD2 | 2.16 | 0.46 |
| 7:5A:912:VAL:CG1 | 7:5A:918:ILE:HG13 | 2.45 | 0.46 |
| 7:5A:1438:LEU:HD12 | 7:5A:1438:LEU:C | 2.41 | 0.46 |
| 7:5A:1443:LYS:C | 7:5A:1443:LYS:CD | 2.85 | 0.46 |
| 7:5A:1452:HIS:ND1 | 7:5A:1452:HIS:C | 2.74 | 0.46 |
| 7:5A:1490:LYS:HD3 | 7:5A:1490:LYS:HA | 1.41 | 0.46 |
| 7:5A:1530:ILE:HD13 | 7:5A:1571:MET:SD | 2.56 | 0.46 |
| 7:5B:1490:LYS:HD3 | 7:5B:1490:LYS:HA | 1.40 | 0.46 |
| 7:5B:1530:ILE:HD13 | 7:5B:1571:MET:SD | 2.56 | 0.46 |
| 7:5C:839:GLU:HA | 8:6C:109:ILE:H | 1.80 | 0.46 |
| 7:5C:1438:LEU:HD12 | 7:5C:1438:LEU:C | 2.41 | 0.46 |
| 7:5C:1530:ILE:HD13 | 7:5C:1571:MET:SD | 2.56 | 0.46 |
| 10:8D:33:UNK:C | 10:8D:35:UNK:N | 2.76 | 0.46 |
| 1:AC:60:LYS:NZ | 1:BC:283:HIS:CE1 | 2.84 | 0.46 |
| 2:AD:287:PRO:HA | 2:AD:290:THR:HG22 | 1.98 | 0.46 |
| 1:AE:188:ILE:HD12 | 1:AE:425:LEU:CD1 | 2.45 | 0.46 |
| 1:BA:224:TYR:CE2 | 2:BB:246:LEU:HD11 | 2.48 | 0.46 |
| 1:BC:2:ARG:HD2 | 1:BC:242:LEU:O | 2.15 | 0.46 |
| 1:BE:258:ASN:ND2 | 1:BE:352:LYS:HD3 | 2.30 | 0.46 |
| 1:CA:282:TYR:HE2 | 10:8D:18:UNK:HA | 1.79 | 0.46 |
| 1:CC:394:LYS:NZ | 2:CD:347:ASN:OD1 | 2.49 | 0.46 |
| 2:CF:287:PRO:HA | 2:CF:290:THR:HG22 | 1.98 | 0.46 |
| 13:EB:501:GDP:H8 | 1:EC:248:LEU:CD1 | 2.29 | 0.46 |
| 2:ED:179:VAL:HG22 | 1:EE:258:ASN:CB | 2.46 | 0.46 |
| 1:EE:430:LYS:HZ2 | 7:5B:834:ASN:CB | 2.26 | 0.46 |
| 2:FB:106:TYR:CD1 | 7:5C:1295:LYS:N | 2.83 | 0.46 |
| 1:FE:188:ILE:HD12 | 1:FE:425:LEU:CD1 | 2.45 | 0.46 |
| 2:FF:287:PRO:HA | 2:FF:290:THR:HG22 | 1.98 | 0.46 |
| 2:HB:248:SER:HA | 2:HB:252:LYS:HE2 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:HE:2:ARG:HD2 | 1:HE:242:LEU:O | 2.15 | 0.46 |
| 1:HE:241:SER:OG | 1:HE:250:VAL:O | 2.23 | 0.46 |
| 1:HE:282:TYR:CD1 | 10:8U:15:UNK:CA | 2.95 | 0.46 |
| 1:IA:401:LYS:HE3 | 1:IA:401:LYS:HB2 | 1.74 | 0.46 |
| 2:IB:257:LEU:HA | 2:IB:312:THR:HG21 | 1.96 | 0.46 |
| 1:IC:241:SER:OG | 1:IC:250:VAL:O | 2.23 | 0.46 |
| 2:LB:248:SER:HA | 2:LB:252:LYS:HE2 | 1.97 | 0.46 |
| 1:LE:222:PRO:HD2 | 2:LF:324:LYS:CG | 2.46 | 0.46 |
| 2:LF:25:SER:HG | 2:LF:51:TYR:HH | 1.57 | 0.46 |
| 2:MB:178:THR:HA | 1:MC:352:LYS:HD3 | 1.97 | 0.46 |
| 2:MD:226:ASN:ND2 | 13:MD:502:GDP:HN1 | 2.12 | 0.46 |
| 2:MF:287:PRO:HA | 2:MF:290:THR:HG22 | 1.98 | 0.46 |
| 4:2A:12:LEU:HD12 | 4:2A:13:THR:H | 1.80 | 0.46 |
| 4:2B:18:ARG:HH12 | 4:2B:122:GLU:CD | 2.23 | 0.46 |
| 5:3C:165:LEU:HD23 | 5:3C:198:MET:HE3 | 1.97 | 0.46 |
| 6:4A:243:ASP:HB3 | 6:4A:247:LYS:HD2 | 1.68 | 0.46 |
| 6:4B:241:LYS:HD3 | 6:4B:241:LYS:O | 2.15 | 0.46 |
| 6:4C:248:VAL:HG13 | 6:4C:288:TYR:HD2 | 1.80 | 0.46 |
| 6:4C:264:GLY:O | 6:4C:273:ARG:HD2 | 2.16 | 0.46 |
| 7:5B:912:VAL:CG1 | 7:5B:918:ILE:HG13 | 2.45 | 0.46 |
| 7:5B:1030:PHE:CZ | 7:5B:1034:ILE:HD11 | 2.50 | 0.46 |
| 7:5B:1438:LEU:HD12 | 7:5B:1438:LEU:C | 2.41 | 0.46 |
| 7:5B:1452:HIS:ND1 | 7:5B:1452:HIS:C | 2.74 | 0.46 |
| 7:5C:1452:HIS:ND1 | 7:5C:1452:HIS:C | 2.74 | 0.46 |
| 8:6A:84:LEU:HG | 8:6A:88:VAL:HG23 | 1.98 | 0.46 |
| 9:7A:11:TYR:CD1 | 9:7B:23:LEU:HD23 | 2.51 | 0.46 |
| 9:7C:11:TYR:CD1 | 9:7D:23:LEU:HD23 | 2.51 | 0.46 |
| 2:AB:100:ASN:HD22 | 2:AB:103:LYS:HB2 | 1.79 | 0.46 |
| 1:AC:188:ILE:HD12 | 1:AC:425:LEU:CD1 | 2.45 | 0.46 |
| 2:AF:248:SER:HA | 2:AF:252:LYS:HE2 | 1.97 | 0.46 |
| 1:BA:404:PHE:CE2 | 2:BB:345:ILE:HD11 | 2.51 | 0.46 |
| 2:BD:287:PRO:HA | 2:BD:290:THR:HG22 | 1.98 | 0.46 |
| 2:BF:287:PRO:HA | 2:BF:290:THR:HG22 | 1.98 | 0.46 |
| 2:CD:176:SER:HG | 1:CE:349:THR:HG1 | 1.48 | 0.46 |
| 2:CD:287:PRO:HA | 2:CD:290:THR:HG22 | 1.98 | 0.46 |
| 2:DB:248:SER:HA | 2:DB:252:LYS:HE2 | 1.97 | 0.46 |
| 2:DB:287:PRO:HA | 2:DB:290:THR:HG22 | 1.98 | 0.46 |
| 1:DE:404:PHE:CE2 | 2:DF:345:ILE:HD11 | 2.51 | 0.46 |
| 2:DF:84:LEU:O | 2:EF:281:TYR:OH | 2.34 | 0.46 |
| 2:EB:287:PRO:HA | 2:EB:290:THR:HG22 | 1.98 | 0.46 |
| 2:ED:222:TYR:HD2 | 1:EE:247:ALA:HB1 | 1.79 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:FC:188:ILE:HD12 | 1:FC:425:LEU:CD1 | 2.45 | 0.46 |
| 1:FE:181:VAL:HG12 | 2:FF:348:ASN:HA | 1.96 | 0.46 |
| 1:FE:401:LYS:HE3 | 2:FF:344:TRP:CZ3 | 2.51 | 0.46 |
| 1:GC:181:VAL:HG21 | 2:GD:256:ASN:O | 2.16 | 0.46 |
| 2:GD:287:PRO:HA | 2:GD:290:THR:HG22 | 1.98 | 0.46 |
| 1:GE:224:TYR:CE2 | 2:GF:246:LEU:HD11 | 2.46 | 0.46 |
| 2:GF:287:PRO:HA | 2:GF:290:THR:HG22 | 1.98 | 0.46 |
| 1:HA:2:ARG:HD2 | 1:HA:242:LEU:O | 2.15 | 0.46 |
| 2:HB:91:VAL:HG21 | 2:HB:116:VAL:HB | 1.96 | 0.46 |
| 2:HB:287:PRO:HA | 2:HB:290:THR:HG22 | 1.98 | 0.46 |
| 2:HD:248:SER:HA | 2:HD:252:LYS:HE2 | 1.97 | 0.46 |
| 1:IA:258:ASN:ND2 | 1:IA:352:LYS:HD3 | 2.30 | 0.46 |
| 2:JD:248:SER:HA | 2:JD:252:LYS:HE2 | 1.97 | 0.46 |
| 2:JD:287:PRO:HA | 2:JD:290:THR:HG22 | 1.98 | 0.46 |
| 2:KD:287:PRO:HA | 2:KD:290:THR:HG22 | 1.98 | 0.46 |
| 2:LB:331:LEU:HD23 | 4:2C:42:PHE:CE2 | 2.14 | 0.46 |
| 2:LB:331:LEU:CD1 | 4:2C:42:PHE:CZ | 2.92 | 0.46 |
| 4:2C:12:LEU:HD12 | 4:2C:13:THR:H | 1.80 | 0.46 |
| 7:5A:1105:TYR:CD1 | 7:5A:1105:TYR:N | 2.83 | 0.46 |
| 7:5A:1443:LYS:HE3 | 7:5A:1444:LYS:HA | 1.97 | 0.46 |
| 7:5B:1105:TYR:CD1 | 7:5B:1105:TYR:N | 2.83 | 0.46 |
| 7:5B:1404:LYS:NZ | 7:5B:1408:GLU:HB2 | 2.31 | 0.46 |
| 7:5C:1105:TYR:CD1 | 7:5C:1105:TYR:N | 2.83 | 0.46 |
| 7:5C:1399:LYS:C | 7:5C:1399:LYS:HZ2 | 2.23 | 0.46 |
| 7:5C:1491:LEU:HD13 | 7:5C:1491:LEU:HA | 1.82 | 0.46 |
| 8:6B:84:LEU:HG | 8:6B:88:VAL:HG23 | 1.98 | 0.46 |
| 9:7E:2:PHE:HB3 | 9:7E:10:TYR:CE1 | 2.51 | 0.46 |
| 10:8F:33:UNK:C | 10:8F:35:UNK:N | 2.76 | 0.46 |
| 1:AA:188:ILE:HD12 | 1:AA:425:LEU:CD1 | 2.45 | 0.46 |
| 2:AB:287:PRO:HA | 2:AB:290:THR:HG22 | 1.98 | 0.46 |
| 2:AF:100:ASN:HD22 | 2:AF:103:LYS:HB2 | 1.79 | 0.46 |
| 2:AF:287:PRO:HA | 2:AF:290:THR:HG22 | 1.98 | 0.46 |
| 1:BA:2:ARG:HD2 | 1:BA:242:LEU:O | 2.15 | 0.46 |
| 1:BA:147:SER:HB2 | 1:BA:190:SER:HB3 | 1.97 | 0.46 |
| 1:BC:60:LYS:HZ2 | 1:CC:283:HIS:CD2 | 2.34 | 0.46 |
| 2:BD:179:VAL:HG22 | 1:BE:258:ASN:CG | 2.41 | 0.46 |
| 1:CA:370:LYS:HE3 | 10:8D:17:UNK:CB | 2.27 | 0.46 |
| 2:CB:11:GLN:O | 2:CB:15:GLN:HG2 | 2.15 | 0.46 |
| 2:CB:287:PRO:HA | 2:CB:290:THR:HG22 | 1.98 | 0.46 |
| 2:CF:91:VAL:HG21 | 2:CF:116:VAL:HB | 1.96 | 0.46 |
| 2:DD:91:VAL:HG21 | 2:DD:116:VAL:HB | 1.96 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:DD:287:PRO:HA | 2:DD:290:THR:HG22 | 1.98 | 0.46 |
| 2:DF:91:VAL:HG21 | 2:DF:116:VAL:HB | 1.96 | 0.46 |
| 2:FD:287:PRO:HA | 2:FD:290:THR:HG22 | 1.98 | 0.46 |
| 1:GC:2:ARG:HD2 | 1:GC:242:LEU:O | 2.15 | 0.46 |
| 1:HA:100:ALA:HB1 | 2:HB:252:LYS:CA | 2.46 | 0.46 |
| 1:HC:2:ARG:HD2 | 1:HC:242:LEU:O | 2.15 | 0.46 |
| 2:HD:287:PRO:HA | 2:HD:290:THR:HG22 | 1.98 | 0.46 |
| 1:HE:100:ALA:HB1 | 2:HF:252:LYS:CA | 2.46 | 0.46 |
| 2:ID:257:LEU:HA | 2:ID:312:THR:HG21 | 1.96 | 0.46 |
| 1:IE:147:SER:HB2 | 1:IE:190:SER:HB3 | 1.97 | 0.46 |
| 1:IE:222:PRO:HG3 | 2:IF:324:LYS:HD3 | 1.95 | 0.46 |
| 2:IF:424:GLN:NE2 | 7:5B:1413:GLN:NE2 | 0.60 | 0.46 |
| 1:JA:258:ASN:ND2 | 1:JA:352:LYS:HD3 | 2.30 | 0.46 |
| 1:JC:181:VAL:HG21 | 2:JD:256:ASN:O | 2.16 | 0.46 |
| 2:JD:257:LEU:HA | 2:JD:312:THR:HG21 | 1.96 | 0.46 |
| 1:JE:222:PRO:HG3 | 2:JF:324:LYS:HD3 | 1.95 | 0.46 |
| 1:KC:79:ARG:C | 1:LC:280:LYS:HE2 | 2.31 | 0.46 |
| 1:LE:222:PRO:HG2 | 2:LF:324:LYS:CD | 2.40 | 0.46 |
| 1:ME:188:ILE:HD12 | 1:ME:425:LEU:CD1 | 2.45 | 0.46 |
| 4:2A:164:ARG:NE | 4:2A:164:ARG:CA | 2.73 | 0.46 |
| 4:2C:164:ARG:NE | 4:2C:164:ARG:CA | 2.73 | 0.46 |
| 6:4A:108:LYS:HE2 | 6:4A:108:LYS:HB3 | 1.36 | 0.46 |
| 6:4A:248:VAL:HG13 | 6:4A:288:TYR:HD2 | 1.80 | 0.46 |
| 6:4B:108:LYS:HE2 | 6:4B:108:LYS:HB3 | 1.36 | 0.46 |
| 6:4D:265:TYR:C | 6:4D:265:TYR:CD2 | 2.94 | 0.46 |
| 7:5A:942:LYS:HB3 | 7:5A:1034:ILE:HG23 | 1.98 | 0.46 |
| 7:5A:1404:LYS:NZ | 7:5A:1408:GLU:HB2 | 2.31 | 0.46 |
| 7:5A:1436:ARG:C | 7:5A:1436:ARG:CD | 2.89 | 0.46 |
| 7:5B:887:TYR:HD1 | 7:5B:890:ILE:HD12 | 1.81 | 0.46 |
| 7:5C:942:LYS:HB3 | 7:5C:1034:ILE:HG23 | 1.98 | 0.46 |
| 7:5C:1436:ARG:C | 7:5C:1436:ARG:CD | 2.89 | 0.46 |
| 7:5C:1521:PHE:HZ | 7:5C:1571:MET:N | 2.14 | 0.46 |
| 8:6C:130:ASN:C | 8:6C:136:LEU:HD12 | 2.40 | 0.46 |
| 1:AA:100:ALA:HB1 | 2:AB:252:LYS:CA | 2.46 | 0.46 |
| 2:AD:100:ASN:HD22 | 2:AD:103:LYS:HB2 | 1.79 | 0.46 |
| 2:AD:372:THR:HA | 2:AD:422:TYR:CE2 | 2.48 | 0.46 |
| 2:BB:287:PRO:HA | 2:BB:290:THR:HG22 | 1.98 | 0.46 |
| 2:BF:105:HIS:CE1 | 2:BF:150:LEU:HD12 | 2.51 | 0.46 |
| 2:DB:91:VAL:HG21 | 2:DB:116:VAL:HB | 1.96 | 0.46 |
| 2:EB:177:ASP:OD2 | 1:EC:353:VAL:HG11 | 2.02 | 0.46 |
| 2:EB:222:TYR:HD2 | 1:EC:247:ALA:HB1 | 1.80 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:FA:188:ILE:HD12 | 1:FA:425:LEU:CD1 | 2.45 | 0.46 |
| 1:FC:56:THR:C | 1:GC:285:GLN:CB | 2.89 | 0.46 |
| 1:GE:2:ARG:HD2 | 1:GE:242:LEU:O | 2.15 | 0.46 |
| 2:HD:91:VAL:HG21 | 2:HD:116:VAL:HB | 1.96 | 0.46 |
| 2:HF:287:PRO:HA | 2:HF:290:THR:HG22 | 1.98 | 0.46 |
| 2:ID:287:PRO:HA | 2:ID:290:THR:HG22 | 1.98 | 0.46 |
| 2:IF:287:PRO:HA | 2:IF:290:THR:HG22 | 1.98 | 0.46 |
| 2:JB:100:ASN:HD22 | 2:JB:103:LYS:HB2 | 1.80 | 0.46 |
| 2:JB:248:SER:HA | 2:JB:252:LYS:HE2 | 1.97 | 0.46 |
| 2:JB:287:PRO:HA | 2:JB:290:THR:HG22 | 1.98 | 0.46 |
| 1:KA:100:ALA:HB1 | 2:KB:252:LYS:CA | 2.45 | 0.46 |
| 2:KB:217:LEU:HB2 | 6:4A:263:CYS:SG | 2.56 | 0.46 |
| 2:LB:388:MET:HA | 1:LC:346:TRP:O | 2.16 | 0.46 |
| 2:LD:248:SER:HA | 2:LD:252:LYS:HE2 | 1.97 | 0.46 |
| 2:LF:287:PRO:HA | 2:LF:290:THR:HG22 | 1.98 | 0.46 |
| 1:MA:147:SER:HB2 | 1:MA:190:SER:HB3 | 1.97 | 0.46 |
| 2:MB:287:PRO:HA | 2:MB:290:THR:HG22 | 1.98 | 0.46 |
| 1:MC:147:SER:HB2 | 1:MC:190:SER:HB3 | 1.97 | 0.46 |
| 2:MD:221:THR:CB | 6:4B:189:ARG:NH1 | 2.79 | 0.46 |
| 2:MD:287:PRO:HA | 2:MD:290:THR:HG22 | 1.98 | 0.46 |
| 2:MD:391:ARG:O | 1:ME:262:TYR:OH | 2.19 | 0.46 |
| 6:4A:241:LYS:C | 6:4A:241:LYS:CD | 2.89 | 0.46 |
| 6:4B:248:VAL:HG13 | 6:4B:288:TYR:HD2 | 1.80 | 0.46 |
| 6:4C:241:LYS:C | 6:4C:241:LYS:CD | 2.89 | 0.46 |
| 6:4D:248:VAL:HG13 | 6:4D:288:TYR:HD2 | 1.80 | 0.46 |
| 7:5A:887:TYR:HD1 | 7:5A:890:ILE:HD12 | 1.81 | 0.46 |
| 7:5B:942:LYS:HB3 | 7:5B:1034:ILE:HG23 | 1.98 | 0.46 |
| 7:5B:1436:ARG:C | 7:5B:1436:ARG:CD | 2.89 | 0.46 |
| 7:5C:887:TYR:HD1 | 7:5C:890:ILE:HD12 | 1.81 | 0.46 |
| 7:5C:1415:GLU:CD | 7:5C:1415:GLU:C | 2.83 | 0.46 |
| 7:5C:1443:LYS:HE3 | 7:5C:1444:LYS:HA | 1.98 | 0.46 |
| 8:6C:81:GLU:HA | 8:6C:85:GLU:OE1 | 2.15 | 0.46 |
| 10:8C:33:UNK:C | 10:8C:35:UNK:N | 2.76 | 0.46 |
| 2:BB:105:HIS:CE1 | 2:BB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:BB:203:ASP:O | 2:BB:207:LEU:HG | 2.16 | 0.45 |
| 1:BC:258:ASN:ND2 | 1:BC:352:LYS:HD3 | 2.30 | 0.45 |
| 2:BD:105:HIS:CE1 | 2:BD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:EA:402:ARG:CD | 7:5C:824:ARG:HH22 | 2.22 | 0.45 |
| 2:EB:105:HIS:CE1 | 2:EB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:EB:220:PRO:HD2 | 1:EC:326:LYS:CD | 2.46 | 0.45 |
| 2:ED:105:HIS:CE1 | 2:ED:150:LEU:HD12 | 2.52 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:ED:203:ASP:O | 2:ED:207:LEU:HG | 2.17 | 0.45 |
| 1:EE:32:PRO:HB3 | 1:EE:83:TYR:CE1 | 2.52 | 0.45 |
| 2:EF:226:ASN:ND2 | 13:EF:501:GDP:HN1 | 2.12 | 0.45 |
| 1:FA:176:GLN:O | 2:FB:347:ASN:ND2 | 2.40 | 0.45 |
| 2:FD:91:VAL:HG21 | 2:FD:116:VAL:HB | 1.96 | 0.45 |
| 2:FD:179:VAL:HG21 | 1:FE:258:ASN:C | 2.32 | 0.45 |
| 1:GC:71:GLU:CD | 2:GD:247:ASN:ND2 | 2.74 | 0.45 |
| 1:GC:147:SER:HB2 | 1:GC:190:SER:HB3 | 1.97 | 0.45 |
| 2:GD:105:HIS:CE1 | 2:GD:150:LEU:HD12 | 2.52 | 0.45 |
| 2:GD:212:PHE:CZ | 1:GE:326:LYS:CE | 2.98 | 0.45 |
| 2:GF:91:VAL:HG21 | 2:GF:116:VAL:HB | 1.96 | 0.45 |
| 1:HC:71:GLU:CD | 2:HD:247:ASN:ND2 | 2.74 | 0.45 |
| 1:HC:278:ALA:HB3 | 10:8T:21:UNK:C | 2.42 | 0.45 |
| 2:HD:394:PHE:CD1 | 1:HE:261:PRO:HA | 2.52 | 0.45 |
| 1:IA:71:GLU:HA | 1:IA:72:PRO:HD3 | 1.84 | 0.45 |
| 2:ID:86:ARG:NH1 | 2:JD:281:TYR:CA | 2.58 | 0.45 |
| 1:JA:188:ILE:HD12 | 1:JA:425:LEU:CD1 | 2.45 | 0.45 |
| 2:JB:203:ASP:O | 2:JB:207:LEU:HG | 2.16 | 0.45 |
| 2:JF:287:PRO:HA | 2:JF:290:THR:HG22 | 1.98 | 0.45 |
| 1:KA:245:ASP:CB | 6:4C:253:ARG:HE | 2.27 | 0.45 |
| 2:KB:158:GLU:HB3 | 4:2C:34:ASN:HB3 | 0.79 | 0.45 |
| 2:KB:287:PRO:HA | 2:KB:290:THR:HG22 | 1.98 | 0.45 |
| 1:KE:100:ALA:HB1 | 2:KF:252:LYS:CA | 2.46 | 0.45 |
| 1:KE:179:THR:O | 2:KF:350:LYS:HA | 2.15 | 0.45 |
| 2:KF:287:PRO:HA | 2:KF:290:THR:HG22 | 1.98 | 0.45 |
| 2:LB:287:PRO:HA | 2:LB:290:THR:HG22 | 1.98 | 0.45 |
| 2:LB:390:ARG:HD3 | 1:LC:439:THR:HG21 | 1.97 | 0.45 |
| 1:LC:222:PRO:CG | 2:LD:324:LYS:HB2 | 2.38 | 0.45 |
| 2:LD:25:SER:HG | 2:LD:51:TYR:HH | 1.56 | 0.45 |
| 2:LD:287:PRO:HA | 2:LD:290:THR:HG22 | 1.98 | 0.45 |
| 1:MC:188:ILE:HD12 | 1:MC:425:LEU:CD1 | 2.45 | 0.45 |
| 1:ME:71:GLU:CD | 2:MF:247:ASN:HD22 | 2.23 | 0.45 |
| 2:MF:105:HIS:CE1 | 2:MF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:MF:221:THR:CB | 6:4D:189:ARG:NH2 | 2.77 | 0.45 |
| 5:3A:165:LEU:HD23 | 5:3A:198:MET:HE3 | 1.97 | 0.45 |
| 6:4A:101:ARG:NH2 | 6:4A:101:ARG:CG | 2.76 | 0.45 |
| 6:4A:241:LYS:HD3 | 6:4A:241:LYS:HA | 1.52 | 0.45 |
| 6:4B:241:LYS:C | 6:4B:241:LYS:CD | 2.89 | 0.45 |
| 6:4C:167:ARG:CB | 6:4C:167:ARG:NH1 | 2.79 | 0.45 |
| 6:4D:161:LYS:HA | 6:4D:161:LYS:HD3 | 1.78 | 0.45 |
| 6:4D:230:TYR:OH | 6:4D:240:LYS:CG | 2.51 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5A:1030:PHE:CZ | 7:5A:1034:ILE:HD11 | 2.50 | 0.45 |
| 7:5A:1272:ILE:HD11 | 9:7B:11:TYR:CD2 | 2.50 | 0.45 |
| 7:5A:1425:LYS:CD | 7:5A:1425:LYS:C | 2.88 | 0.45 |
| 7:5A:1499:LYS:NZ | 7:5A:1513:ASP:O | 2.46 | 0.45 |
| 7:5A:1521:PHE:HZ | 7:5A:1571:MET:N | 2.14 | 0.45 |
| 7:5B:827:GLU:HA | 7:5B:841:VAL:HG13 | 1.98 | 0.45 |
| 7:5B:1348:LYS:N | 7:5B:1348:LYS:CD | 2.73 | 0.45 |
| 7:5B:1425:LYS:CD | 7:5B:1425:LYS:C | 2.88 | 0.45 |
| 7:5B:1443:LYS:HE3 | 7:5B:1444:LYS:HA | 1.98 | 0.45 |
| 7:5B:1499:LYS:NZ | 7:5B:1513:ASP:O | 2.47 | 0.45 |
| 7:5C:841:VAL:CG1 | 8:6C:9:LEU:HD23 | 2.46 | 0.45 |
| 7:5C:1407:GLN:HA | 7:5C:1407:GLN:HE21 | 1.81 | 0.45 |
| 7:5C:1425:LYS:CD | 7:5C:1425:LYS:C | 2.88 | 0.45 |
| 8:6A:130:ASN:C | 8:6A:136:LEU:HD12 | 2.40 | 0.45 |
| 2:AB:203:ASP:O | 2:AB:207:LEU:HG | 2.17 | 0.45 |
| 2:AD:105:HIS:CE1 | 2:AD:150:LEU:HD12 | 2.52 | 0.45 |
| 2:AF:105:HIS:CE1 | 2:AF:150:LEU:HD12 | 2.52 | 0.45 |
| 1:BC:32:PRO:HB3 | 1:BC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:BD:220:PRO:CD | 1:BE:326:LYS:HG2 | 2.37 | 0.45 |
| 1:BE:32:PRO:HB3 | 1:BE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:CA:179:THR:O | 2:CB:350:LYS:HA | 2.15 | 0.45 |
| 1:CA:221:ARG:NH1 | 2:CB:324:LYS:N | 2.64 | 0.45 |
| 2:CD:220:PRO:HD2 | 1:CE:326:LYS:CD | 2.46 | 0.45 |
| 2:DB:179:VAL:HG22 | 1:DC:258:ASN:CB | 2.46 | 0.45 |
| 1:EA:32:PRO:HB3 | 1:EA:83:TYR:CE1 | 2.52 | 0.45 |
| 1:EC:32:PRO:HB3 | 1:EC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:ED:226:ASN:ND2 | 13:ED:502:GDP:HN1 | 2.12 | 0.45 |
| 2:EF:105:HIS:CE1 | 2:EF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:EF:203:ASP:O | 2:EF:207:LEU:HG | 2.17 | 0.45 |
| 1:FA:422:ARG:CZ | 7:5C:1170:THR:HA | 2.38 | 0.45 |
| 2:FF:91:VAL:HG21 | 2:FF:116:VAL:HB | 1.96 | 0.45 |
| 1:GA:32:PRO:HB3 | 1:GA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:GB:91:VAL:HG21 | 2:GB:116:VAL:HB | 1.96 | 0.45 |
| 2:GB:105:HIS:CE1 | 2:GB:150:LEU:HD12 | 2.52 | 0.45 |
| 1:GC:32:PRO:HB3 | 1:GC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:GF:105:HIS:CE1 | 2:GF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:IB:203:ASP:O | 2:IB:207:LEU:HG | 2.17 | 0.45 |
| 13:IB:501:GDP:C8 | 1:IC:248:LEU:CD1 | 2.99 | 0.45 |
| 1:IC:181:VAL:HG21 | 2:ID:256:ASN:O | 2.16 | 0.45 |
| 13:JB:501:GDP:C8 | 1:JC:248:LEU:CD1 | 2.99 | 0.45 |
| 1:JC:188:ILE:HD12 | 1:JC:425:LEU:CD1 | 2.45 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:JD:394:PHE:CD1 | 1:JE:261:PRO:HA | 2.52 | 0.45 |
| 2:JF:87:PRO:HD2 | 2:KF:281:TYR:HD2 | 1.27 | 0.45 |
| 1:KA:88:HIS:HA | 1:LA:284:GLU:HA | 1.85 | 0.45 |
| 2:LB:105:HIS:CE1 | 2:LB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:LD:105:HIS:CE1 | 2:LD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:LE:100:ALA:O | 2:LF:255:VAL:HG21 | 2.15 | 0.45 |
| 2:LF:105:HIS:CE1 | 2:LF:150:LEU:HD12 | 2.52 | 0.45 |
| 1:MA:32:PRO:HB3 | 1:MA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:MB:105:HIS:CE1 | 2:MB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:MB:226:ASN:ND2 | 13:MB:502:GDP:HN1 | 2.12 | 0.45 |
| 1:MC:32:PRO:HB3 | 1:MC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:MD:105:HIS:CE1 | 2:MD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:ME:32:PRO:HB3 | 1:ME:83:TYR:CE1 | 2.52 | 0.45 |
| 6:4A:167:ARG:NH1 | 6:4A:167:ARG:CB | 2.79 | 0.45 |
| 6:4A:230:TYR:OH | 6:4A:240:LYS:CG | 2.51 | 0.45 |
| 6:4B:230:TYR:OH | 6:4B:240:LYS:CG | 2.51 | 0.45 |
| 7:5A:1348:LYS:N | 7:5A:1348:LYS:CD | 2.73 | 0.45 |
| 7:5A:1415:GLU:CD | 7:5A:1415:GLU:C | 2.83 | 0.45 |
| 7:5C:1404:LYS:NZ | 7:5C:1408:GLU:HB2 | 2.31 | 0.45 |
| 8:6B:130:ASN:C | 8:6B:136:LEU:HD12 | 2.40 | 0.45 |
| 9:7F:18:VAL:HG11 | 9:7F:42:LEU:HD23 | 1.93 | 0.45 |
| 1:AA:32:PRO:HB3 | 1:AA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:AB:105:HIS:CE1 | 2:AB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:AD:203:ASP:O | 2:AD:207:LEU:HG | 2.17 | 0.45 |
| 1:AE:32:PRO:HB3 | 1:AE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:AE:100:ALA:HB1 | 2:AF:252:LYS:CA | 2.46 | 0.45 |
| 1:AE:179:THR:O | 2:AF:350:LYS:HA | 2.15 | 0.45 |
| 1:BC:147:SER:HB2 | 1:BC:190:SER:HB3 | 1.97 | 0.45 |
| 2:BD:203:ASP:O | 2:BD:207:LEU:HG | 2.17 | 0.45 |
| 2:BF:226:ASN:ND2 | 13:BF:501:GDP:HN1 | 2.12 | 0.45 |
| 1:CA:32:PRO:HB3 | 1:CA:83:TYR:CE1 | 2.52 | 0.45 |
| 1:CC:32:PRO:HB3 | 1:CC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:EB:203:ASP:O | 2:EB:207:LEU:HG | 2.17 | 0.45 |
| 1:FA:60:LYS:CG | 1:GA:283:HIS:HA | 2.31 | 0.45 |
| 2:FF:203:ASP:O | 2:FF:207:LEU:HG | 2.17 | 0.45 |
| 1:GC:222:PRO:HG3 | 2:GD:324:LYS:HD3 | 1.95 | 0.45 |
| 1:GE:32:PRO:HB3 | 1:GE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:GE:147:SER:HB2 | 1:GE:190:SER:HB3 | 1.97 | 0.45 |
| 2:HF:91:VAL:HG21 | 2:HF:116:VAL:HB | 1.96 | 0.45 |
| 2:HF:105:HIS:CE1 | 2:HF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:IB:287:PRO:HA | 2:IB:290:THR:HG22 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:IE:278:ALA:HB3 | 10:8X:22:UNK:N | 2.24 | 0.45 |
| 1:JC:71:GLU:CD | 2:JD:247:ASN:ND2 | 2.74 | 0.45 |
| 1:JE:188:ILE:HD12 | 1:JE:425:LEU:CD1 | 2.45 | 0.45 |
| 1:KC:181:VAL:HG21 | 2:KD:256:ASN:O | 2.16 | 0.45 |
| 2:KF:203:ASP:O | 2:KF:207:LEU:HG | 2.17 | 0.45 |
| 2:LD:413:SER:HB2 | 4:2A:171:VAL:HG22 | 1.97 | 0.45 |
| 1:LE:32:PRO:HB3 | 1:LE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:LE:188:ILE:HD12 | 1:LE:425:LEU:CD1 | 2.45 | 0.45 |
| 1:MA:188:ILE:HD12 | 1:MA:425:LEU:CD1 | 2.45 | 0.45 |
| 1:MC:279:GLU:HB2 | 6:4A:110:LYS:NZ | 2.32 | 0.45 |
| 5:3B:165:LEU:HD23 | 5:3B:198:MET:HE3 | 1.97 | 0.45 |
| 6:4B:167:ARG:NH1 | 6:4B:167:ARG:CB | 2.79 | 0.45 |
| 6:4C:101:ARG:NH2 | 6:4C:101:ARG:CG | 2.76 | 0.45 |
| 6:4C:108:LYS:HE2 | 6:4C:108:LYS:HB3 | 1.36 | 0.45 |
| 7:5A:1491:LEU:HD13 | 7:5A:1491:LEU:HA | 1.82 | 0.45 |
| 7:5B:1521:PHE:HZ | 7:5B:1571:MET:N | 2.14 | 0.45 |
| 7:5C:841:VAL:HG12 | 8:6C:9:LEU:HD23 | 1.98 | 0.45 |
| 7:5C:1348:LYS:N | 7:5C:1348:LYS:CD | 2.73 | 0.45 |
| 7:5C:1499:LYS:NZ | 7:5C:1513:ASP:O | 2.47 | 0.45 |
| 10:9A:33:UNK:C | 10:9A:35:UNK:N | 2.76 | 0.45 |
| 1:AC:32:PRO:HB3 | 1:AC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:AD:54:ALA:HB1 | 2:BD:281:TYR:O | 2.17 | 0.45 |
| 2:AF:203:ASP:O | 2:AF:207:LEU:HG | 2.17 | 0.45 |
| 1:BA:32:PRO:HB3 | 1:BA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:BB:55:THR:HG23 | 2:CB:283:ALA:HA | 1.99 | 0.45 |
| 2:CD:208:TYR:CD2 | 1:CE:326:LYS:HB3 | 2.52 | 0.45 |
| 1:DA:179:THR:O | 2:DB:350:LYS:HA | 2.16 | 0.45 |
| 2:DF:105:HIS:CE1 | 2:DF:150:LEU:HD12 | 2.51 | 0.45 |
| 1:FA:419:SER:HB2 | 7:5C:1256:ARG:CZ | 2.30 | 0.45 |
| 2:FB:203:ASP:O | 2:FB:207:LEU:HG | 2.17 | 0.45 |
| 1:FC:71:GLU:CD | 2:FD:247:ASN:HD22 | 2.23 | 0.45 |
| 2:FD:203:ASP:O | 2:FD:207:LEU:HG | 2.17 | 0.45 |
| 1:FE:32:PRO:HB3 | 1:FE:83:TYR:CE1 | 2.51 | 0.45 |
| 2:FF:105:HIS:CE1 | 2:FF:150:LEU:HD12 | 2.52 | 0.45 |
| 1:GA:100:ALA:HB1 | 2:GB:252:LYS:CA | 2.45 | 0.45 |
| 2:GD:91:VAL:HG21 | 2:GD:116:VAL:HB | 1.96 | 0.45 |
| 2:GD:394:PHE:CD1 | 1:GE:261:PRO:HA | 2.52 | 0.45 |
| 13:HB:501:GDP:C8 | 1:HC:248:LEU:CD1 | 2.99 | 0.45 |
| 1:HC:181:VAL:HG21 | 2:HD:256:ASN:O | 2.16 | 0.45 |
| 1:HC:222:PRO:HG3 | 2:HD:324:LYS:HD3 | 1.95 | 0.45 |
| 2:HD:105:HIS:CE1 | 2:HD:150:LEU:HD12 | 2.52 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:HD:212:PHE:CZ | 1:HE:326:LYS:CE | 2.98 | 0.45 |
| 1:IA:282:TYR:CE1 | 10:8V:14:UNK:O | 2.70 | 0.45 |
| 2:ID:203:ASP:O | 2:ID:207:LEU:HG | 2.17 | 0.45 |
| 1:IE:100:ALA:HB1 | 2:IF:252:LYS:CA | 2.46 | 0.45 |
| 1:JA:278:ALA:HB1 | 10:8Y:18:UNK:O | 2.17 | 0.45 |
| 2:JD:203:ASP:O | 2:JD:207:LEU:HG | 2.17 | 0.45 |
| 2:KB:203:ASP:O | 2:KB:207:LEU:HG | 2.16 | 0.45 |
| 2:KB:221:THR:HB | 6:4A:261:SER:HA | 1.11 | 0.45 |
| 2:KB:276:ARG:NH2 | 6:4A:265:TYR:C | 2.74 | 0.45 |
| 13:KB:501:GDP:C8 | 1:KC:248:LEU:CD1 | 2.99 | 0.45 |
| 2:KD:203:ASP:O | 2:KD:207:LEU:HG | 2.17 | 0.45 |
| 1:LA:32:PRO:HB3 | 1:LA:83:TYR:CE1 | 2.52 | 0.45 |
| 1:LC:32:PRO:HB3 | 1:LC:83:TYR:CE1 | 2.52 | 0.45 |
| 1:LC:188:ILE:HD12 | 1:LC:425:LEU:CD1 | 2.45 | 0.45 |
| 1:LC:222:PRO:HD2 | 2:LD:324:LYS:CG | 2.46 | 0.45 |
| 2:LF:228:LEU:HD21 | 6:4D:225:PRO:HB2 | 1.97 | 0.45 |
| 2:MD:177:ASP:C | 1:ME:352:LYS:HA | 2.42 | 0.45 |
| 4:2A:171:VAL:HB | 4:2A:176:ARG:HE | 1.81 | 0.45 |
| 4:2B:171:VAL:HB | 4:2B:176:ARG:HE | 1.81 | 0.45 |
| 6:4B:243:ASP:HB3 | 6:4B:247:LYS:HD2 | 1.68 | 0.45 |
| 6:4C:230:TYR:OH | 6:4C:240:LYS:CG | 2.51 | 0.45 |
| 6:4D:167:ARG:NH1 | 6:4D:167:ARG:CB | 2.79 | 0.45 |
| 7:5A:827:GLU:HA | 7:5A:841:VAL:HG13 | 1.98 | 0.45 |
| 7:5A:835:GLN:HE21 | 7:5A:835:GLN:HA | 1.80 | 0.45 |
| 7:5A:1093:LEU:HD21 | 7:5A:1107:LYS:HE2 | 1.98 | 0.45 |
| 7:5A:1407:GLN:HA | 7:5A:1407:GLN:HE21 | 1.81 | 0.45 |
| 7:5B:1407:GLN:HA | 7:5B:1407:GLN:HE21 | 1.81 | 0.45 |
| 7:5B:1475:PHE:CZ | 7:5B:1565:GLU:OE2 | 2.56 | 0.45 |
| 7:5C:1093:LEU:HD21 | 7:5C:1107:LYS:HE2 | 1.98 | 0.45 |
| 2:AD:394:PHE:CD1 | 1:AE:261:PRO:HA | 2.52 | 0.45 |
| 2:AF:372:THR:HA | 2:AF:422:TYR:CE2 | 2.48 | 0.45 |
| 1:BA:60:LYS:HD3 | 1:CA:283:HIS:CD2 | 2.51 | 0.45 |
| 2:BB:220:PRO:HD2 | 1:BC:326:LYS:CE | 2.42 | 0.45 |
| 2:BD:176:SER:CB | 1:BE:349:THR:OG1 | 2.64 | 0.45 |
| 1:BE:147:SER:HB2 | 1:BE:190:SER:HB3 | 1.97 | 0.45 |
| 2:BF:203:ASP:O | 2:BF:207:LEU:HG | 2.17 | 0.45 |
| 1:CA:401:LYS:HE3 | 1:CA:401:LYS:HB2 | 1.74 | 0.45 |
| 2:CB:105:HIS:CE1 | 2:CB:150:LEU:HD12 | 2.52 | 0.45 |
| 1:CC:224:TYR:CE2 | 2:CD:246:LEU:HD11 | 2.48 | 0.45 |
| 2:DD:84:LEU:O | 2:ED:281:TYR:OH | 2.35 | 0.45 |
| 1:DE:401:LYS:HE3 | 1:DE:401:LYS:HB2 | 1.74 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:DF:203:ASP:O | 2:DF:207:LEU:HG | 2.16 | 0.45 |
| 2:EB:102:ALA:HB2 | 2:EB:403:MET:HE3 | 1.99 | 0.45 |
| 2:EB:179:VAL:HG21 | 1:EC:258:ASN:C | 2.31 | 0.45 |
| 2:EB:226:ASN:ND2 | 13:EB:501:GDP:HN1 | 2.12 | 0.45 |
| 1:EE:222:PRO:HG2 | 2:EF:324:LYS:HD3 | 1.93 | 0.45 |
| 2:EF:102:ALA:HB2 | 2:EF:403:MET:HE3 | 1.99 | 0.45 |
| 2:FB:102:ALA:HB2 | 2:FB:403:MET:HE3 | 1.99 | 0.45 |
| 2:FD:102:ALA:HB2 | 2:FD:403:MET:HE3 | 1.99 | 0.45 |
| 1:GC:222:PRO:HD2 | 2:GD:324:LYS:HD3 | 1.99 | 0.45 |
| 2:ID:394:PHE:CD1 | 1:IE:261:PRO:HA | 2.52 | 0.45 |
| 2:IF:203:ASP:O | 2:IF:207:LEU:HG | 2.17 | 0.45 |
| 2:JB:222:TYR:HD2 | 1:JC:247:ALA:HB1 | 1.82 | 0.45 |
| 2:JF:203:ASP:O | 2:JF:207:LEU:HG | 2.17 | 0.45 |
| 2:KD:55:THR:HG21 | 2:LD:363:MET:HE3 | 1.83 | 0.45 |
| 2:KD:394:PHE:CD1 | 1:KE:261:PRO:HA | 2.52 | 0.45 |
| 1:KE:84:ARG:NE | 1:LE:283:HIS:HE1 | 2.10 | 0.45 |
| 2:KF:273:LEU:CB | 6:4D:268:LEU:CD2 | 2.82 | 0.45 |
| 1:LA:188:ILE:HD12 | 1:LA:425:LEU:CD1 | 2.45 | 0.45 |
| 2:LB:178:THR:HA | 1:LC:352:LYS:CD | 2.45 | 0.45 |
| 2:MB:203:ASP:O | 2:MB:207:LEU:HG | 2.17 | 0.45 |
| 2:MD:203:ASP:O | 2:MD:207:LEU:HG | 2.17 | 0.45 |
| 1:ME:147:SER:HB2 | 1:ME:190:SER:HB3 | 1.97 | 0.45 |
| 4:2C:171:VAL:HB | 4:2C:176:ARG:HE | 1.81 | 0.45 |
| 6:4B:101:ARG:NH2 | 6:4B:101:ARG:CG | 2.77 | 0.45 |
| 7:5B:840:GLY:HA3 | 8:6B:109:ILE:HD13 | 0.48 | 0.45 |
| 7:5B:1093:LEU:HD21 | 7:5B:1107:LYS:HE2 | 1.98 | 0.45 |
| 7:5B:1491:LEU:HD13 | 7:5B:1491:LEU:HA | 1.82 | 0.45 |
| 7:5C:826:LEU:O | 7:5C:841:VAL:HG13 | 2.17 | 0.45 |
| 7:5C:1455:LYS:HD2 | 7:5C:1455:LYS:HA | 1.42 | 0.45 |
| 9:7A:2:PHE:HB3 | 9:7A:10:TYR:CE1 | 2.51 | 0.45 |
| 2:BD:226:ASN:ND2 | 13:BD:501:GDP:HN1 | 2.12 | 0.45 |
| 2:CD:105:HIS:CE1 | 2:CD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:CE:32:PRO:HB3 | 1:CE:83:TYR:CE1 | 2.52 | 0.45 |
| 2:CF:102:ALA:HB2 | 2:CF:403:MET:HE3 | 1.99 | 0.45 |
| 1:DA:394:LYS:NZ | 2:DB:347:ASN:OD1 | 2.49 | 0.45 |
| 2:DF:102:ALA:HB2 | 2:DF:403:MET:HE3 | 1.99 | 0.45 |
| 1:EA:404:PHE:CE2 | 2:EB:345:ILE:HD11 | 2.52 | 0.45 |
| 1:EA:430:LYS:HZ2 | 7:5C:834:ASN:ND2 | 0.96 | 0.45 |
| 1:EC:430:LYS:HZ2 | 7:5A:834:ASN:ND2 | 0.95 | 0.45 |
| 1:EE:422:ARG:HE | 7:5B:821:LEU:HD13 | 1.81 | 0.45 |
| 1:FA:181:VAL:CG1 | 2:FB:348:ASN:HA | 2.46 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:FD:105:HIS:CE1 | 2:FD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:FE:420:GLU:HA | 7:5B:1256:ARG:HH22 | 1.81 | 0.45 |
| 2:GB:102:ALA:HB2 | 2:GB:403:MET:HE3 | 1.99 | 0.45 |
| 2:GD:102:ALA:HB2 | 2:GD:403:MET:HE3 | 1.99 | 0.45 |
| 1:GE:89:PRO:HG3 | 1:HE:280:LYS:CD | 2.46 | 0.45 |
| 2:HB:203:ASP:O | 2:HB:207:LEU:HG | 2.17 | 0.45 |
| 1:IA:100:ALA:HB1 | 2:IB:252:LYS:CA | 2.45 | 0.45 |
| 1:IA:279:GLU:N | 10:8V:22:UNK:CB | 2.80 | 0.45 |
| 1:IA:402:ARG:NH2 | 7:5C:1418:GLN:CA | 2.71 | 0.45 |
| 1:IC:268:MET:HB2 | 1:IC:379:SER:O | 2.17 | 0.45 |
| 2:ID:102:ALA:HB2 | 2:ID:403:MET:HE3 | 1.99 | 0.45 |
| 1:JA:88:HIS:ND1 | 1:KA:280:LYS:CD | 2.69 | 0.45 |
| 1:JE:179:THR:O | 2:JF:350:LYS:HA | 2.15 | 0.45 |
| 2:LB:379:LYS:C | 4:2C:166:ILE:HD13 | 2.24 | 0.45 |
| 2:LD:270:PHE:CE2 | 6:4B:226:ILE:CG2 | 2.96 | 0.45 |
| 2:LF:295:ASP:HA | 4:2B:149:ILE:HA | 1.98 | 0.45 |
| 1:ME:178:SER:OG | 2:MF:347:ASN:HB3 | 2.16 | 0.45 |
| 4:2C:16:GLN:O | 4:2C:19:MET:CB | 2.64 | 0.45 |
| 6:4D:110:LYS:HD2 | 6:4D:110:LYS:N | 2.32 | 0.45 |
| 7:5A:943:LEU:HD11 | 7:5A:951:LEU:HD12 | 1.97 | 0.45 |
| 7:5A:1359:ALA:HA | 7:5A:1362:MET:SD | 2.57 | 0.45 |
| 7:5A:1562:LEU:H | 7:5A:1562:LEU:CD1 | 2.11 | 0.45 |
| 7:5B:1366:TRP:CE3 | 7:5B:1366:TRP:N | 2.85 | 0.45 |
| 7:5B:1415:GLU:CD | 7:5B:1415:GLU:C | 2.83 | 0.45 |
| 7:5C:827:GLU:HA | 7:5C:841:VAL:HG13 | 1.98 | 0.45 |
| 7:5C:848:SER:C | 7:5C:850:GLU:N | 2.73 | 0.45 |
| 7:5C:943:LEU:HD11 | 7:5C:951:LEU:HD12 | 1.97 | 0.45 |
| 7:5C:1030:PHE:CZ | 7:5C:1034:ILE:HD11 | 2.50 | 0.45 |
| 7:5C:1359:ALA:HA | 7:5C:1362:MET:SD | 2.57 | 0.45 |
| 9:7C:2:PHE:HB3 | 9:7C:10:TYR:CE1 | 2.51 | 0.45 |
| 9:7E:42:LEU:CD1 | 9:7F:39:GLY:HA3 | 2.47 | 0.45 |
| 1:BC:224:TYR:CE2 | 2:BD:246:LEU:HD11 | 2.49 | 0.45 |
| 1:DA:224:TYR:CE2 | 2:DB:246:LEU:HD11 | 2.47 | 0.45 |
| 2:DD:203:ASP:O | 2:DD:207:LEU:HG | 2.16 | 0.45 |
| 2:DD:220:PRO:HD3 | 1:DE:326:LYS:HE2 | 1.96 | 0.45 |
| 1:EA:179:THR:O | 2:EB:350:LYS:HA | 2.16 | 0.45 |
| 2:ED:102:ALA:HB2 | 2:ED:403:MET:HE3 | 1.99 | 0.45 |
| 2:EF:55:THR:HG23 | 2:FF:283:ALA:C | 2.39 | 0.45 |
| 2:FF:55:THR:OG1 | 2:GF:282:ARG:O | 2.31 | 0.45 |
| 13:GB:501:GDP:C8 | 1:GC:248:LEU:CD1 | 2.99 | 0.45 |
| 2:GF:102:ALA:HB2 | 2:GF:403:MET:HE3 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:HB:105:HIS:CE1 | 2:HB:150:LEU:HD12 | 2.52 | 0.45 |
| 1:HE:32:PRO:HB3 | 1:HE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:IC:222:PRO:HG3 | 2:ID:324:LYS:HD3 | 1.95 | 0.45 |
| 2:ID:212:PHE:CZ | 1:IE:326:LYS:CE | 2.98 | 0.45 |
| 1:IE:389:SER:CB | 5:3A:307:LYS:CD | 2.55 | 0.45 |
| 1:JA:32:PRO:HB3 | 1:JA:83:TYR:CE1 | 2.51 | 0.45 |
| 1:JA:128:ASN:ND2 | 1:KA:285:GLN:NE2 | 2.45 | 0.45 |
| 2:JF:105:HIS:CE1 | 2:JF:150:LEU:HD12 | 2.52 | 0.45 |
| 4:2A:16:GLN:O | 4:2A:19:MET:CB | 2.64 | 0.45 |
| 6:4B:110:LYS:HD2 | 6:4B:110:LYS:N | 2.32 | 0.45 |
| 6:4B:161:LYS:HA | 6:4B:161:LYS:HD3 | 1.78 | 0.45 |
| 6:4C:241:LYS:HD3 | 6:4C:241:LYS:HA | 1.51 | 0.45 |
| 7:5A:826:LEU:O | 7:5A:841:VAL:HG13 | 2.17 | 0.45 |
| 7:5A:1272:ILE:CD1 | 9:7B:11:TYR:CD2 | 2.99 | 0.45 |
| 7:5A:1366:TRP:CE3 | 7:5A:1366:TRP:N | 2.85 | 0.45 |
| 7:5B:1359:ALA:HA | 7:5B:1362:MET:SD | 2.57 | 0.45 |
| 7:5C:1366:TRP:CE3 | 7:5C:1366:TRP:N | 2.85 | 0.45 |
| 7:5C:1412:LYS:HE2 | 7:5C:1416:LYS:CB | 2.47 | 0.45 |
| 7:5C:1488:GLU:O | 7:5C:1491:LEU:HB2 | 2.17 | 0.45 |
| 8:6C:131:ASP:OD1 | 8:6C:134:LYS:N | 2.50 | 0.45 |
| 9:7C:11:TYR:CD1 | 9:7D:23:LEU:CD2 | 3.00 | 0.45 |
| 2:BB:262:ARG:NH1 | 2:BB:421:GLU:OE1 | 2.50 | 0.45 |
| 1:BE:404:PHE:CE2 | 2:BF:345:ILE:HD11 | 2.52 | 0.45 |
| 2:CB:203:ASP:O | 2:CB:207:LEU:HG | 2.17 | 0.45 |
| 2:CD:102:ALA:HB2 | 2:CD:403:MET:HE3 | 1.99 | 0.45 |
| 2:CD:203:ASP:O | 2:CD:207:LEU:HG | 2.16 | 0.45 |
| 1:CE:100:ALA:HB1 | 2:CF:252:LYS:CA | 2.47 | 0.45 |
| 2:CF:203:ASP:O | 2:CF:207:LEU:HG | 2.17 | 0.45 |
| 2:DB:102:ALA:HB2 | 2:DB:403:MET:HE3 | 1.99 | 0.45 |
| 2:DD:87:PRO:HD2 | 2:ED:281:TYR:CE2 | 2.52 | 0.45 |
| 2:DD:102:ALA:HB2 | 2:DD:403:MET:HE3 | 1.99 | 0.45 |
| 2:DD:105:HIS:CE1 | 2:DD:150:LEU:HD12 | 2.52 | 0.45 |
| 1:DE:32:PRO:HB3 | 1:DE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:DE:128:ASN:ND2 | 1:EE:285:GLN:NE2 | 2.64 | 0.45 |
| 2:DF:86:ARG:N | 2:EF:281:TYR:HE1 | 2.09 | 0.45 |
| 2:EB:176:SER:CB | 1:EC:349:THR:OG1 | 2.65 | 0.45 |
| 2:EF:25:SER:HG | 2:EF:51:TYR:HH | 1.58 | 0.45 |
| 1:FA:423:GLU:CG | 7:5C:1256:ARG:NH2 | 2.79 | 0.45 |
| 2:FB:55:THR:HG21 | 2:GB:284:LEU:CB | 2.46 | 0.45 |
| 1:FC:32:PRO:HB3 | 1:FC:83:TYR:CE1 | 2.51 | 0.45 |
| 2:FD:179:VAL:HG12 | 1:FE:350:GLY:C | 2.42 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:FF:102:ALA:HB2 | 2:FF:403:MET:HE3 | 1.99 | 0.45 |
| 2:GB:55:THR:OG1 | 2:HB:283:ALA:HA | 2.14 | 0.45 |
| 1:GE:100:ALA:HB1 | 2:GF:252:LYS:CA | 2.46 | 0.45 |
| 1:HA:32:PRO:HB3 | 1:HA:83:TYR:CE1 | 2.51 | 0.45 |
| 2:HF:203:ASP:O | 2:HF:207:LEU:HG | 2.17 | 0.45 |
| 2:IB:102:ALA:HB2 | 2:IB:403:MET:HE3 | 1.99 | 0.45 |
| 1:IE:268:MET:HB2 | 1:IE:379:SER:O | 2.17 | 0.45 |
| 2:IF:102:ALA:HB2 | 2:IF:403:MET:HE3 | 1.99 | 0.45 |
| 1:JA:100:ALA:HB1 | 2:JB:252:LYS:CA | 2.46 | 0.45 |
| 2:JB:262:ARG:NH1 | 2:JB:421:GLU:OE1 | 2.50 | 0.45 |
| 1:JC:222:PRO:HD2 | 2:JD:324:LYS:HD3 | 1.99 | 0.45 |
| 1:JE:32:PRO:HB3 | 1:JE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:KA:32:PRO:HB3 | 1:KA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:KB:55:THR:CG2 | 2:LB:363:MET:HE3 | 2.30 | 0.45 |
| 2:LB:203:ASP:O | 2:LB:207:LEU:HG | 2.17 | 0.45 |
| 5:3B:21:PHE:CE2 | 5:3B:24:MET:HE2 | 2.52 | 0.45 |
| 6:4A:110:LYS:HD2 | 6:4A:110:LYS:N | 2.32 | 0.45 |
| 6:4B:229:GLU:N | 6:4B:229:GLU:OE1 | 2.50 | 0.45 |
| 6:4D:101:ARG:NH2 | 6:4D:101:ARG:CG | 2.77 | 0.45 |
| 6:4D:229:GLU:N | 6:4D:229:GLU:OE1 | 2.50 | 0.45 |
| 7:5A:1412:LYS:HE2 | 7:5A:1416:LYS:CB | 2.47 | 0.45 |
| 7:5A:1429:GLN:CD | 7:5A:1429:GLN:C | 2.85 | 0.45 |
| 7:5A:1488:GLU:O | 7:5A:1491:LEU:HB2 | 2.17 | 0.45 |
| 7:5B:826:LEU:O | 7:5B:841:VAL:HG13 | 2.17 | 0.45 |
| 7:5B:943:LEU:HD11 | 7:5B:951:LEU:HD12 | 1.97 | 0.45 |
| 7:5B:1412:LYS:HE2 | 7:5B:1416:LYS:CB | 2.47 | 0.45 |
| 7:5B:1429:GLN:CD | 7:5B:1429:GLN:C | 2.85 | 0.45 |
| 7:5C:835:GLN:HE21 | 7:5C:835:GLN:HA | 1.80 | 0.45 |
| 1:AA:71:GLU:HA | 1:AA:72:PRO:HD3 | 1.84 | 0.45 |
| 2:AB:102:ALA:HB2 | 2:AB:403:MET:HE3 | 1.99 | 0.45 |
| 1:AC:340:THR:HG23 | 1:AC:341:ILE:HG13 | 1.99 | 0.45 |
| 1:AE:340:THR:HG23 | 1:AE:341:ILE:HG13 | 1.99 | 0.45 |
| 2:BB:226:ASN:ND2 | 13:BB:501:GDP:HN1 | 2.12 | 0.45 |
| 2:CB:102:ALA:HB2 | 2:CB:403:MET:HE3 | 1.99 | 0.45 |
| 2:CB:391:ARG:HG3 | 1:CC:346:TRP:CD1 | 2.52 | 0.45 |
| 2:CF:105:HIS:CE1 | 2:CF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:DB:84:LEU:C | 2:EB:281:TYR:OH | 2.60 | 0.45 |
| 2:DB:203:ASP:O | 2:DB:207:LEU:HG | 2.16 | 0.45 |
| 1:DE:222:PRO:CG | 2:DF:324:LYS:CD | 2.90 | 0.45 |
| 1:DE:340:THR:HG23 | 1:DE:341:ILE:HG13 | 1.99 | 0.45 |
| 2:ED:177:ASP:HA | 1:EE:353:VAL:HG12 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:EE:71:GLU:OE2 | 1:EE:73:THR:OG1 | 2.28 | 0.45 |
| 2:FB:105:HIS:CE1 | 2:FB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:FB:179:VAL:CG2 | 1:FC:258:ASN:HA | 2.47 | 0.45 |
| 1:FC:268:MET:HB2 | 1:FC:379:SER:O | 2.17 | 0.45 |
| 1:FE:268:MET:HB2 | 1:FE:379:SER:O | 2.17 | 0.45 |
| 1:GC:19:ALA:HA | 1:GC:22:GLU:OE1 | 2.17 | 0.45 |
| 1:GE:19:ALA:HA | 1:GE:22:GLU:OE1 | 2.17 | 0.45 |
| 1:HC:32:PRO:HB3 | 1:HC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:HF:102:ALA:HB2 | 2:HF:403:MET:HE3 | 1.99 | 0.45 |
| 1:IA:268:MET:HB2 | 1:IA:379:SER:O | 2.17 | 0.45 |
| 1:IE:32:PRO:HB3 | 1:IE:83:TYR:CE1 | 2.52 | 0.45 |
| 1:IE:60:LYS:NZ | 1:JE:283:HIS:CE1 | 2.85 | 0.45 |
| 2:IF:105:HIS:CE1 | 2:IF:150:LEU:HD12 | 2.52 | 0.45 |
| 2:JB:102:ALA:HB2 | 2:JB:403:MET:HE3 | 1.99 | 0.45 |
| 2:JD:105:HIS:CE1 | 2:JD:150:LEU:HD12 | 2.52 | 0.45 |
| 2:KB:102:ALA:HB2 | 2:KB:403:MET:HE3 | 1.99 | 0.45 |
| 2:KD:102:ALA:HB2 | 2:KD:403:MET:HE3 | 1.99 | 0.45 |
| 2:KD:262:ARG:NH1 | 2:KD:421:GLU:OE1 | 2.50 | 0.45 |
| 2:KF:102:ALA:HB2 | 2:KF:403:MET:HE3 | 1.99 | 0.45 |
| 1:LA:407:TRP:CE3 | 2:LB:255:VAL:CG1 | 2.75 | 0.45 |
| 2:LD:100:ASN:HB2 | 1:LE:257:THR:HG21 | 1.98 | 0.45 |
| 1:ME:222:PRO:HG2 | 2:MF:324:LYS:HD3 | 1.98 | 0.45 |
| 2:MF:203:ASP:O | 2:MF:207:LEU:HG | 2.17 | 0.45 |
| 5:3A:21:PHE:CE2 | 5:3A:24:MET:HE2 | 2.52 | 0.45 |
| 5:3C:21:PHE:CE2 | 5:3C:24:MET:HE2 | 2.52 | 0.45 |
| 6:4C:110:LYS:HD2 | 6:4C:110:LYS:N | 2.32 | 0.45 |
| 7:5A:1105:TYR:O | 7:5A:1166:LEU:HD12 | 2.16 | 0.45 |
| 7:5A:1152:GLU:OE1 | 8:6A:66:ARG:NH2 | 2.49 | 0.45 |
| 7:5A:1475:PHE:CZ | 7:5A:1565:GLU:OE2 | 2.56 | 0.45 |
| 7:5B:839:GLU:CD | 8:6B:109:ILE:CG1 | 2.86 | 0.45 |
| 7:5B:1459:GLU:CD | 7:5B:1459:GLU:C | 2.85 | 0.45 |
| 7:5C:1429:GLN:CD | 7:5C:1429:GLN:C | 2.85 | 0.45 |
| 7:5C:1490:LYS:HE3 | 7:5C:1494:LEU:HD22 | 1.98 | 0.45 |
| 8:6A:81:GLU:HA | 8:6A:85:GLU:OE1 | 2.15 | 0.45 |
| 8:6A:131:ASP:OD1 | 8:6A:134:LYS:N | 2.50 | 0.45 |
| 8:6B:131:ASP:OD1 | 8:6B:134:LYS:N | 2.50 | 0.45 |
| 1:AA:340:THR:HG23 | 1:AA:341:ILE:HG13 | 1.99 | 0.45 |
| 1:AC:222:PRO:HD2 | 2:AD:324:LYS:HD3 | 1.99 | 0.45 |
| 2:AD:102:ALA:HB2 | 2:AD:403:MET:HE3 | 1.99 | 0.45 |
| 2:AF:262:ARG:NH1 | 2:AF:421:GLU:OE1 | 2.50 | 0.45 |
| 2:BB:98:GLY:CA | 1:BC:254:GLU:CG | 2.56 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:BC:179:THR:O | 2:BD:350:LYS:HA | 2.17 | 0.45 |
| 2:BF:102:ALA:HB2 | 2:BF:403:MET:HE3 | 1.99 | 0.45 |
| 1:CC:179:THR:O | 2:CD:350:LYS:HA | 2.16 | 0.45 |
| 1:CE:340:THR:HG23 | 1:CE:341:ILE:HG13 | 1.99 | 0.45 |
| 2:DB:105:HIS:CE1 | 2:DB:150:LEU:HD12 | 2.52 | 0.45 |
| 1:DC:32:PRO:HB3 | 1:DC:83:TYR:CE1 | 2.52 | 0.45 |
| 1:DC:340:THR:HG23 | 1:DC:341:ILE:HG13 | 1.99 | 0.45 |
| 1:FA:268:MET:HB2 | 1:FA:379:SER:O | 2.17 | 0.45 |
| 1:GC:89:PRO:HG3 | 1:HC:280:LYS:HE3 | 1.98 | 0.45 |
| 2:GF:203:ASP:O | 2:GF:207:LEU:HG | 2.17 | 0.45 |
| 2:GF:262:ARG:NH1 | 2:GF:421:GLU:OE1 | 2.50 | 0.45 |
| 2:HD:102:ALA:HB2 | 2:HD:403:MET:HE3 | 1.99 | 0.45 |
| 2:HD:203:ASP:O | 2:HD:207:LEU:HG | 2.17 | 0.45 |
| 1:HE:268:MET:HB2 | 1:HE:379:SER:O | 2.17 | 0.45 |
| 1:IA:32:PRO:HB3 | 1:IA:83:TYR:CE1 | 2.52 | 0.45 |
| 2:ID:56:GLY:H | 10:8Z:36:UNK:HA | 1.82 | 0.45 |
| 2:IF:262:ARG:NH1 | 2:IF:421:GLU:OE1 | 2.50 | 0.45 |
| 1:JA:222:PRO:CG | 2:JB:324:LYS:CD | 2.91 | 0.45 |
| 1:JA:398:MET:SD | 2:JB:345:ILE:CG1 | 2.90 | 0.45 |
| 2:JB:220:PRO:HD2 | 1:JC:326:LYS:CE | 2.44 | 0.45 |
| 1:JC:32:PRO:HB3 | 1:JC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:JD:220:PRO:HD2 | 1:JE:326:LYS:CE | 2.44 | 0.45 |
| 2:KB:105:HIS:CE1 | 2:KB:150:LEU:HD12 | 2.52 | 0.45 |
| 2:KB:262:ARG:NH1 | 2:KB:421:GLU:OE1 | 2.50 | 0.45 |
| 1:KC:32:PRO:HB3 | 1:KC:83:TYR:CE1 | 2.52 | 0.45 |
| 2:LD:203:ASP:O | 2:LD:207:LEU:HG | 2.17 | 0.45 |
| 2:LD:306:ARG:HH22 | 4:2A:151:VAL:CG2 | 2.08 | 0.45 |
| 2:LF:416:ASN:O | 4:2B:168:LEU:HD12 | 1.94 | 0.45 |
| 2:MB:102:ALA:HB2 | 2:MB:403:MET:HE3 | 1.99 | 0.45 |
| 2:MD:102:ALA:HB2 | 2:MD:403:MET:HE3 | 1.99 | 0.45 |
| 4:2B:16:GLN:O | 4:2B:19:MET:CB | 2.64 | 0.45 |
| 6:4A:229:GLU:N | 6:4A:229:GLU:OE1 | 2.50 | 0.45 |
| 6:4C:206:PHE:O | 6:4C:206:PHE:CD2 | 2.70 | 0.45 |
| 6:4C:229:GLU:N | 6:4C:229:GLU:OE1 | 2.50 | 0.45 |
| 7:5A:1459:GLU:CD | 7:5A:1459:GLU:C | 2.85 | 0.45 |
| 7:5A:1490:LYS:HE3 | 7:5A:1494:LEU:HD22 | 1.98 | 0.45 |
| 7:5B:1488:GLU:O | 7:5B:1491:LEU:HB2 | 2.17 | 0.45 |
| 7:5B:1490:LYS:HE3 | 7:5B:1494:LEU:HD22 | 1.98 | 0.45 |
| 7:5C:1105:TYR:O | 7:5C:1166:LEU:HD12 | 2.16 | 0.45 |
| 7:5C:1543:LEU:C | 7:5C:1573:ARG:CD | 2.90 | 0.45 |
| 9:7E:18:VAL:HG11 | 9:7F:35:ILE:HG23 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:AB:501:GDP:C8 | 1:AC:248:LEU:CD1 | 2.99 | 0.44 |
| 2:AD:262:ARG:NH1 | 2:AD:421:GLU:OE1 | 2.50 | 0.44 |
| 2:AF:54:ALA:HB1 | 2:BF:281:TYR:O | 2.18 | 0.44 |
| 2:AF:102:ALA:HB2 | 2:AF:403:MET:HE3 | 1.99 | 0.44 |
| 1:BA:71:GLU:HA | 1:BA:72:PRO:HD3 | 1.84 | 0.44 |
| 2:BB:102:ALA:HB2 | 2:BB:403:MET:HE3 | 1.99 | 0.44 |
| 2:BD:102:ALA:HB2 | 2:BD:403:MET:HE3 | 1.99 | 0.44 |
| 1:BE:340:THR:HG23 | 1:BE:341:ILE:HG13 | 1.99 | 0.44 |
| 2:CB:391:ARG:HA | 2:CB:391:ARG:HD2 | 1.79 | 0.44 |
| 1:CC:71:GLU:CD | 2:CD:247:ASN:ND2 | 2.75 | 0.44 |
| 1:CC:340:THR:HG23 | 1:CC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:DA:340:THR:HG23 | 1:DA:341:ILE:HG13 | 1.99 | 0.44 |
| 1:EE:19:ALA:HA | 1:EE:22:GLU:OE1 | 2.17 | 0.44 |
| 1:EE:430:LYS:CD | 7:5B:834:ASN:HD22 | 2.23 | 0.44 |
| 1:FA:423:GLU:HG3 | 7:5C:1256:ARG:NH2 | 2.32 | 0.44 |
| 2:FD:179:VAL:CG2 | 1:FE:258:ASN:O | 2.40 | 0.44 |
| 2:GD:262:ARG:NH1 | 2:GD:421:GLU:OE1 | 2.50 | 0.44 |
| 1:GE:60:LYS:HD2 | 1:HE:283:HIS:CG | 2.42 | 0.44 |
| 2:HB:102:ALA:HB2 | 2:HB:403:MET:HE3 | 1.99 | 0.44 |
| 1:HC:268:MET:HB2 | 1:HC:379:SER:O | 2.17 | 0.44 |
| 2:HF:262:ARG:NH1 | 2:HF:421:GLU:OE1 | 2.50 | 0.44 |
| 2:ID:105:HIS:CE1 | 2:ID:150:LEU:HD12 | 2.52 | 0.44 |
| 2:JB:105:HIS:CE1 | 2:JB:150:LEU:HD12 | 2.52 | 0.44 |
| 2:JD:102:ALA:HB2 | 2:JD:403:MET:HE3 | 1.99 | 0.44 |
| 1:JE:100:ALA:HB1 | 2:JF:252:LYS:CA | 2.46 | 0.44 |
| 1:JE:224:TYR:CE2 | 2:JF:246:LEU:HD11 | 2.46 | 0.44 |
| 2:JF:102:ALA:HB2 | 2:JF:403:MET:HE3 | 1.99 | 0.44 |
| 1:KA:79:ARG:C | 1:LA:280:LYS:CE | 2.69 | 0.44 |
| 2:KD:54:ALA:HA | 2:LD:285:THR:HG22 | 1.95 | 0.44 |
| 2:KD:105:HIS:CE1 | 2:KD:150:LEU:HD12 | 2.52 | 0.44 |
| 1:KE:88:HIS:CG | 1:LE:284:GLU:HB2 | 2.52 | 0.44 |
| 2:KF:125:GLU:HA | 4:2B:37:GLY:O | 2.17 | 0.44 |
| 1:LC:100:ALA:O | 2:LD:255:VAL:HG21 | 2.16 | 0.44 |
| 2:LF:55:THR:HG1 | 2:MF:282:ARG:C | 2.13 | 0.44 |
| 2:MB:111:GLU:CB | 3:1A:62:SER:HA | 2.47 | 0.44 |
| 2:MF:262:ARG:NH1 | 2:MF:421:GLU:OE1 | 2.50 | 0.44 |
| 4:2A:12:LEU:HB3 | 4:2A:17:ILE:HG13 | 1.98 | 0.44 |
| 5:3A:230:ILE:HG21 | 5:3A:332:MET:SD | 2.54 | 0.44 |
| 6:4A:206:PHE:O | 6:4A:206:PHE:CD2 | 2.70 | 0.44 |
| 7:5A:1543:LEU:C | 7:5A:1573:ARG:CD | 2.90 | 0.44 |
| 7:5B:1253:ILE:CD1 | 7:5B:1261:ALA:HB1 | 2.47 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5B:1543:LEU:C | 7:5B:1573:ARG:CD | 2.90 | 0.44 |
| 7:5B:1572:LEU:HG | 7:5B:1576:ILE:HD11 | 1.93 | 0.44 |
| 7:5C:826:LEU:C | 7:5C:840:GLY:O | 2.60 | 0.44 |
| 7:5C:846:PHE:CD1 | 7:5C:846:PHE:O | 2.70 | 0.44 |
| 7:5C:1459:GLU:CD | 7:5C:1459:GLU:C | 2.85 | 0.44 |
| 2:AD:55:THR:CG2 | 2:BD:283:ALA:CA | 2.76 | 0.44 |
| 1:BA:268:MET:HB2 | 1:BA:379:SER:O | 2.17 | 0.44 |
| 1:BA:398:MET:SD | 2:BB:345:ILE:CG1 | 2.90 | 0.44 |
| 1:BC:340:THR:HG23 | 1:BC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:BE:394:LYS:NZ | 2:BF:347:ASN:OD1 | 2.51 | 0.44 |
| 1:CA:340:THR:HG23 | 1:CA:341:ILE:HG13 | 1.99 | 0.44 |
| 1:DA:32:PRO:HB3 | 1:DA:83:TYR:CE1 | 2.52 | 0.44 |
| 1:DC:402:ARG:CD | 7:5A:777:ALA:HB1 | 2.46 | 0.44 |
| 1:EA:19:ALA:HA | 1:EA:22:GLU:OE1 | 2.17 | 0.44 |
| 1:EA:268:MET:HB2 | 1:EA:379:SER:O | 2.17 | 0.44 |
| 1:EA:340:THR:HG23 | 1:EA:341:ILE:HG13 | 1.99 | 0.44 |
| 1:EC:19:ALA:HA | 1:EC:22:GLU:OE1 | 2.17 | 0.44 |
| 1:EC:340:THR:HG23 | 1:EC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:EE:181:VAL:HG12 | 2:EF:348:ASN:HA | 1.99 | 0.44 |
| 2:EF:391:ARG:HA | 2:EF:391:ARG:HD2 | 1.79 | 0.44 |
| 1:FA:340:THR:HG23 | 1:FA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:FB:58:ARG:HD3 | 2:GB:280:GLN:O | 2.17 | 0.44 |
| 2:FB:384:GLN:HB3 | 1:FC:348:PRO:HG2 | 1.99 | 0.44 |
| 2:FD:106:TYR:HA | 7:5A:1294:ILE:HG21 | 1.24 | 0.44 |
| 2:FD:179:VAL:HG22 | 1:FE:258:ASN:CB | 2.48 | 0.44 |
| 1:FE:401:LYS:HE3 | 1:FE:401:LYS:HB2 | 1.74 | 0.44 |
| 1:GA:222:PRO:CG | 2:GB:324:LYS:CD | 2.91 | 0.44 |
| 2:HB:55:THR:HG23 | 2:IB:283:ALA:CB | 2.47 | 0.44 |
| 1:HC:19:ALA:HA | 1:HC:22:GLU:OE1 | 2.17 | 0.44 |
| 1:HE:19:ALA:HA | 1:HE:22:GLU:OE1 | 2.17 | 0.44 |
| 1:HE:176:GLN:O | 2:HF:347:ASN:ND2 | 2.40 | 0.44 |
| 1:IC:32:PRO:HB3 | 1:IC:83:TYR:CE1 | 2.52 | 0.44 |
| 2:ID:87:PRO:HD2 | 2:JD:281:TYR:CD2 | 2.52 | 0.44 |
| 2:ID:262:ARG:NH1 | 2:ID:421:GLU:OE1 | 2.50 | 0.44 |
| 1:JA:268:MET:HB2 | 1:JA:379:SER:O | 2.17 | 0.44 |
| 1:LA:176:GLN:HG3 | 4:2C:42:PHE:CD1 | 2.52 | 0.44 |
| 2:LD:102:ALA:HB2 | 2:LD:403:MET:HE3 | 1.99 | 0.44 |
| 2:LF:102:ALA:HB2 | 2:LF:403:MET:HE3 | 1.99 | 0.44 |
| 1:MA:282:TYR:CE1 | 6:4C:98:PRO:HB3 | 2.51 | 0.44 |
| 1:MC:340:THR:HG23 | 1:MC:341:ILE:HG13 | 1.99 | 0.44 |
| 2:MF:79:GLY:C | 6:4D:179:ARG:CD | 2.90 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:MF:102:ALA:HB2 | 2:MF:403:MET:HE3 | 1.99 | 0.44 |
| 4:2B:12:LEU:HB3 | 4:2B:17:ILE:HG13 | 1.98 | 0.44 |
| 5:3B:230:ILE:HG21 | 5:3B:332:MET:SD | 2.54 | 0.44 |
| 5:3C:230:ILE:HG21 | 5:3C:332:MET:SD | 2.54 | 0.44 |
| 6:4A:161:LYS:HA | 6:4A:161:LYS:HD3 | 1.78 | 0.44 |
| 6:4B:206:PHE:O | 6:4B:206:PHE:CD2 | 2.71 | 0.44 |
| 6:4D:206:PHE:O | 6:4D:206:PHE:CD2 | 2.70 | 0.44 |
| 6:4D:239:LEU:HD13 | 6:4D:239:LEU:HA | 1.83 | 0.44 |
| 7:5A:826:LEU:C | 7:5A:840:GLY:O | 2.60 | 0.44 |
| 7:5A:1253:ILE:CD1 | 7:5A:1261:ALA:HB1 | 2.47 | 0.44 |
| 7:5B:846:PHE:O | 7:5B:846:PHE:CG | 2.69 | 0.44 |
| 7:5B:1079:PHE:CZ | 7:5B:1164:GLN:HG2 | 2.52 | 0.44 |
| 7:5B:1105:TYR:O | 7:5B:1166:LEU:HD12 | 2.16 | 0.44 |
| 7:5C:1253:ILE:CD1 | 7:5C:1261:ALA:HB1 | 2.47 | 0.44 |
| 7:5C:1416:LYS:HD3 | 7:5C:1416:LYS:C | 2.42 | 0.44 |
| 7:5C:1475:PHE:CZ | 7:5C:1565:GLU:OE2 | 2.56 | 0.44 |
| 7:5C:1577:LYS:HA | 7:5C:1577:LYS:HD2 | 1.80 | 0.44 |
| 2:AB:262:ARG:NH1 | 2:AB:421:GLU:OE1 | 2.50 | 0.44 |
| 1:AC:268:MET:HB2 | 1:AC:379:SER:O | 2.17 | 0.44 |
| 1:BC:268:MET:HB2 | 1:BC:379:SER:O | 2.17 | 0.44 |
| 1:BE:60:LYS:NZ | 1:CE:283:HIS:CE1 | 2.85 | 0.44 |
| 1:CE:268:MET:HB2 | 1:CE:379:SER:O | 2.17 | 0.44 |
| 1:DA:128:ASN:HD21 | 1:EA:285:GLN:NE2 | 2.16 | 0.44 |
| 2:DB:20:PHE:O | 2:DB:24:ILE:HG12 | 2.18 | 0.44 |
| 1:DC:100:ALA:HB1 | 2:DD:252:LYS:CA | 2.48 | 0.44 |
| 1:DC:398:MET:SD | 2:DD:345:ILE:CG1 | 2.92 | 0.44 |
| 1:DC:404:PHE:CE2 | 2:DD:345:ILE:HD11 | 2.53 | 0.44 |
| 2:DD:20:PHE:O | 2:DD:24:ILE:HG12 | 2.18 | 0.44 |
| 1:EC:268:MET:HB2 | 1:EC:379:SER:O | 2.17 | 0.44 |
| 1:EC:393:HIS:ND1 | 7:5A:814:LYS:CG | 2.81 | 0.44 |
| 1:EE:340:THR:HG23 | 1:EE:341:ILE:HG13 | 1.99 | 0.44 |
| 1:GA:19:ALA:HA | 1:GA:22:GLU:OE1 | 2.17 | 0.44 |
| 2:GD:203:ASP:O | 2:GD:207:LEU:HG | 2.17 | 0.44 |
| 1:HC:100:ALA:HB1 | 2:HD:252:LYS:CA | 2.47 | 0.44 |
| 2:HF:226:ASN:ND2 | 13:HF:501:GDP:HN1 | 2.12 | 0.44 |
| 2:IB:105:HIS:CE1 | 2:IB:150:LEU:HD12 | 2.52 | 0.44 |
| 1:IC:279:GLU:CD | 10:8W:22:UNK:HA | 2.42 | 0.44 |
| 1:JC:128:ASN:HA | 1:KC:285:GLN:HE22 | 1.82 | 0.44 |
| 1:JC:268:MET:HB2 | 1:JC:379:SER:O | 2.17 | 0.44 |
| 1:KA:248:LEU:HD12 | 1:KA:248:LEU:HA | 1.89 | 0.44 |
| 2:KB:127:CYS:N | 4:2C:38:VAL:HB | 1.94 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:KD:28:HIS:C | 2:KD:43:GLN:HE21 | 2.26 | 0.44 |
| 1:KE:32:PRO:HB3 | 1:KE:83:TYR:CE1 | 2.52 | 0.44 |
| 2:KF:105:HIS:CE1 | 2:KF:150:LEU:HD12 | 2.52 | 0.44 |
| 2:LB:102:ALA:HB2 | 2:LB:403:MET:HE3 | 1.99 | 0.44 |
| 2:LD:55:THR:OG1 | 2:MD:283:ALA:HA | 2.17 | 0.44 |
| 2:LF:203:ASP:O | 2:LF:207:LEU:HG | 2.17 | 0.44 |
| 2:LF:262:ARG:NH1 | 2:LF:421:GLU:OE1 | 2.50 | 0.44 |
| 1:MC:224:TYR:CE2 | 2:MD:246:LEU:HD11 | 2.45 | 0.44 |
| 1:ME:11:GLN:HE22 | 2:MF:246:LEU:HA | 1.82 | 0.44 |
| 1:ME:340:THR:HG23 | 1:ME:341:ILE:HG13 | 1.99 | 0.44 |
| 4:2C:12:LEU:HB3 | 4:2C:17:ILE:HG13 | 1.98 | 0.44 |
| 6:4D:243:ASP:HB3 | 6:4D:247:LYS:HD2 | 1.68 | 0.44 |
| 7:5A:846:PHE:CD1 | 7:5A:846:PHE:O | 2.70 | 0.44 |
| 7:5A:1079:PHE:CZ | 7:5A:1164:GLN:HG2 | 2.52 | 0.44 |
| 7:5A:1416:LYS:NZ | 7:5A:1419:GLU:HB3 | 2.32 | 0.44 |
| 7:5B:1120:ASP:HB2 | 7:5B:1125:LEU:HD12 | 1.98 | 0.44 |
| 7:5B:1373:PHE:HA | 7:5B:1376:GLN:HG3 | 1.98 | 0.44 |
| 7:5C:1079:PHE:CZ | 7:5C:1164:GLN:HG2 | 2.52 | 0.44 |
| 8:6B:81:GLU:HA | 8:6B:85:GLU:OE1 | 2.15 | 0.44 |
| 1:AE:268:MET:HB2 | 1:AE:379:SER:O | 2.17 | 0.44 |
| 1:BA:340:THR:HG23 | 1:BA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:BB:20:PHE:O | 2:BB:24:ILE:HG12 | 2.18 | 0.44 |
| 2:BF:20:PHE:O | 2:BF:24:ILE:HG12 | 2.18 | 0.44 |
| 2:CB:28:HIS:C | 2:CB:43:GLN:HE21 | 2.26 | 0.44 |
| 1:CE:60:LYS:CE | 1:DE:283:HIS:CD2 | 3.01 | 0.44 |
| 1:CE:407:TRP:CZ3 | 2:CF:255:VAL:O | 2.31 | 0.44 |
| 2:CF:28:HIS:C | 2:CF:43:GLN:HE21 | 2.26 | 0.44 |
| 1:DC:60:LYS:HD3 | 1:EC:283:HIS:HD2 | 1.14 | 0.44 |
| 1:EA:60:LYS:HD3 | 1:FA:283:HIS:HA | 1.99 | 0.44 |
| 1:EE:268:MET:HB2 | 1:EE:379:SER:O | 2.17 | 0.44 |
| 1:FA:19:ALA:HA | 1:FA:22:GLU:OE1 | 2.17 | 0.44 |
| 1:FA:32:PRO:HB3 | 1:FA:83:TYR:CE1 | 2.52 | 0.44 |
| 2:FD:332:ASN:CG | 7:5A:909:ASN:ND2 | 2.73 | 0.44 |
| 2:FD:391:ARG:HD2 | 2:FD:391:ARG:HA | 1.79 | 0.44 |
| 1:FE:420:GLU:HA | 7:5B:1256:ARG:NH2 | 2.33 | 0.44 |
| 1:GA:268:MET:HB2 | 1:GA:379:SER:O | 2.17 | 0.44 |
| 1:GA:340:THR:HG23 | 1:GA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:GB:262:ARG:NH1 | 2:GB:421:GLU:OE1 | 2.50 | 0.44 |
| 1:GC:268:MET:HB2 | 1:GC:379:SER:O | 2.17 | 0.44 |
| 1:GC:340:THR:HG23 | 1:GC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:GE:340:THR:HG23 | 1:GE:341:ILE:HG13 | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:HA:268:MET:HB2 | 1:HA:379:SER:O | 2.17 | 0.44 |
| 2:HD:262:ARG:NH1 | 2:HD:421:GLU:OE1 | 2.50 | 0.44 |
| 1:HE:282:TYR:CE1 | 10:8U:15:UNK:CA | 2.97 | 0.44 |
| 2:IB:86:ARG:HD3 | 2:JB:281:TYR:HB3 | 1.51 | 0.44 |
| 2:IB:262:ARG:NH1 | 2:IB:421:GLU:OE1 | 2.50 | 0.44 |
| 1:IC:222:PRO:HD2 | 2:ID:324:LYS:HD3 | 1.99 | 0.44 |
| 13:ID:501:GDP:C8 | 1:IE:248:LEU:CD1 | 3.00 | 0.44 |
| 1:IE:19:ALA:HA | 1:IE:22:GLU:OE1 | 2.17 | 0.44 |
| 2:JB:177:ASP:CG | 1:JC:353:VAL:HG13 | 1.99 | 0.44 |
| 1:JC:279:GLU:OE1 | 10:8Z:22:UNK:CA | 2.64 | 0.44 |
| 1:LA:19:ALA:HA | 1:LA:22:GLU:OE1 | 2.17 | 0.44 |
| 2:LB:179:VAL:HG21 | 1:LC:258:ASN:CA | 2.46 | 0.44 |
| 1:LE:340:THR:HG23 | 1:LE:341:ILE:HG13 | 1.99 | 0.44 |
| 1:MA:340:THR:HG23 | 1:MA:341:ILE:HG13 | 1.99 | 0.44 |
| 6:4B:265:TYR:CD2 | 6:4B:265:TYR:O | 2.70 | 0.44 |
| 6:4C:265:TYR:CD2 | 6:4C:265:TYR:O | 2.70 | 0.44 |
| 7:5A:846:PHE:O | 7:5A:846:PHE:CG | 2.69 | 0.44 |
| 7:5A:907:PHE:CE2 | 7:5A:921:HIS:HD2 | 2.35 | 0.44 |
| 7:5A:1148:PHE:CZ | 7:5A:1150:ILE:HG22 | 2.52 | 0.44 |
| 7:5A:1416:LYS:HD3 | 7:5A:1416:LYS:C | 2.42 | 0.44 |
| 7:5A:1439:GLU:CD | 7:5A:1439:GLU:C | 2.86 | 0.44 |
| 7:5A:1455:LYS:HD2 | 7:5A:1455:LYS:HA | 1.42 | 0.44 |
| 7:5A:1572:LEU:HG | 7:5A:1576:ILE:HD11 | 1.92 | 0.44 |
| 7:5B:826:LEU:C | 7:5B:840:GLY:O | 2.60 | 0.44 |
| 7:5B:907:PHE:CE2 | 7:5B:921:HIS:HD2 | 2.35 | 0.44 |
| 7:5B:1148:PHE:CZ | 7:5B:1150:ILE:HG22 | 2.52 | 0.44 |
| 7:5B:1347:LEU:HD13 | 7:5B:1347:LEU:H | 1.81 | 0.44 |
| 7:5B:1416:LYS:NZ | 7:5B:1419:GLU:HB3 | 2.32 | 0.44 |
| 7:5B:1416:LYS:HD3 | 7:5B:1416:LYS:C | 2.42 | 0.44 |
| 7:5B:1436:ARG:HG3 | 7:5B:1436:ARG:NH1 | 2.30 | 0.44 |
| 7:5B:1531:TYR:HB2 | 7:5B:1541:ILE:HD11 | 1.99 | 0.44 |
| 7:5B:1562:LEU:H | 7:5B:1562:LEU:CD1 | 2.11 | 0.44 |
| 7:5C:841:VAL:N | 8:6C:109:ILE:CD1 | 2.44 | 0.44 |
| 7:5C:1148:PHE:CZ | 7:5C:1150:ILE:HG22 | 2.52 | 0.44 |
| 7:5C:1416:LYS:NZ | 7:5C:1419:GLU:HB3 | 2.32 | 0.44 |
| 7:5C:1439:GLU:CD | 7:5C:1439:GLU:C | 2.86 | 0.44 |
| 9:7A:11:TYR:CD1 | 9:7B:23:LEU:CD2 | 3.00 | 0.44 |
| 1:AC:19:ALA:HA | 1:AC:22:GLU:OE1 | 2.17 | 0.44 |
| 1:AC:386:GLU:CD | 3:1C:76:ARG:NH2 | 2.75 | 0.44 |
| 1:BA:19:ALA:HA | 1:BA:22:GLU:OE1 | 2.17 | 0.44 |
| 1:BA:100:ALA:HB1 | 2:BB:252:LYS:CA | 2.48 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:BD:20:PHE:O | 2:BD:24:ILE:HG12 | 2.18 | 0.44 |
| 1:BE:268:MET:HB2 | 1:BE:379:SER:O | 2.17 | 0.44 |
| 1:CC:268:MET:HB2 | 1:CC:379:SER:O | 2.17 | 0.44 |
| 1:CC:401:LYS:HE3 | 1:CC:401:LYS:HB2 | 1.74 | 0.44 |
| 2:CD:28:HIS:C | 2:CD:43:GLN:HE21 | 2.26 | 0.44 |
| 2:DF:20:PHE:O | 2:DF:24:ILE:HG12 | 2.18 | 0.44 |
| 2:EF:262:ARG:NH1 | 2:EF:421:GLU:OE1 | 2.50 | 0.44 |
| 2:FB:394:PHE:CE2 | 1:FC:258:ASN:C | 2.95 | 0.44 |
| 1:FC:340:THR:HG23 | 1:FC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:FE:340:THR:HG23 | 1:FE:341:ILE:HG13 | 1.99 | 0.44 |
| 2:GB:203:ASP:O | 2:GB:207:LEU:HG | 2.16 | 0.44 |
| 1:GE:268:MET:HB2 | 1:GE:379:SER:O | 2.17 | 0.44 |
| 1:HA:60:LYS:HZ2 | 1:IA:283:HIS:CD2 | 2.35 | 0.44 |
| 2:HB:262:ARG:NH1 | 2:HB:421:GLU:OE1 | 2.50 | 0.44 |
| 1:HC:415:GLU:CB | 5:3C:235:LEU:HB2 | 2.45 | 0.44 |
| 1:JC:19:ALA:HA | 1:JC:22:GLU:OE1 | 2.17 | 0.44 |
| 13:JD:501:GDP:C8 | 1:JE:248:LEU:CD1 | 3.00 | 0.44 |
| 1:JE:19:ALA:HA | 1:JE:22:GLU:OE1 | 2.17 | 0.44 |
| 1:KA:268:MET:HB2 | 1:KA:379:SER:O | 2.17 | 0.44 |
| 1:KA:340:THR:HG23 | 1:KA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:KB:28:HIS:C | 2:KB:43:GLN:HE21 | 2.26 | 0.44 |
| 1:KC:87:PHE:C | 1:LC:283:HIS:O | 2.58 | 0.44 |
| 1:KC:248:LEU:HD12 | 1:KC:248:LEU:HA | 1.89 | 0.44 |
| 1:KC:268:MET:HB2 | 1:KC:379:SER:O | 2.17 | 0.44 |
| 1:KC:340:THR:HG23 | 1:KC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:KE:340:THR:HG23 | 1:KE:341:ILE:HG13 | 1.99 | 0.44 |
| 2:KF:28:HIS:C | 2:KF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:KF:276:ARG:HH21 | 6:4D:265:TYR:C | 2.23 | 0.44 |
| 1:MA:164:LYS:HA | 1:MA:164:LYS:HD3 | 1.85 | 0.44 |
| 2:MB:179:VAL:CG2 | 1:MC:258:ASN:O | 2.40 | 0.44 |
| 2:MB:179:VAL:HG22 | 1:MC:258:ASN:CB | 2.48 | 0.44 |
| 1:MC:19:ALA:HA | 1:MC:22:GLU:OE1 | 2.17 | 0.44 |
| 2:MD:262:ARG:NH1 | 2:MD:421:GLU:OE1 | 2.50 | 0.44 |
| 2:MF:28:HIS:C | 2:MF:43:GLN:HE21 | 2.26 | 0.44 |
| 4:2B:144:ASN:ND2 | 4:2B:144:ASN:H | 2.15 | 0.44 |
| 6:4A:145:PHE:CD2 | 6:4A:145:PHE:O | 2.70 | 0.44 |
| 6:4A:265:TYR:CD2 | 6:4A:265:TYR:O | 2.70 | 0.44 |
| 6:4C:145:PHE:O | 6:4C:145:PHE:CD2 | 2.70 | 0.44 |
| 6:4D:116:THR:HA | 6:4D:119:ASN:ND2 | 2.32 | 0.44 |
| 6:4D:265:TYR:CD2 | 6:4D:265:TYR:O | 2.70 | 0.44 |
| 7:5A:1120:ASP:HB2 | 7:5A:1125:LEU:HD12 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5A:1532:PRO:HG2 | 7:5A:1608:ASN:HD21 | 1.83 | 0.44 |
| 7:5B:1439:GLU:CD | 7:5B:1439:GLU:C | 2.86 | 0.44 |
| 7:5B:1532:PRO:HG2 | 7:5B:1608:ASN:HD21 | 1.83 | 0.44 |
| 7:5C:1531:TYR:HB2 | 7:5C:1541:ILE:HD11 | 1.99 | 0.44 |
| 1:AA:268:MET:HB2 | 1:AA:379:SER:O | 2.17 | 0.44 |
| 2:AB:222:TYR:HD2 | 1:AC:247:ALA:HB1 | 1.82 | 0.44 |
| 1:AE:19:ALA:HA | 1:AE:22:GLU:OE1 | 2.17 | 0.44 |
| 1:AE:280:LYS:CE | 2:MB:86:ARG:HH21 | 2.30 | 0.44 |
| 2:BB:415:MET:O | 2:BB:419:VAL:HG23 | 2.18 | 0.44 |
| 1:BC:19:ALA:HA | 1:BC:22:GLU:OE1 | 2.17 | 0.44 |
| 2:BD:415:MET:O | 2:BD:419:VAL:HG23 | 2.18 | 0.44 |
| 1:BE:19:ALA:HA | 1:BE:22:GLU:OE1 | 2.17 | 0.44 |
| 2:BF:55:THR:HG23 | 2:CF:283:ALA:HA | 2.00 | 0.44 |
| 1:CA:100:ALA:HB1 | 2:CB:252:LYS:CA | 2.48 | 0.44 |
| 1:DE:19:ALA:HA | 1:DE:22:GLU:OE1 | 2.17 | 0.44 |
| 1:EC:71:GLU:OE2 | 1:EC:73:THR:OG1 | 2.28 | 0.44 |
| 2:FB:20:PHE:O | 2:FB:24:ILE:HG12 | 2.18 | 0.44 |
| 2:FB:28:HIS:C | 2:FB:43:GLN:HE21 | 2.26 | 0.44 |
| 1:FC:19:ALA:HA | 1:FC:22:GLU:OE1 | 2.17 | 0.44 |
| 1:FC:423:GLU:OE2 | 7:5A:1256:ARG:NH1 | 2.47 | 0.44 |
| 2:FD:388:MET:HA | 1:FE:346:TRP:O | 2.17 | 0.44 |
| 2:FF:226:ASN:ND2 | 13:FF:501:GDP:HN1 | 2.12 | 0.44 |
| 2:GB:379:LYS:HZ1 | 7:5C:1316:LEU:HD11 | 1.82 | 0.44 |
| 2:GB:415:MET:O | 2:GB:419:VAL:HG23 | 2.18 | 0.44 |
| 2:GD:415:MET:O | 2:GD:419:VAL:HG23 | 2.18 | 0.44 |
| 2:GF:415:MET:O | 2:GF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:HA:340:THR:HG23 | 1:HA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:HB:20:PHE:O | 2:HB:24:ILE:HG12 | 2.18 | 0.44 |
| 2:HD:20:PHE:O | 2:HD:24:ILE:HG12 | 2.18 | 0.44 |
| 2:HD:226:ASN:ND2 | 13:HD:501:GDP:HN1 | 2.12 | 0.44 |
| 1:IC:19:ALA:HA | 1:IC:22:GLU:OE1 | 2.17 | 0.44 |
| 2:ID:28:HIS:C | 2:ID:43:GLN:HE21 | 2.26 | 0.44 |
| 2:IF:28:HIS:C | 2:IF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:IF:55:THR:HB | 10:9A:36:UNK:O | 2.17 | 0.44 |
| 1:JA:340:THR:HG23 | 1:JA:341:ILE:HG13 | 1.99 | 0.44 |
| 1:JC:340:THR:HG23 | 1:JC:341:ILE:HG13 | 1.99 | 0.44 |
| 2:JD:28:HIS:C | 2:JD:43:GLN:HE21 | 2.26 | 0.44 |
| 2:JD:415:MET:O | 2:JD:419:VAL:HG23 | 2.18 | 0.44 |
| 1:JE:340:THR:HG23 | 1:JE:341:ILE:HG13 | 1.99 | 0.44 |
| 2:JF:415:MET:O | 2:JF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:KA:224:TYR:CE2 | 2:KB:246:LEU:HD11 | 2.44 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:KC:100:ALA:HB1 | 2:KD:252:LYS:CA | 2.47 | 0.44 |
| 2:KD:55:THR:H | 2:LD:285:THR:HG22 | 1.82 | 0.44 |
| 2:KD:126:GLY:C | 4:2A:39:ALA:H | 2.26 | 0.44 |
| 2:KD:215:LEU:HD12 | 6:4B:267:ILE:HG22 | 1.85 | 0.44 |
| 1:KE:127:ASP:OD2 | 1:LE:334:THR:HG23 | 2.17 | 0.44 |
| 1:LA:340:THR:HG23 | 1:LA:341:ILE:HG13 | 1.99 | 0.44 |
| 2:LB:379:LYS:O | 4:2C:166:ILE:HD13 | 2.17 | 0.44 |
| 2:LB:391:ARG:HA | 2:LB:391:ARG:HD2 | 1.79 | 0.44 |
| 2:LB:415:MET:O | 2:LB:419:VAL:HG23 | 2.18 | 0.44 |
| 2:LD:262:ARG:NH1 | 2:LD:421:GLU:OE1 | 2.50 | 0.44 |
| 1:MA:19:ALA:HA | 1:MA:22:GLU:OE1 | 2.17 | 0.44 |
| 1:ME:19:ALA:HA | 1:ME:22:GLU:OE1 | 2.17 | 0.44 |
| 1:ME:268:MET:HB2 | 1:ME:379:SER:O | 2.17 | 0.44 |
| 4:2A:144:ASN:ND2 | 4:2A:144:ASN:H | 2.15 | 0.44 |
| 4:2B:129:GLU:OE2 | 4:2B:135:LYS:HD3 | 2.17 | 0.44 |
| 4:2C:144:ASN:ND2 | 4:2C:144:ASN:H | 2.15 | 0.44 |
| 6:4A:260:ARG:HH22 | 6:4A:295:LYS:CE | 2.31 | 0.44 |
| 6:4B:145:PHE:O | 6:4B:145:PHE:CD2 | 2.70 | 0.44 |
| 7:5A:1347:LEU:HD13 | 7:5A:1347:LEU:H | 1.81 | 0.44 |
| 7:5A:1373:PHE:HA | 7:5A:1376:GLN:HG3 | 1.98 | 0.44 |
| 7:5A:1531:TYR:HB2 | 7:5A:1541:ILE:HD11 | 1.99 | 0.44 |
| 7:5B:846:PHE:O | 7:5B:846:PHE:CD1 | 2.70 | 0.44 |
| 7:5B:1268:LEU:CD2 | 9:7D:19:LEU:HD13 | 2.47 | 0.44 |
| 7:5C:846:PHE:O | 7:5C:846:PHE:CG | 2.69 | 0.44 |
| 7:5C:907:PHE:CE2 | 7:5C:921:HIS:HD2 | 2.35 | 0.44 |
| 7:5C:1589:LEU:HG | 7:5C:1595:LEU:HD12 | 1.99 | 0.44 |
| 2:AF:356:ILE:HD12 | 6:4A:152:PHE:HD1 | 1.75 | 0.44 |
| 1:CA:268:MET:HB2 | 1:CA:379:SER:O | 2.17 | 0.44 |
| 2:CB:415:MET:O | 2:CB:419:VAL:HG23 | 2.18 | 0.44 |
| 1:DA:268:MET:HB2 | 1:DA:379:SER:O | 2.17 | 0.44 |
| 1:DC:19:ALA:HA | 1:DC:22:GLU:OE1 | 2.17 | 0.44 |
| 2:EB:86:ARG:HA | 2:FB:281:TYR:CZ | 2.52 | 0.44 |
| 2:ED:28:HIS:C | 2:ED:43:GLN:HE21 | 2.26 | 0.44 |
| 2:ED:262:ARG:NH1 | 2:ED:421:GLU:OE1 | 2.50 | 0.44 |
| 1:EE:221:ARG:NH1 | 2:EF:324:LYS:N | 2.66 | 0.44 |
| 2:EF:28:HIS:C | 2:EF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:FB:332:ASN:CG | 7:5C:909:ASN:OD1 | 2.61 | 0.44 |
| 2:FB:391:ARG:HA | 2:FB:391:ARG:HD2 | 1.79 | 0.44 |
| 2:FD:20:PHE:O | 2:FD:24:ILE:HG12 | 2.18 | 0.44 |
| 2:FD:28:HIS:C | 2:FD:43:GLN:HE21 | 2.26 | 0.44 |
| 2:FD:177:ASP:OD1 | 1:FE:353:VAL:HG12 | 1.87 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:FD:178:THR:HA | 1:FE:352:LYS:CD | 2.48 | 0.44 |
| 1:FE:19:ALA:HA | 1:FE:22:GLU:OE1 | 2.17 | 0.44 |
| 2:FF:20:PHE:O | 2:FF:24:ILE:HG12 | 2.18 | 0.44 |
| 1:HA:19:ALA:HA | 1:HA:22:GLU:OE1 | 2.17 | 0.44 |
| 1:HC:222:PRO:HD2 | 2:HD:324:LYS:HD3 | 1.99 | 0.44 |
| 1:HE:370:LYS:NZ | 10:8U:16:UNK:CB | 2.81 | 0.44 |
| 2:HF:20:PHE:O | 2:HF:24:ILE:HG12 | 2.18 | 0.44 |
| 2:IB:28:HIS:C | 2:IB:43:GLN:HE21 | 2.26 | 0.44 |
| 2:IB:391:ARG:HA | 2:IB:391:ARG:HD2 | 1.79 | 0.44 |
| 1:IC:340:THR:HG23 | 1:IC:341:ILE:HG13 | 1.99 | 0.44 |
| 2:ID:178:THR:HA | 1:IE:352:LYS:CD | 2.48 | 0.44 |
| 1:IE:340:THR:HG23 | 1:IE:341:ILE:HG13 | 1.99 | 0.44 |
| 2:IF:424:GLN:HE21 | 7:5B:1413:GLN:CG | 2.25 | 0.44 |
| 2:JB:28:HIS:C | 2:JB:43:GLN:HE21 | 2.26 | 0.44 |
| 1:JC:222:PRO:HG3 | 2:JD:324:LYS:HD3 | 1.95 | 0.44 |
| 2:KB:415:MET:O | 2:KB:419:VAL:HG23 | 2.18 | 0.44 |
| 1:KC:84:ARG:CZ | 1:LC:283:HIS:NE2 | 2.81 | 0.44 |
| 2:KD:415:MET:O | 2:KD:419:VAL:HG23 | 2.18 | 0.44 |
| 13:KD:501:GDP:C8 | 1:KE:248:LEU:CD1 | 3.00 | 0.44 |
| 2:LB:340:TYR:CB | 4:2C:147:PHE:CB | 2.77 | 0.44 |
| 1:LC:19:ALA:HA | 1:LC:22:GLU:OE1 | 2.17 | 0.44 |
| 1:LC:340:THR:HG23 | 1:LC:341:ILE:HG13 | 1.99 | 0.44 |
| 1:LC:407:TRP:CE3 | 2:LD:255:VAL:CG1 | 2.76 | 0.44 |
| 2:LD:177:ASP:O | 1:LE:352:LYS:HA | 2.17 | 0.44 |
| 2:LD:415:MET:O | 2:LD:419:VAL:HG23 | 2.18 | 0.44 |
| 1:LE:19:ALA:HA | 1:LE:22:GLU:OE1 | 2.17 | 0.44 |
| 2:LF:20:PHE:O | 2:LF:24:ILE:HG12 | 2.18 | 0.44 |
| 2:LF:415:MET:O | 2:LF:419:VAL:HG23 | 2.18 | 0.44 |
| 2:MB:78:ALA:HB1 | 6:4A:178:HIS:NE2 | 2.31 | 0.44 |
| 2:MB:262:ARG:NH1 | 2:MB:421:GLU:OE1 | 2.50 | 0.44 |
| 2:MD:28:HIS:C | 2:MD:43:GLN:HE21 | 2.26 | 0.44 |
| 4:2C:129:GLU:OE2 | 4:2C:135:LYS:HD3 | 2.17 | 0.44 |
| 6:4A:222:PRO:HG2 | 6:4A:235:ALA:O | 2.18 | 0.44 |
| 6:4B:116:THR:HA | 6:4B:119:ASN:ND2 | 2.32 | 0.44 |
| 6:4B:222:PRO:HG2 | 6:4B:235:ALA:O | 2.18 | 0.44 |
| 6:4B:260:ARG:HH22 | 6:4B:295:LYS:CE | 2.31 | 0.44 |
| 6:4C:260:ARG:HH22 | 6:4C:295:LYS:CE | 2.31 | 0.44 |
| 6:4D:222:PRO:HG2 | 6:4D:235:ALA:O | 2.18 | 0.44 |
| 7:5A:1436:ARG:HG3 | 7:5A:1436:ARG:NH1 | 2.30 | 0.44 |
| 7:5B:1589:LEU:HG | 7:5B:1595:LEU:HD12 | 1.99 | 0.44 |
| 7:5C:1120:ASP:HB2 | 7:5C:1125:LEU:HD12 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5C:1373:PHE:HA | 7:5C:1376:GLN:HG3 | 1.98 | 0.44 |
| 7:5C:1532:PRO:HG2 | 7:5C:1608:ASN:HD21 | 1.83 | 0.44 |
| 1:AA:19:ALA:HA | 1:AA:22:GLU:OE1 | 2.17 | 0.44 |
| 2:AD:280:GLN:HE22 | 6:4C:141:LYS:HB3 | 1.77 | 0.44 |
| 2:AD:390:ARG:HD2 | 1:AE:439:THR:HG21 | 2.00 | 0.44 |
| 2:BF:415:MET:O | 2:BF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:CA:394:LYS:NZ | 2:CB:347:ASN:OD1 | 2.51 | 0.44 |
| 1:CC:68:LEU:HD22 | 1:CC:153:LEU:HD11 | 2.00 | 0.44 |
| 1:CC:221:ARG:NH1 | 2:CD:324:LYS:N | 2.66 | 0.44 |
| 2:CF:415:MET:O | 2:CF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:DC:268:MET:HB2 | 1:DC:379:SER:O | 2.17 | 0.44 |
| 1:DE:68:LEU:HD22 | 1:DE:153:LEU:HD11 | 2.00 | 0.44 |
| 1:DE:100:ALA:HB1 | 2:DF:252:LYS:CA | 2.48 | 0.44 |
| 1:DE:268:MET:HB2 | 1:DE:379:SER:O | 2.17 | 0.44 |
| 2:EB:28:HIS:C | 2:EB:43:GLN:HE21 | 2.26 | 0.44 |
| 2:EB:55:THR:HG23 | 2:FB:284:LEU:H | 1.81 | 0.44 |
| 1:EC:179:THR:O | 2:ED:350:LYS:HA | 2.17 | 0.44 |
| 2:EF:157:GLU:HA | 7:5B:945:LYS:HZ1 | 1.80 | 0.44 |
| 2:EF:415:MET:O | 2:EF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:FA:96:LYS:HE2 | 2:FB:1:MET:HE3 | 2.00 | 0.44 |
| 2:FB:106:TYR:HA | 7:5C:1294:ILE:HG21 | 1.25 | 0.44 |
| 2:FD:226:ASN:ND2 | 13:FD:502:GDP:HN1 | 2.12 | 0.44 |
| 2:FF:28:HIS:C | 2:FF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:FF:106:TYR:HA | 7:5B:1294:ILE:HG21 | 1.28 | 0.44 |
| 2:GB:222:TYR:HD2 | 1:GC:247:ALA:HB1 | 1.82 | 0.44 |
| 2:HB:415:MET:O | 2:HB:419:VAL:HG23 | 2.18 | 0.44 |
| 1:HC:340:THR:HG23 | 1:HC:341:ILE:HG13 | 1.99 | 0.44 |
| 13:HD:501:GDP:C8 | 1:HE:248:LEU:CD1 | 3.00 | 0.44 |
| 1:HE:68:LEU:HD22 | 1:HE:153:LEU:HD11 | 2.00 | 0.44 |
| 1:IC:409:VAL:HG21 | 7:5A:1421:PHE:HZ | 1.82 | 0.44 |
| 2:JB:415:MET:O | 2:JB:419:VAL:HG23 | 2.18 | 0.44 |
| 2:JF:28:HIS:C | 2:JF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:KD:125:GLU:CD | 2:LD:336:LYS:NZ | 2.54 | 0.44 |
| 2:KD:178:THR:HA | 1:KE:352:LYS:CD | 2.48 | 0.44 |
| 2:KD:179:VAL:HG23 | 1:KE:258:ASN:HA | 1.97 | 0.44 |
| 1:LA:268:MET:HB2 | 1:LA:379:SER:O | 2.17 | 0.44 |
| 2:LB:20:PHE:O | 2:LB:24:ILE:HG12 | 2.18 | 0.44 |
| 2:LB:28:HIS:C | 2:LB:43:GLN:HE21 | 2.26 | 0.44 |
| 2:LB:262:ARG:NH1 | 2:LB:421:GLU:OE1 | 2.50 | 0.44 |
| 1:LC:68:LEU:HD22 | 1:LC:153:LEU:HD11 | 2.00 | 0.44 |
| 2:LD:20:PHE:O | 2:LD:24:ILE:HG12 | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LE:268:MET:HB2 | 1:LE:379:SER:O | 2.17 | 0.44 |
| 2:LF:28:HIS:C | 2:LF:43:GLN:HE21 | 2.26 | 0.44 |
| 2:MB:28:HIS:C | 2:MB:43:GLN:HE21 | 2.26 | 0.44 |
| 1:MC:101:ASN:HA | 1:MC:144:GLY:H | 1.83 | 0.44 |
| 4:2A:129:GLU:OE2 | 4:2A:135:LYS:HD3 | 2.18 | 0.44 |
| 4:2B:112:GLU:OE2 | 4:2B:123:LYS:NZ | 2.50 | 0.44 |
| 6:4D:145:PHE:O | 6:4D:145:PHE:CD2 | 2.70 | 0.44 |
| 6:4D:260:ARG:HH22 | 6:4D:295:LYS:CE | 2.31 | 0.44 |
| 7:5A:1152:GLU:CD | 8:6A:66:ARG:NH2 | 2.76 | 0.44 |
| 7:5A:1577:LYS:HA | 7:5A:1577:LYS:HD2 | 1.80 | 0.44 |
| 7:5A:1589:LEU:HG | 7:5A:1595:LEU:HD12 | 1.99 | 0.44 |
| 7:5B:1119:LEU:CD1 | 7:5B:1135:TYR:CE1 | 3.00 | 0.44 |
| 7:5C:1246:LEU:HG | 9:7F:12:GLU:CG | 2.48 | 0.44 |
| 7:5C:1400:GLU:N | 7:5C:1400:GLU:OE2 | 2.51 | 0.44 |
| 7:5C:1562:LEU:H | 7:5C:1562:LEU:CD1 | 2.11 | 0.44 |
| 7:5C:1572:LEU:HG | 7:5C:1576:ILE:HD11 | 1.93 | 0.44 |
| 8:6A:64:LEU:HG | 8:6A:247:ILE:CD1 | 2.48 | 0.44 |
| 8:6B:64:LEU:HG | 8:6B:247:ILE:CD1 | 2.48 | 0.44 |
| 9:7E:39:GLY:HA3 | 9:7F:43:LEU:CD2 | 2.47 | 0.44 |
| 2:AB:390:ARG:HD2 | 1:AC:439:THR:HG21 | 2.00 | 0.44 |
| 1:AC:100:ALA:HB1 | 2:AD:252:LYS:CA | 2.47 | 0.44 |
| 2:AF:415:MET:O | 2:AF:419:VAL:HG23 | 2.18 | 0.44 |
| 2:BF:28:HIS:C | 2:BF:43:GLN:HE21 | 2.26 | 0.44 |
| 1:CA:68:LEU:HD22 | 1:CA:153:LEU:HD11 | 2.00 | 0.44 |
| 2:CD:415:MET:O | 2:CD:419:VAL:HG23 | 2.18 | 0.44 |
| 1:CE:68:LEU:HD22 | 1:CE:153:LEU:HD11 | 2.00 | 0.44 |
| 2:CF:262:ARG:NH1 | 2:CF:421:GLU:OE1 | 2.50 | 0.44 |
| 2:FB:415:MET:O | 2:FB:419:VAL:HG23 | 2.18 | 0.44 |
| 2:FF:391:ARG:HD2 | 2:FF:391:ARG:HA | 1.79 | 0.44 |
| 2:GB:390:ARG:HD2 | 1:GC:439:THR:HG21 | 2.00 | 0.44 |
| 2:GF:412:GLU:OE2 | 7:5B:1323:MET:HE2 | 2.15 | 0.44 |
| 2:HB:390:ARG:HD2 | 1:HC:439:THR:HG21 | 2.00 | 0.44 |
| 2:HD:178:THR:HA | 1:HE:352:LYS:CD | 2.48 | 0.44 |
| 1:HE:224:TYR:CE2 | 2:HF:246:LEU:HD11 | 2.46 | 0.44 |
| 1:IC:100:ALA:HB1 | 2:ID:252:LYS:CA | 2.47 | 0.44 |
| 1:IC:101:ASN:HA | 1:IC:144:GLY:H | 1.83 | 0.44 |
| 2:ID:424:GLN:HE22 | 7:5A:1413:GLN:NE2 | 0.56 | 0.44 |
| 2:JB:390:ARG:HD2 | 1:JC:439:THR:HG21 | 2.00 | 0.44 |
| 1:JC:101:ASN:HA | 1:JC:144:GLY:H | 1.83 | 0.44 |
| 1:JE:268:MET:HB2 | 1:JE:379:SER:O | 2.17 | 0.44 |
| 1:KA:88:HIS:HD1 | 1:KA:90:GLU:H | 1.64 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KC:101:ASN:HA | 1:KC:144:GLY:H | 1.83 | 0.44 |
| 2:KD:77:ARG:CD | 2:LD:281:TYR:CE2 | 3.01 | 0.44 |
| 1:KE:88:HIS:HD1 | 1:KE:90:GLU:H | 1.64 | 0.44 |
| 1:KE:101:ASN:HA | 1:KE:144:GLY:H | 1.83 | 0.44 |
| 1:KE:268:MET:HB2 | 1:KE:379:SER:O | 2.17 | 0.44 |
| 2:KF:415:MET:O | 2:KF:419:VAL:HG23 | 2.18 | 0.44 |
| 1:LA:68:LEU:HD22 | 1:LA:153:LEU:HD11 | 2.00 | 0.44 |
| 1:LA:176:GLN:NE2 | 4:2C:42:PHE:HB2 | 2.25 | 0.44 |
| 1:LC:268:MET:HB2 | 1:LC:379:SER:O | 2.17 | 0.44 |
| 2:LD:28:HIS:C | 2:LD:43:GLN:HE21 | 2.26 | 0.44 |
| 1:LE:68:LEU:HD22 | 1:LE:153:LEU:HD11 | 2.00 | 0.44 |
| 2:MB:20:PHE:O | 2:MB:24:ILE:HG12 | 2.18 | 0.44 |
| 2:MD:20:PHE:O | 2:MD:24:ILE:HG12 | 2.18 | 0.44 |
| 1:ME:101:ASN:HA | 1:ME:144:GLY:H | 1.83 | 0.44 |
| 2:MF:20:PHE:O | 2:MF:24:ILE:HG12 | 2.18 | 0.44 |
| 5:3B:64:ASN:CG | 5:3B:93:LYS:HE2 | 2.43 | 0.44 |
| 6:4A:116:THR:HA | 6:4A:119:ASN:ND2 | 2.32 | 0.44 |
| 6:4D:230:TYR:CD2 | 6:4D:230:TYR:N | 2.74 | 0.44 |
| 6:4D:263:CYS:HB3 | 6:4D:265:TYR:CE1 | 2.53 | 0.44 |
| 7:5A:1400:GLU:N | 7:5A:1400:GLU:OE2 | 2.51 | 0.44 |
| 7:5A:1532:PRO:HG2 | 7:5A:1608:ASN:ND2 | 2.33 | 0.44 |
| 7:5B:1400:GLU:N | 7:5B:1400:GLU:OE2 | 2.51 | 0.44 |
| 7:5B:1532:PRO:HG2 | 7:5B:1608:ASN:ND2 | 2.33 | 0.44 |
| 7:5B:1535:ILE:CG1 | 7:5B:1574:ILE:C | 2.86 | 0.44 |
| 7:5C:1283:ALA:O | 7:5C:1284:PHE:CG | 2.70 | 0.44 |
| 2:AD:322:SER:N | 6:4C:156:PHE:CD2 | 2.85 | 0.43 |
| 2:BB:212:PHE:CE2 | 1:BC:326:LYS:HB2 | 2.53 | 0.43 |
| 2:BD:28:HIS:C | 2:BD:43:GLN:HE21 | 2.26 | 0.43 |
| 1:CA:19:ALA:HA | 1:CA:22:GLU:OE1 | 2.17 | 0.43 |
| 2:CD:262:ARG:NH1 | 2:CD:421:GLU:OE1 | 2.50 | 0.43 |
| 1:CE:171:ILE:HG23 | 1:CE:204:LEU:O | 2.18 | 0.43 |
| 1:DA:19:ALA:HA | 1:DA:22:GLU:OE1 | 2.17 | 0.43 |
| 1:DA:68:LEU:HD22 | 1:DA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:DC:68:LEU:HD22 | 1:DC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:EB:208:TYR:CE2 | 1:EC:326:LYS:HB3 | 2.52 | 0.43 |
| 2:ED:212:PHE:HE2 | 1:EE:326:LYS:HB2 | 1.82 | 0.43 |
| 2:ED:415:MET:O | 2:ED:419:VAL:HG23 | 2.18 | 0.43 |
| 1:EE:68:LEU:HD22 | 1:EE:153:LEU:HD11 | 2.00 | 0.43 |
| 2:FD:384:GLN:HB3 | 1:FE:348:PRO:HG2 | 1.98 | 0.43 |
| 1:HA:68:LEU:HD22 | 1:HA:153:LEU:HD11 | 2.00 | 0.43 |
| 2:HD:99:ASN:HA | 2:HD:142:GLY:H | 1.83 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:HD:362:LYS:HD3 | 10:8T:36:UNK:O | 2.18 | 0.43 |
| 2:HD:415:MET:O | 2:HD:419:VAL:HG23 | 2.18 | 0.43 |
| 1:HE:340:THR:HG23 | 1:HE:341:ILE:HG13 | 1.99 | 0.43 |
| 1:IA:19:ALA:HA | 1:IA:22:GLU:OE1 | 2.17 | 0.43 |
| 1:IA:224:TYR:CE2 | 2:IB:246:LEU:HD11 | 2.44 | 0.43 |
| 1:IA:340:THR:HG23 | 1:IA:341:ILE:HG13 | 1.99 | 0.43 |
| 1:IE:248:LEU:HD12 | 1:IE:248:LEU:HA | 1.89 | 0.43 |
| 1:JA:19:ALA:HA | 1:JA:22:GLU:OE1 | 2.17 | 0.43 |
| 1:JC:68:LEU:HD22 | 1:JC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:JD:99:ASN:HA | 2:JD:142:GLY:H | 1.83 | 0.43 |
| 1:JE:68:LEU:HD22 | 1:JE:153:LEU:HD11 | 2.00 | 0.43 |
| 1:JE:89:PRO:HD3 | 1:KE:283:HIS:NE2 | 2.22 | 0.43 |
| 1:JE:101:ASN:HA | 1:JE:144:GLY:H | 1.83 | 0.43 |
| 1:JE:398:MET:SD | 2:JF:345:ILE:CG1 | 2.92 | 0.43 |
| 1:KA:68:LEU:HD22 | 1:KA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:KA:101:ASN:HA | 1:KA:144:GLY:H | 1.84 | 0.43 |
| 2:KB:178:THR:HA | 1:KC:352:LYS:CD | 2.48 | 0.43 |
| 1:KC:88:HIS:HD1 | 1:KC:90:GLU:H | 1.65 | 0.43 |
| 1:KC:124:LYS:CD | 1:LC:290:GLU:HA | 2.47 | 0.43 |
| 2:KD:125:GLU:O | 4:2A:39:ALA:N | 2.50 | 0.43 |
| 1:KE:19:ALA:HA | 1:KE:22:GLU:OE1 | 2.17 | 0.43 |
| 1:KE:68:LEU:HD22 | 1:KE:153:LEU:HD11 | 2.00 | 0.43 |
| 2:LB:99:ASN:HA | 2:LB:142:GLY:H | 1.83 | 0.43 |
| 2:LF:391:ARG:HA | 2:LF:391:ARG:HD2 | 1.78 | 0.43 |
| 1:MC:268:MET:HB2 | 1:MC:379:SER:O | 2.17 | 0.43 |
| 2:MF:391:ARG:HA | 2:MF:391:ARG:HD2 | 1.79 | 0.43 |
| 2:MF:415:MET:O | 2:MF:419:VAL:HG23 | 2.18 | 0.43 |
| 6:4A:263:CYS:HB3 | 6:4A:265:TYR:CE1 | 2.53 | 0.43 |
| 6:4B:263:CYS:HB3 | 6:4B:265:TYR:CE1 | 2.53 | 0.43 |
| 6:4C:193:MET:HE3 | 6:4C:193:MET:HB3 | 1.83 | 0.43 |
| 6:4C:222:PRO:HG2 | 6:4C:235:ALA:O | 2.18 | 0.43 |
| 7:5A:1042:LEU:HD11 | 7:5A:1053:LYS:HD2 | 2.00 | 0.43 |
| 7:5A:1283:ALA:O | 7:5A:1284:PHE:CG | 2.70 | 0.43 |
| 7:5C:1042:LEU:HD11 | 7:5C:1053:LYS:HD2 | 2.00 | 0.43 |
| 7:5C:1126:PRO:CG | 8:6C:246:TYR:HH | 2.29 | 0.43 |
| 7:5C:1347:LEU:HD13 | 7:5C:1347:LEU:H | 1.81 | 0.43 |
| 7:5C:1399:LYS:HB3 | 7:5C:1399:LYS:HE3 | 1.66 | 0.43 |
| 7:5C:1532:PRO:HG2 | 7:5C:1608:ASN:ND2 | 2.33 | 0.43 |
| 1:AA:181:VAL:HG21 | 2:AB:256:ASN:O | 2.18 | 0.43 |
| 2:AD:99:ASN:HA | 2:AD:142:GLY:H | 1.84 | 0.43 |
| 2:AD:415:MET:O | 2:AD:419:VAL:HG23 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:BA:171:ILE:HG23 | 1:BA:204:LEU:O | 2.18 | 0.43 |
| 2:BB:28:HIS:C | 2:BB:43:GLN:HE21 | 2.26 | 0.43 |
| 2:BD:208:TYR:CD2 | 1:BE:326:LYS:HB3 | 2.53 | 0.43 |
| 1:CA:171:ILE:HG23 | 1:CA:204:LEU:O | 2.18 | 0.43 |
| 1:CC:171:ILE:HG23 | 1:CC:204:LEU:O | 2.18 | 0.43 |
| 1:DC:179:THR:O | 2:DD:350:LYS:HA | 2.18 | 0.43 |
| 2:EB:262:ARG:NH1 | 2:EB:421:GLU:OE1 | 2.50 | 0.43 |
| 2:ED:391:ARG:HA | 2:ED:391:ARG:HD2 | 1.79 | 0.43 |
| 1:FA:221:ARG:HH11 | 2:FB:325:GLU:H | 1.66 | 0.43 |
| 1:FC:401:LYS:HE3 | 1:FC:401:LYS:HB2 | 1.74 | 0.43 |
| 2:FF:106:TYR:O | 7:5B:1298:LYS:CD | 2.65 | 0.43 |
| 1:GC:171:ILE:HG23 | 1:GC:204:LEU:O | 2.18 | 0.43 |
| 13:GD:501:GDP:C8 | 1:GE:248:LEU:CD1 | 3.00 | 0.43 |
| 1:HC:68:LEU:HD22 | 1:HC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:HD:28:HIS:C | 2:HD:43:GLN:HE21 | 2.26 | 0.43 |
| 2:HD:261:PRO:CG | 5:3C:337:ARG:NH2 | 2.68 | 0.43 |
| 1:HE:415:GLU:HG3 | 5:3A:235:LEU:CG | 2.47 | 0.43 |
| 2:HF:28:HIS:C | 2:HF:43:GLN:HE21 | 2.26 | 0.43 |
| 1:IA:101:ASN:HA | 1:IA:144:GLY:H | 1.84 | 0.43 |
| 1:IE:101:ASN:HA | 1:IE:144:GLY:H | 1.83 | 0.43 |
| 1:JA:68:LEU:HD22 | 1:JA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:JA:181:VAL:HG21 | 2:JB:256:ASN:O | 2.18 | 0.43 |
| 2:JD:176:SER:HG | 1:JE:349:THR:HG1 | 1.61 | 0.43 |
| 1:KC:68:LEU:HD22 | 1:KC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:KD:86:ARG:CG | 2:LD:288:GLU:CD | 2.91 | 0.43 |
| 2:KD:212:PHE:CZ | 1:KE:326:LYS:CE | 2.98 | 0.43 |
| 1:KE:248:LEU:HD12 | 1:KE:248:LEU:HA | 1.89 | 0.43 |
| 1:LA:176:GLN:HE22 | 4:2C:42:PHE:HB2 | 1.80 | 0.43 |
| 2:LD:19:LYS:NZ | 6:4B:217:ASN:O | 2.49 | 0.43 |
| 2:LD:99:ASN:HA | 2:LD:142:GLY:H | 1.83 | 0.43 |
| 1:LE:89:PRO:CB | 1:ME:280:LYS:HZ2 | 2.31 | 0.43 |
| 1:MA:101:ASN:HA | 1:MA:144:GLY:H | 1.84 | 0.43 |
| 2:MD:415:MET:O | 2:MD:419:VAL:HG23 | 2.18 | 0.43 |
| 4:2A:112:GLU:OE2 | 4:2A:123:LYS:NZ | 2.50 | 0.43 |
| 4:2C:112:GLU:OE2 | 4:2C:123:LYS:NZ | 2.50 | 0.43 |
| 6:4C:97:GLN:HA | 6:4C:98:PRO:HD3 | 1.58 | 0.43 |
| 6:4C:116:THR:HA | 6:4C:119:ASN:ND2 | 2.32 | 0.43 |
| 6:4C:263:CYS:HB3 | 6:4C:265:TYR:CE1 | 2.53 | 0.43 |
| 7:5A:1119:LEU:CD1 | 7:5A:1135:TYR:CE1 | 3.00 | 0.43 |
| 7:5B:1042:LEU:HD11 | 7:5B:1053:LYS:HD2 | 2.00 | 0.43 |
| 7:5B:1283:ALA:O | 7:5B:1284:PHE:CG | 2.70 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:1424:GLN:NE2 | 7:5B:1424:GLN:C | 2.73 | 0.43 |
| 7:5B:1455:LYS:HD2 | 7:5B:1455:LYS:HA | 1.42 | 0.43 |
| 7:5C:1442:GLN:CD | 7:5C:1442:GLN:C | 2.86 | 0.43 |
| 9:7C:18:VAL:HG12 | 9:7C:42:LEU:HD21 | 1.95 | 0.43 |
| 2:AB:99:ASN:HA | 2:AB:142:GLY:H | 1.84 | 0.43 |
| 1:AC:101:ASN:HA | 1:AC:144:GLY:H | 1.83 | 0.43 |
| 1:AE:68:LEU:HD22 | 1:AE:153:LEU:HD11 | 2.00 | 0.43 |
| 2:AF:99:ASN:HA | 2:AF:142:GLY:H | 1.84 | 0.43 |
| 1:BC:171:ILE:HG23 | 1:BC:204:LEU:O | 2.18 | 0.43 |
| 1:CC:60:LYS:HD3 | 1:DC:283:HIS:CD2 | 2.53 | 0.43 |
| 1:CC:100:ALA:HB1 | 2:CD:252:LYS:CA | 2.48 | 0.43 |
| 2:CD:179:VAL:HG22 | 1:CE:258:ASN:CB | 2.48 | 0.43 |
| 2:DB:28:HIS:C | 2:DB:43:GLN:HE21 | 2.26 | 0.43 |
| 2:DF:415:MET:O | 2:DF:419:VAL:HG23 | 2.18 | 0.43 |
| 2:EB:55:THR:H | 2:FB:283:ALA:HA | 1.83 | 0.43 |
| 2:EB:415:MET:O | 2:EB:419:VAL:HG23 | 2.18 | 0.43 |
| 2:FB:226:ASN:ND2 | 13:FB:502:GDP:HN1 | 2.12 | 0.43 |
| 1:FC:68:LEU:HD22 | 1:FC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:FD:415:MET:O | 2:FD:419:VAL:HG23 | 2.18 | 0.43 |
| 1:GA:404:PHE:CE2 | 2:GB:345:ILE:HD11 | 2.54 | 0.43 |
| 2:GF:28:HIS:C | 2:GF:43:GLN:HE21 | 2.26 | 0.43 |
| 2:HB:99:ASN:HA | 2:HB:142:GLY:H | 1.84 | 0.43 |
| 2:HB:178:THR:HA | 1:HC:352:LYS:CD | 2.49 | 0.43 |
| 2:HB:226:ASN:ND2 | 13:HB:501:GDP:HN1 | 2.12 | 0.43 |
| 2:HD:68:LEU:HD12 | 2:HD:68:LEU:HA | 1.90 | 0.43 |
| 2:HF:99:ASN:HA | 2:HF:142:GLY:H | 1.84 | 0.43 |
| 1:IA:404:PHE:CE2 | 2:IB:345:ILE:HD11 | 2.54 | 0.43 |
| 2:IB:178:THR:HA | 1:IC:352:LYS:CD | 2.49 | 0.43 |
| 2:IB:390:ARG:HD2 | 1:IC:439:THR:HG21 | 2.00 | 0.43 |
| 2:IF:86:ARG:HD3 | 2:JF:281:TYR:HB3 | 1.37 | 0.43 |
| 1:JA:101:ASN:HA | 1:JA:144:GLY:H | 1.84 | 0.43 |
| 2:JB:99:ASN:HA | 2:JB:142:GLY:H | 1.84 | 0.43 |
| 2:JD:20:PHE:O | 2:JD:24:ILE:HG12 | 2.18 | 0.43 |
| 2:JD:178:THR:HA | 1:JE:352:LYS:CD | 2.48 | 0.43 |
| 2:JF:20:PHE:O | 2:JF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:JF:68:LEU:HD12 | 2:JF:68:LEU:HA | 1.90 | 0.43 |
| 2:JF:99:ASN:HA | 2:JF:142:GLY:H | 1.84 | 0.43 |
| 1:KA:124:LYS:HD2 | 1:LA:290:GLU:HA | 1.98 | 0.43 |
| 1:KA:401:LYS:HE3 | 1:KA:401:LYS:HB2 | 1.74 | 0.43 |
| 2:KD:159:TYR:HE2 | 4:2A:35:VAL:O | 1.94 | 0.43 |
| 1:KE:359:PRO:CG | 6:4B:299:TYR:CD2 | 2.90 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:LB:19:LYS:NZ | 6:4A:217:ASN:O | 2.51 | 0.43 |
| 2:LF:99:ASN:HA | 2:LF:142:GLY:H | 1.84 | 0.43 |
| 1:MA:171:ILE:HG23 | 1:MA:204:LEU:O | 2.18 | 0.43 |
| 2:MB:232:ALA:HB1 | 2:MB:268:ILE:HD12 | 2.00 | 0.43 |
| 1:MC:171:ILE:HG23 | 1:MC:204:LEU:O | 2.18 | 0.43 |
| 1:MC:357:TYR:CE1 | 6:4A:185:ARG:NH1 | 2.85 | 0.43 |
| 2:MD:179:VAL:HG23 | 1:ME:258:ASN:HA | 1.98 | 0.43 |
| 3:1C:33:ASP:HB3 | 3:1C:39:MET:SD | 2.58 | 0.43 |
| 5:3A:64:ASN:CG | 5:3A:93:LYS:HE2 | 2.43 | 0.43 |
| 5:3C:231:THR:N | 5:3C:335:LYS:HD2 | 1.73 | 0.43 |
| 6:4C:161:LYS:HA | 6:4C:161:LYS:HD3 | 1.78 | 0.43 |
| 7:5A:1271:ILE:HD13 | 9:7A:23:LEU:HD12 | 2.00 | 0.43 |
| 7:5B:1442:GLN:CD | 7:5B:1442:GLN:C | 2.86 | 0.43 |
| 7:5C:1119:LEU:CD1 | 7:5C:1135:TYR:CE1 | 3.00 | 0.43 |
| 8:6A:14:ARG:NH2 | 8:6A:89:ILE:O | 2.52 | 0.43 |
| 8:6C:64:LEU:HG | 8:6C:247:ILE:CD1 | 2.48 | 0.43 |
| 9:7E:18:VAL:HG12 | 9:7E:42:LEU:HD21 | 1.95 | 0.43 |
| 1:AA:401:LYS:HE3 | 1:AA:401:LYS:HB2 | 1.74 | 0.43 |
| 2:AB:232:ALA:HB1 | 2:AB:268:ILE:HD12 | 2.00 | 0.43 |
| 2:AD:212:PHE:CZ | 1:AE:326:LYS:CE | 2.98 | 0.43 |
| 2:AD:232:ALA:HB1 | 2:AD:268:ILE:HD12 | 2.00 | 0.43 |
| 13:AD:501:GDP:C8 | 1:AE:248:LEU:CD1 | 3.00 | 0.43 |
| 1:AE:101:ASN:HA | 1:AE:144:GLY:H | 1.83 | 0.43 |
| 1:BC:404:PHE:CE2 | 2:BD:345:ILE:HD11 | 2.54 | 0.43 |
| 1:CC:19:ALA:HA | 1:CC:22:GLU:OE1 | 2.17 | 0.43 |
| 1:CC:407:TRP:CZ3 | 2:CD:255:VAL:O | 2.32 | 0.43 |
| 2:CD:99:ASN:HA | 2:CD:142:GLY:H | 1.84 | 0.43 |
| 1:CE:394:LYS:NZ | 2:CF:347:ASN:OD1 | 2.52 | 0.43 |
| 2:CF:99:ASN:HA | 2:CF:142:GLY:H | 1.84 | 0.43 |
| 2:DB:212:PHE:CE2 | 1:DC:326:LYS:HB2 | 2.52 | 0.43 |
| 1:EA:68:LEU:HD22 | 1:EA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:EA:426:ALA:CB | 7:5C:833:PHE:CG | 2.97 | 0.43 |
| 2:EB:54:ALA:HB2 | 2:FB:281:TYR:O | 2.16 | 0.43 |
| 2:EB:390:ARG:CD | 1:EC:439:THR:HG21 | 2.48 | 0.43 |
| 1:EC:68:LEU:HD22 | 1:EC:153:LEU:HD11 | 2.00 | 0.43 |
| 1:EC:430:LYS:HZ2 | 7:5A:834:ASN:HB2 | 1.79 | 0.43 |
| 1:FA:423:GLU:HG3 | 7:5C:1256:ARG:HH21 | 1.83 | 0.43 |
| 2:FB:99:ASN:HA | 2:FB:142:GLY:H | 1.84 | 0.43 |
| 1:FE:68:LEU:HD22 | 1:FE:153:LEU:HD11 | 2.00 | 0.43 |
| 1:FE:401:LYS:CE | 2:FF:344:TRP:CZ3 | 2.80 | 0.43 |
| 1:GA:171:ILE:HG23 | 1:GA:204:LEU:O | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:GA:181:VAL:HG21 | 2:GB:256:ASN:O | 2.18 | 0.43 |
| 2:GD:28:HIS:C | 2:GD:43:GLN:HE21 | 2.26 | 0.43 |
| 2:HB:28:HIS:C | 2:HB:43:GLN:HE21 | 2.26 | 0.43 |
| 2:HD:390:ARG:HD2 | 1:HE:439:THR:HG21 | 2.00 | 0.43 |
| 2:HF:415:MET:O | 2:HF:419:VAL:HG23 | 2.18 | 0.43 |
| 1:IE:60:LYS:HZ3 | 1:JE:283:HIS:CD2 | 2.31 | 0.43 |
| 1:IE:164:LYS:HA | 1:IE:164:LYS:HD3 | 1.85 | 0.43 |
| 1:JA:278:ALA:O | 10:8Y:18:UNK:O | 2.37 | 0.43 |
| 2:JB:20:PHE:O | 2:JB:24:ILE:HG12 | 2.18 | 0.43 |
| 2:JB:55:THR:HG21 | 2:KB:362:LYS:HZ3 | 0.60 | 0.43 |
| 2:JB:86:ARG:NH1 | 2:KB:280:GLN:CB | 2.64 | 0.43 |
| 2:JB:391:ARG:HA | 2:JB:391:ARG:HD2 | 1.78 | 0.43 |
| 1:JC:124:LYS:HD3 | 1:KC:284:GLU:OE1 | 2.18 | 0.43 |
| 1:JC:171:ILE:HG23 | 1:JC:204:LEU:O | 2.18 | 0.43 |
| 2:JD:390:ARG:HD2 | 1:JE:439:THR:HG21 | 2.00 | 0.43 |
| 1:JE:171:ILE:HG23 | 1:JE:204:LEU:O | 2.18 | 0.43 |
| 2:JF:226:ASN:ND2 | 13:JF:501:GDP:HN1 | 2.12 | 0.43 |
| 1:KA:404:PHE:CE2 | 2:KB:345:ILE:HD11 | 2.54 | 0.43 |
| 2:KB:390:ARG:HD2 | 1:KC:439:THR:HG21 | 2.00 | 0.43 |
| 1:KC:19:ALA:HA | 1:KC:22:GLU:OE1 | 2.17 | 0.43 |
| 1:KC:222:PRO:HD2 | 2:KD:324:LYS:HD3 | 1.99 | 0.43 |
| 1:KC:359:PRO:CG | 6:4A:299:TYR:CE2 | 3.02 | 0.43 |
| 2:KD:276:ARG:HD3 | 6:4B:270:GLY:HA3 | 1.30 | 0.43 |
| 2:KF:226:ASN:ND2 | 13:KF:501:GDP:HN1 | 2.12 | 0.43 |
| 2:LD:180:VAL:HG12 | 1:LE:258:ASN:OD1 | 2.19 | 0.43 |
| 11:MA:501:GTP:O1G | 2:MB:252:LYS:NZ | 2.42 | 0.43 |
| 2:MD:232:ALA:HB1 | 2:MD:268:ILE:HD12 | 2.00 | 0.43 |
| 1:ME:179:THR:O | 2:MF:350:LYS:HA | 2.17 | 0.43 |
| 1:ME:282:TYR:HD2 | 6:4B:104:ARG:CZ | 1.98 | 0.43 |
| 6:4B:239:LEU:HD13 | 6:4B:239:LEU:HA | 1.83 | 0.43 |
| 7:5A:1535:ILE:CG1 | 7:5A:1574:ILE:C | 2.86 | 0.43 |
| 7:5B:1064:LYS:C | 7:5B:1066:GLY:N | 2.76 | 0.43 |
| 7:5C:943:LEU:HD22 | 7:5C:1030:PHE:HE2 | 1.84 | 0.43 |
| 8:6B:14:ARG:NH2 | 8:6B:89:ILE:O | 2.52 | 0.43 |
| 8:6C:14:ARG:NH2 | 8:6C:89:ILE:O | 2.52 | 0.43 |
| 1:AC:68:LEU:HD22 | 1:AC:153:LEU:HD11 | 2.00 | 0.43 |
| 2:AD:222:TYR:CE2 | 1:AE:325:PRO:HG2 | 2.54 | 0.43 |
| 1:AE:342:GLN:NE2 | 3:1A:55:HIS:ND1 | 2.45 | 0.43 |
| 2:AF:232:ALA:HB1 | 2:AF:268:ILE:HD12 | 2.00 | 0.43 |
| 1:BE:171:ILE:HG23 | 1:BE:204:LEU:O | 2.19 | 0.43 |
| 2:CB:99:ASN:HA | 2:CB:142:GLY:H | 1.84 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:262:ARG:NH1 | 2:CB:421:GLU:OE1 | 2.50 | 0.43 |
| 1:CC:398:MET:SD | 2:CD:345:ILE:CG1 | 2.93 | 0.43 |
| 2:CD:212:PHE:CE2 | 1:CE:326:LYS:HB2 | 2.54 | 0.43 |
| 2:CD:397:TRP:CB | 1:CE:256:GLN:HE22 | 2.21 | 0.43 |
| 1:CE:19:ALA:HA | 1:CE:22:GLU:OE1 | 2.17 | 0.43 |
| 2:DD:28:HIS:C | 2:DD:43:GLN:HE21 | 2.26 | 0.43 |
| 2:DF:28:HIS:C | 2:DF:43:GLN:HE21 | 2.26 | 0.43 |
| 2:DF:60:VAL:HG23 | 2:EF:281:TYR:CE1 | 2.53 | 0.43 |
| 1:EE:176:GLN:O | 2:EF:347:ASN:ND2 | 2.41 | 0.43 |
| 2:EF:86:ARG:HD3 | 2:FF:281:TYR:HB3 | 1.76 | 0.43 |
| 2:FB:180:VAL:CG1 | 1:FC:258:ASN:OD1 | 2.67 | 0.43 |
| 1:FC:222:PRO:HG2 | 2:FD:324:LYS:HB2 | 1.99 | 0.43 |
| 1:FE:71:GLU:CD | 2:FF:247:ASN:HD22 | 2.25 | 0.43 |
| 2:FF:415:MET:O | 2:FF:419:VAL:HG23 | 2.18 | 0.43 |
| 2:GB:179:VAL:HG23 | 1:GC:258:ASN:HA | 2.00 | 0.43 |
| 2:GD:390:ARG:HD2 | 1:GE:439:THR:HG21 | 2.00 | 0.43 |
| 1:GE:171:ILE:HG23 | 1:GE:204:LEU:O | 2.19 | 0.43 |
| 2:HF:261:PRO:CG | 5:3A:337:ARG:NH2 | 2.61 | 0.43 |
| 1:IA:171:ILE:HG23 | 1:IA:204:LEU:O | 2.18 | 0.43 |
| 1:IC:171:ILE:HG23 | 1:IC:204:LEU:O | 2.18 | 0.43 |
| 1:JA:171:ILE:HG23 | 1:JA:204:LEU:O | 2.19 | 0.43 |
| 1:JC:100:ALA:HB1 | 2:JD:252:LYS:CA | 2.47 | 0.43 |
| 1:KA:171:ILE:HG23 | 1:KA:204:LEU:O | 2.18 | 0.43 |
| 2:KB:232:ALA:HB1 | 2:KB:268:ILE:HD12 | 2.00 | 0.43 |
| 1:KC:86:LEU:C | 1:LC:283:HIS:O | 2.61 | 0.43 |
| 2:KD:390:ARG:HD2 | 1:KE:439:THR:HG21 | 2.00 | 0.43 |
| 2:KF:232:ALA:HB1 | 2:KF:268:ILE:HD12 | 2.00 | 0.43 |
| 1:LA:101:ASN:HA | 1:LA:144:GLY:H | 1.84 | 0.43 |
| 2:LD:295:ASP:OD1 | 4:2A:150:GLN:OE1 | 2.36 | 0.43 |
| 2:LF:55:THR:HG22 | 2:MF:283:ALA:HB1 | 1.95 | 0.43 |
| 1:MA:268:MET:HB2 | 1:MA:379:SER:O | 2.17 | 0.43 |
| 2:MB:208:TYR:OH | 1:MC:325:PRO:HB2 | 2.18 | 0.43 |
| 2:MB:415:MET:O | 2:MB:419:VAL:HG23 | 2.18 | 0.43 |
| 1:MC:372:MET:CE | 6:4A:96:VAL:CB | 2.95 | 0.43 |
| 1:ME:171:ILE:HG23 | 1:ME:204:LEU:O | 2.19 | 0.43 |
| 2:MF:232:ALA:HB1 | 2:MF:268:ILE:HD12 | 2.00 | 0.43 |
| 4:2A:164:ARG:NH1 | 4:2A:164:ARG:CG | 2.73 | 0.43 |
| 4:2B:15:GLU:C | 4:2B:19:MET:HG2 | 2.40 | 0.43 |
| 4:2C:164:ARG:NH1 | 4:2C:164:ARG:CG | 2.73 | 0.43 |
| 6:4D:258:ASP:O | 6:4D:262:ASN:HB2 | 2.18 | 0.43 |
| 7:5A:1442:GLN:CD | 7:5A:1442:GLN:C | 2.86 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5B:836:ARG:NH2 | 7:5B:837:ASP:HB3 | 2.32 | 0.43 |
| 7:5B:1577:LYS:HA | 7:5B:1577:LYS:HD2 | 1.80 | 0.43 |
| 7:5C:836:ARG:NH2 | 7:5C:837:ASP:HB3 | 2.32 | 0.43 |
| 7:5C:1392:LEU:C | 7:5C:1392:LEU:CD1 | 2.89 | 0.43 |
| 1:AA:68:LEU:HD22 | 1:AA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:AA:101:ASN:HA | 1:AA:144:GLY:H | 1.83 | 0.43 |
| 2:AB:415:MET:O | 2:AB:419:VAL:HG23 | 2.18 | 0.43 |
| 1:BA:68:LEU:HD22 | 1:BA:153:LEU:HD11 | 2.00 | 0.43 |
| 2:BB:232:ALA:HB1 | 2:BB:268:ILE:HD12 | 2.00 | 0.43 |
| 1:CA:60:LYS:HD3 | 1:DA:283:HIS:HD2 | 1.84 | 0.43 |
| 1:CE:282:TYR:CE2 | 10:8F:18:UNK:HA | 2.48 | 0.43 |
| 2:DD:415:MET:O | 2:DD:419:VAL:HG23 | 2.18 | 0.43 |
| 2:EB:212:PHE:HE2 | 1:EC:326:LYS:HB2 | 1.83 | 0.43 |
| 2:ED:20:PHE:O | 2:ED:24:ILE:HG12 | 2.18 | 0.43 |
| 2:ED:220:PRO:HD3 | 1:EE:326:LYS:HE2 | 1.97 | 0.43 |
| 2:EF:20:PHE:O | 2:EF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:FB:73:MET:CE | 2:FB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:FD:99:ASN:HA | 2:FD:142:GLY:H | 1.84 | 0.43 |
| 2:FF:99:ASN:HA | 2:FF:142:GLY:H | 1.84 | 0.43 |
| 2:GB:28:HIS:C | 2:GB:43:GLN:HE21 | 2.26 | 0.43 |
| 2:GD:222:TYR:CE2 | 1:GE:325:PRO:HG2 | 2.54 | 0.43 |
| 1:HC:101:ASN:HA | 1:HC:144:GLY:H | 1.83 | 0.43 |
| 1:HE:60:LYS:HZ2 | 1:IE:283:HIS:CE1 | 2.36 | 0.43 |
| 1:IA:68:LEU:HD22 | 1:IA:153:LEU:HD11 | 2.00 | 0.43 |
| 2:IB:415:MET:O | 2:IB:419:VAL:HG23 | 2.18 | 0.43 |
| 2:ID:390:ARG:HD2 | 1:IE:439:THR:HG21 | 2.00 | 0.43 |
| 1:IE:171:ILE:HG23 | 1:IE:204:LEU:O | 2.19 | 0.43 |
| 2:IF:391:ARG:HA | 2:IF:391:ARG:HD2 | 1.79 | 0.43 |
| 2:JF:232:ALA:HB1 | 2:JF:268:ILE:HD12 | 2.00 | 0.43 |
| 2:KB:77:ARG:CD | 2:LB:281:TYR:CE2 | 3.02 | 0.43 |
| 1:KC:171:ILE:HG23 | 1:KC:204:LEU:O | 2.18 | 0.43 |
| 2:KD:222:TYR:CE2 | 1:KE:325:PRO:HG2 | 2.54 | 0.43 |
| 2:KD:228:LEU:HG | 6:4B:267:ILE:HD12 | 1.99 | 0.43 |
| 2:LB:232:ALA:HB1 | 2:LB:268:ILE:HD12 | 2.00 | 0.43 |
| 1:LC:101:ASN:HA | 1:LC:144:GLY:H | 1.84 | 0.43 |
| 1:LE:176:GLN:O | 2:LF:347:ASN:CG | 2.61 | 0.43 |
| 1:MA:68:LEU:HD22 | 1:MA:153:LEU:HD11 | 2.00 | 0.43 |
| 2:MF:73:MET:CE | 2:MF:92:PHE:HB3 | 2.49 | 0.43 |
| 5:3B:21:PHE:CG | 5:3B:24:MET:HE2 | 2.52 | 0.43 |
| 5:3C:64:ASN:CG | 5:3C:93:LYS:HE2 | 2.43 | 0.43 |
| 6:4C:97:GLN:HE21 | 6:4C:97:GLN:HB2 | 1.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:4C:277:GLU:H | 6:4C:277:GLU:HG3 | 1.57 | 0.43 |
| 6:4D:179:ARG:NH1 | 6:4D:179:ARG:HB3 | 2.34 | 0.43 |
| 7:5A:836:ARG:NH2 | 7:5A:837:ASP:HB3 | 2.32 | 0.43 |
| 7:5A:943:LEU:HD22 | 7:5A:1030:PHE:HE2 | 1.84 | 0.43 |
| 7:5A:1120:ASP:OD2 | 7:5A:1125:LEU:HB2 | 2.19 | 0.43 |
| 7:5B:841:VAL:HG23 | 8:6B:11:PRO:CG | 2.49 | 0.43 |
| 7:5C:1120:ASP:OD2 | 7:5C:1125:LEU:HB2 | 2.19 | 0.43 |
| 9:7F:18:VAL:HG11 | 9:7F:42:LEU:HD22 | 2.00 | 0.43 |
| 2:BD:232:ALA:HB1 | 2:BD:268:ILE:HD12 | 2.00 | 0.43 |
| 2:CB:179:VAL:HG23 | 1:CC:258:ASN:HA | 1.97 | 0.43 |
| 1:CE:401:LYS:HE3 | 1:CE:401:LYS:HB2 | 1.74 | 0.43 |
| 2:CF:20:PHE:O | 2:CF:24:ILE:HG12 | 2.18 | 0.43 |
| 1:DE:171:ILE:HG23 | 1:DE:204:LEU:O | 2.18 | 0.43 |
| 2:DF:73:MET:CE | 2:DF:92:PHE:HB3 | 2.49 | 0.43 |
| 2:EB:20:PHE:O | 2:EB:24:ILE:HG12 | 2.18 | 0.43 |
| 2:EB:125:GLU:C | 7:5C:903:PHE:HE2 | 2.05 | 0.43 |
| 1:EE:62:VAL:CG2 | 1:FE:283:HIS:O | 2.64 | 0.43 |
| 1:FA:68:LEU:HD22 | 1:FA:153:LEU:HD11 | 2.00 | 0.43 |
| 1:FA:210:TYR:CD1 | 2:FB:324:LYS:HD2 | 2.54 | 0.43 |
| 1:FA:248:LEU:HD12 | 1:FA:248:LEU:HA | 1.89 | 0.43 |
| 2:FB:178:THR:HA | 1:FC:352:LYS:CD | 2.49 | 0.43 |
| 1:FC:422:ARG:NE | 7:5A:1170:THR:C | 2.77 | 0.43 |
| 2:FF:73:MET:CE | 2:FF:92:PHE:HB3 | 2.49 | 0.43 |
| 1:GC:100:ALA:HB1 | 2:GD:252:LYS:CA | 2.47 | 0.43 |
| 2:GD:178:THR:HA | 1:GE:352:LYS:CD | 2.48 | 0.43 |
| 2:GF:20:PHE:O | 2:GF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:GF:73:MET:CE | 2:GF:92:PHE:HB3 | 2.49 | 0.43 |
| 1:HE:71:GLU:OE2 | 1:HE:73:THR:OG1 | 2.28 | 0.43 |
| 2:IB:220:PRO:HD2 | 1:IC:326:LYS:CE | 2.44 | 0.43 |
| 1:IC:68:LEU:HD22 | 1:IC:153:LEU:HD11 | 2.00 | 0.43 |
| 1:IC:317:MET:HE2 | 1:IC:319:TYR:CE1 | 2.54 | 0.43 |
| 2:ID:222:TYR:CE2 | 1:IE:325:PRO:HG2 | 2.54 | 0.43 |
| 1:IE:317:MET:HE2 | 1:IE:319:TYR:CE1 | 2.54 | 0.43 |
| 2:IF:87:PRO:HD2 | 2:JF:281:TYR:CD2 | 2.52 | 0.43 |
| 2:JD:179:VAL:HG23 | 1:JE:258:ASN:HA | 1.97 | 0.43 |
| 2:JD:222:TYR:CE2 | 1:JE:325:PRO:HG2 | 2.54 | 0.43 |
| 1:JE:322:ASP:OD1 | 1:JE:373:ARG:NH1 | 2.52 | 0.43 |
| 2:KD:20:PHE:O | 2:KD:24:ILE:HG12 | 2.18 | 0.43 |
| 2:KD:226:ASN:ND2 | 13:KD:501:GDP:HN1 | 2.12 | 0.43 |
| 2:KD:232:ALA:HB1 | 2:KD:268:ILE:HD12 | 2.00 | 0.43 |
| 1:KE:171:ILE:HG23 | 1:KE:204:LEU:O | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:KE:317:MET:HE2 | 1:KE:319:TYR:CE1 | 2.54 | 0.43 |
| 2:KF:20:PHE:O | 2:KF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:LB:220:PRO:HD2 | 1:LC:326:LYS:HE2 | 2.00 | 0.43 |
| 2:LD:232:ALA:HB1 | 2:LD:268:ILE:HD12 | 2.00 | 0.43 |
| 1:LE:71:GLU:OE2 | 1:LE:73:THR:OG1 | 2.28 | 0.43 |
| 1:LE:171:ILE:HG23 | 1:LE:204:LEU:O | 2.18 | 0.43 |
| 1:MA:101:ASN:ND2 | 2:MB:252:LYS:HG3 | 2.10 | 0.43 |
| 2:MD:73:MET:CE | 2:MD:92:PHE:HB3 | 2.49 | 0.43 |
| 6:4B:179:ARG:NH1 | 6:4B:179:ARG:HB3 | 2.34 | 0.43 |
| 6:4D:260:ARG:HH22 | 6:4D:295:LYS:HE2 | 1.82 | 0.43 |
| 7:5A:847:GLY:N | 8:6A:7:ASP:OD1 | 2.37 | 0.43 |
| 7:5A:887:TYR:CD2 | 7:5A:1055:PHE:CD2 | 3.07 | 0.43 |
| 7:5A:1064:LYS:C | 7:5A:1066:GLY:N | 2.76 | 0.43 |
| 7:5A:1399:LYS:HB3 | 7:5A:1399:LYS:HE3 | 1.67 | 0.43 |
| 7:5A:1424:GLN:NE2 | 7:5A:1424:GLN:C | 2.73 | 0.43 |
| 7:5B:887:TYR:CD2 | 7:5B:1055:PHE:CD2 | 3.07 | 0.43 |
| 7:5B:943:LEU:HD22 | 7:5B:1030:PHE:HE2 | 1.84 | 0.43 |
| 7:5B:1449:LEU:HD22 | 7:5B:1449:LEU:HA | 1.75 | 0.43 |
| 7:5C:887:TYR:CD2 | 7:5C:1055:PHE:CD2 | 3.07 | 0.43 |
| 2:AB:28:HIS:C | 2:AB:43:GLN:HE21 | 2.26 | 0.43 |
| 1:BC:100:ALA:HB1 | 2:BD:252:LYS:CA | 2.49 | 0.43 |
| 2:CD:20:PHE:O | 2:CD:24:ILE:HG12 | 2.18 | 0.43 |
| 1:CE:181:VAL:HG21 | 2:CF:256:ASN:O | 2.19 | 0.43 |
| 2:DB:99:ASN:HA | 2:DB:142:GLY:H | 1.84 | 0.43 |
| 2:DD:99:ASN:HA | 2:DD:142:GLY:H | 1.84 | 0.43 |
| 1:DE:101:ASN:HA | 1:DE:144:GLY:H | 1.83 | 0.43 |
| 2:EB:55:THR:HG23 | 2:FB:284:LEU:N | 2.33 | 0.43 |
| 2:EB:99:ASN:HA | 2:EB:142:GLY:H | 1.84 | 0.43 |
| 2:ED:99:ASN:HA | 2:ED:142:GLY:H | 1.84 | 0.43 |
| 1:FA:207:GLU:OE1 | 7:5C:915:PHE:CG | 2.72 | 0.43 |
| 2:FB:391:ARG:CG | 1:FC:346:TRP:CD1 | 2.85 | 0.43 |
| 1:FE:101:ASN:HA | 1:FE:144:GLY:H | 1.83 | 0.43 |
| 2:GB:20:PHE:O | 2:GB:24:ILE:HG12 | 2.18 | 0.43 |
| 1:GC:401:LYS:HE3 | 1:GC:401:LYS:HB2 | 1.74 | 0.43 |
| 2:GD:20:PHE:O | 2:GD:24:ILE:HG12 | 2.18 | 0.43 |
| 2:GF:416:ASN:HD22 | 7:5B:1327:LYS:HE3 | 1.81 | 0.43 |
| 1:HA:101:ASN:HA | 1:HA:144:GLY:H | 1.83 | 0.43 |
| 1:HA:317:MET:HE2 | 1:HA:319:TYR:CE1 | 2.54 | 0.43 |
| 1:HA:404:PHE:CE2 | 2:HB:345:ILE:HD11 | 2.54 | 0.43 |
| 2:HB:222:TYR:HD2 | 1:HC:247:ALA:HB1 | 1.82 | 0.43 |
| 1:HC:171:ILE:HG23 | 1:HC:204:LEU:O | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:IA:181:VAL:HG21 | 2:IB:256:ASN:O | 2.18 | 0.43 |
| 1:IA:317:MET:HE2 | 1:IA:319:TYR:CE1 | 2.54 | 0.43 |
| 2:ID:220:PRO:HD2 | 1:IE:326:LYS:CE | 2.44 | 0.43 |
| 2:ID:220:PRO:HD2 | 1:IE:326:LYS:CG | 2.44 | 0.43 |
| 2:ID:415:MET:O | 2:ID:419:VAL:HG23 | 2.18 | 0.43 |
| 2:IF:232:ALA:HB1 | 2:IF:268:ILE:HD12 | 2.00 | 0.43 |
| 2:IF:415:MET:O | 2:IF:419:VAL:HG23 | 2.18 | 0.43 |
| 2:JD:226:ASN:ND2 | 13:JD:501:GDP:HN1 | 2.12 | 0.43 |
| 2:JD:232:ALA:HB1 | 2:JD:268:ILE:HD12 | 2.00 | 0.43 |
| 1:JE:279:GLU:OE2 | 10:9A:21:UNK:O | 2.36 | 0.43 |
| 1:KA:19:ALA:HA | 1:KA:22:GLU:OE1 | 2.17 | 0.43 |
| 1:KA:85:GLN:CG | 1:LA:283:HIS:HD2 | 2.29 | 0.43 |
| 2:KB:20:PHE:O | 2:KB:24:ILE:HG12 | 2.18 | 0.43 |
| 2:KB:276:ARG:HH21 | 6:4A:265:TYR:HB2 | 1.78 | 0.43 |
| 1:LE:101:ASN:HA | 1:LE:144:GLY:H | 1.84 | 0.43 |
| 4:2A:15:GLU:C | 4:2A:19:MET:HG2 | 2.40 | 0.43 |
| 5:3C:21:PHE:CG | 5:3C:24:MET:HE2 | 2.52 | 0.43 |
| 6:4A:97:GLN:HE21 | 6:4A:97:GLN:HB2 | 1.49 | 0.43 |
| 6:4C:117:ARG:HA | 6:4C:120:GLN:CD | 2.43 | 0.43 |
| 6:4C:179:ARG:NH1 | 6:4C:179:ARG:HB3 | 2.34 | 0.43 |
| 6:4D:135:LEU:H | 6:4D:135:LEU:HD23 | 1.83 | 0.43 |
| 6:4D:241:LYS:C | 6:4D:241:LYS:CD | 2.89 | 0.43 |
| 7:5A:1424:GLN:HE21 | 7:5A:1424:GLN:HA | 1.84 | 0.43 |
| 7:5B:1120:ASP:OD2 | 7:5B:1125:LEU:HB2 | 2.19 | 0.43 |
| 7:5B:1424:GLN:HE21 | 7:5B:1424:GLN:HA | 1.84 | 0.43 |
| 7:5C:826:LEU:CB | 7:5C:840:GLY:O | 2.66 | 0.43 |
| 7:5C:836:ARG:NH1 | 7:5C:836:ARG:HG3 | 2.32 | 0.43 |
| 7:5C:1460:ARG:HE | 7:5C:1460:ARG:HB3 | 1.69 | 0.43 |
| 2:AD:20:PHE:O | 2:AD:24:ILE:HG12 | 2.18 | 0.43 |
| 2:AD:28:HIS:C | 2:AD:43:GLN:HE21 | 2.26 | 0.43 |
| 2:AD:178:THR:HA | 1:AE:352:LYS:CD | 2.48 | 0.43 |
| 2:AD:274:THR:O | 6:4C:134:LEU:CD1 | 2.66 | 0.43 |
| 2:AF:20:PHE:O | 2:AF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:AF:28:HIS:C | 2:AF:43:GLN:HE21 | 2.26 | 0.43 |
| 1:BC:68:LEU:HD22 | 1:BC:153:LEU:HD11 | 2.00 | 0.43 |
| 1:BC:101:ASN:HA | 1:BC:144:GLY:H | 1.84 | 0.43 |
| 1:BC:322:ASP:OD1 | 1:BC:373:ARG:NH1 | 2.52 | 0.43 |
| 1:BE:100:ALA:HB1 | 2:BF:252:LYS:CA | 2.49 | 0.43 |
| 1:BE:101:ASN:HA | 1:BE:144:GLY:H | 1.84 | 0.43 |
| 2:CB:20:PHE:O | 2:CB:24:ILE:HG12 | 2.18 | 0.43 |
| 1:CC:101:ASN:HA | 1:CC:144:GLY:H | 1.83 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CC:181:VAL:HG21 | 2:CD:256:ASN:O | 2.19 | 0.43 |
| 1:CE:101:ASN:HA | 1:CE:144:GLY:H | 1.84 | 0.43 |
| 2:CF:232:ALA:HB1 | 2:CF:268:ILE:HD12 | 2.00 | 0.43 |
| 1:DA:322:ASP:OD1 | 1:DA:373:ARG:NH1 | 2.51 | 0.43 |
| 1:DA:356:ASN:OD1 | 1:DA:357:TYR:N | 2.51 | 0.43 |
| 2:DB:177:ASP:CA | 1:DC:353:VAL:HG12 | 2.49 | 0.43 |
| 2:DB:415:MET:O | 2:DB:419:VAL:HG23 | 2.18 | 0.43 |
| 1:DC:101:ASN:HA | 1:DC:144:GLY:H | 1.83 | 0.43 |
| 1:DC:171:ILE:HG23 | 1:DC:204:LEU:O | 2.19 | 0.43 |
| 1:DC:356:ASN:OD1 | 1:DC:357:TYR:N | 2.51 | 0.43 |
| 2:DD:73:MET:CE | 2:DD:92:PHE:HB3 | 2.49 | 0.43 |
| 2:DF:68:LEU:HD12 | 2:DF:68:LEU:HA | 1.90 | 0.43 |
| 2:DF:99:ASN:HA | 2:DF:142:GLY:H | 1.84 | 0.43 |
| 1:EE:394:LYS:NZ | 2:EF:347:ASN:OD1 | 2.52 | 0.43 |
| 2:EF:99:ASN:HA | 2:EF:142:GLY:H | 1.84 | 0.43 |
| 1:FA:171:ILE:HG23 | 1:FA:204:LEU:O | 2.18 | 0.43 |
| 1:FC:101:ASN:HA | 1:FC:144:GLY:H | 1.83 | 0.43 |
| 2:FD:73:MET:CE | 2:FD:92:PHE:HB3 | 2.49 | 0.43 |
| 1:GA:68:LEU:HD22 | 1:GA:153:LEU:HD11 | 2.00 | 0.43 |
| 2:GB:232:ALA:HB1 | 2:GB:268:ILE:HD12 | 2.00 | 0.43 |
| 2:GD:73:MET:CE | 2:GD:92:PHE:HB3 | 2.49 | 0.43 |
| 2:GD:99:ASN:HA | 2:GD:142:GLY:H | 1.83 | 0.43 |
| 1:GE:317:MET:HE2 | 1:GE:319:TYR:CE1 | 2.54 | 0.43 |
| 2:GF:99:ASN:HA | 2:GF:142:GLY:H | 1.84 | 0.43 |
| 2:HB:73:MET:CE | 2:HB:92:PHE:HB3 | 2.49 | 0.43 |
| 1:HC:317:MET:HE2 | 1:HC:319:TYR:CE1 | 2.54 | 0.43 |
| 2:HD:222:TYR:CE2 | 1:HE:325:PRO:HG2 | 2.54 | 0.43 |
| 1:HE:101:ASN:HA | 1:HE:144:GLY:H | 1.83 | 0.43 |
| 1:HE:171:ILE:HG23 | 1:HE:204:LEU:O | 2.19 | 0.43 |
| 1:HE:317:MET:HE2 | 1:HE:319:TYR:CE1 | 2.54 | 0.43 |
| 2:IB:179:VAL:HG23 | 1:IC:258:ASN:HA | 2.00 | 0.43 |
| 2:ID:20:PHE:O | 2:ID:24:ILE:HG12 | 2.18 | 0.43 |
| 1:IE:68:LEU:HD22 | 1:IE:153:LEU:HD11 | 2.00 | 0.43 |
| 2:JB:73:MET:CE | 2:JB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:JB:232:ALA:HB1 | 2:JB:268:ILE:HD12 | 2.00 | 0.43 |
| 1:KA:181:VAL:HG21 | 2:KB:256:ASN:O | 2.18 | 0.43 |
| 1:KA:317:MET:HE2 | 1:KA:319:TYR:CE1 | 2.54 | 0.43 |
| 1:KC:79:ARG:C | 1:LC:280:LYS:CE | 2.90 | 0.43 |
| 1:KC:317:MET:HE2 | 1:KC:319:TYR:CE1 | 2.54 | 0.43 |
| 2:KF:276:ARG:CZ | 6:4D:265:TYR:HB2 | 2.47 | 0.43 |
| 2:LB:73:MET:CE | 2:LB:92:PHE:HB3 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:LC:171:ILE:HG23 | 1:LC:204:LEU:O | 2.19 | 0.43 |
| 1:MA:279:GLU:OE1 | 6:4C:107:MET:CG | 2.67 | 0.43 |
| 1:MA:317:MET:HE2 | 1:MA:319:TYR:CE1 | 2.54 | 0.43 |
| 2:MB:73:MET:CE | 2:MB:92:PHE:HB3 | 2.49 | 0.43 |
| 1:MC:68:LEU:HD22 | 1:MC:153:LEU:HD11 | 2.00 | 0.43 |
| 1:MC:317:MET:HE2 | 1:MC:319:TYR:CE1 | 2.54 | 0.43 |
| 2:MD:111:GLU:CB | 3:1B:62:SER:HA | 2.49 | 0.43 |
| 3:1A:33:ASP:HB3 | 3:1A:39:MET:SD | 2.58 | 0.43 |
| 4:2B:164:ARG:NH1 | 4:2B:164:ARG:CG | 2.73 | 0.43 |
| 6:4A:117:ARG:HA | 6:4A:120:GLN:CD | 2.43 | 0.43 |
| 6:4B:230:TYR:CD2 | 6:4B:230:TYR:N | 2.74 | 0.43 |
| 6:4B:258:ASP:O | 6:4B:262:ASN:HB2 | 2.18 | 0.43 |
| 6:4B:260:ARG:HH22 | 6:4B:295:LYS:HE2 | 1.82 | 0.43 |
| 6:4C:113:ILE:HB | 6:4C:117:ARG:NH2 | 2.34 | 0.43 |
| 7:5A:826:LEU:CB | 7:5A:840:GLY:O | 2.66 | 0.43 |
| 7:5A:836:ARG:NH1 | 7:5A:836:ARG:HG3 | 2.32 | 0.43 |
| 7:5A:841:VAL:N | 8:6A:109:ILE:CD1 | 2.66 | 0.43 |
| 7:5B:872:GLU:CD | 8:6B:90:ARG:NH1 | 2.77 | 0.43 |
| 7:5B:1399:LYS:HB3 | 7:5B:1399:LYS:HE3 | 1.67 | 0.43 |
| 7:5C:1445:LEU:HD13 | 7:5C:1445:LEU:HA | 1.78 | 0.43 |
| 7:5C:1535:ILE:CG1 | 7:5C:1574:ILE:C | 2.86 | 0.43 |
| 2:AB:20:PHE:O | 2:AB:24:ILE:HG12 | 2.18 | 0.43 |
| 1:BA:101:ASN:HA | 1:BA:144:GLY:H | 1.84 | 0.43 |
| 2:BB:73:MET:CE | 2:BB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:BB:99:ASN:HA | 2:BB:142:GLY:H | 1.84 | 0.43 |
| 2:BD:73:MET:CE | 2:BD:92:PHE:HB3 | 2.49 | 0.43 |
| 2:BD:99:ASN:HA | 2:BD:142:GLY:H | 1.84 | 0.43 |
| 2:BD:179:VAL:HG23 | 1:BE:258:ASN:HA | 1.98 | 0.43 |
| 2:BF:73:MET:CE | 2:BF:92:PHE:HB3 | 2.49 | 0.43 |
| 2:BF:232:ALA:HB1 | 2:BF:268:ILE:HD12 | 2.00 | 0.43 |
| 1:CA:101:ASN:HA | 1:CA:144:GLY:H | 1.84 | 0.43 |
| 2:CB:69:GLU:HA | 2:CB:70:PRO:HD3 | 1.89 | 0.43 |
| 2:CB:73:MET:CE | 2:CB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:CD:73:MET:CE | 2:CD:92:PHE:HB3 | 2.49 | 0.43 |
| 1:DA:171:ILE:HG23 | 1:DA:204:LEU:O | 2.18 | 0.43 |
| 1:DE:356:ASN:OD1 | 1:DE:357:TYR:N | 2.51 | 0.43 |
| 2:EB:73:MET:CE | 2:EB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:EB:232:ALA:HB1 | 2:EB:268:ILE:HD12 | 2.00 | 0.43 |
| 2:ED:55:THR:N | 2:FD:283:ALA:CB | 2.82 | 0.43 |
| 1:EE:259:LEU:HD11 | 1:EE:316:SER:HB3 | 2.01 | 0.43 |
| 2:EF:73:MET:CE | 2:EF:92:PHE:HB3 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:FC:171:ILE:HG23 | 1:FC:204:LEU:O | 2.18 | 0.43 |
| 1:GA:317:MET:HE2 | 1:GA:319:TYR:CE1 | 2.54 | 0.43 |
| 2:GB:73:MET:CE | 2:GB:92:PHE:HB3 | 2.49 | 0.43 |
| 2:GB:99:ASN:HA | 2:GB:142:GLY:H | 1.84 | 0.43 |
| 1:GC:101:ASN:HA | 1:GC:144:GLY:H | 1.83 | 0.43 |
| 1:GE:101:ASN:HA | 1:GE:144:GLY:H | 1.83 | 0.43 |
| 2:GF:232:ALA:HB1 | 2:GF:268:ILE:HD12 | 2.00 | 0.43 |
| 1:HA:181:VAL:HG21 | 2:HB:256:ASN:O | 2.18 | 0.43 |
| 2:HB:397:TRP:HE3 | 1:HC:257:THR:HG22 | 1.34 | 0.43 |
| 2:HD:73:MET:CE | 2:HD:92:PHE:HB3 | 2.49 | 0.43 |
| 2:HD:179:VAL:HG23 | 1:HE:258:ASN:HA | 1.97 | 0.43 |
| 2:HF:68:LEU:HD12 | 2:HF:68:LEU:HA | 1.90 | 0.43 |
| 2:HF:232:ALA:HB1 | 2:HF:268:ILE:HD12 | 2.00 | 0.43 |
| 2:IB:20:PHE:O | 2:IB:24:ILE:HG12 | 2.18 | 0.43 |
| 1:IC:164:LYS:HA | 1:IC:164:LYS:HD3 | 1.85 | 0.43 |
| 2:ID:391:ARG:HA | 2:ID:391:ARG:HD2 | 1.79 | 0.43 |
| 2:IF:20:PHE:O | 2:IF:24:ILE:HG12 | 2.18 | 0.43 |
| 2:IF:73:MET:CE | 2:IF:92:PHE:HB3 | 2.49 | 0.43 |
| 1:JE:279:GLU:CD | 10:9A:22:UNK:O | 2.57 | 0.43 |
| 1:JE:401:LYS:HE3 | 1:JE:401:LYS:HB2 | 1.74 | 0.43 |
| 2:KB:124:ALA:O | 4:2C:38:VAL:HA | 2.19 | 0.43 |
| 2:KB:391:ARG:HD2 | 2:KB:391:ARG:HA | 1.79 | 0.43 |
| 2:KD:276:ARG:NH2 | 6:4B:265:TYR:C | 2.76 | 0.43 |
| 1:KE:71:GLU:HA | 1:KE:72:PRO:HD3 | 1.84 | 0.43 |
| 1:KE:88:HIS:HA | 1:LE:284:GLU:HA | 1.97 | 0.43 |
| 2:KF:121:ARG:NH2 | 4:2B:144:ASN:CG | 2.77 | 0.43 |
| 1:LA:171:ILE:HG23 | 1:LA:204:LEU:O | 2.18 | 0.43 |
| 2:LD:73:MET:CE | 2:LD:92:PHE:HB3 | 2.49 | 0.43 |
| 2:LF:232:ALA:HB1 | 2:LF:268:ILE:HD12 | 2.00 | 0.43 |
| 2:LF:294:PHE:O | 4:2B:148:ASN:O | 2.36 | 0.43 |
| 1:ME:317:MET:HE2 | 1:ME:319:TYR:CE1 | 2.54 | 0.43 |
| 3:1B:33:ASP:HB3 | 3:1B:39:MET:SD | 2.58 | 0.43 |
| 4:2B:143:LEU:HD12 | 4:2B:143:LEU:HA | 1.82 | 0.43 |
| 4:2C:15:GLU:C | 4:2C:19:MET:HG2 | 2.40 | 0.43 |
| 5:3A:21:PHE:CG | 5:3A:24:MET:HE2 | 2.52 | 0.43 |
| 6:4A:135:LEU:HD23 | 6:4A:135:LEU:H | 1.83 | 0.43 |
| 6:4A:179:ARG:NH1 | 6:4A:179:ARG:HB3 | 2.34 | 0.43 |
| 6:4A:258:ASP:O | 6:4A:262:ASN:HB2 | 2.18 | 0.43 |
| 6:4B:135:LEU:HD23 | 6:4B:135:LEU:H | 1.83 | 0.43 |
| 7:5A:1445:LEU:HD13 | 7:5A:1445:LEU:HA | 1.78 | 0.43 |
| 7:5A:1449:LEU:HD22 | 7:5A:1449:LEU:HA | 1.75 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5B:1125:LEU:CD2 | 8:6B:246:TYR:CE2 | 3.02 | 0.43 |
| 7:5B:1316:LEU:HA | 7:5B:1316:LEU:HD13 | 1.87 | 0.43 |
| 7:5C:839:GLU:OE2 | 8:6C:11:PRO:HG2 | 2.18 | 0.43 |
| 7:5C:1267:CYS:C | 7:5C:1270:ASP:H | 2.24 | 0.43 |
| 7:5C:1388:GLN:O | 7:5C:1392:LEU:N | 2.43 | 0.43 |
| 7:5C:1424:GLN:HE21 | 7:5C:1424:GLN:HA | 1.84 | 0.43 |
| 7:5C:1490:LYS:CG | 7:5C:1494:LEU:CG | 2.95 | 0.43 |
| 1:AA:60:LYS:CD | 1:BA:283:HIS:CD2 | 3.01 | 0.42 |
| 1:AA:404:PHE:CE2 | 2:AB:345:ILE:HD11 | 2.54 | 0.42 |
| 2:AD:321:MET:CA | 6:4C:156:PHE:CD2 | 3.02 | 0.42 |
| 1:AE:171:ILE:HG23 | 1:AE:204:LEU:O | 2.19 | 0.42 |
| 1:BA:248:LEU:HD12 | 1:BA:248:LEU:HA | 1.89 | 0.42 |
| 1:BE:68:LEU:HD22 | 1:BE:153:LEU:HD11 | 2.00 | 0.42 |
| 1:BE:322:ASP:OD1 | 1:BE:373:ARG:NH1 | 2.52 | 0.42 |
| 2:BF:99:ASN:HA | 2:BF:142:GLY:H | 1.84 | 0.42 |
| 2:BF:391:ARG:HA | 2:BF:391:ARG:HD2 | 1.78 | 0.42 |
| 1:CA:356:ASN:OD1 | 1:CA:357:TYR:N | 2.51 | 0.42 |
| 2:CB:232:ALA:HB1 | 2:CB:268:ILE:HD12 | 2.00 | 0.42 |
| 2:CF:73:MET:CE | 2:CF:92:PHE:HB3 | 2.49 | 0.42 |
| 1:DA:101:ASN:HA | 1:DA:144:GLY:H | 1.83 | 0.42 |
| 2:DB:73:MET:CE | 2:DB:92:PHE:HB3 | 2.49 | 0.42 |
| 1:DC:322:ASP:OD1 | 1:DC:373:ARG:NH1 | 2.52 | 0.42 |
| 1:DE:394:LYS:NZ | 2:DF:347:ASN:OD1 | 2.52 | 0.42 |
| 1:EC:259:LEU:HD11 | 1:EC:316:SER:HB3 | 2.01 | 0.42 |
| 2:ED:73:MET:CE | 2:ED:92:PHE:HB3 | 2.49 | 0.42 |
| 2:ED:125:GLU:C | 7:5A:903:PHE:HE2 | 2.01 | 0.42 |
| 2:ED:232:ALA:HB1 | 2:ED:268:ILE:HD12 | 2.00 | 0.42 |
| 1:EE:101:ASN:HA | 1:EE:144:GLY:H | 1.84 | 0.42 |
| 1:FA:101:ASN:HA | 1:FA:144:GLY:H | 1.83 | 0.42 |
| 1:FE:317:MET:HE2 | 1:FE:319:TYR:CE1 | 2.54 | 0.42 |
| 1:GC:68:LEU:HD22 | 1:GC:153:LEU:HD11 | 2.00 | 0.42 |
| 2:GD:232:ALA:HB1 | 2:GD:268:ILE:HD12 | 2.00 | 0.42 |
| 1:HA:171:ILE:HG23 | 1:HA:204:LEU:O | 2.18 | 0.42 |
| 2:HF:73:MET:CE | 2:HF:92:PHE:HB3 | 2.49 | 0.42 |
| 2:ID:73:MET:CE | 2:ID:92:PHE:HB3 | 2.49 | 0.42 |
| 2:JB:178:THR:HA | 1:JC:352:LYS:CD | 2.49 | 0.42 |
| 2:JF:391:ARG:HD2 | 2:JF:391:ARG:HA | 1.79 | 0.42 |
| 1:KA:222:PRO:CG | 2:KB:324:LYS:CD | 2.91 | 0.42 |
| 2:KB:215:LEU:HD12 | 6:4A:267:ILE:CG2 | 2.31 | 0.42 |
| 2:KB:217:LEU:HD13 | 6:4A:263:CYS:HG | 1.84 | 0.42 |
| 2:KB:222:TYR:HD2 | 1:KC:247:ALA:HB1 | 1.82 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:KD:87:PRO:CD | 2:LD:282:ARG:CG | 2.92 | 0.42 |
| 1:LC:222:PRO:HG2 | 2:LD:324:LYS:CD | 2.41 | 0.42 |
| 1:LE:356:ASN:OD1 | 1:LE:357:TYR:N | 2.51 | 0.42 |
| 2:MB:179:VAL:HG22 | 1:MC:258:ASN:CG | 2.44 | 0.42 |
| 1:ME:282:TYR:CD2 | 6:4B:104:ARG:CZ | 2.65 | 0.42 |
| 4:2A:143:LEU:HD12 | 4:2A:143:LEU:HA | 1.82 | 0.42 |
| 6:4A:193:MET:HE3 | 6:4A:193:MET:HB3 | 1.83 | 0.42 |
| 6:4A:260:ARG:HH22 | 6:4A:295:LYS:HE2 | 1.82 | 0.42 |
| 6:4B:107:MET:O | 6:4B:109:ASP:N | 2.52 | 0.42 |
| 6:4B:117:ARG:HA | 6:4B:120:GLN:CD | 2.43 | 0.42 |
| 7:5A:1267:CYS:C | 7:5A:1270:ASP:H | 2.24 | 0.42 |
| 7:5B:826:LEU:CB | 7:5B:840:GLY:O | 2.66 | 0.42 |
| 7:5B:847:GLY:N | 8:6B:7:ASP:OD1 | 2.40 | 0.42 |
| 7:5B:1253:ILE:HD12 | 7:5B:1261:ALA:CB | 2.47 | 0.42 |
| 7:5B:1428:GLU:CD | 7:5B:1428:GLU:C | 2.85 | 0.42 |
| 9:7D:12:GLU:CA | 9:7D:16:THR:HG1 | 2.17 | 0.42 |
| 1:AA:259:LEU:HD11 | 1:AA:316:SER:HB3 | 2.02 | 0.42 |
| 2:AB:73:MET:CE | 2:AB:92:PHE:HB3 | 2.49 | 0.42 |
| 1:AC:171:ILE:HG23 | 1:AC:204:LEU:O | 2.18 | 0.42 |
| 1:AC:259:LEU:HD11 | 1:AC:316:SER:HB3 | 2.02 | 0.42 |
| 2:AD:321:MET:CA | 6:4C:156:PHE:CE2 | 3.02 | 0.42 |
| 2:CD:87:PRO:HD3 | 2:DD:281:TYR:CZ | 2.51 | 0.42 |
| 2:CD:232:ALA:HB1 | 2:CD:268:ILE:HD12 | 2.00 | 0.42 |
| 1:DA:259:LEU:HD11 | 1:DA:316:SER:HB3 | 2.02 | 0.42 |
| 1:DC:259:LEU:HD11 | 1:DC:316:SER:HB3 | 2.02 | 0.42 |
| 1:DE:259:LEU:HD11 | 1:DE:316:SER:HB3 | 2.01 | 0.42 |
| 1:DE:398:MET:SD | 2:DF:345:ILE:CG1 | 2.93 | 0.42 |
| 2:DF:232:ALA:HB1 | 2:DF:268:ILE:HD12 | 2.00 | 0.42 |
| 1:EA:171:ILE:HG23 | 1:EA:204:LEU:O | 2.18 | 0.42 |
| 1:EA:259:LEU:HD11 | 1:EA:316:SER:HB3 | 2.01 | 0.42 |
| 1:EA:317:MET:HE2 | 1:EA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:EC:101:ASN:HA | 1:EC:144:GLY:H | 1.84 | 0.42 |
| 1:EC:317:MET:HE2 | 1:EC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:EE:401:LYS:HE3 | 1:EE:401:LYS:HB2 | 1.74 | 0.42 |
| 2:EF:232:ALA:HB1 | 2:EF:268:ILE:HD12 | 2.00 | 0.42 |
| 2:FB:208:TYR:CE2 | 1:FC:326:LYS:HB3 | 2.54 | 0.42 |
| 2:FB:232:ALA:HB1 | 2:FB:268:ILE:HD12 | 2.00 | 0.42 |
| 1:FC:317:MET:HE2 | 1:FC:319:TYR:CE1 | 2.54 | 0.42 |
| 13:FD:502:GDP:H8 | 1:FE:248:LEU:CD1 | 2.31 | 0.42 |
| 1:FE:171:ILE:HG23 | 1:FE:204:LEU:O | 2.18 | 0.42 |
| 1:GA:356:ASN:OD1 | 1:GA:357:TYR:N | 2.51 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:GC:317:MET:HE2 | 1:GC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:HC:60:LYS:HZ2 | 1:IC:283:HIS:CE1 | 2.37 | 0.42 |
| 1:HC:259:LEU:HD11 | 1:HC:316:SER:HB3 | 2.02 | 0.42 |
| 1:HC:404:PHE:CE2 | 2:HD:345:ILE:HD11 | 2.54 | 0.42 |
| 2:HD:232:ALA:HB1 | 2:HD:268:ILE:HD12 | 2.00 | 0.42 |
| 2:IB:73:MET:CE | 2:IB:92:PHE:HB3 | 2.49 | 0.42 |
| 2:IB:232:ALA:HB1 | 2:IB:268:ILE:HD12 | 2.00 | 0.42 |
| 1:IC:404:PHE:CE2 | 2:ID:345:ILE:HD11 | 2.54 | 0.42 |
| 2:ID:232:ALA:HB1 | 2:ID:268:ILE:HD12 | 2.00 | 0.42 |
| 2:JD:73:MET:CE | 2:JD:92:PHE:HB3 | 2.49 | 0.42 |
| 2:JF:73:MET:CE | 2:JF:92:PHE:HB3 | 2.49 | 0.42 |
| 2:JF:86:ARG:NH1 | 2:KF:280:GLN:CA | 2.79 | 0.42 |
| 2:KB:226:ASN:ND2 | 13:KB:501:GDP:HN1 | 2.12 | 0.42 |
| 1:KE:245:ASP:OD2 | 6:4B:257:LEU:HD11 | 2.19 | 0.42 |
| 2:LB:220:PRO:O | 1:LC:324:VAL:HG11 | 2.19 | 0.42 |
| 1:LE:259:LEU:HD11 | 1:LE:316:SER:HB3 | 2.01 | 0.42 |
| 2:LF:73:MET:CE | 2:LF:92:PHE:HB3 | 2.49 | 0.42 |
| 2:MD:212:PHE:CZ | 1:ME:326:LYS:CD | 2.42 | 0.42 |
| 1:ME:68:LEU:HD22 | 1:ME:153:LEU:HD11 | 2.00 | 0.42 |
| 2:MF:221:THR:HG21 | 6:4D:189:ARG:NH1 | 2.27 | 0.42 |
| 4:2C:143:LEU:HD12 | 4:2C:143:LEU:HA | 1.82 | 0.42 |
| 4:2C:164:ARG:O | 4:2C:164:ARG:HG3 | 2.19 | 0.42 |
| 6:4A:107:MET:O | 6:4A:109:ASP:N | 2.52 | 0.42 |
| 6:4A:113:ILE:HB | 6:4A:117:ARG:NH2 | 2.34 | 0.42 |
| 6:4C:107:MET:O | 6:4C:109:ASP:N | 2.52 | 0.42 |
| 6:4C:135:LEU:HD23 | 6:4C:135:LEU:H | 1.83 | 0.42 |
| 6:4D:107:MET:O | 6:4D:109:ASP:N | 2.52 | 0.42 |
| 6:4D:108:LYS:O | 6:4D:108:LYS:CG | 2.67 | 0.42 |
| 7:5A:1253:ILE:HD12 | 7:5A:1261:ALA:CB | 2.47 | 0.42 |
| 7:5A:1263:GLN:HB3 | 9:7A:8:ARG:HD2 | 2.01 | 0.42 |
| 7:5A:1490:LYS:CG | 7:5A:1494:LEU:CG | 2.95 | 0.42 |
| 7:5B:1397:GLU:CD | 7:5B:1397:GLU:N | 2.77 | 0.42 |
| 7:5B:1445:LEU:HD13 | 7:5B:1445:LEU:HA | 1.77 | 0.42 |
| 7:5B:1471:ILE:H | 7:5B:1471:ILE:CD1 | 2.17 | 0.42 |
| 7:5C:1424:GLN:NE2 | 7:5C:1424:GLN:C | 2.73 | 0.42 |
| 7:5C:1449:LEU:HD22 | 7:5C:1449:LEU:HA | 1.75 | 0.42 |
| 9:7B:45:ARG:HA | 9:7B:45:ARG:HD2 | 1.85 | 0.42 |
| 1:AA:171:ILE:HG23 | 1:AA:204:LEU:O | 2.18 | 0.42 |
| 1:AE:259:LEU:HD11 | 1:AE:316:SER:HB3 | 2.02 | 0.42 |
| 1:CC:356:ASN:OD1 | 1:CC:357:TYR:N | 2.51 | 0.42 |
| 2:DB:55:THR:HG23 | 2:EB:283:ALA:HA | 2.00 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:DB:390:ARG:CD | 1:DC:439:THR:HG21 | 2.49 | 0.42 |
| 2:DD:179:VAL:HG23 | 1:DE:258:ASN:HA | 1.98 | 0.42 |
| 2:DD:232:ALA:HB1 | 2:DD:268:ILE:HD12 | 2.00 | 0.42 |
| 1:EA:101:ASN:HA | 1:EA:144:GLY:H | 1.84 | 0.42 |
| 2:EB:176:SER:OG | 1:EC:349:THR:OG1 | 2.25 | 0.42 |
| 2:EB:179:VAL:HG22 | 1:EC:258:ASN:CB | 2.50 | 0.42 |
| 2:EB:391:ARG:HD2 | 2:EB:391:ARG:HA | 1.79 | 0.42 |
| 1:EC:100:ALA:HB1 | 2:ED:252:LYS:N | 2.34 | 0.42 |
| 1:EE:317:MET:HE2 | 1:EE:319:TYR:CE1 | 2.54 | 0.42 |
| 1:FA:401:LYS:HE3 | 1:FA:401:LYS:HB2 | 1.74 | 0.42 |
| 2:GD:55:THR:HG21 | 2:HD:284:LEU:H | 1.11 | 0.42 |
| 1:HA:259:LEU:HD11 | 1:HA:316:SER:HB3 | 2.02 | 0.42 |
| 2:HB:232:ALA:HB1 | 2:HB:268:ILE:HD12 | 2.00 | 0.42 |
| 2:IB:99:ASN:HA | 2:IB:142:GLY:H | 1.84 | 0.42 |
| 1:JA:404:PHE:CE2 | 2:JB:345:ILE:HD11 | 2.54 | 0.42 |
| 2:JB:226:ASN:ND2 | 13:JB:501:GDP:HN1 | 2.12 | 0.42 |
| 1:JC:259:LEU:HD11 | 1:JC:316:SER:HB3 | 2.02 | 0.42 |
| 2:JD:69:GLU:HA | 2:JD:70:PRO:HD3 | 1.89 | 0.42 |
| 1:JE:259:LEU:HD11 | 1:JE:316:SER:HB3 | 2.02 | 0.42 |
| 1:JE:317:MET:HE2 | 1:JE:319:TYR:CE1 | 2.54 | 0.42 |
| 2:KB:73:MET:CE | 2:KB:92:PHE:HB3 | 2.49 | 0.42 |
| 1:KC:259:LEU:HD11 | 1:KC:316:SER:HB3 | 2.02 | 0.42 |
| 2:KF:77:ARG:CD | 2:LF:281:TYR:CE2 | 3.01 | 0.42 |
| 1:LA:259:LEU:HD11 | 1:LA:316:SER:HB3 | 2.02 | 0.42 |
| 1:LA:317:MET:HE2 | 1:LA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:LC:176:GLN:O | 2:LD:347:ASN:CG | 2.61 | 0.42 |
| 1:LC:259:LEU:HD11 | 1:LC:316:SER:HB3 | 2.02 | 0.42 |
| 1:LC:356:ASN:OD1 | 1:LC:357:TYR:N | 2.51 | 0.42 |
| 2:LF:226:ASN:ND2 | 13:LF:501:GDP:HN1 | 2.12 | 0.42 |
| 2:MB:69:GLU:HA | 2:MB:70:PRO:HD3 | 1.89 | 0.42 |
| 6:4B:97:GLN:HE21 | 6:4B:97:GLN:HB2 | 1.49 | 0.42 |
| 6:4C:258:ASP:O | 6:4C:262:ASN:HB2 | 2.18 | 0.42 |
| 6:4D:117:ARG:HA | 6:4D:120:GLN:CD | 2.43 | 0.42 |
| 7:5A:1397:GLU:N | 7:5A:1397:GLU:CD | 2.77 | 0.42 |
| 7:5A:1406:PHE:O | 7:5A:1409:PHE:N | 2.53 | 0.42 |
| 7:5A:1436:ARG:NH2 | 7:5A:1437:ASN:HA | 2.33 | 0.42 |
| 7:5B:829:GLY:HA2 | 8:6B:109:ILE:HG21 | 2.01 | 0.42 |
| 7:5B:1267:CYS:C | 7:5B:1270:ASP:H | 2.24 | 0.42 |
| 7:5B:1386:LYS:N | 7:5B:1386:LYS:HZ2 | 2.17 | 0.42 |
| 7:5B:1406:PHE:O | 7:5B:1409:PHE:N | 2.53 | 0.42 |
| 7:5B:1436:ARG:NH2 | 7:5B:1437:ASN:HA | 2.33 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5B:1530:ILE:CG2 | 7:5B:1574:ILE:HG21 | 2.50 | 0.42 |
| 7:5C:1253:ILE:HD12 | 7:5C:1261:ALA:CB | 2.47 | 0.42 |
| 7:5C:1397:GLU:N | 7:5C:1397:GLU:CD | 2.77 | 0.42 |
| 7:5C:1406:PHE:O | 7:5C:1409:PHE:N | 2.53 | 0.42 |
| 7:5C:1436:ARG:NH2 | 7:5C:1437:ASN:HA | 2.33 | 0.42 |
| 2:AD:73:MET:CE | 2:AD:92:PHE:HB3 | 2.49 | 0.42 |
| 1:AE:386:GLU:CD | 3:1A:76:ARG:HH21 | 2.26 | 0.42 |
| 2:AF:357:PRO:HG2 | 6:4A:151:ARG:CD | 2.49 | 0.42 |
| 1:BE:356:ASN:OD1 | 1:BE:357:TYR:N | 2.51 | 0.42 |
| 1:CA:164:LYS:HA | 1:CA:164:LYS:HD3 | 1.85 | 0.42 |
| 1:DA:317:MET:HE2 | 1:DA:319:TYR:CE1 | 2.54 | 0.42 |
| 2:DD:60:VAL:HG23 | 2:ED:281:TYR:CE1 | 2.54 | 0.42 |
| 1:DE:322:ASP:OD1 | 1:DE:373:ARG:NH1 | 2.52 | 0.42 |
| 2:DF:86:ARG:CA | 2:EF:281:TYR:CZ | 2.83 | 0.42 |
| 1:EC:171:ILE:HG23 | 1:EC:204:LEU:O | 2.19 | 0.42 |
| 1:FA:317:MET:HE2 | 1:FA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:FA:394:LYS:HG2 | 2:FB:346:PRO:CG | 2.49 | 0.42 |
| 1:FC:259:LEU:HD11 | 1:FC:316:SER:HB3 | 2.02 | 0.42 |
| 2:FD:232:ALA:HB1 | 2:FD:268:ILE:HD12 | 2.00 | 0.42 |
| 1:FE:259:LEU:HD11 | 1:FE:316:SER:HB3 | 2.02 | 0.42 |
| 2:FF:232:ALA:HB1 | 2:FF:268:ILE:HD12 | 2.00 | 0.42 |
| 1:GA:101:ASN:HA | 1:GA:144:GLY:H | 1.83 | 0.42 |
| 2:GB:68:LEU:HD12 | 2:GB:68:LEU:HA | 1.90 | 0.42 |
| 1:GC:356:ASN:OD1 | 1:GC:357:TYR:N | 2.51 | 0.42 |
| 1:GE:68:LEU:HD22 | 1:GE:153:LEU:HD11 | 2.00 | 0.42 |
| 1:GE:356:ASN:OD1 | 1:GE:357:TYR:N | 2.51 | 0.42 |
| 2:HB:391:ARG:HD2 | 2:HB:391:ARG:HA | 1.79 | 0.42 |
| 1:HE:259:LEU:HD11 | 1:HE:316:SER:HB3 | 2.02 | 0.42 |
| 2:HF:362:LYS:HD3 | 10:8U:37:UNK:CB | 2.49 | 0.42 |
| 2:ID:99:ASN:HA | 2:ID:142:GLY:H | 1.83 | 0.42 |
| 2:IF:99:ASN:HA | 2:IF:142:GLY:H | 1.83 | 0.42 |
| 1:JA:226:ASN:ND2 | 1:JA:367:ASP:OD2 | 2.51 | 0.42 |
| 1:JA:259:LEU:HD11 | 1:JA:316:SER:HB3 | 2.02 | 0.42 |
| 1:JC:317:MET:HE2 | 1:JC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:JC:404:PHE:CE2 | 2:JD:345:ILE:HD11 | 2.54 | 0.42 |
| 1:KA:259:LEU:HD11 | 1:KA:316:SER:HB3 | 2.02 | 0.42 |
| 2:KB:55:THR:CB | 2:LB:363:MET:HE3 | 2.49 | 0.42 |
| 2:KD:87:PRO:HG2 | 2:LD:282:ARG:HD2 | 2.01 | 0.42 |
| 1:KE:259:LEU:HD11 | 1:KE:316:SER:HB3 | 2.02 | 0.42 |
| 2:KF:276:ARG:HD3 | 6:4D:270:GLY:HA3 | 1.22 | 0.42 |
| 1:LA:356:ASN:OD1 | 1:LA:357:TYR:N | 2.51 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LB:294:PHE:O | 4:2C:148:ASN:O | 2.37 | 0.42 |
| 1:MA:100:ALA:HB1 | 2:MB:252:LYS:N | 2.34 | 0.42 |
| 2:MB:212:PHE:CZ | 1:MC:326:LYS:CD | 2.48 | 0.42 |
| 1:MC:356:ASN:OD1 | 1:MC:357:TYR:N | 2.51 | 0.42 |
| 1:MC:357:TYR:CE2 | 6:4A:185:ARG:NH2 | 2.76 | 0.42 |
| 1:ME:356:ASN:OD1 | 1:ME:357:TYR:N | 2.51 | 0.42 |
| 4:2A:164:ARG:O | 4:2A:164:ARG:HG3 | 2.19 | 0.42 |
| 7:5A:1374:ASP:HA | 7:5A:1377:LYS:CE | 2.45 | 0.42 |
| 7:5A:1428:GLU:CD | 7:5A:1428:GLU:C | 2.85 | 0.42 |
| 7:5B:1399:LYS:C | 7:5B:1399:LYS:HZ2 | 2.27 | 0.42 |
| 7:5C:1036:SER:HB2 | 7:5C:1043:ARG:HD3 | 2.02 | 0.42 |
| 7:5C:1416:LYS:HB2 | 7:5C:1416:LYS:HE2 | 1.63 | 0.42 |
| 8:6C:107:PRO:HA | 8:6C:118:GLU:CD | 2.44 | 0.42 |
| 1:AA:328:VAL:O | 1:AA:332:ILE:HG12 | 2.20 | 0.42 |
| 1:AA:356:ASN:OD1 | 1:AA:357:TYR:N | 2.51 | 0.42 |
| 2:AB:222:TYR:CE2 | 1:AC:325:PRO:HG2 | 2.55 | 0.42 |
| 2:AF:73:MET:CE | 2:AF:92:PHE:HB3 | 2.49 | 0.42 |
| 1:BC:356:ASN:OD1 | 1:BC:357:TYR:N | 2.51 | 0.42 |
| 2:BD:212:PHE:CE2 | 1:BE:326:LYS:HB2 | 2.55 | 0.42 |
| 1:BE:224:TYR:CE2 | 2:BF:246:LEU:HD11 | 2.52 | 0.42 |
| 1:CA:93:ILE:H | 1:CA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:CC:317:MET:HE2 | 1:CC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:CE:356:ASN:OD1 | 1:CE:357:TYR:N | 2.51 | 0.42 |
| 2:DB:222:TYR:CE2 | 1:DC:325:PRO:HG2 | 2.53 | 0.42 |
| 2:DB:232:ALA:HB1 | 2:DB:268:ILE:HD12 | 2.00 | 0.42 |
| 1:DC:317:MET:HE2 | 1:DC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:EA:221:ARG:NH1 | 2:EB:324:LYS:N | 2.67 | 0.42 |
| 1:EE:171:ILE:HG23 | 1:EE:204:LEU:O | 2.18 | 0.42 |
| 1:FA:259:LEU:HD11 | 1:FA:316:SER:HB3 | 2.02 | 0.42 |
| 2:FB:69:GLU:HA | 2:FB:70:PRO:HD3 | 1.89 | 0.42 |
| 2:FD:55:THR:OG1 | 2:GD:282:ARG:O | 2.35 | 0.42 |
| 2:GB:178:THR:HA | 1:GC:352:LYS:CD | 2.49 | 0.42 |
| 2:GB:222:TYR:CE2 | 1:GC:325:PRO:HG2 | 2.54 | 0.42 |
| 1:HE:60:LYS:NZ | 1:IE:283:HIS:CE1 | 2.87 | 0.42 |
| 1:IA:60:LYS:NZ | 1:JA:283:HIS:CE1 | 2.87 | 0.42 |
| 1:IC:93:ILE:HD12 | 1:IC:93:ILE:H | 1.85 | 0.42 |
| 2:ID:69:GLU:HA | 2:ID:70:PRO:HD3 | 1.89 | 0.42 |
| 1:JA:89:PRO:HD3 | 1:KA:283:HIS:NE2 | 2.22 | 0.42 |
| 1:JA:328:VAL:O | 1:JA:332:ILE:HG12 | 2.20 | 0.42 |
| 2:JD:177:ASP:CG | 1:JE:353:VAL:HG13 | 2.00 | 0.42 |
| 1:JE:226:ASN:ND2 | 1:JE:367:ASP:OD2 | 2.51 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:KA:87:PHE:O | 1:LA:284:GLU:N | 2.51 | 0.42 |
| 2:KB:99:ASN:HA | 2:KB:142:GLY:H | 1.84 | 0.42 |
| 1:KC:401:LYS:HE3 | 1:KC:401:LYS:HB2 | 1.74 | 0.42 |
| 1:KE:224:TYR:CE2 | 2:KF:246:LEU:HD11 | 2.46 | 0.42 |
| 1:LC:317:MET:HE2 | 1:LC:319:TYR:CE1 | 2.54 | 0.42 |
| 2:LD:18:ALA:CB | 6:4B:217:ASN:ND2 | 2.76 | 0.42 |
| 2:LD:391:ARG:HA | 2:LD:391:ARG:HD2 | 1.79 | 0.42 |
| 1:LE:56:THR:OG1 | 1:ME:284:GLU:CA | 2.67 | 0.42 |
| 1:LE:60:LYS:HE3 | 6:4B:101:ARG:CZ | 2.49 | 0.42 |
| 2:LF:227:HIS:CE1 | 6:4D:226:ILE:CD1 | 3.03 | 0.42 |
| 1:MA:356:ASN:OD1 | 1:MA:357:TYR:N | 2.51 | 0.42 |
| 2:MD:222:TYR:CD2 | 1:ME:247:ALA:HB1 | 2.55 | 0.42 |
| 2:MD:391:ARG:HA | 2:MD:391:ARG:HD2 | 1.79 | 0.42 |
| 1:ME:164:LYS:HA | 1:ME:164:LYS:HD3 | 1.85 | 0.42 |
| 6:4C:113:ILE:H | 6:4C:113:ILE:HG13 | 1.44 | 0.42 |
| 6:4C:260:ARG:HH22 | 6:4C:295:LYS:HE2 | 1.82 | 0.42 |
| 6:4D:118:ILE:HA | 6:4D:121:ARG:HD2 | 2.02 | 0.42 |
| 7:5A:1036:SER:HB2 | 7:5A:1043:ARG:HD3 | 2.02 | 0.42 |
| 7:5A:1388:GLN:O | 7:5A:1392:LEU:N | 2.43 | 0.42 |
| 7:5A:1399:LYS:C | 7:5A:1399:LYS:HZ3 | 2.27 | 0.42 |
| 7:5A:1530:ILE:CG2 | 7:5A:1574:ILE:HG21 | 2.50 | 0.42 |
| 7:5B:1036:SER:HB2 | 7:5B:1043:ARG:HD3 | 2.02 | 0.42 |
| 7:5B:1407:GLN:NE2 | 7:5B:1407:GLN:HA | 2.35 | 0.42 |
| 7:5C:1548:VAL:HB | 7:5C:1566:GLU:HA | 1.92 | 0.42 |
| 8:6C:19:VAL:HG11 | 8:6C:34:LEU:HD11 | 2.01 | 0.42 |
| 2:AD:380:ARG:HE | 2:AD:380:ARG:HB3 | 1.72 | 0.42 |
| 1:AE:317:MET:HE2 | 1:AE:319:TYR:CE1 | 2.54 | 0.42 |
| 1:BE:328:VAL:O | 1:BE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:CA:248:LEU:HD12 | 1:CA:248:LEU:HA | 1.89 | 0.42 |
| 1:CA:259:LEU:HD11 | 1:CA:316:SER:HB3 | 2.02 | 0.42 |
| 1:CA:317:MET:HE2 | 1:CA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:CC:93:ILE:H | 1:CC:93:ILE:HD12 | 1.85 | 0.42 |
| 2:CF:226:ASN:ND2 | 13:CF:501:GDP:HN1 | 2.12 | 0.42 |
| 1:DA:262:TYR:HB2 | 1:DA:265:ILE:HD12 | 2.02 | 0.42 |
| 1:DE:262:TYR:HB2 | 1:DE:265:ILE:HD12 | 2.02 | 0.42 |
| 1:DE:317:MET:HE2 | 1:DE:319:TYR:CE1 | 2.54 | 0.42 |
| 1:EE:93:ILE:H | 1:EE:93:ILE:HD12 | 1.85 | 0.42 |
| 1:EE:356:ASN:OD1 | 1:EE:357:TYR:N | 2.51 | 0.42 |
| 2:FB:55:THR:HG21 | 2:GB:284:LEU:HB2 | 2.01 | 0.42 |
| 1:FC:248:LEU:HD12 | 1:FC:248:LEU:HA | 1.89 | 0.42 |
| 2:FF:262:ARG:NH1 | 2:FF:421:GLU:OE1 | 2.50 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:GA:328:VAL:O | 1:GA:332:ILE:HG12 | 2.20 | 0.42 |
| 1:GC:404:PHE:CE2 | 2:GD:345:ILE:HD11 | 2.55 | 0.42 |
| 1:HC:71:GLU:OE2 | 1:HC:73:THR:OG1 | 2.28 | 0.42 |
| 1:JC:226:ASN:ND2 | 1:JC:367:ASP:OD2 | 2.51 | 0.42 |
| 1:KC:245:ASP:OD2 | 6:4A:257:LEU:HD12 | 2.20 | 0.42 |
| 2:KD:73:MET:CE | 2:KD:92:PHE:HB3 | 2.49 | 0.42 |
| 2:KF:221:THR:HB | 6:4D:261:SER:HA | 1.57 | 0.42 |
| 1:LA:248:LEU:HD12 | 1:LA:248:LEU:HA | 1.89 | 0.42 |
| 2:MB:99:ASN:HA | 2:MB:142:GLY:H | 1.83 | 0.42 |
| 2:MD:177:ASP:CA | 1:ME:353:VAL:HG12 | 2.49 | 0.42 |
| 4:2B:164:ARG:HG3 | 4:2B:164:ARG:O | 2.19 | 0.42 |
| 6:4A:239:LEU:HD13 | 6:4A:239:LEU:HA | 1.83 | 0.42 |
| 6:4C:266:ASN:HB2 | 6:4C:273:ARG:NE | 2.34 | 0.42 |
| 7:5A:1407:GLN:NE2 | 7:5A:1407:GLN:HA | 2.35 | 0.42 |
| 7:5B:1490:LYS:CG | 7:5B:1494:LEU:CG | 2.95 | 0.42 |
| 7:5C:1407:GLN:NE2 | 7:5C:1407:GLN:HA | 2.35 | 0.42 |
| 7:5C:1530:ILE:CG2 | 7:5C:1574:ILE:HG21 | 2.50 | 0.42 |
| 8:6A:107:PRO:HA | 8:6A:118:GLU:CD | 2.44 | 0.42 |
| 9:7D:18:VAL:HG11 | 9:7D:42:LEU:HD22 | 2.00 | 0.42 |
| 2:AB:178:THR:HA | 1:AC:352:LYS:CD | 2.49 | 0.42 |
| 1:AC:262:TYR:HB2 | 1:AC:265:ILE:HD12 | 2.02 | 0.42 |
| 1:AC:317:MET:HE2 | 1:AC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:AC:328:VAL:O | 1:AC:332:ILE:HG12 | 2.20 | 0.42 |
| 1:AC:356:ASN:OD1 | 1:AC:357:TYR:N | 2.51 | 0.42 |
| 1:AE:328:VAL:O | 1:AE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:AE:356:ASN:OD1 | 1:AE:357:TYR:N | 2.51 | 0.42 |
| 1:BA:317:MET:HE2 | 1:BA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:BA:328:VAL:O | 1:BA:332:ILE:HG12 | 2.20 | 0.42 |
| 1:CC:259:LEU:HD11 | 1:CC:316:SER:HB3 | 2.01 | 0.42 |
| 2:CD:222:TYR:CE2 | 1:CE:325:PRO:HG2 | 2.54 | 0.42 |
| 1:CE:93:ILE:H | 1:CE:93:ILE:HD12 | 1.85 | 0.42 |
| 1:CE:328:VAL:O | 1:CE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:CE:398:MET:SD | 2:CF:345:ILE:CG1 | 2.94 | 0.42 |
| 2:CF:268:ILE:HG13 | 2:CF:300:MET:HG3 | 2.02 | 0.42 |
| 1:DC:262:TYR:HB2 | 1:DC:265:ILE:HD12 | 2.02 | 0.42 |
| 1:DC:328:VAL:O | 1:DC:332:ILE:HG12 | 2.20 | 0.42 |
| 1:DC:394:LYS:NZ | 2:DD:347:ASN:OD1 | 2.53 | 0.42 |
| 1:DE:328:VAL:O | 1:DE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:EA:60:LYS:HD3 | 1:FA:283:HIS:HD2 | 1.27 | 0.42 |
| 1:EA:93:ILE:H | 1:EA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:EA:248:LEU:HD12 | 1:EA:248:LEU:HA | 1.89 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:EA:328:VAL:O | 1:EA:332:ILE:HG12 | 2.20 | 0.42 |
| 1:EC:328:VAL:O | 1:EC:332:ILE:HG12 | 2.20 | 0.42 |
| 2:ED:55:THR:H | 2:FD:283:ALA:HB2 | 1.85 | 0.42 |
| 1:EE:328:VAL:O | 1:EE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:FA:164:LYS:HA | 1:FA:164:LYS:HD3 | 1.85 | 0.42 |
| 1:FA:328:VAL:O | 1:FA:332:ILE:HG12 | 2.20 | 0.42 |
| 2:FB:55:THR:HG21 | 2:GB:284:LEU:CA | 2.46 | 0.42 |
| 1:FE:356:ASN:OD1 | 1:FE:357:TYR:N | 2.51 | 0.42 |
| 2:GB:380:ARG:HE | 2:GB:380:ARG:HB3 | 1.72 | 0.42 |
| 1:HA:164:LYS:HA | 1:HA:164:LYS:HD3 | 1.85 | 0.42 |
| 1:HA:222:PRO:CG | 2:HB:324:LYS:CD | 2.91 | 0.42 |
| 1:HC:93:ILE:H | 1:HC:93:ILE:HD12 | 1.85 | 0.42 |
| 1:HC:415:GLU:HG3 | 5:3C:235:LEU:CG | 2.48 | 0.42 |
| 1:IC:393:HIS:CB | 5:3C:308:PHE:CD2 | 3.02 | 0.42 |
| 1:JA:93:ILE:H | 1:JA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:JA:317:MET:HE2 | 1:JA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:JC:93:ILE:H | 1:JC:93:ILE:HD12 | 1.85 | 0.42 |
| 1:JC:328:VAL:O | 1:JC:332:ILE:HG12 | 2.20 | 0.42 |
| 2:JD:87:PRO:HD2 | 2:KD:281:TYR:HD2 | 1.21 | 0.42 |
| 2:JD:391:ARG:HD2 | 2:JD:391:ARG:HA | 1.79 | 0.42 |
| 1:JE:328:VAL:O | 1:JE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:KC:85:GLN:HA | 1:LC:283:HIS:N | 2.31 | 0.42 |
| 2:KD:99:ASN:HA | 2:KD:142:GLY:H | 1.84 | 0.42 |
| 2:KF:73:MET:CE | 2:KF:92:PHE:HB3 | 2.49 | 0.42 |
| 2:KF:99:ASN:HA | 2:KF:142:GLY:H | 1.84 | 0.42 |
| 1:LC:71:GLU:OE2 | 1:LC:73:THR:OG1 | 2.28 | 0.42 |
| 1:LE:181:VAL:HG12 | 2:LF:348:ASN:HA | 2.00 | 0.42 |
| 1:LE:328:VAL:O | 1:LE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:MA:279:GLU:OE1 | 6:4C:106:ALA:HB3 | 2.19 | 0.42 |
| 2:MB:177:ASP:HA | 1:MC:353:VAL:HG12 | 2.02 | 0.42 |
| 2:MB:220:PRO:HD2 | 1:MC:326:LYS:CG | 2.42 | 0.42 |
| 2:MD:99:ASN:HA | 2:MD:142:GLY:H | 1.83 | 0.42 |
| 4:2A:144:ASN:H | 4:2A:144:ASN:HD22 | 1.68 | 0.42 |
| 4:2B:144:ASN:H | 4:2B:144:ASN:HD22 | 1.68 | 0.42 |
| 4:2C:144:ASN:H | 4:2C:144:ASN:HD22 | 1.68 | 0.42 |
| 6:4A:118:ILE:HA | 6:4A:121:ARG:HD2 | 2.02 | 0.42 |
| 6:4A:266:ASN:HB2 | 6:4A:273:ARG:NE | 2.34 | 0.42 |
| 6:4B:118:ILE:HA | 6:4B:121:ARG:HD2 | 2.02 | 0.42 |
| 6:4D:178:HIS:ND1 | 6:4D:178:HIS:C | 2.72 | 0.42 |
| 7:5A:1460:ARG:HE | 7:5A:1460:ARG:HB3 | 1.69 | 0.42 |
| 7:5B:1272:ILE:HD11 | 9:7D:11:TYR:CD2 | 2.53 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1428:GLU:CD | 7:5C:1428:GLU:C | 2.85 | 0.42 |
| 8:6B:107:PRO:HA | 8:6B:118:GLU:CD | 2.44 | 0.42 |
| 9:7A:39:GLY:CA | 9:7B:43:LEU:HG | 2.47 | 0.42 |
| 10:8R:13:UNK:C | 10:8R:15:UNK:N | 2.83 | 0.42 |
| 1:AA:317:MET:HE2 | 1:AA:319:TYR:CE1 | 2.54 | 0.42 |
| 1:AE:262:TYR:HB2 | 1:AE:265:ILE:HD12 | 2.02 | 0.42 |
| 2:BB:179:VAL:HG22 | 1:BC:258:ASN:CA | 2.49 | 0.42 |
| 1:BC:222:PRO:CG | 2:BD:324:LYS:CD | 2.89 | 0.42 |
| 1:BC:248:LEU:HD12 | 1:BC:248:LEU:HA | 1.89 | 0.42 |
| 1:BC:328:VAL:O | 1:BC:332:ILE:HG12 | 2.20 | 0.42 |
| 2:BD:55:THR:HG23 | 2:CD:283:ALA:HA | 2.02 | 0.42 |
| 1:CA:328:VAL:O | 1:CA:332:ILE:HG12 | 2.20 | 0.42 |
| 2:CB:208:TYR:CD2 | 1:CC:326:LYS:HB3 | 2.55 | 0.42 |
| 2:CB:268:ILE:HG13 | 2:CB:300:MET:HG3 | 2.02 | 0.42 |
| 1:CC:328:VAL:O | 1:CC:332:ILE:HG12 | 2.20 | 0.42 |
| 1:CE:317:MET:HE2 | 1:CE:319:TYR:CE1 | 2.54 | 0.42 |
| 1:DA:71:GLU:CD | 2:DB:247:ASN:ND2 | 2.78 | 0.42 |
| 1:DA:328:VAL:O | 1:DA:332:ILE:HG12 | 2.20 | 0.42 |
| 2:DB:179:VAL:HG22 | 1:DC:258:ASN:CG | 2.45 | 0.42 |
| 2:DB:268:ILE:HG13 | 2:DB:300:MET:HG3 | 2.02 | 0.42 |
| 2:DD:176:SER:HG | 1:DE:349:THR:HG1 | 1.51 | 0.42 |
| 2:DD:268:ILE:HG13 | 2:DD:300:MET:HG3 | 2.02 | 0.42 |
| 2:DF:268:ILE:HG13 | 2:DF:300:MET:HG3 | 2.02 | 0.42 |
| 1:EC:93:ILE:H | 1:EC:93:ILE:HD12 | 1.85 | 0.42 |
| 1:EE:262:TYR:HB2 | 1:EE:265:ILE:HD12 | 2.02 | 0.42 |
| 1:FA:322:ASP:OD1 | 1:FA:373:ARG:NH1 | 2.52 | 0.42 |
| 1:FC:328:VAL:O | 1:FC:332:ILE:HG12 | 2.20 | 0.42 |
| 2:FD:179:VAL:HG22 | 1:FE:258:ASN:CG | 2.45 | 0.42 |
| 1:FE:328:VAL:O | 1:FE:332:ILE:HG12 | 2.20 | 0.42 |
| 1:GA:401:LYS:HE3 | 1:GA:401:LYS:HB2 | 1.74 | 0.42 |
| 1:GE:328:VAL:O | 1:GE:332:ILE:HG12 | 2.20 | 0.42 |
| 2:HB:220:PRO:HD2 | 1:HC:326:LYS:CE | 2.44 | 0.42 |
| 1:HE:68:LEU:HD21 | 1:HE:118:CYS:SG | 2.60 | 0.42 |
| 1:HE:93:ILE:H | 1:HE:93:ILE:HD12 | 1.85 | 0.42 |
| 1:IA:226:ASN:ND2 | 1:IA:367:ASP:OD2 | 2.51 | 0.42 |
| 2:IB:222:TYR:CE2 | 1:IC:325:PRO:HG2 | 2.55 | 0.42 |
| 1:IE:93:ILE:HD12 | 1:IE:93:ILE:H | 1.85 | 0.42 |
| 1:IE:278:ALA:HB1 | 10:8X:18:UNK:C | 2.39 | 0.42 |
| 2:JB:222:TYR:CE2 | 1:JC:325:PRO:HG2 | 2.54 | 0.42 |
| 1:KA:84:ARG:NH2 | 1:LA:279:GLU:O | 2.48 | 0.42 |
| 2:KB:222:TYR:CE2 | 1:KC:325:PRO:HG2 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:KC:404:PHE:CE2 | 2:KD:345:ILE:HD11 | 2.55 | 0.42 |
| 2:KF:217:LEU:HB2 | 6:4D:265:TYR:OH | 2.03 | 0.42 |
| 2:LB:375:GLN:O | 2:LB:379:LYS:HG3 | 2.20 | 0.42 |
| 1:LC:328:VAL:O | 1:LC:332:ILE:HG12 | 2.20 | 0.42 |
| 1:LE:89:PRO:CA | 1:ME:280:LYS:HZ2 | 2.33 | 0.42 |
| 1:LE:262:TYR:HB2 | 1:LE:265:ILE:HD12 | 2.02 | 0.42 |
| 1:LE:317:MET:HE2 | 1:LE:319:TYR:CE1 | 2.54 | 0.42 |
| 2:MF:99:ASN:HA | 2:MF:142:GLY:H | 1.84 | 0.42 |
| 6:4B:266:ASN:HB2 | 6:4B:273:ARG:NE | 2.34 | 0.42 |
| 6:4D:266:ASN:HB2 | 6:4D:273:ARG:NE | 2.34 | 0.42 |
| 7:5A:891:LEU:HD13 | 7:5A:1024:LEU:CD2 | 2.49 | 0.42 |
| 7:5A:1316:LEU:HA | 7:5A:1316:LEU:HD13 | 1.87 | 0.42 |
| 7:5B:891:LEU:HD13 | 7:5B:1024:LEU:CD2 | 2.49 | 0.42 |
| 7:5B:1436:ARG:CB | 7:5B:1436:ARG:NH1 | 2.78 | 0.42 |
| 7:5C:1374:ASP:HA | 7:5C:1377:LYS:CE | 2.45 | 0.42 |
| 8:6B:48:ASN:OD1 | 8:6B:145:LYS:HE2 | 2.19 | 0.42 |
| 8:6B:103:CYS:HB3 | 8:6B:138:TRP:NE1 | 2.35 | 0.42 |
| 9:7A:39:GLY:H | 9:7B:43:LEU:HD21 | 1.84 | 0.42 |
| 9:7E:18:VAL:CG1 | 9:7E:42:LEU:HD22 | 2.36 | 0.42 |
| 10:8Q:13:UNK:C | 10:8Q:15:UNK:N | 2.83 | 0.42 |
| 2:AB:68:LEU:HD12 | 2:AB:68:LEU:HA | 1.90 | 0.42 |
| 2:AD:179:VAL:HG23 | 1:AE:258:ASN:HA | 1.97 | 0.42 |
| 1:AE:296:PHE:CE2 | 1:AE:335:ILE:HG21 | 2.55 | 0.42 |
| 1:AE:401:LYS:HE3 | 1:AE:401:LYS:HB2 | 1.74 | 0.42 |
| 1:BA:356:ASN:OD1 | 1:BA:357:TYR:N | 2.51 | 0.42 |
| 1:CA:398:MET:SD | 2:CB:345:ILE:CG1 | 2.94 | 0.42 |
| 2:CD:268:ILE:HG13 | 2:CD:300:MET:HG3 | 2.02 | 0.42 |
| 2:DD:176:SER:CB | 1:DE:349:THR:HG1 | 2.31 | 0.42 |
| 1:EA:262:TYR:HB2 | 1:EA:265:ILE:HD12 | 2.02 | 0.42 |
| 1:EE:71:GLU:HA | 1:EE:72:PRO:HD3 | 1.84 | 0.42 |
| 2:EF:293:MET:HE3 | 2:EF:294:PHE:CD1 | 2.55 | 0.42 |
| 2:FD:131:GLN:O | 2:FD:163:ILE:HG12 | 2.20 | 0.42 |
| 2:FD:262:ARG:NH1 | 2:FD:421:GLU:OE1 | 2.50 | 0.42 |
| 1:GC:328:VAL:O | 1:GC:332:ILE:HG12 | 2.20 | 0.42 |
| 1:HA:68:LEU:HD21 | 1:HA:118:CYS:SG | 2.60 | 0.42 |
| 2:HB:222:TYR:CE2 | 1:HC:325:PRO:HG2 | 2.54 | 0.42 |
| 1:HC:68:LEU:HD21 | 1:HC:118:CYS:SG | 2.60 | 0.42 |
| 2:HD:220:PRO:HD2 | 1:HE:326:LYS:CE | 2.44 | 0.42 |
| 1:HE:58:ALA:HB3 | 10:8X:13:UNK:HA | 2.01 | 0.42 |
| 1:IA:93:ILE:H | 1:IA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:IA:259:LEU:HD11 | 1:IA:316:SER:HB3 | 2.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:IB:85:PHE:C | 2:JB:281:TYR:HH | 2.15 | 0.42 |
| 1:IC:279:GLU:CG | 10:8W:22:UNK:HA | 2.48 | 0.42 |
| 2:ID:131:GLN:O | 2:ID:163:ILE:HG12 | 2.20 | 0.42 |
| 2:ID:424:GLN:HE21 | 7:5A:1413:GLN:NE2 | 0.96 | 0.42 |
| 1:IE:226:ASN:ND2 | 1:IE:367:ASP:OD2 | 2.51 | 0.42 |
| 1:JC:401:LYS:HE3 | 1:JC:401:LYS:HB2 | 1.74 | 0.42 |
| 2:JD:212:PHE:CZ | 1:JE:326:LYS:CE | 2.98 | 0.42 |
| 1:KA:226:ASN:ND2 | 1:KA:367:ASP:OD2 | 2.51 | 0.42 |
| 1:KC:71:GLU:HA | 1:KC:72:PRO:HD3 | 1.85 | 0.42 |
| 1:KE:296:PHE:CE2 | 1:KE:335:ILE:HG21 | 2.55 | 0.42 |
| 2:KF:77:ARG:HD3 | 2:LF:281:TYR:CZ | 2.54 | 0.42 |
| 2:KF:125:GLU:C | 4:2B:38:VAL:HA | 2.45 | 0.42 |
| 1:LC:248:LEU:HD12 | 1:LC:248:LEU:HA | 1.89 | 0.42 |
| 1:LC:262:TYR:HB2 | 1:LC:265:ILE:HD12 | 2.02 | 0.42 |
| 2:LD:226:ASN:ND2 | 13:LD:501:GDP:HN1 | 2.12 | 0.42 |
| 2:LF:294:PHE:HD2 | 4:2B:147:PHE:CE2 | 2.35 | 0.42 |
| 2:MB:218:THR:OG1 | 6:4A:196:GLN:NE2 | 2.49 | 0.42 |
| 1:MC:279:GLU:OE1 | 6:4A:107:MET:CB | 2.67 | 0.42 |
| 6:4A:110:LYS:O | 6:4A:110:LYS:HD3 | 2.20 | 0.42 |
| 6:4A:230:TYR:CD2 | 6:4A:230:TYR:N | 2.74 | 0.42 |
| 6:4B:193:MET:HE3 | 6:4B:193:MET:HB3 | 1.83 | 0.42 |
| 6:4C:110:LYS:O | 6:4C:110:LYS:HD3 | 2.20 | 0.42 |
| 6:4C:118:ILE:HA | 6:4C:121:ARG:HD2 | 2.02 | 0.42 |
| 6:4D:97:GLN:HE21 | 6:4D:97:GLN:HB2 | 1.49 | 0.42 |
| 6:4D:105:GLU:OE2 | 6:4D:105:GLU:HA | 2.17 | 0.42 |
| 6:4D:113:ILE:HB | 6:4D:117:ARG:NH2 | 2.34 | 0.42 |
| 7:5A:1548:VAL:HB | 7:5A:1566:GLU:HA | 1.91 | 0.42 |
| 7:5B:827:GLU:HG3 | 7:5B:849:ARG:HH22 | 1.84 | 0.42 |
| 7:5B:1105:TYR:HB2 | 7:5B:1165:PRO:C | 2.45 | 0.42 |
| 7:5C:891:LEU:HD13 | 7:5C:1024:LEU:CD2 | 2.49 | 0.42 |
| 8:6A:48:ASN:OD1 | 8:6A:145:LYS:HE2 | 2.20 | 0.42 |
| 8:6A:60:PHE:CZ | 8:6A:243:ILE:HG12 | 2.55 | 0.42 |
| 8:6A:142:THR:HG21 | 8:6A:180:GLU:HA | 2.02 | 0.42 |
| 8:6C:23:ASP:OD2 | 8:6C:132:LYS:HE3 | 2.20 | 0.42 |
| 8:6C:34:LEU:HD21 | 8:6C:127:PHE:HE1 | 1.84 | 0.42 |
| 8:6C:103:CYS:HB3 | 8:6C:138:TRP:NE1 | 2.35 | 0.42 |
| 9:7E:11:TYR:OH | 9:7F:27:GLY:CA | 2.67 | 0.42 |
| 10:8K:13:UNK:C | 10:8K:15:UNK:N | 2.83 | 0.42 |
| 1:AA:262:TYR:HB2 | 1:AA:265:ILE:HD12 | 2.02 | 0.42 |
| 1:AA:407:TRP:HE3 | 2:AB:255:VAL:HG13 | 0.97 | 0.42 |
| 2:AB:293:MET:HE3 | 2:AB:294:PHE:CD1 | 2.55 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AD:179:VAL:HG21 | 1:AE:258:ASN:CA | 2.50 | 0.42 |
| 2:AF:69:GLU:HA | 2:AF:70:PRO:HD3 | 1.89 | 0.42 |
| 1:BA:222:PRO:CG | 2:BB:324:LYS:CD | 2.90 | 0.42 |
| 1:BC:259:LEU:HD11 | 1:BC:316:SER:HB3 | 2.01 | 0.42 |
| 1:BC:317:MET:HE2 | 1:BC:319:TYR:CE1 | 2.54 | 0.42 |
| 1:BE:259:LEU:HD11 | 1:BE:316:SER:HB3 | 2.02 | 0.42 |
| 1:CA:262:TYR:HB2 | 1:CA:265:ILE:HD12 | 2.02 | 0.42 |
| 2:CB:179:VAL:HG22 | 1:CC:258:ASN:HA | 1.99 | 0.42 |
| 2:CB:375:GLN:O | 2:CB:379:LYS:HG3 | 2.20 | 0.42 |
| 2:CD:226:ASN:ND2 | 13:CD:501:GDP:HN1 | 2.12 | 0.42 |
| 2:CD:375:GLN:O | 2:CD:379:LYS:HG3 | 2.20 | 0.42 |
| 1:CE:259:LEU:HD11 | 1:CE:316:SER:HB3 | 2.02 | 0.42 |
| 2:CF:375:GLN:O | 2:CF:379:LYS:HG3 | 2.20 | 0.42 |
| 1:EC:71:GLU:CD | 2:ED:247:ASN:HD22 | 2.27 | 0.42 |
| 1:EC:262:TYR:HB2 | 1:EC:265:ILE:HD12 | 2.02 | 0.42 |
| 1:EC:356:ASN:OD1 | 1:EC:357:TYR:N | 2.51 | 0.42 |
| 2:ED:293:MET:HE3 | 2:ED:294:PHE:CD1 | 2.55 | 0.42 |
| 2:FB:131:GLN:O | 2:FB:163:ILE:HG12 | 2.20 | 0.42 |
| 1:FC:356:ASN:OD1 | 1:FC:357:TYR:N | 2.51 | 0.42 |
| 1:FE:262:TYR:HB2 | 1:FE:265:ILE:HD12 | 2.02 | 0.42 |
| 1:GC:93:ILE:H | 1:GC:93:ILE:HD12 | 1.85 | 0.42 |
| 1:GE:398:MET:SD | 2:GF:345:ILE:CG1 | 2.92 | 0.42 |
| 1:HA:93:ILE:H | 1:HA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:HA:356:ASN:OD1 | 1:HA:357:TYR:N | 2.51 | 0.42 |
| 2:HB:131:GLN:O | 2:HB:163:ILE:HG12 | 2.20 | 0.42 |
| 1:HC:262:TYR:HB2 | 1:HC:265:ILE:HD12 | 2.02 | 0.42 |
| 2:HD:131:GLN:O | 2:HD:163:ILE:HG12 | 2.20 | 0.42 |
| 1:HE:356:ASN:OD1 | 1:HE:357:TYR:N | 2.51 | 0.42 |
| 2:IB:131:GLN:O | 2:IB:163:ILE:HG12 | 2.20 | 0.42 |
| 2:IB:220:PRO:HD2 | 1:IC:326:LYS:CG | 2.46 | 0.42 |
| 1:IC:226:ASN:ND2 | 1:IC:367:ASP:OD2 | 2.51 | 0.42 |
| 1:IC:434:GLU:CG | 5:3C:61:SER:HA | 2.50 | 0.42 |
| 1:IE:224:TYR:CE2 | 2:IF:246:LEU:HD11 | 2.46 | 0.42 |
| 2:IF:131:GLN:O | 2:IF:163:ILE:HG12 | 2.20 | 0.42 |
| 2:JB:69:GLU:HA | 2:JB:70:PRO:HD3 | 1.89 | 0.42 |
| 2:JB:85:PHE:O | 2:KB:281:TYR:CE2 | 2.62 | 0.42 |
| 2:JB:131:GLN:O | 2:JB:163:ILE:HG12 | 2.20 | 0.42 |
| 1:JE:93:ILE:H | 1:JE:93:ILE:HD12 | 1.85 | 0.42 |
| 1:JE:356:ASN:OD1 | 1:JE:357:TYR:N | 2.51 | 0.42 |
| 1:KC:262:TYR:HB2 | 1:KC:265:ILE:HD12 | 2.02 | 0.42 |
| 2:KD:117:LEU:HD21 | 4:2A:144:ASN:OD1 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KE:356:ASN:OD1 | 1:KE:357:TYR:N | 2.51 | 0.42 |
| 1:LA:93:ILE:H | 1:LA:93:ILE:HD12 | 1.85 | 0.42 |
| 1:LA:100:ALA:O | 2:LB:255:VAL:HG21 | 2.19 | 0.42 |
| 1:LA:262:TYR:HB2 | 1:LA:265:ILE:HD12 | 2.02 | 0.42 |
| 1:LA:328:VAL:O | 1:LA:332:ILE:HG12 | 2.20 | 0.42 |
| 1:MA:296:PHE:CE2 | 1:MA:335:ILE:HG21 | 2.55 | 0.42 |
| 2:MB:375:GLN:O | 2:MB:379:LYS:HG3 | 2.20 | 0.42 |
| 1:ME:224:TYR:CE2 | 2:MF:246:LEU:HD11 | 2.47 | 0.42 |
| 6:4A:113:ILE:H | 6:4A:113:ILE:HG13 | 1.44 | 0.42 |
| 6:4B:105:GLU:OE2 | 6:4B:105:GLU:HA | 2.17 | 0.42 |
| 6:4B:113:ILE:HB | 6:4B:117:ARG:NH2 | 2.34 | 0.42 |
| 6:4C:266:ASN:CG | 6:4C:269:THR:HG23 | 2.45 | 0.42 |
| 7:5A:1471:ILE:H | 7:5A:1471:ILE:CD1 | 2.18 | 0.42 |
| 7:5B:1259:TYR:O | 7:5B:1263:GLN:HG2 | 2.19 | 0.42 |
| 7:5B:1370:LYS:HD3 | 7:5B:1370:LYS:HA | 1.61 | 0.42 |
| 7:5B:1388:GLN:O | 7:5B:1392:LEU:N | 2.43 | 0.42 |
| 7:5C:930:MET:HE1 | 7:5C:1018:PHE:CE2 | 2.55 | 0.42 |
| 8:6A:103:CYS:HB3 | 8:6A:138:TRP:NE1 | 2.35 | 0.42 |
| 8:6B:60:PHE:CZ | 8:6B:243:ILE:HG12 | 2.55 | 0.42 |
| 8:6B:142:THR:HG21 | 8:6B:180:GLU:HA | 2.02 | 0.42 |
| 8:6C:48:ASN:OD1 | 8:6C:145:LYS:HE2 | 2.20 | 0.42 |
| 8:6C:142:THR:HG21 | 8:6C:180:GLU:HA | 2.02 | 0.42 |
| 8:6C:206:ASN:O | 8:6C:214:LYS:HE2 | 2.20 | 0.42 |
| 9:7E:11:TYR:CE1 | 9:7F:26:LEU:CG | 2.89 | 0.42 |
| 9:7E:39:GLY:CA | 9:7F:43:LEU:HD11 | 2.48 | 0.42 |
| 10:8L:13:UNK:C | 10:8L:15:UNK:N | 2.83 | 0.42 |
| 10:8P:13:UNK:C | 10:8P:15:UNK:N | 2.83 | 0.42 |
| 1:AA:226:ASN:ND2 | 1:AA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:AD:293:MET:HE3 | 2:AD:294:PHE:CD1 | 2.55 | 0.41 |
| 2:BD:222:TYR:CE2 | 1:BE:325:PRO:HG2 | 2.55 | 0.41 |
| 2:BD:391:ARG:HA | 2:BD:391:ARG:HD2 | 1.78 | 0.41 |
| 1:BE:317:MET:HE2 | 1:BE:319:TYR:CE1 | 2.54 | 0.41 |
| 1:CC:248:LEU:HD12 | 1:CC:248:LEU:HA | 1.89 | 0.41 |
| 1:CE:262:TYR:HB2 | 1:CE:265:ILE:HD12 | 2.02 | 0.41 |
| 1:CE:296:PHE:CE2 | 1:CE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:DA:296:PHE:CE2 | 1:DA:335:ILE:HG21 | 2.55 | 0.41 |
| 1:DA:407:TRP:HE3 | 2:DB:255:VAL:HG13 | 1.06 | 0.41 |
| 2:DB:391:ARG:HD2 | 2:DB:391:ARG:HA | 1.79 | 0.41 |
| 2:DD:390:ARG:CD | 1:DE:439:THR:HG21 | 2.50 | 0.41 |
| 1:DE:128:ASN:HD21 | 1:EE:285:GLN:NE2 | 2.18 | 0.41 |
| 1:EA:356:ASN:OD1 | 1:EA:357:TYR:N | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:EB:293:MET:HE3 | 2:EB:294:PHE:CD1 | 2.55 | 0.41 |
| 1:FC:62:VAL:CG2 | 1:GC:283:HIS:O | 2.68 | 0.41 |
| 1:FC:221:ARG:NH1 | 2:FD:324:LYS:N | 2.68 | 0.41 |
| 1:FC:262:TYR:HB2 | 1:FC:265:ILE:HD12 | 2.02 | 0.41 |
| 1:FE:226:ASN:ND2 | 1:FE:367:ASP:OD2 | 2.51 | 0.41 |
| 1:FE:248:LEU:HD12 | 1:FE:248:LEU:HA | 1.89 | 0.41 |
| 2:FF:131:GLN:O | 2:FF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:GB:131:GLN:O | 2:GB:163:ILE:HG12 | 2.20 | 0.41 |
| 1:GE:93:ILE:H | 1:GE:93:ILE:HD12 | 1.85 | 0.41 |
| 1:HC:356:ASN:OD1 | 1:HC:357:TYR:N | 2.51 | 0.41 |
| 1:HE:262:TYR:HB2 | 1:HE:265:ILE:HD12 | 2.02 | 0.41 |
| 2:HF:131:GLN:O | 2:HF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:HF:268:ILE:HG13 | 2:HF:300:MET:HG3 | 2.02 | 0.41 |
| 1:IA:164:LYS:HA | 1:IA:164:LYS:HD3 | 1.86 | 0.41 |
| 1:IA:328:VAL:O | 1:IA:332:ILE:HG12 | 2.20 | 0.41 |
| 1:IC:259:LEU:HD11 | 1:IC:316:SER:HB3 | 2.02 | 0.41 |
| 1:JA:68:LEU:HD21 | 1:JA:118:CYS:SG | 2.60 | 0.41 |
| 2:JD:131:GLN:O | 2:JD:163:ILE:HG12 | 2.20 | 0.41 |
| 2:JF:131:GLN:O | 2:JF:163:ILE:HG12 | 2.20 | 0.41 |
| 1:KA:356:ASN:OD1 | 1:KA:357:TYR:N | 2.51 | 0.41 |
| 1:KC:356:ASN:OD1 | 1:KC:357:TYR:N | 2.51 | 0.41 |
| 1:KE:262:TYR:HB2 | 1:KE:265:ILE:HD12 | 2.02 | 0.41 |
| 2:KF:131:GLN:O | 2:KF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:LD:375:GLN:O | 2:LD:379:LYS:HG3 | 2.20 | 0.41 |
| 2:LF:268:ILE:HG13 | 2:LF:300:MET:HG3 | 2.02 | 0.41 |
| 1:MA:96:LYS:HE2 | 2:MB:1:MET:CE | 2.50 | 0.41 |
| 1:MA:226:ASN:ND2 | 1:MA:367:ASP:OD2 | 2.51 | 0.41 |
| 1:MC:226:ASN:ND2 | 1:MC:367:ASP:OD2 | 2.51 | 0.41 |
| 6:4B:110:LYS:O | 6:4B:110:LYS:HD3 | 2.20 | 0.41 |
| 6:4B:266:ASN:CG | 6:4B:269:THR:HG23 | 2.45 | 0.41 |
| 6:4C:230:TYR:CD2 | 6:4C:230:TYR:N | 2.74 | 0.41 |
| 6:4D:95:SER:O | 6:4D:95:SER:OG | 2.38 | 0.41 |
| 7:5A:827:GLU:HG3 | 7:5A:849:ARG:HH22 | 1.84 | 0.41 |
| 7:5A:1105:TYR:HB2 | 7:5A:1165:PRO:C | 2.45 | 0.41 |
| 7:5C:1244:LEU:O | 7:5C:1246:LEU:N | 2.53 | 0.41 |
| 7:5C:1490:LYS:CE | 7:5C:1494:LEU:CD2 | 2.98 | 0.41 |
| 8:6A:34:LEU:HD21 | 8:6A:127:PHE:HE1 | 1.84 | 0.41 |
| 8:6B:34:LEU:HD21 | 8:6B:127:PHE:HE1 | 1.84 | 0.41 |
| 9:7A:15:VAL:HG11 | 9:7B:35:ILE:HA | 1.97 | 0.41 |
| 10:8B:13:UNK:C | 10:8B:15:UNK:N | 2.83 | 0.41 |
| 1:AC:296:PHE:CE2 | 1:AC:335:ILE:HG21 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:404:PHE:CE2 | 2:AD:345:ILE:HD11 | 2.54 | 0.41 |
| 2:AD:274:THR:O | 6:4C:134:LEU:HD11 | 2.20 | 0.41 |
| 1:AE:226:ASN:ND2 | 1:AE:367:ASP:OD2 | 2.51 | 0.41 |
| 2:AF:55:THR:CG2 | 2:BF:283:ALA:CA | 2.80 | 0.41 |
| 2:AF:293:MET:HE3 | 2:AF:294:PHE:CD1 | 2.55 | 0.41 |
| 2:BB:293:MET:HE3 | 2:BB:294:PHE:CD1 | 2.56 | 0.41 |
| 1:BC:93:ILE:H | 1:BC:93:ILE:HD12 | 1.85 | 0.41 |
| 1:BC:296:PHE:CE2 | 1:BC:335:ILE:HG21 | 2.55 | 0.41 |
| 1:BE:93:ILE:H | 1:BE:93:ILE:HD12 | 1.85 | 0.41 |
| 1:CA:181:VAL:HG21 | 2:CB:256:ASN:O | 2.20 | 0.41 |
| 1:CC:262:TYR:HB2 | 1:CC:265:ILE:HD12 | 2.02 | 0.41 |
| 1:CC:296:PHE:CE2 | 1:CC:335:ILE:HG21 | 2.55 | 0.41 |
| 2:DB:179:VAL:HG22 | 1:DC:258:ASN:CA | 2.50 | 0.41 |
| 1:DC:296:PHE:CE2 | 1:DC:335:ILE:HG21 | 2.55 | 0.41 |
| 1:DE:212:ILE:HD11 | 1:DE:300:ASN:HA | 2.03 | 0.41 |
| 2:EB:394:PHE:CD1 | 1:EC:261:PRO:HA | 2.55 | 0.41 |
| 1:EC:407:TRP:HE3 | 2:ED:255:VAL:HG13 | 0.90 | 0.41 |
| 2:ED:268:ILE:HG13 | 2:ED:300:MET:HG3 | 2.02 | 0.41 |
| 2:EF:268:ILE:HG13 | 2:EF:300:MET:HG3 | 2.02 | 0.41 |
| 1:FA:356:ASN:OD1 | 1:FA:357:TYR:N | 2.51 | 0.41 |
| 1:FC:226:ASN:ND2 | 1:FC:367:ASP:OD2 | 2.51 | 0.41 |
| 2:FD:293:MET:HE1 | 2:FD:330:MET:HE1 | 2.02 | 0.41 |
| 1:FE:56:THR:O | 1:GE:285:GLN:HA | 2.20 | 0.41 |
| 2:GF:44:LEU:HD23 | 2:GF:44:LEU:HA | 1.93 | 0.41 |
| 2:GF:416:ASN:HB3 | 7:5B:1327:LYS:CE | 2.50 | 0.41 |
| 1:HA:248:LEU:HD12 | 1:HA:248:LEU:HA | 1.89 | 0.41 |
| 1:HA:262:TYR:HB2 | 1:HA:265:ILE:HD12 | 2.02 | 0.41 |
| 1:HC:60:LYS:NZ | 1:IC:283:HIS:CE1 | 2.88 | 0.41 |
| 1:HE:328:VAL:O | 1:HE:332:ILE:HG12 | 2.20 | 0.41 |
| 2:IB:293:MET:HE3 | 2:IB:294:PHE:CD1 | 2.55 | 0.41 |
| 2:JB:293:MET:HE3 | 2:JB:294:PHE:CD1 | 2.56 | 0.41 |
| 2:JB:394:PHE:CD1 | 1:JC:261:PRO:HA | 2.55 | 0.41 |
| 1:JC:68:LEU:HD21 | 1:JC:118:CYS:SG | 2.60 | 0.41 |
| 1:JC:262:TYR:HB2 | 1:JC:265:ILE:HD12 | 2.02 | 0.41 |
| 2:JD:212:PHE:HZ | 1:JE:326:LYS:CE | 2.19 | 0.41 |
| 2:JD:222:TYR:HD2 | 1:JE:247:ALA:HB1 | 1.86 | 0.41 |
| 2:JD:293:MET:HE3 | 2:JD:294:PHE:CD1 | 2.55 | 0.41 |
| 1:JE:262:TYR:HB2 | 1:JE:265:ILE:HD12 | 2.02 | 0.41 |
| 1:JE:296:PHE:CE2 | 1:JE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:KA:124:LYS:HD3 | 1:LA:293:ASN:HB2 | 2.00 | 0.41 |
| 1:KA:262:TYR:HB2 | 1:KA:265:ILE:HD12 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:KA:296:PHE:CE2 | 1:KA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:KB:293:MET:HE3 | 2:KB:294:PHE:CD1 | 2.55 | 0.41 |
| 1:KC:226:ASN:ND2 | 1:KC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:KC:296:PHE:CE2 | 1:KC:335:ILE:HG21 | 2.55 | 0.41 |
| 2:KD:217:LEU:CD1 | 6:4B:263:CYS:SG | 3.08 | 0.41 |
| 2:KD:293:MET:HE3 | 2:KD:294:PHE:CD1 | 2.55 | 0.41 |
| 1:KE:226:ASN:ND2 | 1:KE:367:ASP:OD2 | 2.51 | 0.41 |
| 2:KF:293:MET:HE3 | 2:KF:294:PHE:CD1 | 2.56 | 0.41 |
| 1:LA:33:ASP:O | 6:4C:101:ARG:NE | 2.54 | 0.41 |
| 1:LA:222:PRO:HG2 | 2:LB:324:LYS:CD | 2.42 | 0.41 |
| 2:LB:379:LYS:HE3 | 4:2C:166:ILE:HG13 | 2.01 | 0.41 |
| 1:LC:93:ILE:H | 1:LC:93:ILE:HD12 | 1.85 | 0.41 |
| 2:LD:268:ILE:HG13 | 2:LD:300:MET:HG3 | 2.02 | 0.41 |
| 2:LD:379:LYS:HZ1 | 4:2A:166:ILE:CA | 2.32 | 0.41 |
| 1:LE:60:LYS:CE | 6:4B:101:ARG:NH2 | 2.80 | 0.41 |
| 2:LF:270:PHE:CE2 | 6:4D:226:ILE:CG2 | 2.97 | 0.41 |
| 2:MB:293:MET:HE3 | 2:MB:294:PHE:CD1 | 2.55 | 0.41 |
| 11:MC:501:GTP:O1G | 2:MD:252:LYS:NZ | 2.43 | 0.41 |
| 2:MD:375:GLN:O | 2:MD:379:LYS:HG3 | 2.20 | 0.41 |
| 6:4A:266:ASN:CG | 6:4A:269:THR:HG23 | 2.45 | 0.41 |
| 6:4C:239:LEU:HD13 | 6:4C:239:LEU:HA | 1.83 | 0.41 |
| 6:4D:110:LYS:O | 6:4D:110:LYS:HD3 | 2.20 | 0.41 |
| 6:4D:202:VAL:HA | 6:4D:205:GLN:CD | 2.46 | 0.41 |
| 6:4D:266:ASN:CG | 6:4D:269:THR:HG23 | 2.45 | 0.41 |
| 7:5A:930:MET:HE1 | 7:5A:1018:PHE:CE2 | 2.55 | 0.41 |
| 7:5A:1244:LEU:O | 7:5A:1246:LEU:N | 2.53 | 0.41 |
| 7:5A:1259:TYR:O | 7:5A:1263:GLN:HG2 | 2.19 | 0.41 |
| 7:5B:1244:LEU:O | 7:5B:1246:LEU:N | 2.53 | 0.41 |
| 7:5B:1577:LYS:HE3 | 7:5B:1578:GLY:H | 1.86 | 0.41 |
| 7:5C:1391:GLN:HE21 | 7:5C:1391:GLN:HB3 | 1.64 | 0.41 |
| 8:6C:101:GLU:OE2 | 8:6C:130:ASN:ND2 | 2.37 | 0.41 |
| 9:7D:45:ARG:HA | 9:7D:45:ARG:HD2 | 1.85 | 0.41 |
| 10:8A:13:UNK:C | 10:8A:15:UNK:N | 2.83 | 0.41 |
| 10:8C:13:UNK:C | 10:8C:15:UNK:N | 2.83 | 0.41 |
| 1:AA:212:ILE:HD11 | 1:AA:300:ASN:HA | 2.03 | 0.41 |
| 2:AB:375:GLN:O | 2:AB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:AC:212:ILE:HD11 | 1:AC:300:ASN:HA | 2.03 | 0.41 |
| 1:AC:226:ASN:ND2 | 1:AC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:BA:212:ILE:HD11 | 1:BA:300:ASN:HA | 2.03 | 0.41 |
| 1:BA:259:LEU:HD11 | 1:BA:316:SER:HB3 | 2.01 | 0.41 |
| 1:BC:212:ILE:HD11 | 1:BC:300:ASN:HA | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BD:293:MET:HE3 | 2:BD:294:PHE:CD1 | 2.56 | 0.41 |
| 1:BE:212:ILE:HD11 | 1:BE:300:ASN:HA | 2.03 | 0.41 |
| 1:BE:226:ASN:ND2 | 1:BE:367:ASP:OD2 | 2.51 | 0.41 |
| 1:BE:296:PHE:CE2 | 1:BE:335:ILE:HG21 | 2.55 | 0.41 |
| 2:BF:69:GLU:HA | 2:BF:70:PRO:HD3 | 1.89 | 0.41 |
| 2:BF:293:MET:HE3 | 2:BF:294:PHE:CD1 | 2.56 | 0.41 |
| 1:CA:217:LEU:HD23 | 1:CA:217:LEU:HA | 1.92 | 0.41 |
| 1:CE:212:ILE:HD11 | 1:CE:300:ASN:HA | 2.03 | 0.41 |
| 1:DA:212:ILE:HD11 | 1:DA:300:ASN:HA | 2.03 | 0.41 |
| 2:DD:177:ASP:O | 1:DE:352:LYS:CA | 2.64 | 0.41 |
| 2:EB:375:GLN:O | 2:EB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:EC:401:LYS:HE3 | 1:EC:401:LYS:HB2 | 1.74 | 0.41 |
| 1:FA:226:ASN:ND2 | 1:FA:367:ASP:OD2 | 2.51 | 0.41 |
| 1:FA:262:TYR:HB2 | 1:FA:265:ILE:HD12 | 2.02 | 0.41 |
| 2:FB:293:MET:HE1 | 2:FB:330:MET:HE1 | 2.02 | 0.41 |
| 1:FC:296:PHE:CE2 | 1:FC:335:ILE:HG21 | 2.55 | 0.41 |
| 1:FC:322:ASP:OD1 | 1:FC:373:ARG:NH1 | 2.52 | 0.41 |
| 1:FE:222:PRO:HG2 | 2:FF:324:LYS:HB2 | 2.01 | 0.41 |
| 2:FF:293:MET:HE1 | 2:FF:330:MET:HE1 | 2.02 | 0.41 |
| 1:GA:93:ILE:H | 1:GA:93:ILE:HD12 | 1.85 | 0.41 |
| 2:GD:44:LEU:HD23 | 2:GD:44:LEU:HA | 1.93 | 0.41 |
| 2:HB:394:PHE:CD1 | 1:HC:261:PRO:HA | 2.56 | 0.41 |
| 1:HC:328:VAL:O | 1:HC:332:ILE:HG12 | 2.20 | 0.41 |
| 1:HC:407:TRP:HE3 | 2:HD:255:VAL:HG13 | 0.95 | 0.41 |
| 2:IB:69:GLU:HA | 2:IB:70:PRO:HD3 | 1.89 | 0.41 |
| 2:IB:293:MET:HE1 | 2:IB:330:MET:HE1 | 2.02 | 0.41 |
| 1:IC:282:TYR:CG | 10:8W:15:UNK:CA | 3.01 | 0.41 |
| 2:ID:293:MET:HE1 | 2:ID:330:MET:HE1 | 2.02 | 0.41 |
| 1:JA:262:TYR:HB2 | 1:JA:265:ILE:HD12 | 2.02 | 0.41 |
| 1:JA:296:PHE:CE2 | 1:JA:335:ILE:HG21 | 2.55 | 0.41 |
| 1:JC:356:ASN:OD1 | 1:JC:357:TYR:N | 2.51 | 0.41 |
| 2:JD:88:ASP:OD1 | 2:KD:278:SER:OG | 2.28 | 0.41 |
| 1:KA:85:GLN:O | 1:LA:282:TYR:O | 2.38 | 0.41 |
| 1:KC:93:ILE:H | 1:KC:93:ILE:HD12 | 1.85 | 0.41 |
| 2:KD:131:GLN:O | 2:KD:163:ILE:HG12 | 2.20 | 0.41 |
| 1:KE:93:ILE:H | 1:KE:93:ILE:HD12 | 1.85 | 0.41 |
| 2:KF:54:ALA:HA | 2:LF:285:THR:CG2 | 2.50 | 0.41 |
| 2:KF:257:LEU:HD11 | 2:KF:314:SER:HB2 | 2.03 | 0.41 |
| 1:LA:60:LYS:HZ2 | 1:MA:283:HIS:CE1 | 2.38 | 0.41 |
| 2:LB:305:PRO:CG | 4:2C:149:ILE:HD11 | 2.49 | 0.41 |
| 2:LD:221:THR:CG2 | 6:4B:219:ASN:HD22 | 2.32 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:LE:176:GLN:NE2 | 4:2B:42:PHE:CD1 | 2.47 | 0.41 |
| 2:LF:375:GLN:O | 2:LF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:MA:93:ILE:H | 1:MA:93:ILE:HD12 | 1.85 | 0.41 |
| 1:MC:296:PHE:CE2 | 1:MC:335:ILE:HG21 | 2.56 | 0.41 |
| 2:MD:293:MET:HE3 | 2:MD:294:PHE:CD1 | 2.55 | 0.41 |
| 1:ME:226:ASN:ND2 | 1:ME:367:ASP:OD2 | 2.51 | 0.41 |
| 1:ME:279:GLU:CG | 6:4B:110:LYS:HE2 | 2.34 | 0.41 |
| 1:ME:296:PHE:CE2 | 1:ME:335:ILE:HG21 | 2.55 | 0.41 |
| 6:4B:202:VAL:HA | 6:4B:205:GLN:CD | 2.46 | 0.41 |
| 6:4C:219:ASN:HD22 | 6:4C:219:ASN:HA | 1.53 | 0.41 |
| 6:4D:230:TYR:O | 6:4D:230:TYR:CD2 | 2.73 | 0.41 |
| 7:5A:1370:LYS:HD3 | 7:5A:1370:LYS:HA | 1.61 | 0.41 |
| 7:5A:1490:LYS:HD2 | 7:5A:1494:LEU:HD22 | 1.95 | 0.41 |
| 7:5A:1490:LYS:CE | 7:5A:1494:LEU:CD2 | 2.98 | 0.41 |
| 7:5A:1577:LYS:HE3 | 7:5A:1578:GLY:H | 1.86 | 0.41 |
| 7:5B:930:MET:HE1 | 7:5B:1018:PHE:CE2 | 2.55 | 0.41 |
| 7:5B:1460:ARG:HE | 7:5B:1460:ARG:HB3 | 1.69 | 0.41 |
| 7:5B:1490:LYS:HD2 | 7:5B:1494:LEU:HD22 | 1.95 | 0.41 |
| 7:5C:1105:TYR:HB2 | 7:5C:1165:PRO:C | 2.45 | 0.41 |
| 7:5C:1259:TYR:O | 7:5C:1263:GLN:HG2 | 2.19 | 0.41 |
| 7:5C:1386:LYS:N | 7:5C:1386:LYS:HZ3 | 2.18 | 0.41 |
| 8:6A:19:VAL:HG11 | 8:6A:34:LEU:HD11 | 2.01 | 0.41 |
| 8:6A:23:ASP:OD2 | 8:6A:132:LYS:HE3 | 2.20 | 0.41 |
| 10:8J:13:UNK:C | 10:8J:15:UNK:N | 2.83 | 0.41 |
| 1:AA:222:PRO:CG | 2:AB:324:LYS:CD | 2.91 | 0.41 |
| 1:AA:296:PHE:CE2 | 1:AA:335:ILE:HG21 | 2.55 | 0.41 |
| 1:AE:342:GLN:CD | 3:1A:55:HIS:CE1 | 2.97 | 0.41 |
| 2:AF:40:SER:HB3 | 6:4A:152:PHE:CD2 | 2.23 | 0.41 |
| 2:AF:268:ILE:HG13 | 2:AF:300:MET:HG3 | 2.02 | 0.41 |
| 2:AF:279:GLN:O | 6:4A:142:SER:HB3 | 2.21 | 0.41 |
| 2:BB:268:ILE:HG13 | 2:BB:300:MET:HG3 | 2.02 | 0.41 |
| 1:BE:71:GLU:OE2 | 1:BE:73:THR:OG1 | 2.28 | 0.41 |
| 1:BE:179:THR:O | 2:BF:350:LYS:HA | 2.20 | 0.41 |
| 1:BE:248:LEU:HD12 | 1:BE:248:LEU:HA | 1.89 | 0.41 |
| 1:CA:296:PHE:CE2 | 1:CA:335:ILE:HG21 | 2.56 | 0.41 |
| 2:CB:226:ASN:ND2 | 13:CB:501:GDP:HN1 | 2.12 | 0.41 |
| 1:CC:212:ILE:HD11 | 1:CC:300:ASN:HA | 2.03 | 0.41 |
| 2:CD:179:VAL:HG22 | 1:CE:258:ASN:CG | 2.45 | 0.41 |
| 2:DB:131:GLN:O | 2:DB:163:ILE:HG12 | 2.20 | 0.41 |
| 2:DB:177:ASP:HA | 1:DC:353:VAL:HG12 | 2.02 | 0.41 |
| 1:DE:402:ARG:HD2 | 7:5B:777:ALA:HB1 | 2.01 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:EB:268:ILE:HG13 | 2:EB:300:MET:HG3 | 2.02 | 0.41 |
| 1:EC:248:LEU:HD12 | 1:EC:248:LEU:HA | 1.89 | 0.41 |
| 2:ED:375:GLN:O | 2:ED:379:LYS:HG3 | 2.20 | 0.41 |
| 1:EE:212:ILE:HD11 | 1:EE:300:ASN:HA | 2.03 | 0.41 |
| 1:EE:226:ASN:ND2 | 1:EE:367:ASP:OD2 | 2.51 | 0.41 |
| 2:EF:375:GLN:O | 2:EF:379:LYS:HG3 | 2.20 | 0.41 |
| 2:FD:401:GLU:H | 7:5A:1293:VAL:HG21 | 1.84 | 0.41 |
| 1:FE:296:PHE:CE2 | 1:FE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:GA:296:PHE:CE2 | 1:GA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:GB:220:PRO:HD2 | 1:GC:326:LYS:CE | 2.44 | 0.41 |
| 2:GB:394:PHE:CD1 | 1:GC:261:PRO:HA | 2.55 | 0.41 |
| 1:GC:212:ILE:HD11 | 1:GC:300:ASN:HA | 2.02 | 0.41 |
| 1:GC:296:PHE:CE2 | 1:GC:335:ILE:HG21 | 2.55 | 0.41 |
| 2:GD:131:GLN:O | 2:GD:163:ILE:HG12 | 2.20 | 0.41 |
| 1:GE:296:PHE:CE2 | 1:GE:335:ILE:HG21 | 2.55 | 0.41 |
| 2:GF:391:ARG:HA | 2:GF:391:ARG:HD2 | 1.79 | 0.41 |
| 2:HB:375:GLN:O | 2:HB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:HC:248:LEU:HD12 | 1:HC:248:LEU:HA | 1.89 | 0.41 |
| 2:HD:268:ILE:HG13 | 2:HD:300:MET:HG3 | 2.02 | 0.41 |
| 1:IC:328:VAL:O | 1:IC:332:ILE:HG12 | 2.20 | 0.41 |
| 2:ID:293:MET:HE3 | 2:ID:294:PHE:CD1 | 2.55 | 0.41 |
| 1:IE:259:LEU:HD11 | 1:IE:316:SER:HB3 | 2.02 | 0.41 |
| 2:IF:293:MET:HE1 | 2:IF:330:MET:HE1 | 2.02 | 0.41 |
| 1:JA:356:ASN:OD1 | 1:JA:357:TYR:N | 2.51 | 0.41 |
| 1:JE:68:LEU:HD21 | 1:JE:118:CYS:SG | 2.60 | 0.41 |
| 2:JF:293:MET:HE3 | 2:JF:294:PHE:CD1 | 2.55 | 0.41 |
| 2:KB:131:GLN:O | 2:KB:163:ILE:HG12 | 2.20 | 0.41 |
| 2:KB:257:LEU:HD11 | 2:KB:314:SER:HB2 | 2.03 | 0.41 |
| 2:KD:212:PHE:HZ | 1:KE:326:LYS:CE | 2.19 | 0.41 |
| 2:KD:391:ARG:HD2 | 2:KD:391:ARG:HA | 1.79 | 0.41 |
| 1:LC:60:LYS:HB3 | 6:4A:101:ARG:CZ | 2.24 | 0.41 |
| 1:LE:68:LEU:HD21 | 1:LE:118:CYS:SG | 2.60 | 0.41 |
| 1:LE:93:ILE:H | 1:LE:93:ILE:HD12 | 1.85 | 0.41 |
| 1:LE:217:LEU:HD23 | 1:LE:217:LEU:HA | 1.93 | 0.41 |
| 2:LF:221:THR:CG2 | 6:4D:219:ASN:HD22 | 2.31 | 0.41 |
| 2:LF:224:ASP:CG | 6:4D:219:ASN:HD21 | 2.26 | 0.41 |
| 2:LF:227:HIS:HE1 | 6:4D:226:ILE:HG13 | 1.78 | 0.41 |
| 1:MA:68:LEU:HD21 | 1:MA:118:CYS:SG | 2.60 | 0.41 |
| 1:ME:259:LEU:HD11 | 1:ME:316:SER:HB3 | 2.02 | 0.41 |
| 2:MF:293:MET:HE3 | 2:MF:294:PHE:CD1 | 2.55 | 0.41 |
| 4:2B:16:GLN:O | 4:2B:19:MET:HB2 | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:4A:105:GLU:OE2 | 6:4A:105:GLU:HA | 2.17 | 0.41 |
| 6:4A:202:VAL:HA | 6:4A:205:GLN:CD | 2.46 | 0.41 |
| 6:4B:230:TYR:O | 6:4B:230:TYR:CD2 | 2.73 | 0.41 |
| 7:5A:1391:GLN:HE21 | 7:5A:1391:GLN:HB3 | 1.64 | 0.41 |
| 7:5A:1436:ARG:CB | 7:5A:1436:ARG:NH1 | 2.78 | 0.41 |
| 7:5B:1561:GLY:O | 7:5B:1566:GLU:OE2 | 2.38 | 0.41 |
| 7:5C:827:GLU:HG3 | 7:5C:849:ARG:HH22 | 1.84 | 0.41 |
| 7:5C:1064:LYS:C | 7:5C:1066:GLY:N | 2.76 | 0.41 |
| 7:5C:1490:LYS:HD2 | 7:5C:1494:LEU:HD22 | 1.95 | 0.41 |
| 7:5C:1577:LYS:HE3 | 7:5C:1578:GLY:H | 1.86 | 0.41 |
| 8:6B:19:VAL:HG11 | 8:6B:34:LEU:HD11 | 2.01 | 0.41 |
| 8:6C:75:ILE:HD13 | 8:6C:84:LEU:HD21 | 2.01 | 0.41 |
| 9:7A:10:TYR:OH | 9:7B:34:PRO:CB | 2.68 | 0.41 |
| 1:AA:287:SER:O | 1:AA:291:ILE:HG23 | 2.21 | 0.41 |
| 2:AB:394:PHE:CD1 | 1:AC:261:PRO:HA | 2.56 | 0.41 |
| 1:AC:68:LEU:HD21 | 1:AC:118:CYS:SG | 2.60 | 0.41 |
| 1:AC:287:SER:O | 1:AC:291:ILE:HG23 | 2.21 | 0.41 |
| 2:AD:268:ILE:HG13 | 2:AD:300:MET:HG3 | 2.02 | 0.41 |
| 2:AD:375:GLN:O | 2:AD:379:LYS:HG3 | 2.20 | 0.41 |
| 1:AE:68:LEU:HD21 | 1:AE:118:CYS:SG | 2.60 | 0.41 |
| 1:AE:212:ILE:HD11 | 1:AE:300:ASN:HA | 2.03 | 0.41 |
| 2:AF:257:LEU:HD11 | 2:AF:314:SER:HB2 | 2.03 | 0.41 |
| 2:AF:380:ARG:HE | 2:AF:380:ARG:HB3 | 1.72 | 0.41 |
| 1:BA:93:ILE:HD12 | 1:BA:93:ILE:H | 1.85 | 0.41 |
| 1:BA:296:PHE:CE2 | 1:BA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:BD:87:PRO:CD | 2:CD:281:TYR:CE2 | 3.01 | 0.41 |
| 2:BD:268:ILE:HG13 | 2:BD:300:MET:HG3 | 2.02 | 0.41 |
| 1:CA:212:ILE:HD11 | 1:CA:300:ASN:HA | 2.03 | 0.41 |
| 2:CB:293:MET:HE3 | 2:CB:294:PHE:CD1 | 2.55 | 0.41 |
| 1:CE:222:PRO:HG2 | 2:CF:324:LYS:HB2 | 2.02 | 0.41 |
| 1:DC:212:ILE:HD11 | 1:DC:300:ASN:HA | 2.03 | 0.41 |
| 1:DC:224:TYR:CE2 | 2:DD:246:LEU:HD11 | 2.52 | 0.41 |
| 2:DD:131:GLN:O | 2:DD:163:ILE:HG12 | 2.20 | 0.41 |
| 2:DD:179:VAL:HG22 | 1:DE:258:ASN:CG | 2.46 | 0.41 |
| 1:DE:179:THR:O | 2:DF:350:LYS:HA | 2.20 | 0.41 |
| 1:DE:296:PHE:CE2 | 1:DE:335:ILE:HG21 | 2.56 | 0.41 |
| 2:DF:293:MET:HE3 | 2:DF:294:PHE:CD1 | 2.55 | 0.41 |
| 2:EB:179:VAL:HG22 | 1:EC:258:ASN:CG | 2.46 | 0.41 |
| 1:EC:212:ILE:HD11 | 1:EC:300:ASN:HA | 2.03 | 0.41 |
| 1:FA:212:ILE:HD11 | 1:FA:300:ASN:HA | 2.03 | 0.41 |
| 1:FA:296:PHE:CE2 | 1:FA:335:ILE:HG21 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FA:402:ARG:HD3 | 7:5C:1259:TYR:CG | 2.53 | 0.41 |
| 2:FB:262:ARG:NH1 | 2:FB:421:GLU:OE1 | 2.50 | 0.41 |
| 2:FB:293:MET:HE3 | 2:FB:294:PHE:CD1 | 2.55 | 0.41 |
| 13:FB:502:GDP:H8 | 1:FC:248:LEU:CD1 | 2.33 | 0.41 |
| 1:FC:68:LEU:HD21 | 1:FC:118:CYS:SG | 2.60 | 0.41 |
| 1:FC:212:ILE:HD11 | 1:FC:300:ASN:HA | 2.03 | 0.41 |
| 1:FE:68:LEU:HD21 | 1:FE:118:CYS:SG | 2.60 | 0.41 |
| 2:FF:268:ILE:HG13 | 2:FF:300:MET:HG3 | 2.02 | 0.41 |
| 2:FF:375:GLN:O | 2:FF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:GA:259:LEU:HD11 | 1:GA:316:SER:HB3 | 2.02 | 0.41 |
| 2:GD:179:VAL:HG21 | 1:GE:258:ASN:CA | 2.50 | 0.41 |
| 2:GD:220:PRO:HD2 | 1:GE:326:LYS:CG | 2.44 | 0.41 |
| 2:GD:380:ARG:HE | 2:GD:380:ARG:HB3 | 1.72 | 0.41 |
| 1:GE:226:ASN:ND2 | 1:GE:367:ASP:OD2 | 2.51 | 0.41 |
| 1:HA:328:VAL:O | 1:HA:332:ILE:HG12 | 2.20 | 0.41 |
| 2:HB:268:ILE:HG13 | 2:HB:300:MET:HG3 | 2.02 | 0.41 |
| 2:HD:293:MET:HE1 | 2:HD:330:MET:HE1 | 2.02 | 0.41 |
| 2:HD:375:GLN:O | 2:HD:379:LYS:HG3 | 2.20 | 0.41 |
| 2:HD:391:ARG:HD2 | 2:HD:391:ARG:HA | 1.79 | 0.41 |
| 2:HF:293:MET:HE1 | 2:HF:330:MET:HE1 | 2.02 | 0.41 |
| 1:IA:296:PHE:CE2 | 1:IA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:IB:44:LEU:HD23 | 2:IB:44:LEU:HA | 1.93 | 0.41 |
| 2:IB:222:TYR:HD2 | 1:IC:247:ALA:HB1 | 1.82 | 0.41 |
| 2:IB:257:LEU:HD11 | 2:IB:314:SER:HB2 | 2.03 | 0.41 |
| 2:IB:390:ARG:CD | 1:IC:439:THR:HG21 | 2.51 | 0.41 |
| 2:IB:394:PHE:CD1 | 1:IC:261:PRO:HA | 2.55 | 0.41 |
| 1:IE:68:LEU:HD21 | 1:IE:118:CYS:SG | 2.60 | 0.41 |
| 1:JA:287:SER:O | 1:JA:291:ILE:HG23 | 2.21 | 0.41 |
| 2:JB:390:ARG:CD | 1:JC:439:THR:HG21 | 2.51 | 0.41 |
| 1:JC:296:PHE:CE2 | 1:JC:335:ILE:HG21 | 2.56 | 0.41 |
| 2:JF:268:ILE:HG13 | 2:JF:300:MET:HG3 | 2.02 | 0.41 |
| 1:KA:68:LEU:HD21 | 1:KA:118:CYS:SG | 2.60 | 0.41 |
| 1:KA:93:ILE:H | 1:KA:93:ILE:HD12 | 1.85 | 0.41 |
| 2:KB:394:PHE:CD1 | 1:KC:261:PRO:HA | 2.56 | 0.41 |
| 2:KD:268:ILE:HG13 | 2:KD:300:MET:HG3 | 2.02 | 0.41 |
| 2:KF:268:ILE:HG13 | 2:KF:300:MET:HG3 | 2.02 | 0.41 |
| 1:LA:68:LEU:HD21 | 1:LA:118:CYS:SG | 2.60 | 0.41 |
| 2:LB:226:ASN:ND2 | 13:LB:501:GDP:HN1 | 2.12 | 0.41 |
| 2:LB:268:ILE:HG13 | 2:LB:300:MET:HG3 | 2.02 | 0.41 |
| 1:LC:68:LEU:HD21 | 1:LC:118:CYS:SG | 2.60 | 0.41 |
| 1:LC:222:PRO:CG | 2:LD:324:LYS:CB | 2.96 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:LF:294:PHE:O | 4:2B:149:ILE:HG12 | 2.21 | 0.41 |
| 2:MB:257:LEU:HD11 | 2:MB:314:SER:HB2 | 2.03 | 0.41 |
| 1:MC:68:LEU:HD21 | 1:MC:118:CYS:SG | 2.60 | 0.41 |
| 2:MD:257:LEU:HD11 | 2:MD:314:SER:HB2 | 2.03 | 0.41 |
| 2:MF:257:LEU:HD11 | 2:MF:314:SER:HB2 | 2.03 | 0.41 |
| 2:MF:375:GLN:O | 2:MF:379:LYS:HG3 | 2.20 | 0.41 |
| 6:4B:113:ILE:H | 6:4B:113:ILE:HG13 | 1.44 | 0.41 |
| 6:4C:202:VAL:HA | 6:4C:205:GLN:CD | 2.46 | 0.41 |
| 7:5A:772:LEU:HB3 | 7:5A:773:ARG:H | 1.72 | 0.41 |
| 7:5A:1561:GLY:O | 7:5A:1566:GLU:OE2 | 2.38 | 0.41 |
| 7:5B:772:LEU:HB3 | 7:5B:773:ARG:H | 1.72 | 0.41 |
| 7:5C:836:ARG:HD2 | 7:5C:836:ARG:HA | 1.42 | 0.41 |
| 7:5C:1370:LYS:HD3 | 7:5C:1370:LYS:HA | 1.61 | 0.41 |
| 8:6B:23:ASP:OD2 | 8:6B:132:LYS:HE3 | 2.20 | 0.41 |
| 10:8E:13:UNK:C | 10:8E:15:UNK:N | 2.83 | 0.41 |
| 10:8N:13:UNK:C | 10:8N:15:UNK:N | 2.83 | 0.41 |
| 1:AA:68:LEU:HD21 | 1:AA:118:CYS:SG | 2.60 | 0.41 |
| 1:AE:287:SER:O | 1:AE:291:ILE:HG23 | 2.21 | 0.41 |
| 2:AF:276:ARG:HH12 | 6:4A:137:ASN:HB3 | 1.86 | 0.41 |
| 1:BC:226:ASN:ND2 | 1:BC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:CC:226:ASN:ND2 | 1:CC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:CE:71:GLU:OE2 | 1:CE:73:THR:OG1 | 2.28 | 0.41 |
| 1:CE:226:ASN:ND2 | 1:CE:367:ASP:OD2 | 2.51 | 0.41 |
| 2:DD:87:PRO:HD2 | 2:ED:281:TYR:CD2 | 2.56 | 0.41 |
| 1:DE:71:GLU:HA | 1:DE:72:PRO:HD3 | 1.84 | 0.41 |
| 2:DF:131:GLN:O | 2:DF:163:ILE:HG12 | 2.20 | 0.41 |
| 1:EA:212:ILE:HD11 | 1:EA:300:ASN:HA | 2.03 | 0.41 |
| 1:EA:430:LYS:NZ | 7:5C:834:ASN:CB | 2.66 | 0.41 |
| 1:EC:71:GLU:HA | 1:EC:72:PRO:HD3 | 1.85 | 0.41 |
| 1:EC:226:ASN:ND2 | 1:EC:367:ASP:OD2 | 2.51 | 0.41 |
| 2:ED:208:TYR:CE2 | 1:EE:326:LYS:HB3 | 2.55 | 0.41 |
| 1:FA:93:ILE:H | 1:FA:93:ILE:HD12 | 1.85 | 0.41 |
| 1:GA:212:ILE:HD11 | 1:GA:300:ASN:HA | 2.03 | 0.41 |
| 1:GA:226:ASN:ND2 | 1:GA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:GB:375:GLN:O | 2:GB:379:LYS:HG3 | 2.20 | 0.41 |
| 2:GD:68:LEU:HD12 | 2:GD:68:LEU:HA | 1.90 | 0.41 |
| 1:GE:259:LEU:HD11 | 1:GE:316:SER:HB3 | 2.02 | 0.41 |
| 2:GF:131:GLN:O | 2:GF:163:ILE:HG12 | 2.20 | 0.41 |
| 1:HA:71:GLU:OE2 | 1:HA:73:THR:OG1 | 2.28 | 0.41 |
| 2:HB:293:MET:HE3 | 2:HB:294:PHE:CD1 | 2.55 | 0.41 |
| 2:HB:293:MET:HE1 | 2:HB:330:MET:HE1 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:HB:390:ARG:CD | 1:HC:439:THR:HG21 | 2.51 | 0.41 |
| 1:HE:296:PHE:CE2 | 1:HE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:IA:287:SER:O | 1:IA:291:ILE:HG23 | 2.21 | 0.41 |
| 1:IA:356:ASN:OD1 | 1:IA:357:TYR:N | 2.51 | 0.41 |
| 2:IB:375:GLN:O | 2:IB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:IE:328:VAL:O | 1:IE:332:ILE:HG12 | 2.20 | 0.41 |
| 2:IF:293:MET:HE3 | 2:IF:294:PHE:CD1 | 2.56 | 0.41 |
| 2:JB:257:LEU:HD11 | 2:JB:314:SER:HB2 | 2.03 | 0.41 |
| 2:JD:268:ILE:HG13 | 2:JD:300:MET:HG3 | 2.02 | 0.41 |
| 1:JE:124:LYS:HD3 | 1:KE:284:GLU:OE1 | 2.18 | 0.41 |
| 1:JE:287:SER:O | 1:JE:291:ILE:HG23 | 2.21 | 0.41 |
| 2:KB:268:ILE:HG13 | 2:KB:300:MET:HG3 | 2.02 | 0.41 |
| 2:KB:293:MET:HE1 | 2:KB:330:MET:HE1 | 2.02 | 0.41 |
| 2:KB:390:ARG:CD | 1:KC:439:THR:HG21 | 2.51 | 0.41 |
| 2:KD:257:LEU:HD11 | 2:KD:314:SER:HB2 | 2.03 | 0.41 |
| 2:KD:293:MET:HE1 | 2:KD:330:MET:HE1 | 2.02 | 0.41 |
| 1:KE:68:LEU:HD21 | 1:KE:118:CYS:SG | 2.60 | 0.41 |
| 1:KE:71:GLU:OE2 | 1:KE:73:THR:OG1 | 2.28 | 0.41 |
| 1:KE:401:LYS:HE3 | 1:KE:401:LYS:HB2 | 1.74 | 0.41 |
| 2:KF:125:GLU:CD | 2:LF:332:ASN:HD21 | 2.17 | 0.41 |
| 2:KF:293:MET:HE1 | 2:KF:330:MET:HE1 | 2.02 | 0.41 |
| 1:LA:89:PRO:CA | 1:MA:280:LYS:HZ2 | 2.34 | 0.41 |
| 2:LB:293:MET:HE3 | 2:LB:294:PHE:CD1 | 2.56 | 0.41 |
| 1:LE:248:LEU:HD12 | 1:LE:248:LEU:HA | 1.89 | 0.41 |
| 1:MA:287:SER:O | 1:MA:291:ILE:HG23 | 2.21 | 0.41 |
| 1:MA:328:VAL:O | 1:MA:332:ILE:HG12 | 2.20 | 0.41 |
| 1:MC:93:ILE:HD12 | 1:MC:93:ILE:H | 1.85 | 0.41 |
| 1:MC:259:LEU:HD11 | 1:MC:316:SER:HB3 | 2.02 | 0.41 |
| 5:3C:158:LEU:HD21 | 5:3C:243:PHE:CZ | 2.56 | 0.41 |
| 6:4A:230:TYR:O | 6:4A:230:TYR:CD2 | 2.73 | 0.41 |
| 6:4C:118:ILE:O | 6:4C:121:ARG:HB2 | 2.21 | 0.41 |
| 6:4C:148:GLU:OE1 | 6:4C:148:GLU:HA | 2.20 | 0.41 |
| 6:4D:139:ASP:HA | 6:4D:140:PRO:HD3 | 1.85 | 0.41 |
| 7:5A:1416:LYS:HB2 | 7:5A:1416:LYS:HE2 | 1.63 | 0.41 |
| 7:5B:1370:LYS:CA | 7:5B:1370:LYS:HE2 | 2.50 | 0.41 |
| 7:5B:1490:LYS:CE | 7:5B:1494:LEU:CD2 | 2.98 | 0.41 |
| 7:5C:771:LEU:HB3 | 7:5C:772:LEU:H | 1.64 | 0.41 |
| 7:5C:842:LEU:HD23 | 7:5C:843:LEU:CD2 | 2.43 | 0.41 |
| 7:5C:1105:TYR:CG | 7:5C:1165:PRO:CA | 2.84 | 0.41 |
| 7:5C:1316:LEU:HA | 7:5C:1316:LEU:HD13 | 1.87 | 0.41 |
| 7:5C:1343:LYS:N | 7:5C:1343:LYS:HD3 | 2.34 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:5C:1561:GLY:O | 7:5C:1566:GLU:OE2 | 2.38 | 0.41 |
| 10:8F:13:UNK:C | 10:8F:15:UNK:N | 2.83 | 0.41 |
| 1:BA:226:ASN:ND2 | 1:BA:367:ASP:OD2 | 2.51 | 0.41 |
| 1:BA:262:TYR:HB2 | 1:BA:265:ILE:HD12 | 2.02 | 0.41 |
| 1:BC:217:LEU:HD23 | 1:BC:217:LEU:HA | 1.93 | 0.41 |
| 1:BE:124:LYS:HE2 | 1:BE:124:LYS:HB2 | 1.89 | 0.41 |
| 1:BE:221:ARG:NH1 | 2:BF:324:LYS:N | 2.68 | 0.41 |
| 1:BE:287:SER:O | 1:BE:291:ILE:HG23 | 2.21 | 0.41 |
| 2:BF:268:ILE:HG13 | 2:BF:300:MET:HG3 | 2.02 | 0.41 |
| 2:CD:293:MET:HE3 | 2:CD:294:PHE:CD1 | 2.55 | 0.41 |
| 1:CE:248:LEU:HD12 | 1:CE:248:LEU:HA | 1.89 | 0.41 |
| 1:DA:248:LEU:HD12 | 1:DA:248:LEU:HA | 1.89 | 0.41 |
| 2:DB:282:ARG:NH2 | 2:DB:292:GLN:OE1 | 2.54 | 0.41 |
| 2:DD:282:ARG:NH2 | 2:DD:292:GLN:OE1 | 2.54 | 0.41 |
| 2:DD:293:MET:HE3 | 2:DD:294:PHE:CD1 | 2.55 | 0.41 |
| 1:DE:226:ASN:ND2 | 1:DE:367:ASP:OD2 | 2.51 | 0.41 |
| 1:EA:296:PHE:CE2 | 1:EA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:ED:179:VAL:HG22 | 1:EE:258:ASN:CG | 2.46 | 0.41 |
| 2:ED:384:GLN:HB3 | 1:EE:348:PRO:HG2 | 2.03 | 0.41 |
| 1:EE:423:GLU:HG2 | 7:5B:832:ASN:HA | 2.03 | 0.41 |
| 1:FA:68:LEU:HD21 | 1:FA:118:CYS:SG | 2.60 | 0.41 |
| 2:FB:257:LEU:HD11 | 2:FB:314:SER:HB2 | 2.03 | 0.41 |
| 2:FD:293:MET:HE3 | 2:FD:294:PHE:CD1 | 2.55 | 0.41 |
| 2:FD:375:GLN:O | 2:FD:379:LYS:HG3 | 2.20 | 0.41 |
| 1:FE:60:LYS:HD3 | 1:GE:283:HIS:CG | 2.56 | 0.41 |
| 1:FE:212:ILE:HD11 | 1:FE:300:ASN:HA | 2.03 | 0.41 |
| 1:FE:322:ASP:OD1 | 1:FE:373:ARG:NH1 | 2.52 | 0.41 |
| 2:GB:44:LEU:HD23 | 2:GB:44:LEU:HA | 1.93 | 0.41 |
| 2:GB:390:ARG:CD | 1:GC:439:THR:HG21 | 2.51 | 0.41 |
| 1:GC:226:ASN:ND2 | 1:GC:367:ASP:OD2 | 2.51 | 0.41 |
| 2:GD:220:PRO:HD2 | 1:GE:326:LYS:CE | 2.44 | 0.41 |
| 2:GD:282:ARG:NH2 | 2:GD:292:GLN:OE1 | 2.54 | 0.41 |
| 1:GE:212:ILE:HD11 | 1:GE:300:ASN:HA | 2.03 | 0.41 |
| 2:GF:257:LEU:HD11 | 2:GF:314:SER:HB2 | 2.03 | 0.41 |
| 1:HA:226:ASN:ND2 | 1:HA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:HD:73:MET:HE1 | 2:HD:92:PHE:HB3 | 2.02 | 0.41 |
| 2:HD:293:MET:HE3 | 2:HD:294:PHE:CD1 | 2.55 | 0.41 |
| 2:HF:73:MET:HE1 | 2:HF:92:PHE:HB3 | 2.03 | 0.41 |
| 2:IB:86:ARG:NH1 | 2:JB:281:TYR:CA | 2.64 | 0.41 |
| 1:IC:68:LEU:HD21 | 1:IC:118:CYS:SG | 2.60 | 0.41 |
| 2:ID:257:LEU:HD11 | 2:ID:314:SER:HB2 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:IF:257:LEU:HD11 | 2:IF:314:SER:HB2 | 2.02 | 0.41 |
| 2:JB:268:ILE:HG13 | 2:JB:300:MET:HG3 | 2.02 | 0.41 |
| 1:JC:287:SER:O | 1:JC:291:ILE:HG23 | 2.21 | 0.41 |
| 1:KA:124:LYS:HB2 | 1:LA:293:ASN:ND2 | 2.35 | 0.41 |
| 2:KB:375:GLN:O | 2:KB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:KC:68:LEU:HD21 | 1:KC:118:CYS:SG | 2.60 | 0.41 |
| 1:KE:328:VAL:O | 1:KE:332:ILE:HG12 | 2.20 | 0.41 |
| 2:KF:276:ARG:NH2 | 6:4D:265:TYR:C | 2.79 | 0.41 |
| 1:LA:71:GLU:OE2 | 1:LA:73:THR:OG1 | 2.29 | 0.41 |
| 2:LB:257:LEU:HD11 | 2:LB:314:SER:HB2 | 2.03 | 0.41 |
| 2:LD:257:LEU:HD11 | 2:LD:314:SER:HB2 | 2.03 | 0.41 |
| 2:LF:257:LEU:HD11 | 2:LF:314:SER:HB2 | 2.03 | 0.41 |
| 1:MA:259:LEU:HD11 | 1:MA:316:SER:HB3 | 2.02 | 0.41 |
| 2:MB:111:GLU:CD | 3:1A:62:SER:HB2 | 2.45 | 0.41 |
| 2:MB:268:ILE:HG13 | 2:MB:300:MET:HG3 | 2.02 | 0.41 |
| 1:MC:210:TYR:CD1 | 2:MD:324:LYS:HD2 | 2.56 | 0.41 |
| 1:MC:287:SER:O | 1:MC:291:ILE:HG23 | 2.21 | 0.41 |
| 1:MC:328:VAL:O | 1:MC:332:ILE:HG12 | 2.20 | 0.41 |
| 2:MD:268:ILE:HG13 | 2:MD:300:MET:HG3 | 2.02 | 0.41 |
| 1:ME:68:LEU:HD21 | 1:ME:118:CYS:SG | 2.60 | 0.41 |
| 1:ME:93:ILE:H | 1:ME:93:ILE:HD12 | 1.85 | 0.41 |
| 1:ME:287:SER:O | 1:ME:291:ILE:HG23 | 2.21 | 0.41 |
| 5:3A:158:LEU:HD21 | 5:3A:243:PHE:CZ | 2.56 | 0.41 |
| 6:4A:148:GLU:OE1 | 6:4A:148:GLU:HA | 2.20 | 0.41 |
| 6:4B:148:GLU:HA | 6:4B:148:GLU:OE1 | 2.20 | 0.41 |
| 6:4C:105:GLU:OE2 | 6:4C:105:GLU:HA | 2.17 | 0.41 |
| 7:5B:1548:VAL:HB | 7:5B:1566:GLU:HA | 1.92 | 0.41 |
| 7:5C:772:LEU:HB3 | 7:5C:773:ARG:H | 1.72 | 0.41 |
| 7:5C:1471:ILE:H | 7:5C:1471:ILE:CD1 | 2.18 | 0.41 |
| 8:6A:206:ASN:O | 8:6A:214:LYS:HE2 | 2.20 | 0.41 |
| 8:6C:60:PHE:CZ | 8:6C:243:ILE:HG12 | 2.55 | 0.41 |
| 10:8H:13:UNK:C | 10:8H:15:UNK:N | 2.83 | 0.41 |
| 10:8M:13:UNK:C | 10:8M:15:UNK:N | 2.83 | 0.41 |
| 10:8O:13:UNK:C | 10:8O:15:UNK:N | 2.83 | 0.41 |
| 10:8T:13:UNK:C | 10:8T:15:UNK:N | 2.83 | 0.41 |
| 10:8Z:13:UNK:C | 10:8Z:15:UNK:N | 2.83 | 0.41 |
| 2:AB:131:GLN:O | 2:AB:163:ILE:HG12 | 2.20 | 0.41 |
| 2:AB:268:ILE:HG13 | 2:AB:300:MET:HG3 | 2.02 | 0.41 |
| 2:AD:257:LEU:HD11 | 2:AD:314:SER:HB2 | 2.03 | 0.41 |
| 2:BB:282:ARG:NH2 | 2:BB:292:GLN:OE1 | 2.54 | 0.41 |
| 1:BC:247:ALA:HB2 | 1:BC:357:TYR:OH | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:BC:287:SER:O | 1:BC:291:ILE:HG23 | 2.21 | 0.41 |
| 2:BD:257:LEU:HD11 | 2:BD:314:SER:HB2 | 2.03 | 0.41 |
| 2:BD:282:ARG:NH2 | 2:BD:292:GLN:OE1 | 2.54 | 0.41 |
| 2:BF:257:LEU:HD11 | 2:BF:314:SER:HB2 | 2.03 | 0.41 |
| 2:BF:375:GLN:O | 2:BF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:CA:226:ASN:ND2 | 1:CA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:CD:177:ASP:CA | 1:CE:353:VAL:HG12 | 2.51 | 0.41 |
| 2:DB:84:LEU:O | 2:EB:281:TYR:OH | 2.39 | 0.41 |
| 1:DE:68:LEU:HD21 | 1:DE:118:CYS:SG | 2.60 | 0.41 |
| 1:DE:402:ARG:HE | 7:5B:777:ALA:HB3 | 1.57 | 0.41 |
| 2:DF:293:MET:HE1 | 2:DF:330:MET:HE1 | 2.02 | 0.41 |
| 1:EA:226:ASN:ND2 | 1:EA:367:ASP:OD2 | 2.51 | 0.41 |
| 1:EA:401:LYS:HE3 | 1:EA:401:LYS:HB2 | 1.74 | 0.41 |
| 2:EB:257:LEU:HD11 | 2:EB:314:SER:HB2 | 2.03 | 0.41 |
| 2:EF:131:GLN:O | 2:EF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:FD:268:ILE:HG13 | 2:FD:300:MET:HG3 | 2.02 | 0.41 |
| 1:GA:68:LEU:HD21 | 1:GA:118:CYS:SG | 2.60 | 0.41 |
| 1:GA:407:TRP:HE3 | 2:GB:255:VAL:HG13 | 0.97 | 0.41 |
| 1:GC:68:LEU:HD21 | 1:GC:118:CYS:SG | 2.60 | 0.41 |
| 1:GC:259:LEU:HD11 | 1:GC:316:SER:HB3 | 2.02 | 0.41 |
| 2:GD:375:GLN:O | 2:GD:379:LYS:HG3 | 2.20 | 0.41 |
| 1:GE:68:LEU:HD21 | 1:GE:118:CYS:SG | 2.60 | 0.41 |
| 2:HB:257:LEU:HD11 | 2:HB:314:SER:HB2 | 2.03 | 0.41 |
| 2:HD:83:GLN:OE1 | 2:HD:83:GLN:HA | 2.21 | 0.41 |
| 2:HF:83:GLN:OE1 | 2:HF:83:GLN:HA | 2.21 | 0.41 |
| 2:HF:257:LEU:HD11 | 2:HF:314:SER:HB2 | 2.03 | 0.41 |
| 2:HF:375:GLN:O | 2:HF:379:LYS:HG3 | 2.20 | 0.41 |
| 2:IB:268:ILE:HG13 | 2:IB:300:MET:HG3 | 2.02 | 0.41 |
| 1:IC:287:SER:O | 1:IC:291:ILE:HG23 | 2.21 | 0.41 |
| 2:ID:268:ILE:HG13 | 2:ID:300:MET:HG3 | 2.02 | 0.41 |
| 2:ID:375:GLN:O | 2:ID:379:LYS:HG3 | 2.20 | 0.41 |
| 1:IE:287:SER:O | 1:IE:291:ILE:HG23 | 2.21 | 0.41 |
| 1:IE:389:SER:CB | 5:3A:307:LYS:HB3 | 2.50 | 0.41 |
| 2:IF:56:GLY:HA2 | 10:9A:36:UNK:CA | 2.49 | 0.41 |
| 1:JA:203:MET:HE2 | 1:JA:203:MET:HA | 2.03 | 0.41 |
| 2:JF:257:LEU:HD11 | 2:JF:314:SER:HB2 | 2.03 | 0.41 |
| 1:KA:71:GLU:HA | 1:KA:72:PRO:HD3 | 1.84 | 0.41 |
| 1:KA:85:GLN:O | 1:LA:283:HIS:C | 2.64 | 0.41 |
| 1:KA:328:VAL:O | 1:KA:332:ILE:HG12 | 2.20 | 0.41 |
| 1:KC:247:ALA:HB2 | 1:KC:357:TYR:OH | 2.21 | 0.41 |
| 1:KE:84:ARG:NH1 | 1:LE:283:HIS:NE2 | 2.69 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:LA:226:ASN:ND2 | 1:LA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:LB:270:PHE:CE2 | 6:4A:226:ILE:CG2 | 2.97 | 0.41 |
| 1:LC:89:PRO:HD3 | 1:MC:280:LYS:HZ2 | 0.63 | 0.41 |
| 1:LC:203:MET:HA | 1:LC:203:MET:HE2 | 2.02 | 0.41 |
| 2:LD:293:MET:HE3 | 2:LD:294:PHE:CD1 | 2.56 | 0.41 |
| 1:LE:296:PHE:CE2 | 1:LE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:MA:262:TYR:HB2 | 1:MA:265:ILE:HD12 | 2.02 | 0.41 |
| 5:3B:158:LEU:HD21 | 5:3B:243:PHE:CZ | 2.55 | 0.41 |
| 6:4A:118:ILE:O | 6:4A:121:ARG:HB2 | 2.21 | 0.41 |
| 6:4B:215:LYS:HE3 | 6:4B:215:LYS:HB2 | 1.47 | 0.41 |
| 6:4D:148:GLU:HA | 6:4D:148:GLU:OE1 | 2.20 | 0.41 |
| 7:5A:1392:LEU:C | 7:5A:1392:LEU:CD1 | 2.89 | 0.41 |
| 7:5A:1548:VAL:HB | 7:5A:1566:GLU:CA | 2.51 | 0.41 |
| 8:6B:206:ASN:O | 8:6B:214:LYS:HE2 | 2.20 | 0.41 |
| 9:7B:2:PHE:HE1 | 9:7B:13:SER:HB3 | 1.85 | 0.41 |
| 9:7D:26:LEU:HD11 | 9:7D:34:PRO:HA | 2.03 | 0.41 |
| 9:7E:36:GLN:CA | 9:7F:43:LEU:CD2 | 2.86 | 0.41 |
| 10:8D:13:UNK:C | 10:8D:15:UNK:N | 2.83 | 0.41 |
| 10:8I:13:UNK:C | 10:8I:15:UNK:N | 2.83 | 0.41 |
| 10:8S:13:UNK:C | 10:8S:15:UNK:N | 2.83 | 0.41 |
| 10:8U:13:UNK:C | 10:8U:15:UNK:N | 2.83 | 0.41 |
| 10:8W:13:UNK:C | 10:8W:15:UNK:N | 2.83 | 0.41 |
| 10:9A:13:UNK:C | 10:9A:15:UNK:N | 2.83 | 0.41 |
| 1:AA:93:ILE:H | 1:AA:93:ILE:HD12 | 1.85 | 0.41 |
| 1:AA:248:LEU:HD12 | 1:AA:248:LEU:HA | 1.89 | 0.41 |
| 2:AB:257:LEU:HD11 | 2:AB:314:SER:HB2 | 2.03 | 0.41 |
| 1:AC:93:ILE:H | 1:AC:93:ILE:HD12 | 1.85 | 0.41 |
| 1:AC:247:ALA:HB2 | 1:AC:357:TYR:OH | 2.21 | 0.41 |
| 1:AC:401:LYS:HE3 | 1:AC:401:LYS:HB2 | 1.74 | 0.41 |
| 2:AD:68:LEU:HD12 | 2:AD:68:LEU:HA | 1.90 | 0.41 |
| 2:AD:69:GLU:HA | 2:AD:70:PRO:HD3 | 1.89 | 0.41 |
| 2:AD:220:PRO:HD2 | 1:AE:326:LYS:CE | 2.44 | 0.41 |
| 2:AD:282:ARG:NH2 | 2:AD:292:GLN:OE1 | 2.54 | 0.41 |
| 1:AE:222:PRO:CG | 2:AF:324:LYS:CD | 2.95 | 0.41 |
| 1:AE:247:ALA:HB2 | 1:AE:357:TYR:OH | 2.21 | 0.41 |
| 1:AE:398:MET:SD | 2:AF:345:ILE:CG1 | 2.92 | 0.41 |
| 2:AF:131:GLN:O | 2:AF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:AF:375:GLN:O | 2:AF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:BA:247:ALA:HB2 | 1:BA:357:TYR:OH | 2.21 | 0.41 |
| 1:BA:287:SER:O | 1:BA:291:ILE:HG23 | 2.21 | 0.41 |
| 2:BB:257:LEU:HD11 | 2:BB:314:SER:HB2 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:BB:293:MET:HE1 | 2:BB:330:MET:HE1 | 2.02 | 0.41 |
| 2:BB:390:ARG:CD | 1:BC:439:THR:HG21 | 2.51 | 0.41 |
| 1:BC:398:MET:SD | 2:BD:345:ILE:CG1 | 2.93 | 0.41 |
| 2:BD:293:MET:HE1 | 2:BD:330:MET:HE1 | 2.02 | 0.41 |
| 1:BE:247:ALA:HB2 | 1:BE:357:TYR:OH | 2.21 | 0.41 |
| 2:BF:293:MET:HE1 | 2:BF:330:MET:HE1 | 2.02 | 0.41 |
| 1:CA:404:PHE:CE2 | 2:CB:345:ILE:HD11 | 2.56 | 0.41 |
| 1:CC:217:LEU:HD23 | 1:CC:217:LEU:HA | 1.93 | 0.41 |
| 2:CD:176:SER:CB | 1:CE:349:THR:HG1 | 2.34 | 0.41 |
| 1:CE:287:SER:O | 1:CE:291:ILE:HG23 | 2.21 | 0.41 |
| 2:CF:44:LEU:HD23 | 2:CF:44:LEU:HA | 1.93 | 0.41 |
| 2:CF:131:GLN:O | 2:CF:163:ILE:HG12 | 2.20 | 0.41 |
| 2:CF:282:ARG:NH2 | 2:CF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:CF:293:MET:HE3 | 2:CF:294:PHE:CD1 | 2.55 | 0.41 |
| 1:DA:68:LEU:HD21 | 1:DA:118:CYS:SG | 2.60 | 0.41 |
| 1:DA:93:ILE:H | 1:DA:93:ILE:HD12 | 1.85 | 0.41 |
| 1:DA:226:ASN:ND2 | 1:DA:367:ASP:OD2 | 2.51 | 0.41 |
| 2:DB:293:MET:HE3 | 2:DB:294:PHE:CD1 | 2.56 | 0.41 |
| 2:DB:293:MET:HE1 | 2:DB:330:MET:HE1 | 2.02 | 0.41 |
| 1:DC:226:ASN:ND2 | 1:DC:367:ASP:OD2 | 2.51 | 0.41 |
| 2:DD:83:GLN:HA | 2:DD:83:GLN:OE1 | 2.21 | 0.41 |
| 2:DD:293:MET:HE1 | 2:DD:330:MET:HE1 | 2.02 | 0.41 |
| 2:DF:262:ARG:NH1 | 2:DF:421:GLU:OE1 | 2.50 | 0.41 |
| 2:DF:282:ARG:NH2 | 2:DF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:DF:375:GLN:O | 2:DF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:EA:217:LEU:HD23 | 1:EA:217:LEU:HA | 1.93 | 0.41 |
| 2:EB:222:TYR:CE2 | 1:EC:325:PRO:CG | 3.04 | 0.41 |
| 2:EB:325:GLU:HA | 2:EB:328:GLU:HG2 | 2.02 | 0.41 |
| 1:EC:296:PHE:CE2 | 1:EC:335:ILE:HG21 | 2.55 | 0.41 |
| 2:ED:131:GLN:O | 2:ED:163:ILE:HG12 | 2.20 | 0.41 |
| 2:ED:257:LEU:HD11 | 2:ED:314:SER:HB2 | 2.03 | 0.41 |
| 1:EE:248:LEU:HD12 | 1:EE:248:LEU:HA | 1.89 | 0.41 |
| 1:EE:296:PHE:CE2 | 1:EE:335:ILE:HG21 | 2.55 | 0.41 |
| 1:EE:402:ARG:CD | 7:5B:824:ARG:NH2 | 2.75 | 0.41 |
| 2:EF:257:LEU:HD11 | 2:EF:314:SER:HB2 | 2.03 | 0.41 |
| 2:EF:282:ARG:NH2 | 2:EF:292:GLN:OE1 | 2.54 | 0.41 |
| 1:FA:420:GLU:HA | 7:5C:1256:ARG:HH22 | 1.86 | 0.41 |
| 2:FB:73:MET:HE1 | 2:FB:92:PHE:HB3 | 2.03 | 0.41 |
| 2:FB:268:ILE:HG13 | 2:FB:300:MET:HG3 | 2.02 | 0.41 |
| 2:FB:325:GLU:HA | 2:FB:328:GLU:HG2 | 2.03 | 0.41 |
| 2:FB:375:GLN:O | 2:FB:379:LYS:HG3 | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:FC:93:ILE:H | 1:FC:93:ILE:HD12 | 1.85 | 0.41 |
| 1:FC:98:ASP:CG | 1:FC:100:ALA:H | 2.29 | 0.41 |
| 1:FC:221:ARG:HH11 | 2:FD:325:GLU:H | 1.69 | 0.41 |
| 2:FD:83:GLN:OE1 | 2:FD:83:GLN:HA | 2.21 | 0.41 |
| 2:FD:86:ARG:HD2 | 2:GD:281:TYR:HD1 | 1.52 | 0.41 |
| 2:FD:257:LEU:HD11 | 2:FD:314:SER:HB2 | 2.03 | 0.41 |
| 2:FD:325:GLU:HA | 2:FD:328:GLU:HG2 | 2.02 | 0.41 |
| 1:FE:221:ARG:HH11 | 2:FF:325:GLU:H | 1.69 | 0.41 |
| 2:FF:257:LEU:HD11 | 2:FF:314:SER:HB2 | 2.03 | 0.41 |
| 2:FF:293:MET:HE3 | 2:FF:294:PHE:CD1 | 2.55 | 0.41 |
| 2:GB:73:MET:HE1 | 2:GB:92:PHE:HB3 | 2.03 | 0.41 |
| 2:GB:257:LEU:HD11 | 2:GB:314:SER:HB2 | 2.03 | 0.41 |
| 2:GB:268:ILE:HG13 | 2:GB:300:MET:HG3 | 2.02 | 0.41 |
| 2:GB:282:ARG:NH2 | 2:GB:292:GLN:OE1 | 2.54 | 0.41 |
| 2:GB:293:MET:HE1 | 2:GB:330:MET:HE1 | 2.02 | 0.41 |
| 2:GB:325:GLU:HA | 2:GB:328:GLU:HG2 | 2.02 | 0.41 |
| 2:GD:73:MET:HE1 | 2:GD:92:PHE:HB3 | 2.03 | 0.41 |
| 2:GD:257:LEU:HD11 | 2:GD:314:SER:HB2 | 2.03 | 0.41 |
| 2:GD:268:ILE:HG13 | 2:GD:300:MET:HG3 | 2.02 | 0.41 |
| 2:GD:293:MET:HE1 | 2:GD:330:MET:HE1 | 2.02 | 0.41 |
| 2:GD:293:MET:HE3 | 2:GD:294:PHE:CD1 | 2.55 | 0.41 |
| 2:GF:73:MET:HE1 | 2:GF:92:PHE:HB3 | 2.03 | 0.41 |
| 2:GF:282:ARG:NH2 | 2:GF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:GF:293:MET:HE3 | 2:GF:294:PHE:CD1 | 2.55 | 0.41 |
| 2:GF:325:GLU:HA | 2:GF:328:GLU:HG2 | 2.02 | 0.41 |
| 1:HA:203:MET:HE2 | 1:HA:203:MET:HA | 2.03 | 0.41 |
| 2:HB:73:MET:HE1 | 2:HB:92:PHE:HB3 | 2.03 | 0.41 |
| 2:HB:83:GLN:OE1 | 2:HB:83:GLN:HA | 2.21 | 0.41 |
| 2:HD:257:LEU:HD11 | 2:HD:314:SER:HB2 | 2.03 | 0.41 |
| 2:HD:282:ARG:NH2 | 2:HD:292:GLN:OE1 | 2.54 | 0.41 |
| 1:HE:248:LEU:HD12 | 1:HE:248:LEU:HA | 1.89 | 0.41 |
| 1:HE:278:ALA:CB | 10:8U:21:UNK:C | 2.94 | 0.41 |
| 2:HF:282:ARG:NH2 | 2:HF:292:GLN:OE1 | 2.54 | 0.41 |
| 1:IA:68:LEU:HD21 | 1:IA:118:CYS:SG | 2.60 | 0.41 |
| 1:IA:203:MET:HE2 | 1:IA:203:MET:HA | 2.03 | 0.41 |
| 1:IA:262:TYR:HB2 | 1:IA:265:ILE:HD12 | 2.02 | 0.41 |
| 1:IC:296:PHE:CE2 | 1:IC:335:ILE:HG21 | 2.55 | 0.41 |
| 1:IC:356:ASN:OD1 | 1:IC:357:TYR:N | 2.51 | 0.41 |
| 2:ID:282:ARG:NH2 | 2:ID:292:GLN:OE1 | 2.54 | 0.41 |
| 1:IE:203:MET:HE2 | 1:IE:203:MET:HA | 2.03 | 0.41 |
| 1:IE:356:ASN:OD1 | 1:IE:357:TYR:N | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:IF:268:ILE:HG13 | 2:IF:300:MET:HG3 | 2.02 | 0.41 |
| 2:IF:282:ARG:NH2 | 2:IF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:IF:375:GLN:O | 2:IF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:JA:212:ILE:HD11 | 1:JA:300:ASN:HA | 2.03 | 0.41 |
| 1:JA:401:LYS:HE3 | 1:JA:401:LYS:HB2 | 1.74 | 0.41 |
| 2:JB:282:ARG:NH2 | 2:JB:292:GLN:OE1 | 2.54 | 0.41 |
| 1:JC:203:MET:HE2 | 1:JC:203:MET:HA | 2.03 | 0.41 |
| 1:JC:212:ILE:HD11 | 1:JC:300:ASN:HA | 2.03 | 0.41 |
| 2:JD:257:LEU:HD11 | 2:JD:314:SER:HB2 | 2.03 | 0.41 |
| 2:JD:282:ARG:NH2 | 2:JD:292:GLN:OE1 | 2.54 | 0.41 |
| 1:JE:164:LYS:HA | 1:JE:164:LYS:HD3 | 1.85 | 0.41 |
| 1:JE:203:MET:HE2 | 1:JE:203:MET:HA | 2.03 | 0.41 |
| 2:JF:282:ARG:NH2 | 2:JF:292:GLN:OE1 | 2.54 | 0.41 |
| 1:KA:87:PHE:O | 1:LA:284:GLU:CB | 2.67 | 0.41 |
| 1:KA:88:HIS:ND1 | 1:LA:284:GLU:CD | 2.78 | 0.41 |
| 1:KA:247:ALA:HB2 | 1:KA:357:TYR:OH | 2.21 | 0.41 |
| 1:KA:287:SER:O | 1:KA:291:ILE:HG23 | 2.21 | 0.41 |
| 2:KB:179:VAL:HG23 | 1:KC:258:ASN:HA | 2.00 | 0.41 |
| 2:KB:335:ASN:HD22 | 7:5C:1506:ILE:HD13 | 1.77 | 0.41 |
| 1:KC:287:SER:O | 1:KC:291:ILE:HG23 | 2.21 | 0.41 |
| 1:KC:328:VAL:O | 1:KC:332:ILE:HG12 | 2.20 | 0.41 |
| 2:KD:179:VAL:HG21 | 1:KE:258:ASN:CA | 2.50 | 0.41 |
| 2:KD:282:ARG:NH2 | 2:KD:292:GLN:OE1 | 2.54 | 0.41 |
| 2:KD:375:GLN:O | 2:KD:379:LYS:HG3 | 2.20 | 0.41 |
| 1:KE:203:MET:HE2 | 1:KE:203:MET:HA | 2.03 | 0.41 |
| 1:KE:247:ALA:HB2 | 1:KE:357:TYR:OH | 2.21 | 0.41 |
| 1:KE:287:SER:O | 1:KE:291:ILE:HG23 | 2.21 | 0.41 |
| 2:KF:73:MET:HE1 | 2:KF:92:PHE:HB3 | 2.03 | 0.41 |
| 2:KF:125:GLU:HG3 | 2:LF:336:LYS:HE3 | 1.77 | 0.41 |
| 2:KF:375:GLN:O | 2:KF:379:LYS:HG3 | 2.20 | 0.41 |
| 1:LA:89:PRO:HG3 | 1:MA:280:LYS:CG | 2.47 | 0.41 |
| 1:LA:203:MET:HA | 1:LA:203:MET:HE2 | 2.03 | 0.41 |
| 1:LA:222:PRO:CG | 2:LB:324:LYS:HB2 | 2.41 | 0.41 |
| 1:LA:247:ALA:HB2 | 1:LA:357:TYR:OH | 2.21 | 0.41 |
| 2:LB:83:GLN:HA | 2:LB:83:GLN:OE1 | 2.21 | 0.41 |
| 1:LC:56:THR:O | 1:MC:285:GLN:CB | 2.68 | 0.41 |
| 2:LD:83:GLN:HA | 2:LD:83:GLN:OE1 | 2.21 | 0.41 |
| 1:LE:71:GLU:HA | 1:LE:72:PRO:HD3 | 1.84 | 0.41 |
| 2:LF:282:ARG:NH2 | 2:LF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:LF:293:MET:HE3 | 2:LF:294:PHE:CD1 | 2.55 | 0.41 |
| 1:MA:247:ALA:HB2 | 1:MA:357:TYR:OH | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:MB:83:GLN:HA | 2:MB:83:GLN:OE1 | 2.21 | 0.41 |
| 2:MB:131:GLN:O | 2:MB:163:ILE:HG12 | 2.20 | 0.41 |
| 2:MB:293:MET:HE1 | 2:MB:330:MET:HE1 | 2.02 | 0.41 |
| 2:MB:391:ARG:HA | 2:MB:391:ARG:HD2 | 1.79 | 0.41 |
| 1:MC:164:LYS:HA | 1:MC:164:LYS:HD3 | 1.85 | 0.41 |
| 1:MC:247:ALA:HB2 | 1:MC:357:TYR:OH | 2.21 | 0.41 |
| 1:MC:282:TYR:CE1 | 6:4A:98:PRO:HB3 | 2.55 | 0.41 |
| 1:MC:398:MET:SD | 2:MD:345:ILE:CG1 | 2.91 | 0.41 |
| 2:MD:83:GLN:HA | 2:MD:83:GLN:OE1 | 2.21 | 0.41 |
| 2:MD:221:THR:CG2 | 6:4B:189:ARG:CZ | 2.79 | 0.41 |
| 2:MD:293:MET:HE1 | 2:MD:330:MET:HE1 | 2.02 | 0.41 |
| 1:ME:124:LYS:HE2 | 1:ME:124:LYS:HB2 | 1.89 | 0.41 |
| 1:ME:247:ALA:HB2 | 1:ME:357:TYR:OH | 2.21 | 0.41 |
| 1:ME:328:VAL:O | 1:ME:332:ILE:HG12 | 2.20 | 0.41 |
| 2:MF:79:GLY:CA | 6:4D:179:ARG:HD3 | 2.45 | 0.41 |
| 2:MF:83:GLN:OE1 | 2:MF:83:GLN:HA | 2.21 | 0.41 |
| 2:MF:268:ILE:HG13 | 2:MF:300:MET:HG3 | 2.02 | 0.41 |
| 3:1A:23:LEU:HD13 | 3:1A:39:MET:HE2 | 2.03 | 0.41 |
| 3:1B:23:LEU:HD13 | 3:1B:39:MET:HE2 | 2.03 | 0.41 |
| 3:1C:23:LEU:HD13 | 3:1C:39:MET:HE2 | 2.03 | 0.41 |
| 6:4C:230:TYR:O | 6:4C:230:TYR:CD2 | 2.73 | 0.41 |
| 6:4D:113:ILE:H | 6:4D:113:ILE:HG13 | 1.44 | 0.41 |
| 6:4D:193:MET:HE3 | 6:4D:193:MET:HB3 | 1.83 | 0.41 |
| 7:5A:771:LEU:HB3 | 7:5A:772:LEU:H | 1.64 | 0.41 |
| 7:5A:836:ARG:CG | 7:5A:836:ARG:NH1 | 2.71 | 0.41 |
| 7:5A:1343:LYS:N | 7:5A:1343:LYS:HD3 | 2.35 | 0.41 |
| 7:5A:1370:LYS:CA | 7:5A:1370:LYS:HE2 | 2.50 | 0.41 |
| 7:5A:1408:GLU:OE1 | 7:5A:1408:GLU:CA | 2.69 | 0.41 |
| 7:5A:1410:ASN:HD21 | 7:5A:1414:ILE:HD13 | 1.85 | 0.41 |
| 7:5A:1511:ILE:CD1 | 7:5A:1517:SER:HB3 | 2.50 | 0.41 |
| 7:5A:1544:ILE:N | 7:5A:1573:ARG:CD | 2.84 | 0.41 |
| 7:5B:1391:GLN:HE21 | 7:5B:1391:GLN:HB3 | 1.64 | 0.41 |
| 7:5B:1410:ASN:HD21 | 7:5B:1414:ILE:HD13 | 1.86 | 0.41 |
| 7:5B:1511:ILE:CD1 | 7:5B:1517:SER:HB3 | 2.50 | 0.41 |
| 7:5B:1544:ILE:N | 7:5B:1573:ARG:CD | 2.84 | 0.41 |
| 7:5B:1548:VAL:HB | 7:5B:1566:GLU:CA | 2.51 | 0.41 |
| 7:5C:839:GLU:OE2 | 8:6C:109:ILE:HG13 | 2.20 | 0.41 |
| 7:5C:1406:PHE:HA | 7:5C:1409:PHE:HB3 | 2.02 | 0.41 |
| 7:5C:1408:GLU:OE1 | 7:5C:1408:GLU:CA | 2.69 | 0.41 |
| 7:5C:1511:ILE:CD1 | 7:5C:1517:SER:HB3 | 2.50 | 0.41 |
| 8:6C:53:ALA:HB2 | 8:6C:174:THR:HG23 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:6C:202:GLU:OE1 | 8:6C:217:ASN:N | 2.34 | 0.41 |
| 9:7A:18:VAL:HG12 | 9:7A:42:LEU:HD21 | 1.95 | 0.41 |
| 9:7A:35:ILE:CG2 | 9:7B:42:LEU:C | 2.90 | 0.41 |
| 9:7C:35:ILE:CG2 | 9:7D:42:LEU:C | 2.90 | 0.41 |
| 9:7F:26:LEU:HD11 | 9:7F:34:PRO:HA | 2.03 | 0.41 |
| 10:8G:13:UNK:C | 10:8G:15:UNK:N | 2.83 | 0.41 |
| 10:8V:13:UNK:C | 10:8V:15:UNK:N | 2.83 | 0.41 |
| 10:8X:13:UNK:C | 10:8X:15:UNK:N | 2.83 | 0.41 |
| 10:8Y:13:UNK:C | 10:8Y:15:UNK:N | 2.83 | 0.41 |
| 1:AA:203:MET:HE2 | 1:AA:203:MET:HA | 2.03 | 0.41 |
| 1:AA:247:ALA:HB2 | 1:AA:357:TYR:OH | 2.21 | 0.41 |
| 2:AB:83:GLN:HA | 2:AB:83:GLN:OE1 | 2.21 | 0.41 |
| 2:AB:282:ARG:NH2 | 2:AB:292:GLN:OE1 | 2.54 | 0.41 |
| 2:AB:390:ARG:CD | 1:AC:439:THR:HG21 | 2.51 | 0.41 |
| 2:AD:131:GLN:O | 2:AD:163:ILE:HG12 | 2.20 | 0.41 |
| 2:AF:282:ARG:NH2 | 2:AF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:AF:293:MET:HE1 | 2:AF:330:MET:HE1 | 2.02 | 0.41 |
| 2:BB:131:GLN:O | 2:BB:163:ILE:HG12 | 2.20 | 0.41 |
| 1:BC:124:LYS:HE2 | 1:BC:124:LYS:HB2 | 1.89 | 0.41 |
| 1:BC:203:MET:HA | 1:BC:203:MET:HE2 | 2.02 | 0.41 |
| 2:BD:69:GLU:HA | 2:BD:70:PRO:HD3 | 1.89 | 0.41 |
| 2:BD:375:GLN:O | 2:BD:379:LYS:HG3 | 2.20 | 0.41 |
| 1:BE:68:LEU:HD21 | 1:BE:118:CYS:SG | 2.60 | 0.41 |
| 1:BE:115:VAL:HG22 | 1:BE:119:LEU:HD23 | 2.04 | 0.41 |
| 2:BF:282:ARG:NH2 | 2:BF:292:GLN:OE1 | 2.54 | 0.41 |
| 2:CB:179:VAL:HG21 | 1:CC:258:ASN:CA | 2.49 | 0.41 |
| 2:CD:44:LEU:HD23 | 2:CD:44:LEU:HA | 1.93 | 0.41 |
| 2:CD:257:LEU:HD11 | 2:CD:314:SER:HB2 | 2.03 | 0.41 |
| 1:CE:68:LEU:HD21 | 1:CE:118:CYS:SG | 2.60 | 0.41 |
| 2:CF:257:LEU:HD11 | 2:CF:314:SER:HB2 | 2.03 | 0.41 |
| 2:CF:325:GLU:HA | 2:CF:328:GLU:HG2 | 2.02 | 0.41 |
| 1:DA:217:LEU:HD23 | 1:DA:217:LEU:HA | 1.93 | 0.41 |
| 1:DA:222:PRO:HG2 | 2:DB:324:LYS:HB2 | 2.03 | 0.41 |
| 2:DB:257:LEU:HD11 | 2:DB:314:SER:HB2 | 2.03 | 0.41 |
| 1:DC:68:LEU:HD21 | 1:DC:118:CYS:SG | 2.60 | 0.41 |
| 1:DC:205:ASP:OD1 | 1:DC:303:ALA:HA | 2.22 | 0.41 |
| 1:DC:400:ALA:O | 7:5A:775:PRO:CA | 2.67 | 0.41 |
| 2:DD:375:GLN:O | 2:DD:379:LYS:HG3 | 2.20 | 0.41 |
| 2:DD:391:ARG:HD2 | 2:DD:391:ARG:HA | 1.79 | 0.41 |
| 1:DE:93:ILE:H | 1:DE:93:ILE:HD12 | 1.85 | 0.41 |
| 1:EA:71:GLU:HA | 1:EA:72:PRO:HD3 | 1.84 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EA:181:VAL:HG21 | 2:EB:256:ASN:O | 2.21 | 0.41 |
| 2:EB:131:GLN:O | 2:EB:163:ILE:HG12 | 2.20 | 0.41 |
| 2:EB:293:MET:HE1 | 2:EB:330:MET:HE1 | 2.02 | 0.41 |
| 2:ED:325:GLU:HA | 2:ED:328:GLU:HG2 | 2.03 | 0.41 |
| 1:EE:68:LEU:HD21 | 1:EE:118:CYS:SG | 2.60 | 0.41 |
| 2:EF:73:MET:HE1 | 2:EF:92:PHE:HB3 | 2.02 | 0.41 |
| 2:FF:73:MET:HE1 | 2:FF:92:PHE:HB3 | 2.03 | 0.41 |
| 2:FF:325:GLU:HA | 2:FF:328:GLU:HG2 | 2.02 | 0.41 |
| 2:GD:325:GLU:HA | 2:GD:328:GLU:HG2 | 2.03 | 0.41 |
| 1:GE:262:TYR:HB2 | 1:GE:265:ILE:HD12 | 2.02 | 0.41 |
| 2:GF:83:GLN:OE1 | 2:GF:83:GLN:HA | 2.21 | 0.41 |
| 2:GF:375:GLN:O | 2:GF:379:LYS:HG3 | 2.20 | 0.41 |
| 2:HB:282:ARG:NH2 | 2:HB:292:GLN:OE1 | 2.54 | 0.41 |
| 1:HC:203:MET:HE2 | 1:HC:203:MET:HA | 2.03 | 0.41 |
| 1:HC:226:ASN:ND2 | 1:HC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:HC:296:PHE:CE2 | 1:HC:335:ILE:HG21 | 2.55 | 0.41 |
| 1:HE:203:MET:HE2 | 1:HE:203:MET:HA | 2.03 | 0.41 |
| 1:HE:212:ILE:HD11 | 1:HE:300:ASN:HA | 2.03 | 0.41 |
| 1:HE:226:ASN:ND2 | 1:HE:367:ASP:OD2 | 2.51 | 0.41 |
| 2:HF:380:ARG:HE | 2:HF:380:ARG:HB3 | 1.72 | 0.41 |
| 2:IB:83:GLN:OE1 | 2:IB:83:GLN:HA | 2.21 | 0.41 |
| 2:IB:282:ARG:NH2 | 2:IB:292:GLN:OE1 | 2.54 | 0.41 |
| 2:IB:325:GLU:HA | 2:IB:328:GLU:HG2 | 2.02 | 0.41 |
| 1:IC:60:LYS:HZ3 | 1:JC:283:HIS:CD2 | 2.38 | 0.41 |
| 1:IC:203:MET:HE2 | 1:IC:203:MET:HA | 2.03 | 0.41 |
| 1:IC:262:TYR:HB2 | 1:IC:265:ILE:HD12 | 2.02 | 0.41 |
| 2:ID:83:GLN:OE1 | 2:ID:83:GLN:HA | 2.21 | 0.41 |
| 2:ID:390:ARG:CD | 1:IE:439:THR:HG21 | 2.51 | 0.41 |
| 1:IE:296:PHE:CE2 | 1:IE:335:ILE:HG21 | 2.55 | 0.41 |
| 2:JB:83:GLN:HA | 2:JB:83:GLN:OE1 | 2.21 | 0.41 |
| 2:JB:375:GLN:O | 2:JB:379:LYS:HG3 | 2.20 | 0.41 |
| 1:JE:90:GLU:CB | 1:KE:280:LYS:CD | 2.67 | 0.41 |
| 2:JF:83:GLN:HA | 2:JF:83:GLN:OE1 | 2.21 | 0.41 |
| 2:JF:293:MET:HE1 | 2:JF:330:MET:HE1 | 2.02 | 0.41 |
| 1:KA:203:MET:HE2 | 1:KA:203:MET:HA | 2.03 | 0.41 |
| 2:KB:83:GLN:HA | 2:KB:83:GLN:OE1 | 2.21 | 0.41 |
| 2:KB:282:ARG:NH2 | 2:KB:292:GLN:OE1 | 2.54 | 0.41 |
| 1:KC:79:ARG:HD2 | 1:LC:280:LYS:HD2 | 2.03 | 0.41 |
| 2:KD:73:MET:HE1 | 2:KD:92:PHE:HB3 | 2.03 | 0.41 |
| 2:KD:273:LEU:HA | 6:4B:268:LEU:HG | 1.97 | 0.41 |
| 2:KD:390:ARG:CD | 1:KE:439:THR:HG21 | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:KE:85:GLN:HA | 1:LE:283:HIS:HD2 | 1.82 | 0.41 |
| 1:LA:287:SER:O | 1:LA:291:ILE:HG23 | 2.21 | 0.41 |
| 1:LA:296:PHE:CE2 | 1:LA:335:ILE:HG21 | 2.55 | 0.41 |
| 2:LB:383:GLU:OE1 | 4:2C:164:ARG:NH1 | 2.54 | 0.41 |
| 1:LC:226:ASN:ND2 | 1:LC:367:ASP:OD2 | 2.51 | 0.41 |
| 1:LC:247:ALA:HB2 | 1:LC:357:TYR:OH | 2.21 | 0.41 |
| 1:LC:287:SER:O | 1:LC:291:ILE:HG23 | 2.21 | 0.41 |
| 1:LC:296:PHE:CE2 | 1:LC:335:ILE:HG21 | 2.55 | 0.41 |
| 2:LD:73:MET:HE1 | 2:LD:92:PHE:HB3 | 2.03 | 0.41 |
| 1:LE:203:MET:HA | 1:LE:203:MET:HE2 | 2.03 | 0.41 |
| 2:LF:83:GLN:HA | 2:LF:83:GLN:OE1 | 2.21 | 0.41 |
| 1:MA:212:ILE:HD11 | 1:MA:300:ASN:HA | 2.03 | 0.41 |
| 1:MC:212:ILE:HD11 | 1:MC:300:ASN:HA | 2.03 | 0.41 |
| 1:MC:282:TYR:CD2 | 6:4A:104:ARG:CZ | 2.65 | 0.41 |
| 1:ME:203:MET:HA | 1:ME:203:MET:HE2 | 2.03 | 0.41 |
| 2:MF:293:MET:HE1 | 2:MF:330:MET:HE1 | 2.02 | 0.41 |
| 4:2A:149:ILE:O | 4:2A:151:VAL:N | 2.53 | 0.41 |
| 4:2C:149:ILE:O | 4:2C:151:VAL:N | 2.54 | 0.41 |
| 6:4A:219:ASN:HA | 6:4A:219:ASN:HD22 | 1.53 | 0.41 |
| 6:4B:118:ILE:O | 6:4B:121:ARG:HB2 | 2.21 | 0.41 |
| 6:4C:161:LYS:C | 6:4C:161:LYS:CD | 2.93 | 0.41 |
| 6:4D:118:ILE:O | 6:4D:121:ARG:HB2 | 2.21 | 0.41 |
| 7:5A:842:LEU:HD23 | 7:5A:843:LEU:CD2 | 2.43 | 0.41 |
| 7:5A:1406:PHE:HA | 7:5A:1409:PHE:HB3 | 2.02 | 0.41 |
| 7:5A:1419:GLU:OE1 | 7:5A:1419:GLU:CA | 2.69 | 0.41 |
| 7:5B:1419:GLU:OE1 | 7:5B:1419:GLU:CA | 2.69 | 0.41 |
| 7:5C:1061:ILE:O | 7:5C:1065:LYS:HG3 | 2.20 | 0.41 |
| 7:5C:1544:ILE:N | 7:5C:1573:ARG:CD | 2.84 | 0.41 |
| 9:7B:18:VAL:HG11 | 9:7B:42:LEU:HD22 | 2.00 | 0.41 |
| 9:7D:2:PHE:HE1 | 9:7D:13:SER:HB3 | 1.85 | 0.41 |
| 9:7E:15:VAL:CG1 | 9:7F:35:ILE:HA | 2.50 | 0.41 |
| 2:AD:83:GLN:HA | 2:AD:83:GLN:OE1 | 2.21 | 0.40 |
| 2:AD:293:MET:HE1 | 2:AD:330:MET:HE1 | 2.02 | 0.40 |
| 2:AF:83:GLN:HA | 2:AF:83:GLN:OE1 | 2.21 | 0.40 |
| 2:AF:224:ASP:OD1 | 6:4A:132:LYS:CA | 2.63 | 0.40 |
| 1:BA:115:VAL:HG22 | 1:BA:119:LEU:HD23 | 2.04 | 0.40 |
| 1:BC:60:LYS:NZ | 1:CC:283:HIS:CE1 | 2.89 | 0.40 |
| 1:BC:115:VAL:HG22 | 1:BC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:BC:262:TYR:HB2 | 1:BC:265:ILE:HD12 | 2.02 | 0.40 |
| 1:BE:203:MET:HA | 1:BE:203:MET:HE2 | 2.03 | 0.40 |
| 1:BE:217:LEU:HD23 | 1:BE:217:LEU:HA | 1.93 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:203:MET:HA | 1:CA:203:MET:HE2 | 2.03 | 0.40 |
| 1:CA:287:SER:O | 1:CA:291:ILE:HG23 | 2.21 | 0.40 |
| 2:CB:87:PRO:HD3 | 2:DB:281:TYR:CZ | 2.53 | 0.40 |
| 2:CD:131:GLN:O | 2:CD:163:ILE:HG12 | 2.20 | 0.40 |
| 2:CD:282:ARG:NH2 | 2:CD:292:GLN:OE1 | 2.54 | 0.40 |
| 1:CE:115:VAL:HG22 | 1:CE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:CE:217:LEU:HD23 | 1:CE:217:LEU:HA | 1.92 | 0.40 |
| 1:DA:205:ASP:OD1 | 1:DA:303:ALA:HA | 2.22 | 0.40 |
| 2:DB:83:GLN:HA | 2:DB:83:GLN:OE1 | 2.21 | 0.40 |
| 1:DC:93:ILE:H | 1:DC:93:ILE:HD12 | 1.85 | 0.40 |
| 1:DC:248:LEU:HD12 | 1:DC:248:LEU:HA | 1.89 | 0.40 |
| 1:DC:402:ARG:HD2 | 7:5A:777:ALA:HB1 | 2.03 | 0.40 |
| 1:DE:205:ASP:OD1 | 1:DE:303:ALA:HA | 2.22 | 0.40 |
| 2:DF:83:GLN:HA | 2:DF:83:GLN:OE1 | 2.21 | 0.40 |
| 1:EA:115:VAL:HG22 | 1:EA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:ED:282:ARG:NH2 | 2:ED:292:GLN:OE1 | 2.54 | 0.40 |
| 1:FC:89:PRO:CB | 1:GC:280:LYS:HZ1 | 2.32 | 0.40 |
| 1:FC:203:MET:HE2 | 1:FC:203:MET:HA | 2.03 | 0.40 |
| 1:FE:56:THR:OG1 | 1:GE:284:GLU:C | 2.64 | 0.40 |
| 1:FE:93:ILE:H | 1:FE:93:ILE:HD12 | 1.85 | 0.40 |
| 1:FE:98:ASP:CG | 1:FE:100:ALA:H | 2.29 | 0.40 |
| 1:FE:203:MET:HE2 | 1:FE:203:MET:HA | 2.03 | 0.40 |
| 2:GB:293:MET:HE3 | 2:GB:294:PHE:CD1 | 2.55 | 0.40 |
| 2:GF:293:MET:HE1 | 2:GF:330:MET:HE1 | 2.02 | 0.40 |
| 2:HB:325:GLU:HA | 2:HB:328:GLU:HG2 | 2.02 | 0.40 |
| 1:HC:212:ILE:HD11 | 1:HC:300:ASN:HA | 2.03 | 0.40 |
| 2:HF:293:MET:HE3 | 2:HF:294:PHE:CD1 | 2.56 | 0.40 |
| 2:IF:83:GLN:OE1 | 2:IF:83:GLN:HA | 2.21 | 0.40 |
| 2:JD:83:GLN:HA | 2:JD:83:GLN:OE1 | 2.21 | 0.40 |
| 1:JE:90:GLU:OE2 | 1:KE:276:ILE:HD11 | 2.21 | 0.40 |
| 1:JE:247:ALA:HB2 | 1:JE:357:TYR:OH | 2.21 | 0.40 |
| 2:KB:220:PRO:HD2 | 1:KC:326:LYS:CE | 2.44 | 0.40 |
| 1:KC:203:MET:HE2 | 1:KC:203:MET:HA | 2.03 | 0.40 |
| 2:KD:127:CYS:HB2 | 4:2A:38:VAL:HG21 | 1.34 | 0.40 |
| 2:KF:282:ARG:NH2 | 2:KF:292:GLN:OE1 | 2.54 | 0.40 |
| 1:LA:89:PRO:CB | 1:MA:280:LYS:HZ2 | 2.34 | 0.40 |
| 2:LB:73:MET:HE1 | 2:LB:92:PHE:HB3 | 2.03 | 0.40 |
| 2:LB:131:GLN:O | 2:LB:163:ILE:HG12 | 2.20 | 0.40 |
| 2:LD:282:ARG:NH2 | 2:LD:292:GLN:OE1 | 2.54 | 0.40 |
| 1:LE:287:SER:O | 1:LE:291:ILE:HG23 | 2.21 | 0.40 |
| 2:LF:73:MET:HE1 | 2:LF:92:PHE:HB3 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:MA:203:MET:HE2 | 1:MA:203:MET:HA | 2.03 | 0.40 |
| 1:MC:203:MET:HE2 | 1:MC:203:MET:HA | 2.03 | 0.40 |
| 1:MC:262:TYR:HB2 | 1:MC:265:ILE:HD12 | 2.02 | 0.40 |
| 1:ME:212:ILE:HD11 | 1:ME:300:ASN:HA | 2.03 | 0.40 |
| 4:2C:16:GLN:CA | 4:2C:19:MET:CB | 2.30 | 0.40 |
| 6:4A:161:LYS:C | 6:4A:161:LYS:CD | 2.93 | 0.40 |
| 7:5A:1061:ILE:O | 7:5A:1065:LYS:HG3 | 2.20 | 0.40 |
| 7:5A:1386:LYS:N | 7:5A:1386:LYS:HZ3 | 2.19 | 0.40 |
| 7:5B:1343:LYS:N | 7:5B:1343:LYS:HD3 | 2.35 | 0.40 |
| 7:5B:1392:LEU:C | 7:5B:1392:LEU:CD1 | 2.89 | 0.40 |
| 7:5C:1271:ILE:H | 7:5C:1271:ILE:HG13 | 1.43 | 0.40 |
| 7:5C:1410:ASN:HD21 | 7:5C:1414:ILE:HD13 | 1.86 | 0.40 |
| 7:5C:1419:GLU:OE1 | 7:5C:1419:GLU:CA | 2.69 | 0.40 |
| 7:5C:1436:ARG:CB | 7:5C:1436:ARG:NH1 | 2.78 | 0.40 |
| 8:6A:75:ILE:HD13 | 8:6A:84:LEU:HD21 | 2.01 | 0.40 |
| 8:6A:129:VAL:HG21 | 8:6A:141:GLU:HB2 | 2.03 | 0.40 |
| 8:6B:129:VAL:HG21 | 8:6B:141:GLU:HB2 | 2.03 | 0.40 |
| 9:7B:26:LEU:HD11 | 9:7B:34:PRO:HA | 2.03 | 0.40 |
| 9:7F:2:PHE:HE1 | 9:7F:13:SER:HB3 | 1.85 | 0.40 |
| 2:AB:293:MET:HE1 | 2:AB:330:MET:HE1 | 2.02 | 0.40 |
| 1:AC:203:MET:HE2 | 1:AC:203:MET:HA | 2.03 | 0.40 |
| 2:AF:359:LYS:O | 6:4A:136:HIS:CD2 | 2.73 | 0.40 |
| 1:BA:203:MET:HE2 | 1:BA:203:MET:HA | 2.02 | 0.40 |
| 2:BB:375:GLN:O | 2:BB:379:LYS:HG3 | 2.20 | 0.40 |
| 1:BC:68:LEU:HD21 | 1:BC:118:CYS:SG | 2.60 | 0.40 |
| 2:BD:131:GLN:O | 2:BD:163:ILE:HG12 | 2.20 | 0.40 |
| 1:CA:68:LEU:HD21 | 1:CA:118:CYS:SG | 2.60 | 0.40 |
| 1:CA:115:VAL:HG22 | 1:CA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:CB:131:GLN:O | 2:CB:163:ILE:HG12 | 2.20 | 0.40 |
| 2:CB:257:LEU:HD11 | 2:CB:314:SER:HB2 | 2.03 | 0.40 |
| 1:CC:287:SER:O | 1:CC:291:ILE:HG23 | 2.21 | 0.40 |
| 1:CC:404:PHE:CE2 | 2:CD:345:ILE:HD11 | 2.57 | 0.40 |
| 2:CF:68:LEU:HD12 | 2:CF:68:LEU:HA | 1.90 | 0.40 |
| 2:DB:87:PRO:CD | 2:EB:281:TYR:CE2 | 3.04 | 0.40 |
| 2:DB:325:GLU:HA | 2:DB:328:GLU:HG2 | 2.02 | 0.40 |
| 1:DE:287:SER:O | 1:DE:291:ILE:HG23 | 2.21 | 0.40 |
| 2:DF:87:PRO:HA | 2:DF:90:PHE:HD2 | 1.86 | 0.40 |
| 1:EA:247:ALA:HB2 | 1:EA:357:TYR:OH | 2.21 | 0.40 |
| 2:EB:73:MET:HE1 | 2:EB:92:PHE:HB3 | 2.03 | 0.40 |
| 2:EB:282:ARG:NH2 | 2:EB:292:GLN:OE1 | 2.54 | 0.40 |
| 1:EC:68:LEU:HD21 | 1:EC:118:CYS:SG | 2.60 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:EC:115:VAL:HG22 | 1:EC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:EC:203:MET:HA | 1:EC:203:MET:HE2 | 2.02 | 0.40 |
| 1:EC:247:ALA:HB2 | 1:EC:357:TYR:OH | 2.21 | 0.40 |
| 2:ED:293:MET:HE1 | 2:ED:330:MET:HE1 | 2.02 | 0.40 |
| 1:EE:203:MET:HA | 1:EE:203:MET:HE2 | 2.03 | 0.40 |
| 1:EE:222:PRO:HG3 | 2:EF:324:LYS:HD3 | 1.96 | 0.40 |
| 2:EF:325:GLU:HA | 2:EF:328:GLU:HG2 | 2.03 | 0.40 |
| 1:FA:420:GLU:HA | 7:5C:1256:ARG:NH2 | 2.37 | 0.40 |
| 2:FB:83:GLN:HA | 2:FB:83:GLN:OE1 | 2.21 | 0.40 |
| 1:FC:205:ASP:OD1 | 1:FC:303:ALA:HA | 2.22 | 0.40 |
| 1:FC:287:SER:O | 1:FC:291:ILE:HG23 | 2.21 | 0.40 |
| 1:FC:394:LYS:NZ | 2:FD:347:ASN:OD1 | 2.53 | 0.40 |
| 2:FD:73:MET:HE1 | 2:FD:92:PHE:HB3 | 2.03 | 0.40 |
| 1:FE:205:ASP:OD1 | 1:FE:303:ALA:HA | 2.22 | 0.40 |
| 1:FE:287:SER:O | 1:FE:291:ILE:HG23 | 2.21 | 0.40 |
| 2:FF:83:GLN:HA | 2:FF:83:GLN:OE1 | 2.21 | 0.40 |
| 2:GD:83:GLN:OE1 | 2:GD:83:GLN:HA | 2.21 | 0.40 |
| 2:GD:390:ARG:CD | 1:GE:439:THR:HG21 | 2.51 | 0.40 |
| 2:GF:54:ALA:CB | 2:HF:281:TYR:O | 2.69 | 0.40 |
| 2:GF:68:LEU:HD12 | 2:GF:68:LEU:HA | 1.90 | 0.40 |
| 2:GF:226:ASN:ND2 | 13:GF:501:GDP:HN1 | 2.12 | 0.40 |
| 2:GF:380:ARG:HE | 2:GF:380:ARG:HB3 | 1.73 | 0.40 |
| 1:HA:212:ILE:HD11 | 1:HA:300:ASN:HA | 2.03 | 0.40 |
| 1:HA:287:SER:O | 1:HA:291:ILE:HG23 | 2.21 | 0.40 |
| 2:HB:212:PHE:HE2 | 1:HC:326:LYS:HB2 | 1.87 | 0.40 |
| 1:HC:115:VAL:HG22 | 1:HC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:HC:287:SER:O | 1:HC:291:ILE:HG23 | 2.21 | 0.40 |
| 1:HE:115:VAL:HG22 | 1:HE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:IA:222:PRO:CG | 2:IB:324:LYS:CD | 2.91 | 0.40 |
| 1:IC:115:VAL:HG22 | 1:IC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:IE:124:LYS:HE2 | 1:IE:124:LYS:HB2 | 1.89 | 0.40 |
| 2:IF:73:MET:HE1 | 2:IF:92:PHE:HB3 | 2.03 | 0.40 |
| 2:JB:178:THR:HG22 | 2:JB:180:VAL:H | 1.87 | 0.40 |
| 2:JB:293:MET:HE1 | 2:JB:330:MET:HE1 | 2.02 | 0.40 |
| 2:JD:293:MET:HE1 | 2:JD:330:MET:HE1 | 2.02 | 0.40 |
| 2:KB:73:MET:HE1 | 2:KB:92:PHE:HB3 | 2.03 | 0.40 |
| 1:KC:115:VAL:HG22 | 1:KC:119:LEU:HD23 | 2.04 | 0.40 |
| 2:KF:44:LEU:HD23 | 2:KF:44:LEU:HA | 1.93 | 0.40 |
| 2:KF:391:ARG:HD2 | 2:KF:391:ARG:HA | 1.79 | 0.40 |
| 1:LA:115:VAL:HG22 | 1:LA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:LB:180:VAL:HB | 1:LC:257:THR:O | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:LB:282:ARG:NH2 | 2:LB:292:GLN:OE1 | 2.54 | 0.40 |
| 2:LB:293:MET:HE1 | 2:LB:330:MET:HE1 | 2.02 | 0.40 |
| 2:LD:180:VAL:HB | 1:LE:257:THR:O | 2.20 | 0.40 |
| 2:LD:293:MET:HE1 | 2:LD:330:MET:HE1 | 2.02 | 0.40 |
| 1:LE:115:VAL:HG22 | 1:LE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:LE:226:ASN:ND2 | 1:LE:367:ASP:OD2 | 2.51 | 0.40 |
| 2:LF:293:MET:HE1 | 2:LF:330:MET:HE1 | 2.02 | 0.40 |
| 1:MA:115:VAL:HG22 | 1:MA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:MB:68:LEU:HD12 | 2:MB:68:LEU:HA | 1.90 | 0.40 |
| 2:MB:325:GLU:HA | 2:MB:328:GLU:HG2 | 2.02 | 0.40 |
| 1:MC:115:VAL:HG22 | 1:MC:119:LEU:HD23 | 2.04 | 0.40 |
| 2:MD:131:GLN:O | 2:MD:163:ILE:HG12 | 2.20 | 0.40 |
| 2:MD:178:THR:HG22 | 2:MD:180:VAL:H | 1.87 | 0.40 |
| 2:MD:282:ARG:NH2 | 2:MD:292:GLN:OE1 | 2.54 | 0.40 |
| 1:ME:262:TYR:HB2 | 1:ME:265:ILE:HD12 | 2.02 | 0.40 |
| 2:MF:178:THR:HG22 | 2:MF:180:VAL:H | 1.87 | 0.40 |
| 2:MF:282:ARG:NH2 | 2:MF:292:GLN:OE1 | 2.54 | 0.40 |
| 4:2B:149:ILE:O | 4:2B:151:VAL:N | 2.53 | 0.40 |
| 5:3B:158:LEU:HD21 | 5:3B:243:PHE:CE1 | 2.56 | 0.40 |
| 6:4B:161:LYS:C | 6:4B:161:LYS:CD | 2.93 | 0.40 |
| 6:4D:161:LYS:C | 6:4D:161:LYS:CD | 2.93 | 0.40 |
| 7:5A:1271:ILE:H | 7:5A:1271:ILE:HG13 | 1.43 | 0.40 |
| 7:5A:1384:GLN:N | 7:5A:1384:GLN:NE2 | 2.69 | 0.40 |
| 7:5B:1408:GLU:OE1 | 7:5B:1408:GLU:CA | 2.69 | 0.40 |
| 7:5C:1415:GLU:OE1 | 7:5C:1415:GLU:CA | 2.69 | 0.40 |
| 8:6B:75:ILE:HD13 | 8:6B:84:LEU:HD21 | 2.01 | 0.40 |
| 9:7C:39:GLY:CA | 9:7D:43:LEU:HG | 2.47 | 0.40 |
| 9:7C:39:GLY:H | 9:7D:43:LEU:HD21 | 1.85 | 0.40 |
| 2:AB:55:THR:CG2 | 2:BB:283:ALA:HB1 | 2.51 | 0.40 |
| 2:AD:390:ARG:CD | 1:AE:439:THR:HG21 | 2.51 | 0.40 |
| 1:AE:93:ILE:H | 1:AE:93:ILE:HD12 | 1.85 | 0.40 |
| 1:AE:203:MET:HE2 | 1:AE:203:MET:HA | 2.03 | 0.40 |
| 1:BA:68:LEU:HD21 | 1:BA:118:CYS:SG | 2.60 | 0.40 |
| 1:BA:124:LYS:HE2 | 1:BA:124:LYS:HB2 | 1.89 | 0.40 |
| 1:BA:205:ASP:OD1 | 1:BA:303:ALA:HA | 2.22 | 0.40 |
| 2:BB:391:ARG:HA | 2:BB:391:ARG:HD2 | 1.79 | 0.40 |
| 1:BC:181:VAL:HG21 | 2:BD:256:ASN:O | 2.20 | 0.40 |
| 1:BE:205:ASP:OD1 | 1:BE:303:ALA:HA | 2.22 | 0.40 |
| 2:BF:131:GLN:O | 2:BF:163:ILE:HG12 | 2.20 | 0.40 |
| 1:CA:322:ASP:OD1 | 1:CA:373:ARG:NH1 | 2.52 | 0.40 |
| 2:CB:282:ARG:NH2 | 2:CB:292:GLN:OE1 | 2.54 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CC:68:LEU:HD21 | 1:CC:118:CYS:SG | 2.60 | 0.40 |
| 1:CC:115:VAL:HG22 | 1:CC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:CC:203:MET:HA | 1:CC:203:MET:HE2 | 2.03 | 0.40 |
| 1:CE:203:MET:HA | 1:CE:203:MET:HE2 | 2.03 | 0.40 |
| 2:DB:87:PRO:HA | 2:DB:90:PHE:HD2 | 1.87 | 0.40 |
| 1:DC:203:MET:HE2 | 1:DC:203:MET:HA | 2.03 | 0.40 |
| 2:DD:69:GLU:HA | 2:DD:70:PRO:HD3 | 1.89 | 0.40 |
| 2:DD:87:PRO:HA | 2:DD:90:PHE:HD2 | 1.87 | 0.40 |
| 1:DE:115:VAL:HG22 | 1:DE:119:LEU:HD23 | 2.03 | 0.40 |
| 2:DF:178:THR:HG22 | 2:DF:180:VAL:H | 1.87 | 0.40 |
| 1:EA:68:LEU:HD21 | 1:EA:118:CYS:SG | 2.60 | 0.40 |
| 2:EB:84:LEU:O | 2:FB:281:TYR:OH | 2.39 | 0.40 |
| 2:EB:178:THR:HG22 | 2:EB:180:VAL:H | 1.87 | 0.40 |
| 1:EC:217:LEU:HD23 | 1:EC:217:LEU:HA | 1.93 | 0.40 |
| 2:ED:73:MET:HE1 | 2:ED:92:PHE:HB3 | 2.03 | 0.40 |
| 2:ED:83:GLN:OE1 | 2:ED:83:GLN:HA | 2.21 | 0.40 |
| 2:ED:178:THR:HG22 | 2:ED:180:VAL:H | 1.87 | 0.40 |
| 1:EE:181:VAL:CG1 | 2:EF:348:ASN:HA | 2.52 | 0.40 |
| 2:EF:83:GLN:OE1 | 2:EF:83:GLN:HA | 2.21 | 0.40 |
| 2:EF:293:MET:HE1 | 2:EF:330:MET:HE1 | 2.02 | 0.40 |
| 1:FA:115:VAL:HG22 | 1:FA:119:LEU:HD23 | 2.04 | 0.40 |
| 1:FA:205:ASP:OD1 | 1:FA:303:ALA:HA | 2.22 | 0.40 |
| 1:FA:287:SER:O | 1:FA:291:ILE:HG23 | 2.21 | 0.40 |
| 1:FC:85:GLN:O | 1:GC:283:HIS:CE1 | 2.75 | 0.40 |
| 1:FC:115:VAL:HG22 | 1:FC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:FC:181:VAL:CG1 | 2:FD:348:ASN:HA | 2.51 | 0.40 |
| 1:FE:423:GLU:OE2 | 7:5B:1256:ARG:NH1 | 2.50 | 0.40 |
| 2:GB:212:PHE:HE2 | 1:GC:326:LYS:HB2 | 1.87 | 0.40 |
| 1:GC:115:VAL:HG22 | 1:GC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:GC:262:TYR:HB2 | 1:GC:265:ILE:HD12 | 2.02 | 0.40 |
| 2:GD:87:PRO:HA | 2:GD:90:PHE:HD2 | 1.86 | 0.40 |
| 2:GD:391:ARG:HA | 2:GD:391:ARG:HD2 | 1.79 | 0.40 |
| 1:GE:98:ASP:CG | 1:GE:100:ALA:H | 2.29 | 0.40 |
| 1:GE:115:VAL:HG22 | 1:GE:119:LEU:HD23 | 2.04 | 0.40 |
| 2:GF:268:ILE:HG13 | 2:GF:300:MET:HG3 | 2.02 | 0.40 |
| 1:HA:296:PHE:CE2 | 1:HA:335:ILE:HG21 | 2.55 | 0.40 |
| 1:HC:247:ALA:HB2 | 1:HC:357:TYR:OH | 2.21 | 0.40 |
| 2:HD:325:GLU:HA | 2:HD:328:GLU:HG2 | 2.02 | 0.40 |
| 2:HD:390:ARG:CD | 1:HE:439:THR:HG21 | 2.51 | 0.40 |
| 2:HF:325:GLU:HA | 2:HF:328:GLU:HG2 | 2.03 | 0.40 |
| 1:IC:429:GLU:CD | 5:3C:307:LYS:NZ | 2.76 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:ID:73:MET:HE1 | 2:ID:92:PHE:HB3 | 2.03 | 0.40 |
| 1:IE:115:VAL:HG22 | 1:IE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:IE:262:TYR:HB2 | 1:IE:265:ILE:HD12 | 2.02 | 0.40 |
| 2:JB:325:GLU:HA | 2:JB:328:GLU:HG2 | 2.02 | 0.40 |
| 1:JC:247:ALA:HB2 | 1:JC:357:TYR:OH | 2.21 | 0.40 |
| 2:JD:178:THR:HG22 | 2:JD:180:VAL:H | 1.87 | 0.40 |
| 2:JD:375:GLN:O | 2:JD:379:LYS:HG3 | 2.20 | 0.40 |
| 1:JE:212:ILE:HD11 | 1:JE:300:ASN:HA | 2.03 | 0.40 |
| 2:JF:69:GLU:HA | 2:JF:70:PRO:HD3 | 1.89 | 0.40 |
| 2:JF:178:THR:HG22 | 2:JF:180:VAL:H | 1.87 | 0.40 |
| 2:JF:375:GLN:O | 2:JF:379:LYS:HG3 | 2.20 | 0.40 |
| 2:KB:212:PHE:HE2 | 1:KC:326:LYS:HB2 | 1.87 | 0.40 |
| 2:KB:325:GLU:HA | 2:KB:328:GLU:HG2 | 2.02 | 0.40 |
| 2:KD:83:GLN:HA | 2:KD:83:GLN:OE1 | 2.21 | 0.40 |
| 2:KD:87:PRO:HA | 2:KD:90:PHE:HD2 | 1.86 | 0.40 |
| 1:KE:115:VAL:HG22 | 1:KE:119:LEU:HD23 | 2.04 | 0.40 |
| 2:KF:83:GLN:OE1 | 2:KF:83:GLN:HA | 2.21 | 0.40 |
| 2:KF:178:THR:HG22 | 2:KF:180:VAL:H | 1.86 | 0.40 |
| 1:LC:115:VAL:HG22 | 1:LC:119:LEU:HD23 | 2.04 | 0.40 |
| 1:LC:181:VAL:HG12 | 2:LD:348:ASN:HA | 2.02 | 0.40 |
| 1:LE:205:ASP:OD1 | 1:LE:303:ALA:HA | 2.22 | 0.40 |
| 2:MB:178:THR:HG22 | 2:MB:180:VAL:H | 1.87 | 0.40 |
| 2:MB:282:ARG:NH2 | 2:MB:292:GLN:OE1 | 2.54 | 0.40 |
| 1:MC:100:ALA:HB1 | 2:MD:252:LYS:N | 2.36 | 0.40 |
| 1:ME:115:VAL:HG22 | 1:ME:119:LEU:HD23 | 2.04 | 0.40 |
| 2:MF:131:GLN:O | 2:MF:163:ILE:HG12 | 2.20 | 0.40 |
| 5:3A:158:LEU:HD21 | 5:3A:243:PHE:CE1 | 2.56 | 0.40 |
| 5:3C:158:LEU:HD21 | 5:3C:243:PHE:CE1 | 2.56 | 0.40 |
| 6:4A:112:SER:HA | 6:4A:115:LYS:HE2 | 2.03 | 0.40 |
| 6:4B:139:ASP:HA | 6:4B:140:PRO:HD3 | 1.85 | 0.40 |
| 6:4B:219:ASN:HA | 6:4B:219:ASN:HD22 | 1.53 | 0.40 |
| 6:4D:112:SER:HA | 6:4D:115:LYS:HE2 | 2.03 | 0.40 |
| 7:5A:1284:PHE:CE1 | 9:7A:12:GLU:CD | 2.83 | 0.40 |
| 7:5A:1398:GLU:HG3 | 7:5A:1400:GLU:CG | 2.52 | 0.40 |
| 7:5B:1271:ILE:H | 7:5B:1271:ILE:HG13 | 1.43 | 0.40 |
| 7:5B:1316:LEU:CA | 7:5B:1319:HIS:HB2 | 2.47 | 0.40 |
| 7:5B:1406:PHE:HA | 7:5B:1409:PHE:HB3 | 2.02 | 0.40 |
| 7:5C:1370:LYS:CA | 7:5C:1370:LYS:HE2 | 2.50 | 0.40 |
| 7:5C:1398:GLU:HG3 | 7:5C:1400:GLU:CG | 2.52 | 0.40 |
| 7:5C:1425:LYS:O | 7:5C:1425:LYS:CE | 2.69 | 0.40 |
| 7:5C:1474:LEU:CD2 | 7:5C:1576:ILE:CD1 | 2.93 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:212:PHE:HE2 | 1:AC:326:LYS:HB2 | 1.87 | 0.40 |
| 2:AB:325:GLU:HA | 2:AB:328:GLU:HG2 | 2.02 | 0.40 |
| 2:AD:87:PRO:HA | 2:AD:90:PHE:HD2 | 1.86 | 0.40 |
| 2:AD:220:PRO:HD2 | 1:AE:326:LYS:CG | 2.44 | 0.40 |
| 2:AF:325:GLU:HA | 2:AF:328:GLU:HG2 | 2.02 | 0.40 |
| 1:BC:205:ASP:OD1 | 1:BC:303:ALA:HA | 2.22 | 0.40 |
| 1:BE:60:LYS:NZ | 1:CE:283:HIS:CD2 | 2.89 | 0.40 |
| 1:CA:247:ALA:HB2 | 1:CA:357:TYR:OH | 2.21 | 0.40 |
| 2:CB:44:LEU:HD23 | 2:CB:44:LEU:HA | 1.93 | 0.40 |
| 2:CB:293:MET:HE1 | 2:CB:330:MET:HE1 | 2.02 | 0.40 |
| 2:CB:325:GLU:HA | 2:CB:328:GLU:HG2 | 2.02 | 0.40 |
| 2:CD:83:GLN:OE1 | 2:CD:83:GLN:HA | 2.21 | 0.40 |
| 2:CD:177:ASP:HA | 1:CE:353:VAL:HG12 | 2.03 | 0.40 |
| 2:CD:293:MET:HE1 | 2:CD:330:MET:HE1 | 2.02 | 0.40 |
| 2:CD:325:GLU:HA | 2:CD:328:GLU:HG2 | 2.02 | 0.40 |
| 1:CE:247:ALA:HB2 | 1:CE:357:TYR:OH | 2.21 | 0.40 |
| 2:CF:83:GLN:OE1 | 2:CF:83:GLN:HA | 2.21 | 0.40 |
| 2:CF:293:MET:HE1 | 2:CF:330:MET:HE1 | 2.02 | 0.40 |
| 2:DB:375:GLN:O | 2:DB:379:LYS:HG3 | 2.20 | 0.40 |
| 1:DC:287:SER:O | 1:DC:291:ILE:HG23 | 2.21 | 0.40 |
| 2:DD:222:TYR:CE2 | 1:DE:325:PRO:HG2 | 2.56 | 0.40 |
| 2:DD:257:LEU:HD11 | 2:DD:314:SER:HB2 | 2.03 | 0.40 |
| 2:DD:325:GLU:HA | 2:DD:328:GLU:HG2 | 2.02 | 0.40 |
| 1:DE:98:ASP:CG | 1:DE:100:ALA:H | 2.29 | 0.40 |
| 1:DE:203:MET:HE2 | 1:DE:203:MET:HA | 2.03 | 0.40 |
| 1:EA:203:MET:HA | 1:EA:203:MET:HE2 | 2.03 | 0.40 |
| 1:EA:426:ALA:CB | 7:5C:833:PHE:CB | 2.94 | 0.40 |
| 1:EA:430:LYS:H | 7:5C:833:PHE:HE1 | 1.66 | 0.40 |
| 1:EC:430:LYS:HZ2 | 7:5A:834:ASN:HD22 | 0.69 | 0.40 |
| 1:EE:115:VAL:HG22 | 1:EE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:EE:247:ALA:HB2 | 1:EE:357:TYR:OH | 2.21 | 0.40 |
| 2:EF:178:THR:HG22 | 2:EF:180:VAL:H | 1.87 | 0.40 |
| 1:FA:203:MET:HE2 | 1:FA:203:MET:HA | 2.03 | 0.40 |
| 2:FD:208:TYR:CE2 | 1:FE:326:LYS:HB3 | 2.56 | 0.40 |
| 1:FE:115:VAL:HG22 | 1:FE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:GA:115:VAL:HG22 | 1:GA:119:LEU:HD23 | 2.04 | 0.40 |
| 1:GA:203:MET:HE2 | 1:GA:203:MET:HA | 2.03 | 0.40 |
| 2:GB:83:GLN:OE1 | 2:GB:83:GLN:HA | 2.21 | 0.40 |
| 1:HA:115:VAL:HG22 | 1:HA:119:LEU:HD23 | 2.04 | 0.40 |
| 1:HA:247:ALA:HB2 | 1:HA:357:TYR:OH | 2.21 | 0.40 |
| 1:HE:205:ASP:OD1 | 1:HE:303:ALA:HA | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:HE:287:SER:O | 1:HE:291:ILE:HG23 | 2.21 | 0.40 |
| 1:HE:425:LEU:HA | 1:HE:425:LEU:HD23 | 1.86 | 0.40 |
| 1:IA:98:ASP:CG | 1:IA:100:ALA:H | 2.29 | 0.40 |
| 1:IA:115:VAL:HG22 | 1:IA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:IB:73:MET:HE1 | 2:IB:92:PHE:HB3 | 2.03 | 0.40 |
| 1:IC:124:LYS:HE2 | 1:IC:124:LYS:HB2 | 1.88 | 0.40 |
| 2:ID:325:GLU:HA | 2:ID:328:GLU:HG2 | 2.02 | 0.40 |
| 1:IE:98:ASP:CG | 1:IE:100:ALA:H | 2.29 | 0.40 |
| 1:JC:115:VAL:HG22 | 1:JC:119:LEU:HD23 | 2.04 | 0.40 |
| 2:JD:390:ARG:CD | 1:JE:439:THR:HG21 | 2.51 | 0.40 |
| 2:JF:262:ARG:NH1 | 2:JF:421:GLU:OE1 | 2.50 | 0.40 |
| 1:KA:115:VAL:HG22 | 1:KA:119:LEU:HD23 | 2.04 | 0.40 |
| 2:KB:69:GLU:HA | 2:KB:70:PRO:HD3 | 1.89 | 0.40 |
| 2:KB:178:THR:HG22 | 2:KB:180:VAL:H | 1.87 | 0.40 |
| 1:KC:71:GLU:OE2 | 1:KC:73:THR:OG1 | 2.28 | 0.40 |
| 1:KE:398:MET:SD | 2:KF:345:ILE:CG1 | 2.92 | 0.40 |
| 1:LA:205:ASP:OD1 | 1:LA:303:ALA:HA | 2.22 | 0.40 |
| 2:LB:306:ARG:NH2 | 4:2C:151:VAL:CB | 2.84 | 0.40 |
| 1:LC:205:ASP:OD1 | 1:LC:303:ALA:HA | 2.22 | 0.40 |
| 1:LE:212:ILE:HD11 | 1:LE:300:ASN:HA | 2.03 | 0.40 |
| 1:LE:247:ALA:HB2 | 1:LE:357:TYR:OH | 2.21 | 0.40 |
| 1:MC:124:LYS:HE2 | 1:MC:124:LYS:HB2 | 1.89 | 0.40 |
| 2:MD:325:GLU:HA | 2:MD:328:GLU:HG2 | 2.03 | 0.40 |
| 2:MF:325:GLU:HA | 2:MF:328:GLU:HG2 | 2.03 | 0.40 |
| 4:2B:72:TYR:HE2 | 4:2B:111:GLU:HG3 | 1.87 | 0.40 |
| 6:4B:112:SER:HA | 6:4B:115:LYS:HE2 | 2.03 | 0.40 |
| 7:5A:1387:ILE:N | 7:5A:1387:ILE:HD13 | 2.37 | 0.40 |
| 7:5A:1415:GLU:OE1 | 7:5A:1415:GLU:CA | 2.69 | 0.40 |
| 7:5B:1061:ILE:O | 7:5B:1065:LYS:HG3 | 2.20 | 0.40 |
| 7:5B:1398:GLU:HG3 | 7:5B:1400:GLU:CG | 2.52 | 0.40 |
| 7:5C:1250:VAL:HG11 | 7:5C:1262:GLU:CG | 2.51 | 0.40 |
| 7:5C:1384:GLN:N | 7:5C:1384:GLN:NE2 | 2.69 | 0.40 |
| 7:5C:1387:ILE:N | 7:5C:1387:ILE:HD13 | 2.37 | 0.40 |
| 7:5C:1392:LEU:O | 7:5C:1392:LEU:HD22 | 2.21 | 0.40 |
| 1:AA:115:VAL:HG22 | 1:AA:119:LEU:HD23 | 2.04 | 0.40 |
| 1:AC:248:LEU:HD12 | 1:AC:248:LEU:HA | 1.89 | 0.40 |
| 2:AD:325:GLU:HA | 2:AD:328:GLU:HG2 | 2.02 | 0.40 |
| 1:AE:164:LYS:HA | 1:AE:164:LYS:HD3 | 1.85 | 0.40 |
| 1:AE:205:ASP:OD1 | 1:AE:303:ALA:HA | 2.21 | 0.40 |
| 2:AF:391:ARG:HA | 2:AF:391:ARG:HD2 | 1.79 | 0.40 |
| 2:BB:68:LEU:HD12 | 2:BB:68:LEU:HA | 1.90 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BB:73:MET:HE1 | 2:BB:92:PHE:HB3 | 2.03 | 0.40 |
| 2:BB:176:SER:CB | 1:BC:349:THR:OG1 | 2.70 | 0.40 |
| 2:BB:325:GLU:HA | 2:BB:328:GLU:HG2 | 2.02 | 0.40 |
| 1:BC:71:GLU:OE2 | 1:BC:73:THR:OG1 | 2.28 | 0.40 |
| 2:BD:325:GLU:HA | 2:BD:328:GLU:HG2 | 2.02 | 0.40 |
| 1:BE:262:TYR:HB2 | 1:BE:265:ILE:HD12 | 2.02 | 0.40 |
| 1:CA:222:PRO:HG2 | 2:CB:324:LYS:HB2 | 2.03 | 0.40 |
| 1:CC:322:ASP:OD1 | 1:CC:373:ARG:NH1 | 2.52 | 0.40 |
| 2:CD:73:MET:HE1 | 2:CD:92:PHE:HB3 | 2.03 | 0.40 |
| 2:CF:73:MET:HE1 | 2:CF:92:PHE:HB3 | 2.03 | 0.40 |
| 1:DA:115:VAL:HG22 | 1:DA:119:LEU:HD23 | 2.03 | 0.40 |
| 1:DA:203:MET:HE2 | 1:DA:203:MET:HA | 2.03 | 0.40 |
| 1:DA:287:SER:O | 1:DA:291:ILE:HG23 | 2.21 | 0.40 |
| 2:DB:73:MET:HE1 | 2:DB:92:PHE:HB3 | 2.03 | 0.40 |
| 2:DB:85:PHE:C | 2:EB:281:TYR:CE1 | 2.97 | 0.40 |
| 1:DC:128:ASN:HD21 | 1:EC:285:GLN:NE2 | 2.18 | 0.40 |
| 2:DD:73:MET:HE1 | 2:DD:92:PHE:HB3 | 2.03 | 0.40 |
| 2:DD:178:THR:HG22 | 2:DD:180:VAL:H | 1.87 | 0.40 |
| 2:DD:219:THR:HA | 1:DE:326:LYS:HE2 | 2.03 | 0.40 |
| 2:DD:262:ARG:NH1 | 2:DD:421:GLU:OE1 | 2.50 | 0.40 |
| 2:DF:73:MET:HE1 | 2:DF:92:PHE:HB3 | 2.03 | 0.40 |
| 2:DF:257:LEU:HD11 | 2:DF:314:SER:HB2 | 2.03 | 0.40 |
| 2:DF:325:GLU:HA | 2:DF:328:GLU:HG2 | 2.03 | 0.40 |
| 1:FA:222:PRO:HG2 | 2:FB:324:LYS:HB2 | 2.04 | 0.40 |
| 2:FD:106:TYR:O | 7:5A:1298:LYS:HE2 | 2.16 | 0.40 |
| 1:FE:164:LYS:HD3 | 1:FE:164:LYS:HA | 1.86 | 0.40 |
| 2:GB:178:THR:HG22 | 2:GB:180:VAL:H | 1.87 | 0.40 |
| 2:GB:220:PRO:HD2 | 1:GC:326:LYS:CG | 2.46 | 0.40 |
| 1:GC:98:ASP:CG | 1:GC:100:ALA:H | 2.29 | 0.40 |
| 1:GC:203:MET:HE2 | 1:GC:203:MET:HA | 2.03 | 0.40 |
| 1:GC:247:ALA:HB2 | 1:GC:357:TYR:OH | 2.21 | 0.40 |
| 1:GE:60:LYS:CD | 1:HE:283:HIS:CD2 | 2.95 | 0.40 |
| 1:HA:205:ASP:OD1 | 1:HA:303:ALA:HA | 2.22 | 0.40 |
| 1:HC:205:ASP:OD1 | 1:HC:303:ALA:HA | 2.22 | 0.40 |
| 1:HE:247:ALA:HB2 | 1:HE:357:TYR:OH | 2.21 | 0.40 |
| 2:HF:391:ARG:HD2 | 2:HF:391:ARG:HA | 1.79 | 0.40 |
| 1:IA:212:ILE:HD11 | 1:IA:300:ASN:HA | 2.03 | 0.40 |
| 2:IB:212:PHE:HE2 | 1:IC:326:LYS:HB2 | 1.87 | 0.40 |
| 1:IC:98:ASP:CG | 1:IC:100:ALA:H | 2.29 | 0.40 |
| 1:IC:212:ILE:HD11 | 1:IC:300:ASN:HA | 2.02 | 0.40 |
| 2:IF:325:GLU:HA | 2:IF:328:GLU:HG2 | 2.02 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:JA:247:ALA:HB2 | 1:JA:357:TYR:OH | 2.21 | 0.40 |
| 2:JD:262:ARG:NH1 | 2:JD:421:GLU:OE1 | 2.50 | 0.40 |
| 1:JE:115:VAL:HG22 | 1:JE:119:LEU:HD23 | 2.04 | 0.40 |
| 1:KA:372:MET:O | 6:4C:299:TYR:CE2 | 2.72 | 0.40 |
| 2:KB:87:PRO:HA | 2:KB:90:PHE:HD2 | 1.87 | 0.40 |
| 2:KB:176:SER:CB | 1:KC:349:THR:HG1 | 2.34 | 0.40 |
| 1:KC:212:ILE:HD11 | 1:KC:300:ASN:HA | 2.02 | 0.40 |
| 2:KD:178:THR:HG22 | 2:KD:180:VAL:H | 1.87 | 0.40 |
| 2:KD:220:PRO:HD2 | 1:KE:326:LYS:CE | 2.44 | 0.40 |
| 2:KD:325:GLU:HA | 2:KD:328:GLU:HG2 | 2.02 | 0.40 |
| 2:KF:325:GLU:HA | 2:KF:328:GLU:HG2 | 2.02 | 0.40 |
| 2:LB:325:GLU:HA | 2:LB:328:GLU:HG2 | 2.02 | 0.40 |
| 2:LD:131:GLN:O | 2:LD:163:ILE:HG12 | 2.20 | 0.40 |
| 1:MA:357:TYR:CE1 | 6:4C:185:ARG:NH1 | 2.88 | 0.40 |
| 1:ME:372:MET:CE | 6:4B:96:VAL:HB | 2.52 | 0.40 |
| 2:MF:73:MET:HE1 | 2:MF:92:PHE:HB3 | 2.03 | 0.40 |
| 4:2A:16:GLN:CA | 4:2A:19:MET:CB | 2.30 | 0.40 |
| 4:2A:72:TYR:HE2 | 4:2A:111:GLU:HG3 | 1.87 | 0.40 |
| 4:2C:72:TYR:HE2 | 4:2C:111:GLU:HG3 | 1.87 | 0.40 |
| 6:4B:175:LEU:HD13 | 6:4B:175:LEU:HA | 1.74 | 0.40 |
| 7:5A:1392:LEU:O | 7:5A:1392:LEU:HD22 | 2.21 | 0.40 |
| 7:5A:1425:LYS:O | 7:5A:1425:LYS:CE | 2.70 | 0.40 |
| 7:5B:771:LEU:HB3 | 7:5B:772:LEU:H | 1.64 | 0.40 |
| 7:5B:1387:ILE:N | 7:5B:1387:ILE:HD13 | 2.37 | 0.40 |
| 7:5B:1392:LEU:O | 7:5B:1392:LEU:HD22 | 2.21 | 0.40 |
| 7:5B:1425:LYS:O | 7:5B:1425:LYS:CE | 2.69 | 0.40 |
| 7:5C:1397:GLU:OE1 | 7:5C:1397:GLU:CA | 2.70 | 0.40 |
| 8:6A:20:LYS:CE | 8:6A:101:GLU:OE1 | 2.70 | 0.40 |
| 8:6B:20:LYS:CE | 8:6B:101:GLU:OE1 | 2.70 | 0.40 |
| 8:6C:129:VAL:HG21 | 8:6C:141:GLU:HB2 | 2.03 | 0.40 |
| 9:7F:12:GLU:CA | 9:7F:16:THR:HG1 | 2.10 | 0.40 |
| 9:7F:45:ARG:HD2 | 9:7F:45:ARG:HA | 1.85 | 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 | AA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | AC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | AE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | BA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | BC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | BE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | CA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | CC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | CE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | DA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | DC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | DE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | EA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | EC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | EE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | FA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | FC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | FE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | GA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | GC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | GE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | HA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | HC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | HE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | IA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | IC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | IE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | JA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | JC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | JE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | KA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | KC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | KE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | LA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | LC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | LE | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | MA | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | MC | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | ME | 426/449 (95%) | 416 (98%) | 10 (2%) | 0 | 100 | 100 |
| 2 | AB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | AD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | AF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | BB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | BD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | BF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | CB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | CD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | CF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | DB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | DD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | DF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | EB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | ED | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | EF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | FB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | FD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | FF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | GB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | GD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | GF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | HB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | HD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | HF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | IB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | ID | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | IF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | JB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | JD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | JF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | KB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | KD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | KF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | LB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | LD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | LF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | MB | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | MD | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | MF | 428/443 (97%) | 423 (99%) | 5 (1%) | 0 | 100 | 100 |
| 3 | 1A | 138/213 (65%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | 1B | 138/213 (65%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | 1C | 138/213 (65%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 4 | 2A | 186/742 (25%) | 172 (92%) | 9 (5%) | 5 (3%) | 4 | 29 |
| 4 | 2B | 186/742 (25%) | 172 (92%) | 9 (5%) | 5 (3%) | 4 | 29 |
| 4 | 2C | 186/742 (25%) | 172 (92%) | 9 (5%) | 5 (3%) | 4 | 29 |
| 5 | 3A | 327/495 (66%) | 316 (97%) | 10 (3%) | 1 (0%) | 37 | 67 |
| 5 | 3B | 327/495 (66%) | 316 (97%) | 10 (3%) | 1 (0%) | 37 | 67 |
| 5 | 3C | 327/495 (66%) | 316 (97%) | 10 (3%) | 1 (0%) | 37 | 67 |
| 6 | 4A | 183/317 (58%) | 176 (96%) | 4 (2%) | 3 (2%) | 8 | 37 |
| 6 | 4B | 183/317 (58%) | 176 (96%) | 4 (2%) | 3 (2%) | 8 | 37 |
| 6 | 4C | 183/317 (58%) | 176 (96%) | 4 (2%) | 3 (2%) | 8 | 37 |
| 6 | 4D | 183/317 (58%) | 176 (96%) | 4 (2%) | 3 (2%) | 8 | 37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 7 | 5A | 695/1754 (40%) | 650 (94%) | 33 (5%) | 12 (2%) | 7 | 36 |
| 7 | 5B | 695/1754 (40%) | 650 (94%) | 33 (5%) | 12 (2%) | 7 | 36 |
| 7 | 5C | 695/1754 (40%) | 650 (94%) | 33 (5%) | 12 (2%) | 7 | 36 |
| 8 | 6A | 254/346 (73%) | 247 (97%) | 7 (3%) | 0 | 100 | 100 |
| 8 | 6B | 254/346 (73%) | 247 (97%) | 7 (3%) | 0 | 100 | 100 |
| 8 | 6C | 254/346 (73%) | 247 (97%) | 7 (3%) | 0 | 100 | 100 |
| 9 | 7A | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 9 | 7B | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 9 | 7C | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 9 | 7D | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 9 | 7E | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 9 | 7F | 44/101 (44%) | 44 (100%) | 0 | 0 | 100 | 100 |
| All | All | 39102/47312 (83%) | 38252 (98%) | 784 (2%) | 66 (0%) | 45 | 72 |

All (66) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2A | 146 | PRO |
| 4 | 2A | 147 | PHE |
| 4 | 2A | 150 | GLN |
| 4 | 2B | 146 | PRO |
| 4 | 2B | 147 | PHE |
| 4 | 2B | 150 | GLN |
| 4 | 2C | 146 | PRO |
| 4 | 2C | 147 | PHE |
| 4 | 2C | 150 | GLN |
| 6 | 4A | 98 | PRO |
| 6 | 4A | 105 | GLU |
| 6 | 4A | 108 | LYS |
| 6 | 4B | 98 | PRO |
| 6 | 4B | 105 | GLU |
| 6 | 4B | 108 | LYS |
| 6 | 4C | 98 | PRO |
| 6 | 4C | 105 | GLU |
| 6 | 4C | 108 | LYS |
| 6 | 4D | 98 | PRO |
| 6 | 4D | 105 | GLU |
| 6 | 4D | 108 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5A | 774 | ASN |
| 7 | 5A | 811 | GLN |
| 7 | 5A | 812 | LYS |
| 7 | 5A | 846 | PHE |
| 7 | 5A | 1371 | GLU |
| 7 | 5A | 1580 | LYS |
| 7 | 5B | 774 | ASN |
| 7 | 5B | 811 | GLN |
| 7 | 5B | 812 | LYS |
| 7 | 5B | 846 | PHE |
| 7 | 5B | 1371 | GLU |
| 7 | 5B | 1580 | LYS |
| 7 | 5C | 774 | ASN |
| 7 | 5C | 811 | GLN |
| 7 | 5C | 812 | LYS |
| 7 | 5C | 846 | PHE |
| 7 | 5C | 1371 | GLU |
| 7 | 5C | 1580 | LYS |
| 7 | 5A | 1245 | GLY |
| 7 | 5A | 1280 | SER |
| 7 | 5A | 1471 | ILE |
| 7 | 5A | 1578 | GLY |
| 7 | 5B | 1245 | GLY |
| 7 | 5B | 1280 | SER |
| 7 | 5B | 1471 | ILE |
| 7 | 5B | 1578 | GLY |
| 7 | 5C | 1245 | GLY |
| 7 | 5C | 1280 | SER |
| 7 | 5C | 1471 | ILE |
| 7 | 5C | 1578 | GLY |
| 5 | 3A | 23 | SER |
| 5 | 3B | 23 | SER |
| 5 | 3C | 23 | SER |
| 7 | 5A | 1244 | LEU |
| 7 | 5B | 1244 | LEU |
| 7 | 5C | 1244 | LEU |
| 4 | 2A | 148 | ASN |
| 4 | 2B | 148 | ASN |
| 4 | 2C | 148 | ASN |
| 7 | 5A | 909 | ASN |
| 7 | 5B | 909 | ASN |
| 7 | 5C | 909 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2B | 149 | ILE |
| 4 | 2A | 149 | ILE |
| 4 | 2C | 149 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | AA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | AC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | AE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | BA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | BC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | BE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | CA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | CC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | CE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | DA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | DC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | DE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | EA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | EC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | EE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | FA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | FC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | FE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | GA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | GC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | GE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | HA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | HC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | HE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | IA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | IC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | IE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | JA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | JC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | JE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | KA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | KC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | KE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | LA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | LC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | LE | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | MA | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | MC | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 1 | ME | 364/376 (97%) | 364 (100%) | 0 | 100 | 100 |
| 2 | AB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | AD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | AF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | BB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | BD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | BF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | CB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | CD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | CF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | DB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | DD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | DF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | EB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | ED | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | EF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | FB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | FD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | FF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | GB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | GD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | GF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | HB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | HD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | HF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | IB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | ID | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | IF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | JB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | JD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | JF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | KB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | KD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | KF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | LB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | LD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | LF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | MB | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | MD | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 2 | MF | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 3 | 1A | 129/196 (66%) | 128 (99%) | 1 (1%) | 79 | 85 |
| 3 | 1B | 129/196 (66%) | 128 (99%) | 1 (1%) | 79 | 85 |
| 3 | 1C | 129/196 (66%) | 128 (99%) | 1 (1%) | 79 | 85 |
| 4 | 2A | 180/692 (26%) | 162 (90%) | 18 (10%) | 6 | 26 |
| 4 | 2B | 180/692 (26%) | 162 (90%) | 18 (10%) | 6 | 26 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|-------------|-----|
| 4 | 2C | 180/692 (26%) | 162 (90%) | 18 (10%) | 6 | 26 |
| 5 | 3A | 309/457 (68%) | 305 (99%) | 4 (1%) | 65 | 77 |
| 5 | 3B | 309/457 (68%) | 305 (99%) | 4 (1%) | 65 | 77 |
| 5 | 3C | 309/457 (68%) | 305 (99%) | 4 (1%) | 65 | 77 |
| 6 | 4A | 176/286 (62%) | 92 (52%) | 84 (48%) | 0 | 0 |
| 6 | 4B | 176/286 (62%) | 92 (52%) | 84 (48%) | 0 | 0 |
| 6 | 4C | 176/286 (62%) | 92 (52%) | 84 (48%) | 0 | 0 |
| 6 | 4D | 176/286 (62%) | 92 (52%) | 84 (48%) | 0 | 0 |
| 7 | 5A | 663/1625 (41%) | 501 (76%) | 162 (24%) | 0 | 4 |
| 7 | 5B | 663/1625 (41%) | 501 (76%) | 162 (24%) | 0 | 4 |
| 7 | 5C | 663/1625 (41%) | 500 (75%) | 163 (25%) | 0 | 4 |
| 8 | 6A | 229/316 (72%) | 225 (98%) | 4 (2%) | 56 | 73 |
| 8 | 6B | 229/316 (72%) | 225 (98%) | 4 (2%) | 56 | 73 |
| 8 | 6C | 229/316 (72%) | 225 (98%) | 4 (2%) | 56 | 73 |
| 9 | 7A | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| 9 | 7B | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| 9 | 7C | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| 9 | 7D | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| 9 | 7E | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| 9 | 7F | 42/86 (49%) | 42 (100%) | 0 | 100 | 100 |
| All | All | 33917/40846 (83%) | 33013 (97%) | 904 (3%) | 41 | 61 |

All (904) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1A | 1 | MET |
| 3 | 1B | 1 | MET |
| 3 | 1C | 1 | MET |
| 4 | 2A | 10 | LYS |
| 4 | 2A | 13 | THR |
| 4 | 2A | 14 | LYS |
| 4 | 2A | 15 | GLU |
| 4 | 2A | 38 | VAL |
| 4 | 2A | 87 | LEU |
| 4 | 2A | 144 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2A | 147 | PHE |
| 4 | 2A | 148 | ASN |
| 4 | 2A | 149 | ILE |
| 4 | 2A | 151 | VAL |
| 4 | 2A | 152 | LYS |
| 4 | 2A | 160 | PHE |
| 4 | 2A | 162 | GLN |
| 4 | 2A | 164 | ARG |
| 4 | 2A | 178 | LYS |
| 4 | 2A | 192 | LEU |
| 4 | 2A | 197 | LEU |
| 4 | 2B | 10 | LYS |
| 4 | 2B | 13 | THR |
| 4 | 2B | 14 | LYS |
| 4 | 2B | 15 | GLU |
| 4 | 2B | 38 | VAL |
| 4 | 2B | 87 | LEU |
| 4 | 2B | 144 | ASN |
| 4 | 2B | 147 | PHE |
| 4 | 2B | 148 | ASN |
| 4 | 2B | 149 | ILE |
| 4 | 2B | 151 | VAL |
| 4 | 2B | 152 | LYS |
| 4 | 2B | 160 | PHE |
| 4 | 2B | 162 | GLN |
| 4 | 2B | 164 | ARG |
| 4 | 2B | 178 | LYS |
| 4 | 2B | 192 | LEU |
| 4 | 2B | 197 | LEU |
| 4 | 2C | 10 | LYS |
| 4 | 2C | 13 | THR |
| 4 | 2C | 14 | LYS |
| 4 | 2C | 15 | GLU |
| 4 | 2C | 38 | VAL |
| 4 | 2C | 87 | LEU |
| 4 | 2C | 144 | ASN |
| 4 | 2C | 147 | PHE |
| 4 | 2C | 148 | ASN |
| 4 | 2C | 149 | ILE |
| 4 | 2C | 151 | VAL |
| 4 | 2C | 152 | LYS |
| 4 | 2C | 160 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2C | 162 | GLN |
| 4 | 2C | 164 | ARG |
| 4 | 2C | 178 | LYS |
| 4 | 2C | 192 | LEU |
| 4 | 2C | 197 | LEU |
| 5 | 3A | 100 | LEU |
| 5 | 3A | 138 | LEU |
| 5 | 3A | 309 | TRP |
| 5 | 3A | 321 | LEU |
| 5 | 3B | 100 | LEU |
| 5 | 3B | 138 | LEU |
| 5 | 3B | 309 | TRP |
| 5 | 3B | 321 | LEU |
| 5 | 3C | 100 | LEU |
| 5 | 3C | 138 | LEU |
| 5 | 3C | 309 | TRP |
| 5 | 3C | 321 | LEU |
| 6 | 4A | 96 | VAL |
| 6 | 4A | 97 | GLN |
| 6 | 4A | 99 | ARG |
| 6 | 4A | 102 | LEU |
| 6 | 4A | 105 | GLU |
| 6 | 4A | 107 | MET |
| 6 | 4A | 108 | LYS |
| 6 | 4A | 110 | LYS |
| 6 | 4A | 113 | ILE |
| 6 | 4A | 114 | GLU |
| 6 | 4A | 115 | LYS |
| 6 | 4A | 116 | THR |
| 6 | 4A | 121 | ARG |
| 6 | 4A | 132 | LYS |
| 6 | 4A | 135 | LEU |
| 6 | 4A | 137 | ASN |
| 6 | 4A | 141 | LYS |
| 6 | 4A | 142 | SER |
| 6 | 4A | 143 | THR |
| 6 | 4A | 144 | LEU |
| 6 | 4A | 149 | ASN |
| 6 | 4A | 151 | ARG |
| 6 | 4A | 154 | LYS |
| 6 | 4A | 155 | ASP |
| 6 | 4A | 157 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4A | 161 | LYS |
| 6 | 4A | 162 | GLN |
| 6 | 4A | 163 | GLN |
| 6 | 4A | 164 | ARG |
| 6 | 4A | 167 | ARG |
| 6 | 4A | 173 | VAL |
| 6 | 4A | 178 | HIS |
| 6 | 4A | 179 | ARG |
| 6 | 4A | 180 | ILE |
| 6 | 4A | 184 | GLU |
| 6 | 4A | 185 | ARG |
| 6 | 4A | 190 | TRP |
| 6 | 4A | 191 | GLU |
| 6 | 4A | 192 | GLN |
| 6 | 4A | 193 | MET |
| 6 | 4A | 201 | GLN |
| 6 | 4A | 205 | GLN |
| 6 | 4A | 215 | LYS |
| 6 | 4A | 217 | ASN |
| 6 | 4A | 218 | THR |
| 6 | 4A | 219 | ASN |
| 6 | 4A | 221 | MET |
| 6 | 4A | 223 | PHE |
| 6 | 4A | 226 | ILE |
| 6 | 4A | 228 | LEU |
| 6 | 4A | 230 | TYR |
| 6 | 4A | 231 | GLU |
| 6 | 4A | 232 | LYS |
| 6 | 4A | 233 | SER |
| 6 | 4A | 239 | LEU |
| 6 | 4A | 241 | LYS |
| 6 | 4A | 242 | ARG |
| 6 | 4A | 244 | GLU |
| 6 | 4A | 245 | MET |
| 6 | 4A | 247 | LYS |
| 6 | 4A | 252 | VAL |
| 6 | 4A | 253 | ARG |
| 6 | 4A | 257 | LEU |
| 6 | 4A | 258 | ASP |
| 6 | 4A | 262 | ASN |
| 6 | 4A | 267 | ILE |
| 6 | 4A | 268 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4A | 269 | THR |
| 6 | 4A | 273 | ARG |
| 6 | 4A | 274 | ILE |
| 6 | 4A | 277 | GLU |
| 6 | 4A | 278 | TYR |
| 6 | 4A | 280 | VAL |
| 6 | 4A | 282 | ASN |
| 6 | 4A | 283 | HIS |
| 6 | 4A | 285 | ARG |
| 6 | 4A | 287 | ASP |
| 6 | 4A | 289 | LYS |
| 6 | 4A | 290 | THR |
| 6 | 4A | 292 | VAL |
| 6 | 4A | 295 | LYS |
| 6 | 4A | 297 | GLU |
| 6 | 4A | 299 | TYR |
| 6 | 4A | 300 | SER |
| 6 | 4B | 96 | VAL |
| 6 | 4B | 97 | GLN |
| 6 | 4B | 99 | ARG |
| 6 | 4B | 102 | LEU |
| 6 | 4B | 105 | GLU |
| 6 | 4B | 107 | MET |
| 6 | 4B | 108 | LYS |
| 6 | 4B | 110 | LYS |
| 6 | 4B | 113 | ILE |
| 6 | 4B | 114 | GLU |
| 6 | 4B | 115 | LYS |
| 6 | 4B | 116 | THR |
| 6 | 4B | 121 | ARG |
| 6 | 4B | 132 | LYS |
| 6 | 4B | 135 | LEU |
| 6 | 4B | 137 | ASN |
| 6 | 4B | 141 | LYS |
| 6 | 4B | 142 | SER |
| 6 | 4B | 143 | THR |
| 6 | 4B | 144 | LEU |
| 6 | 4B | 149 | ASN |
| 6 | 4B | 151 | ARG |
| 6 | 4B | 154 | LYS |
| 6 | 4B | 155 | ASP |
| 6 | 4B | 157 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4B | 161 | LYS |
| 6 | 4B | 162 | GLN |
| 6 | 4B | 163 | GLN |
| 6 | 4B | 164 | ARG |
| 6 | 4B | 167 | ARG |
| 6 | 4B | 173 | VAL |
| 6 | 4B | 178 | HIS |
| 6 | 4B | 179 | ARG |
| 6 | 4B | 180 | ILE |
| 6 | 4B | 184 | GLU |
| 6 | 4B | 185 | ARG |
| 6 | 4B | 190 | TRP |
| 6 | 4B | 191 | GLU |
| 6 | 4B | 192 | GLN |
| 6 | 4B | 193 | MET |
| 6 | 4B | 201 | GLN |
| 6 | 4B | 205 | GLN |
| 6 | 4B | 215 | LYS |
| 6 | 4B | 217 | ASN |
| 6 | 4B | 218 | THR |
| 6 | 4B | 219 | ASN |
| 6 | 4B | 221 | MET |
| 6 | 4B | 223 | PHE |
| 6 | 4B | 226 | ILE |
| 6 | 4B | 228 | LEU |
| 6 | 4B | 230 | TYR |
| 6 | 4B | 231 | GLU |
| 6 | 4B | 232 | LYS |
| 6 | 4B | 233 | SER |
| 6 | 4B | 239 | LEU |
| 6 | 4B | 241 | LYS |
| 6 | 4B | 242 | ARG |
| 6 | 4B | 244 | GLU |
| 6 | 4B | 245 | MET |
| 6 | 4B | 247 | LYS |
| 6 | 4B | 252 | VAL |
| 6 | 4B | 253 | ARG |
| 6 | 4B | 257 | LEU |
| 6 | 4B | 258 | ASP |
| 6 | 4B | 262 | ASN |
| 6 | 4B | 267 | ILE |
| 6 | 4B | 268 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4B | 269 | THR |
| 6 | 4B | 273 | ARG |
| 6 | 4B | 274 | ILE |
| 6 | 4B | 277 | GLU |
| 6 | 4B | 278 | TYR |
| 6 | 4B | 280 | VAL |
| 6 | 4B | 282 | ASN |
| 6 | 4B | 283 | HIS |
| 6 | 4B | 285 | ARG |
| 6 | 4B | 287 | ASP |
| 6 | 4B | 289 | LYS |
| 6 | 4B | 290 | THR |
| 6 | 4B | 292 | VAL |
| 6 | 4B | 295 | LYS |
| 6 | 4B | 297 | GLU |
| 6 | 4B | 299 | TYR |
| 6 | 4B | 300 | SER |
| 6 | 4C | 96 | VAL |
| 6 | 4C | 97 | GLN |
| 6 | 4C | 99 | ARG |
| 6 | 4C | 102 | LEU |
| 6 | 4C | 105 | GLU |
| 6 | 4C | 107 | MET |
| 6 | 4C | 108 | LYS |
| 6 | 4C | 110 | LYS |
| 6 | 4C | 113 | ILE |
| 6 | 4C | 114 | GLU |
| 6 | 4C | 115 | LYS |
| 6 | 4C | 116 | THR |
| 6 | 4C | 121 | ARG |
| 6 | 4C | 132 | LYS |
| 6 | 4C | 135 | LEU |
| 6 | 4C | 137 | ASN |
| 6 | 4C | 141 | LYS |
| 6 | 4C | 142 | SER |
| 6 | 4C | 143 | THR |
| 6 | 4C | 144 | LEU |
| 6 | 4C | 149 | ASN |
| 6 | 4C | 151 | ARG |
| 6 | 4C | 154 | LYS |
| 6 | 4C | 155 | ASP |
| 6 | 4C | 157 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4C | 161 | LYS |
| 6 | 4C | 162 | GLN |
| 6 | 4C | 163 | GLN |
| 6 | 4C | 164 | ARG |
| 6 | 4C | 167 | ARG |
| 6 | 4C | 173 | VAL |
| 6 | 4C | 178 | HIS |
| 6 | 4C | 179 | ARG |
| 6 | 4C | 180 | ILE |
| 6 | 4C | 184 | GLU |
| 6 | 4C | 185 | ARG |
| 6 | 4C | 190 | TRP |
| 6 | 4C | 191 | GLU |
| 6 | 4C | 192 | GLN |
| 6 | 4C | 193 | MET |
| 6 | 4C | 201 | GLN |
| 6 | 4C | 205 | GLN |
| 6 | 4C | 215 | LYS |
| 6 | 4C | 217 | ASN |
| 6 | 4C | 218 | THR |
| 6 | 4C | 219 | ASN |
| 6 | 4C | 221 | MET |
| 6 | 4C | 223 | PHE |
| 6 | 4C | 226 | ILE |
| 6 | 4C | 228 | LEU |
| 6 | 4C | 230 | TYR |
| 6 | 4C | 231 | GLU |
| 6 | 4C | 232 | LYS |
| 6 | 4C | 233 | SER |
| 6 | 4C | 239 | LEU |
| 6 | 4C | 241 | LYS |
| 6 | 4C | 242 | ARG |
| 6 | 4C | 244 | GLU |
| 6 | 4C | 245 | MET |
| 6 | 4C | 247 | LYS |
| 6 | 4C | 252 | VAL |
| 6 | 4C | 253 | ARG |
| 6 | 4C | 257 | LEU |
| 6 | 4C | 258 | ASP |
| 6 | 4C | 262 | ASN |
| 6 | 4C | 267 | ILE |
| 6 | 4C | 268 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4C | 269 | THR |
| 6 | 4C | 273 | ARG |
| 6 | 4C | 274 | ILE |
| 6 | 4C | 277 | GLU |
| 6 | 4C | 278 | TYR |
| 6 | 4C | 280 | VAL |
| 6 | 4C | 282 | ASN |
| 6 | 4C | 283 | HIS |
| 6 | 4C | 285 | ARG |
| 6 | 4C | 287 | ASP |
| 6 | 4C | 289 | LYS |
| 6 | 4C | 290 | THR |
| 6 | 4C | 292 | VAL |
| 6 | 4C | 295 | LYS |
| 6 | 4C | 297 | GLU |
| 6 | 4C | 299 | TYR |
| 6 | 4C | 300 | SER |
| 6 | 4D | 96 | VAL |
| 6 | 4D | 97 | GLN |
| 6 | 4D | 99 | ARG |
| 6 | 4D | 102 | LEU |
| 6 | 4D | 105 | GLU |
| 6 | 4D | 107 | MET |
| 6 | 4D | 108 | LYS |
| 6 | 4D | 110 | LYS |
| 6 | 4D | 113 | ILE |
| 6 | 4D | 114 | GLU |
| 6 | 4D | 115 | LYS |
| 6 | 4D | 116 | THR |
| 6 | 4D | 121 | ARG |
| 6 | 4D | 132 | LYS |
| 6 | 4D | 135 | LEU |
| 6 | 4D | 137 | ASN |
| 6 | 4D | 141 | LYS |
| 6 | 4D | 142 | SER |
| 6 | 4D | 143 | THR |
| 6 | 4D | 144 | LEU |
| 6 | 4D | 149 | ASN |
| 6 | 4D | 151 | ARG |
| 6 | 4D | 154 | LYS |
| 6 | 4D | 155 | ASP |
| 6 | 4D | 157 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 4D | 161 | LYS |
| 6 | 4D | 162 | GLN |
| 6 | 4D | 163 | GLN |
| 6 | 4D | 164 | ARG |
| 6 | 4D | 167 | ARG |
| 6 | 4D | 173 | VAL |
| 6 | 4D | 178 | HIS |
| 6 | 4D | 179 | ARG |
| 6 | 4D | 180 | ILE |
| 6 | 4D | 184 | GLU |
| 6 | 4D | 185 | ARG |
| 6 | 4D | 190 | TRP |
| 6 | 4D | 191 | GLU |
| 6 | 4D | 192 | GLN |
| 6 | 4D | 193 | MET |
| 6 | 4D | 201 | GLN |
| 6 | 4D | 205 | GLN |
| 6 | 4D | 215 | LYS |
| 6 | 4D | 217 | ASN |
| 6 | 4D | 218 | THR |
| 6 | 4D | 219 | ASN |
| 6 | 4D | 221 | MET |
| 6 | 4D | 223 | PHE |
| 6 | 4D | 226 | ILE |
| 6 | 4D | 228 | LEU |
| 6 | 4D | 230 | TYR |
| 6 | 4D | 231 | GLU |
| 6 | 4D | 232 | LYS |
| 6 | 4D | 233 | SER |
| 6 | 4D | 239 | LEU |
| 6 | 4D | 241 | LYS |
| 6 | 4D | 242 | ARG |
| 6 | 4D | 244 | GLU |
| 6 | 4D | 245 | MET |
| 6 | 4D | 247 | LYS |
| 6 | 4D | 252 | VAL |
| 6 | 4D | 253 | ARG |
| 6 | 4D | 257 | LEU |
| 6 | 4D | 258 | ASP |
| 6 | 4D | 262 | ASN |
| 6 | 4D | 267 | ILE |
| 6 | 4D | 268 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | 4D | 269 | THR |
| 6 | 4D | 273 | ARG |
| 6 | 4D | 274 | ILE |
| 6 | 4D | 277 | GLU |
| 6 | 4D | 278 | TYR |
| 6 | 4D | 280 | VAL |
| 6 | 4D | 282 | ASN |
| 6 | 4D | 283 | HIS |
| 6 | 4D | 285 | ARG |
| 6 | 4D | 287 | ASP |
| 6 | 4D | 289 | LYS |
| 6 | 4D | 290 | THR |
| 6 | 4D | 292 | VAL |
| 6 | 4D | 295 | LYS |
| 6 | 4D | 297 | GLU |
| 6 | 4D | 299 | TYR |
| 6 | 4D | 300 | SER |
| 7 | 5A | 771 | LEU |
| 7 | 5A | 772 | LEU |
| 7 | 5A | 773 | ARG |
| 7 | 5A | 796 | GLU |
| 7 | 5A | 800 | LYS |
| 7 | 5A | 801 | LEU |
| 7 | 5A | 803 | VAL |
| 7 | 5A | 804 | VAL |
| 7 | 5A | 806 | GLN |
| 7 | 5A | 808 | GLN |
| 7 | 5A | 810 | THR |
| 7 | 5A | 811 | GLN |
| 7 | 5A | 817 | LEU |
| 7 | 5A | 832 | ASN |
| 7 | 5A | 835 | GLN |
| 7 | 5A | 836 | ARG |
| 7 | 5A | 839 | GLU |
| 7 | 5A | 841 | VAL |
| 7 | 5A | 842 | LEU |
| 7 | 5A | 843 | LEU |
| 7 | 5A | 915 | PHE |
| 7 | 5A | 1068 | SER |
| 7 | 5A | 1083 | THR |
| 7 | 5A | 1094 | GLU |
| 7 | 5A | 1095 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5A | 1105 | TYR |
| 7 | 5A | 1124 | ILE |
| 7 | 5A | 1125 | LEU |
| 7 | 5A | 1138 | LEU |
| 7 | 5A | 1141 | LEU |
| 7 | 5A | 1148 | PHE |
| 7 | 5A | 1157 | THR |
| 7 | 5A | 1160 | VAL |
| 7 | 5A | 1166 | LEU |
| 7 | 5A | 1243 | ASP |
| 7 | 5A | 1247 | LYS |
| 7 | 5A | 1255 | TYR |
| 7 | 5A | 1260 | THR |
| 7 | 5A | 1269 | ASP |
| 7 | 5A | 1271 | ILE |
| 7 | 5A | 1272 | ILE |
| 7 | 5A | 1274 | SER |
| 7 | 5A | 1279 | ASP |
| 7 | 5A | 1285 | ARG |
| 7 | 5A | 1294 | ILE |
| 7 | 5A | 1295 | LYS |
| 7 | 5A | 1296 | GLU |
| 7 | 5A | 1297 | LYS |
| 7 | 5A | 1298 | LYS |
| 7 | 5A | 1299 | LYS |
| 7 | 5A | 1301 | GLU |
| 7 | 5A | 1309 | LYS |
| 7 | 5A | 1314 | LYS |
| 7 | 5A | 1315 | ARG |
| 7 | 5A | 1316 | LEU |
| 7 | 5A | 1317 | LYS |
| 7 | 5A | 1319 | HIS |
| 7 | 5A | 1321 | PHE |
| 7 | 5A | 1323 | MET |
| 7 | 5A | 1325 | ARG |
| 7 | 5A | 1328 | GLU |
| 7 | 5A | 1331 | GLU |
| 7 | 5A | 1332 | GLN |
| 7 | 5A | 1335 | ASP |
| 7 | 5A | 1338 | LYS |
| 7 | 5A | 1339 | GLN |
| 7 | 5A | 1340 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5A | 1341 | LYS |
| 7 | 5A | 1342 | GLU |
| 7 | 5A | 1343 | LYS |
| 7 | 5A | 1344 | GLU |
| 7 | 5A | 1345 | LEU |
| 7 | 5A | 1346 | GLN |
| 7 | 5A | 1347 | LEU |
| 7 | 5A | 1348 | LYS |
| 7 | 5A | 1349 | LYS |
| 7 | 5A | 1352 | GLU |
| 7 | 5A | 1353 | GLU |
| 7 | 5A | 1355 | GLN |
| 7 | 5A | 1356 | LYS |
| 7 | 5A | 1358 | LYS |
| 7 | 5A | 1362 | MET |
| 7 | 5A | 1366 | TRP |
| 7 | 5A | 1367 | LYS |
| 7 | 5A | 1370 | LYS |
| 7 | 5A | 1371 | GLU |
| 7 | 5A | 1373 | PHE |
| 7 | 5A | 1374 | ASP |
| 7 | 5A | 1376 | GLN |
| 7 | 5A | 1377 | LYS |
| 7 | 5A | 1378 | GLN |
| 7 | 5A | 1380 | LEU |
| 7 | 5A | 1381 | ILE |
| 7 | 5A | 1382 | GLU |
| 7 | 5A | 1384 | GLN |
| 7 | 5A | 1385 | LYS |
| 7 | 5A | 1386 | LYS |
| 7 | 5A | 1387 | ILE |
| 7 | 5A | 1389 | GLU |
| 7 | 5A | 1390 | GLU |
| 7 | 5A | 1391 | GLN |
| 7 | 5A | 1393 | ARG |
| 7 | 5A | 1394 | ARG |
| 7 | 5A | 1396 | GLN |
| 7 | 5A | 1397 | GLU |
| 7 | 5A | 1398 | GLU |
| 7 | 5A | 1399 | LYS |
| 7 | 5A | 1400 | GLU |
| 7 | 5A | 1401 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5A | 1402 | LYS |
| 7 | 5A | 1403 | GLU |
| 7 | 5A | 1404 | LYS |
| 7 | 5A | 1407 | GLN |
| 7 | 5A | 1411 | LYS |
| 7 | 5A | 1412 | LYS |
| 7 | 5A | 1414 | ILE |
| 7 | 5A | 1416 | LYS |
| 7 | 5A | 1417 | GLN |
| 7 | 5A | 1420 | GLU |
| 7 | 5A | 1421 | PHE |
| 7 | 5A | 1422 | LYS |
| 7 | 5A | 1423 | LYS |
| 7 | 5A | 1425 | LYS |
| 7 | 5A | 1426 | GLU |
| 7 | 5A | 1427 | LYS |
| 7 | 5A | 1430 | GLN |
| 7 | 5A | 1431 | GLU |
| 7 | 5A | 1433 | GLU |
| 7 | 5A | 1434 | LYS |
| 7 | 5A | 1435 | GLN |
| 7 | 5A | 1436 | ARG |
| 7 | 5A | 1443 | LYS |
| 7 | 5A | 1444 | LYS |
| 7 | 5A | 1445 | LEU |
| 7 | 5A | 1447 | GLU |
| 7 | 5A | 1449 | LEU |
| 7 | 5A | 1450 | HIS |
| 7 | 5A | 1452 | HIS |
| 7 | 5A | 1453 | ILE |
| 7 | 5A | 1455 | LYS |
| 7 | 5A | 1456 | THR |
| 7 | 5A | 1459 | GLU |
| 7 | 5A | 1461 | ILE |
| 7 | 5A | 1462 | GLU |
| 7 | 5A | 1463 | ILE |
| 7 | 5A | 1464 | GLU |
| 7 | 5A | 1466 | VAL |
| 7 | 5A | 1469 | VAL |
| 7 | 5A | 1471 | ILE |
| 7 | 5A | 1474 | LEU |
| 7 | 5A | 1485 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5A | 1486 | THR |
| 7 | 5A | 1487 | ASN |
| 7 | 5A | 1488 | GLU |
| 7 | 5A | 1489 | PHE |
| 7 | 5A | 1490 | LYS |
| 7 | 5A | 1491 | LEU |
| 7 | 5A | 1492 | SER |
| 7 | 5A | 1562 | LEU |
| 7 | 5A | 1564 | GLU |
| 7 | 5A | 1565 | GLU |
| 7 | 5A | 1577 | LYS |
| 7 | 5B | 771 | LEU |
| 7 | 5B | 772 | LEU |
| 7 | 5B | 773 | ARG |
| 7 | 5B | 796 | GLU |
| 7 | 5B | 800 | LYS |
| 7 | 5B | 801 | LEU |
| 7 | 5B | 803 | VAL |
| 7 | 5B | 804 | VAL |
| 7 | 5B | 806 | GLN |
| 7 | 5B | 808 | GLN |
| 7 | 5B | 810 | THR |
| 7 | 5B | 811 | GLN |
| 7 | 5B | 817 | LEU |
| 7 | 5B | 832 | ASN |
| 7 | 5B | 835 | GLN |
| 7 | 5B | 836 | ARG |
| 7 | 5B | 839 | GLU |
| 7 | 5B | 841 | VAL |
| 7 | 5B | 842 | LEU |
| 7 | 5B | 843 | LEU |
| 7 | 5B | 915 | PHE |
| 7 | 5B | 1068 | SER |
| 7 | 5B | 1083 | THR |
| 7 | 5B | 1094 | GLU |
| 7 | 5B | 1095 | GLU |
| 7 | 5B | 1105 | TYR |
| 7 | 5B | 1124 | ILE |
| 7 | 5B | 1125 | LEU |
| 7 | 5B | 1138 | LEU |
| 7 | 5B | 1141 | LEU |
| 7 | 5B | 1148 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5B | 1157 | THR |
| 7 | 5B | 1160 | VAL |
| 7 | 5B | 1166 | LEU |
| 7 | 5B | 1243 | ASP |
| 7 | 5B | 1247 | LYS |
| 7 | 5B | 1255 | TYR |
| 7 | 5B | 1260 | THR |
| 7 | 5B | 1269 | ASP |
| 7 | 5B | 1271 | ILE |
| 7 | 5B | 1272 | ILE |
| 7 | 5B | 1274 | SER |
| 7 | 5B | 1279 | ASP |
| 7 | 5B | 1285 | ARG |
| 7 | 5B | 1294 | ILE |
| 7 | 5B | 1295 | LYS |
| 7 | 5B | 1296 | GLU |
| 7 | 5B | 1297 | LYS |
| 7 | 5B | 1298 | LYS |
| 7 | 5B | 1299 | LYS |
| 7 | 5B | 1301 | GLU |
| 7 | 5B | 1309 | LYS |
| 7 | 5B | 1314 | LYS |
| 7 | 5B | 1315 | ARG |
| 7 | 5B | 1316 | LEU |
| 7 | 5B | 1317 | LYS |
| 7 | 5B | 1319 | HIS |
| 7 | 5B | 1321 | PHE |
| 7 | 5B | 1323 | MET |
| 7 | 5B | 1325 | ARG |
| 7 | 5B | 1328 | GLU |
| 7 | 5B | 1331 | GLU |
| 7 | 5B | 1332 | GLN |
| 7 | 5B | 1335 | ASP |
| 7 | 5B | 1338 | LYS |
| 7 | 5B | 1339 | GLN |
| 7 | 5B | 1340 | LYS |
| 7 | 5B | 1341 | LYS |
| 7 | 5B | 1342 | GLU |
| 7 | 5B | 1343 | LYS |
| 7 | 5B | 1344 | GLU |
| 7 | 5B | 1345 | LEU |
| 7 | 5B | 1346 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5B | 1347 | LEU |
| 7 | 5B | 1348 | LYS |
| 7 | 5B | 1349 | LYS |
| 7 | 5B | 1352 | GLU |
| 7 | 5B | 1353 | GLU |
| 7 | 5B | 1355 | GLN |
| 7 | 5B | 1356 | LYS |
| 7 | 5B | 1358 | LYS |
| 7 | 5B | 1362 | MET |
| 7 | 5B | 1366 | TRP |
| 7 | 5B | 1367 | LYS |
| 7 | 5B | 1370 | LYS |
| 7 | 5B | 1371 | GLU |
| 7 | 5B | 1373 | PHE |
| 7 | 5B | 1374 | ASP |
| 7 | 5B | 1376 | GLN |
| 7 | 5B | 1377 | LYS |
| 7 | 5B | 1378 | GLN |
| 7 | 5B | 1380 | LEU |
| 7 | 5B | 1381 | ILE |
| 7 | 5B | 1382 | GLU |
| 7 | 5B | 1384 | GLN |
| 7 | 5B | 1385 | LYS |
| 7 | 5B | 1386 | LYS |
| 7 | 5B | 1387 | ILE |
| 7 | 5B | 1389 | GLU |
| 7 | 5B | 1390 | GLU |
| 7 | 5B | 1391 | GLN |
| 7 | 5B | 1393 | ARG |
| 7 | 5B | 1394 | ARG |
| 7 | 5B | 1396 | GLN |
| 7 | 5B | 1397 | GLU |
| 7 | 5B | 1398 | GLU |
| 7 | 5B | 1399 | LYS |
| 7 | 5B | 1400 | GLU |
| 7 | 5B | 1401 | LYS |
| 7 | 5B | 1402 | LYS |
| 7 | 5B | 1403 | GLU |
| 7 | 5B | 1404 | LYS |
| 7 | 5B | 1407 | GLN |
| 7 | 5B | 1411 | LYS |
| 7 | 5B | 1412 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5B | 1414 | ILE |
| 7 | 5B | 1416 | LYS |
| 7 | 5B | 1417 | GLN |
| 7 | 5B | 1420 | GLU |
| 7 | 5B | 1421 | PHE |
| 7 | 5B | 1422 | LYS |
| 7 | 5B | 1423 | LYS |
| 7 | 5B | 1425 | LYS |
| 7 | 5B | 1426 | GLU |
| 7 | 5B | 1427 | LYS |
| 7 | 5B | 1430 | GLN |
| 7 | 5B | 1431 | GLU |
| 7 | 5B | 1433 | GLU |
| 7 | 5B | 1434 | LYS |
| 7 | 5B | 1435 | GLN |
| 7 | 5B | 1436 | ARG |
| 7 | 5B | 1443 | LYS |
| 7 | 5B | 1444 | LYS |
| 7 | 5B | 1445 | LEU |
| 7 | 5B | 1447 | GLU |
| 7 | 5B | 1449 | LEU |
| 7 | 5B | 1450 | HIS |
| 7 | 5B | 1452 | HIS |
| 7 | 5B | 1453 | ILE |
| 7 | 5B | 1455 | LYS |
| 7 | 5B | 1456 | THR |
| 7 | 5B | 1459 | GLU |
| 7 | 5B | 1461 | ILE |
| 7 | 5B | 1462 | GLU |
| 7 | 5B | 1463 | ILE |
| 7 | 5B | 1464 | GLU |
| 7 | 5B | 1466 | VAL |
| 7 | 5B | 1469 | VAL |
| 7 | 5B | 1471 | ILE |
| 7 | 5B | 1474 | LEU |
| 7 | 5B | 1485 | LYS |
| 7 | 5B | 1486 | THR |
| 7 | 5B | 1487 | ASN |
| 7 | 5B | 1488 | GLU |
| 7 | 5B | 1489 | PHE |
| 7 | 5B | 1490 | LYS |
| 7 | 5B | 1491 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5B | 1492 | SER |
| 7 | 5B | 1562 | LEU |
| 7 | 5B | 1564 | GLU |
| 7 | 5B | 1565 | GLU |
| 7 | 5B | 1577 | LYS |
| 7 | 5C | 771 | LEU |
| 7 | 5C | 772 | LEU |
| 7 | 5C | 773 | ARG |
| 7 | 5C | 796 | GLU |
| 7 | 5C | 800 | LYS |
| 7 | 5C | 801 | LEU |
| 7 | 5C | 803 | VAL |
| 7 | 5C | 804 | VAL |
| 7 | 5C | 806 | GLN |
| 7 | 5C | 808 | GLN |
| 7 | 5C | 810 | THR |
| 7 | 5C | 811 | GLN |
| 7 | 5C | 817 | LEU |
| 7 | 5C | 832 | ASN |
| 7 | 5C | 835 | GLN |
| 7 | 5C | 836 | ARG |
| 7 | 5C | 837 | ASP |
| 7 | 5C | 839 | GLU |
| 7 | 5C | 841 | VAL |
| 7 | 5C | 842 | LEU |
| 7 | 5C | 843 | LEU |
| 7 | 5C | 915 | PHE |
| 7 | 5C | 1068 | SER |
| 7 | 5C | 1083 | THR |
| 7 | 5C | 1094 | GLU |
| 7 | 5C | 1095 | GLU |
| 7 | 5C | 1105 | TYR |
| 7 | 5C | 1124 | ILE |
| 7 | 5C | 1125 | LEU |
| 7 | 5C | 1138 | LEU |
| 7 | 5C | 1141 | LEU |
| 7 | 5C | 1148 | PHE |
| 7 | 5C | 1157 | THR |
| 7 | 5C | 1160 | VAL |
| 7 | 5C | 1166 | LEU |
| 7 | 5C | 1243 | ASP |
| 7 | 5C | 1247 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5C | 1255 | TYR |
| 7 | 5C | 1260 | THR |
| 7 | 5C | 1269 | ASP |
| 7 | 5C | 1271 | ILE |
| 7 | 5C | 1272 | ILE |
| 7 | 5C | 1274 | SER |
| 7 | 5C | 1279 | ASP |
| 7 | 5C | 1285 | ARG |
| 7 | 5C | 1294 | ILE |
| 7 | 5C | 1295 | LYS |
| 7 | 5C | 1296 | GLU |
| 7 | 5C | 1297 | LYS |
| 7 | 5C | 1298 | LYS |
| 7 | 5C | 1299 | LYS |
| 7 | 5C | 1301 | GLU |
| 7 | 5C | 1309 | LYS |
| 7 | 5C | 1314 | LYS |
| 7 | 5C | 1315 | ARG |
| 7 | 5C | 1316 | LEU |
| 7 | 5C | 1317 | LYS |
| 7 | 5C | 1319 | HIS |
| 7 | 5C | 1321 | PHE |
| 7 | 5C | 1323 | MET |
| 7 | 5C | 1325 | ARG |
| 7 | 5C | 1328 | GLU |
| 7 | 5C | 1331 | GLU |
| 7 | 5C | 1332 | GLN |
| 7 | 5C | 1335 | ASP |
| 7 | 5C | 1338 | LYS |
| 7 | 5C | 1339 | GLN |
| 7 | 5C | 1340 | LYS |
| 7 | 5C | 1341 | LYS |
| 7 | 5C | 1342 | GLU |
| 7 | 5C | 1343 | LYS |
| 7 | 5C | 1344 | GLU |
| 7 | 5C | 1345 | LEU |
| 7 | 5C | 1346 | GLN |
| 7 | 5C | 1347 | LEU |
| 7 | 5C | 1348 | LYS |
| 7 | 5C | 1349 | LYS |
| 7 | 5C | 1352 | GLU |
| 7 | 5C | 1353 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5C | 1355 | GLN |
| 7 | 5C | 1356 | LYS |
| 7 | 5C | 1358 | LYS |
| 7 | 5C | 1362 | MET |
| 7 | 5C | 1366 | TRP |
| 7 | 5C | 1367 | LYS |
| 7 | 5C | 1370 | LYS |
| 7 | 5C | 1371 | GLU |
| 7 | 5C | 1373 | PHE |
| 7 | 5C | 1374 | ASP |
| 7 | 5C | 1376 | GLN |
| 7 | 5C | 1377 | LYS |
| 7 | 5C | 1378 | GLN |
| 7 | 5C | 1380 | LEU |
| 7 | 5C | 1381 | ILE |
| 7 | 5C | 1382 | GLU |
| 7 | 5C | 1384 | GLN |
| 7 | 5C | 1385 | LYS |
| 7 | 5C | 1386 | LYS |
| 7 | 5C | 1387 | ILE |
| 7 | 5C | 1389 | GLU |
| 7 | 5C | 1390 | GLU |
| 7 | 5C | 1391 | GLN |
| 7 | 5C | 1393 | ARG |
| 7 | 5C | 1394 | ARG |
| 7 | 5C | 1396 | GLN |
| 7 | 5C | 1397 | GLU |
| 7 | 5C | 1398 | GLU |
| 7 | 5C | 1399 | LYS |
| 7 | 5C | 1400 | GLU |
| 7 | 5C | 1401 | LYS |
| 7 | 5C | 1402 | LYS |
| 7 | 5C | 1403 | GLU |
| 7 | 5C | 1404 | LYS |
| 7 | 5C | 1407 | GLN |
| 7 | 5C | 1411 | LYS |
| 7 | 5C | 1412 | LYS |
| 7 | 5C | 1414 | ILE |
| 7 | 5C | 1416 | LYS |
| 7 | 5C | 1417 | GLN |
| 7 | 5C | 1420 | GLU |
| 7 | 5C | 1421 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5C | 1422 | LYS |
| 7 | 5C | 1423 | LYS |
| 7 | 5C | 1425 | LYS |
| 7 | 5C | 1426 | GLU |
| 7 | 5C | 1427 | LYS |
| 7 | 5C | 1430 | GLN |
| 7 | 5C | 1431 | GLU |
| 7 | 5C | 1433 | GLU |
| 7 | 5C | 1434 | LYS |
| 7 | 5C | 1435 | GLN |
| 7 | 5C | 1436 | ARG |
| 7 | 5C | 1443 | LYS |
| 7 | 5C | 1444 | LYS |
| 7 | 5C | 1445 | LEU |
| 7 | 5C | 1447 | GLU |
| 7 | 5C | 1449 | LEU |
| 7 | 5C | 1450 | HIS |
| 7 | 5C | 1452 | HIS |
| 7 | 5C | 1453 | ILE |
| 7 | 5C | 1455 | LYS |
| 7 | 5C | 1456 | THR |
| 7 | 5C | 1459 | GLU |
| 7 | 5C | 1461 | ILE |
| 7 | 5C | 1462 | GLU |
| 7 | 5C | 1463 | ILE |
| 7 | 5C | 1464 | GLU |
| 7 | 5C | 1466 | VAL |
| 7 | 5C | 1469 | VAL |
| 7 | 5C | 1471 | ILE |
| 7 | 5C | 1474 | LEU |
| 7 | 5C | 1485 | LYS |
| 7 | 5C | 1486 | THR |
| 7 | 5C | 1487 | ASN |
| 7 | 5C | 1488 | GLU |
| 7 | 5C | 1489 | PHE |
| 7 | 5C | 1490 | LYS |
| 7 | 5C | 1491 | LEU |
| 7 | 5C | 1492 | SER |
| 7 | 5C | 1562 | LEU |
| 7 | 5C | 1564 | GLU |
| 7 | 5C | 1565 | GLU |
| 7 | 5C | 1577 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | 6A | 136 | LEU |
| 8 | 6A | 178 | LEU |
| 8 | 6A | 225 | GLU |
| 8 | 6A | 252 | THR |
| 8 | 6B | 136 | LEU |
| 8 | 6B | 178 | LEU |
| 8 | 6B | 225 | GLU |
| 8 | 6B | 252 | THR |
| 8 | 6C | 136 | LEU |
| 8 | 6C | 178 | LEU |
| 8 | 6C | 225 | GLU |
| 8 | 6C | 252 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (386) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 101 | ASN |
| 1 | AA | 192 | HIS |
| 2 | AB | 100 | ASN |
| 2 | AB | 227 | HIS |
| 2 | AB | 334 | GLN |
| 1 | AC | 101 | ASN |
| 1 | AC | 192 | HIS |
| 1 | AC | 256 | GLN |
| 1 | AC | 342 | GLN |
| 2 | AD | 100 | ASN |
| 2 | AD | 227 | HIS |
| 2 | AD | 334 | GLN |
| 1 | AE | 101 | ASN |
| 1 | AE | 192 | HIS |
| 1 | AE | 256 | GLN |
| 1 | AE | 342 | GLN |
| 2 | AF | 100 | ASN |
| 2 | AF | 227 | HIS |
| 2 | AF | 334 | GLN |
| 1 | BA | 101 | ASN |
| 1 | BA | 192 | HIS |
| 2 | BB | 100 | ASN |
| 2 | BB | 227 | HIS |
| 2 | BB | 334 | GLN |
| 1 | BC | 101 | ASN |
| 1 | BC | 192 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BC | 256 | GLN |
| 2 | BD | 100 | ASN |
| 2 | BD | 227 | HIS |
| 2 | BD | 334 | GLN |
| 1 | BE | 101 | ASN |
| 1 | BE | 192 | HIS |
| 1 | BE | 256 | GLN |
| 2 | BF | 100 | ASN |
| 2 | BF | 227 | HIS |
| 2 | BF | 334 | GLN |
| 1 | CA | 101 | ASN |
| 1 | CA | 192 | HIS |
| 2 | CB | 100 | ASN |
| 2 | CB | 227 | HIS |
| 2 | CB | 334 | GLN |
| 1 | CC | 101 | ASN |
| 1 | CC | 192 | HIS |
| 1 | CC | 256 | GLN |
| 2 | CD | 100 | ASN |
| 2 | CD | 227 | HIS |
| 2 | CD | 334 | GLN |
| 1 | CE | 101 | ASN |
| 1 | CE | 192 | HIS |
| 1 | CE | 256 | GLN |
| 2 | CF | 100 | ASN |
| 2 | CF | 227 | HIS |
| 2 | CF | 334 | GLN |
| 1 | DA | 101 | ASN |
| 1 | DA | 128 | ASN |
| 1 | DA | 192 | HIS |
| 2 | DB | 100 | ASN |
| 2 | DB | 227 | HIS |
| 2 | DB | 334 | GLN |
| 1 | DC | 101 | ASN |
| 1 | DC | 128 | ASN |
| 1 | DC | 192 | HIS |
| 1 | DC | 256 | GLN |
| 2 | DD | 100 | ASN |
| 2 | DD | 227 | HIS |
| 2 | DD | 334 | GLN |
| 1 | DE | 101 | ASN |
| 1 | DE | 128 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | DE | 192 | HIS |
| 1 | DE | 256 | GLN |
| 1 | DE | 285 | GLN |
| 2 | DF | 100 | ASN |
| 2 | DF | 334 | GLN |
| 1 | EA | 101 | ASN |
| 1 | EA | 192 | HIS |
| 1 | EA | 285 | GLN |
| 2 | EB | 100 | ASN |
| 2 | EB | 227 | HIS |
| 2 | EB | 334 | GLN |
| 1 | EC | 101 | ASN |
| 1 | EC | 192 | HIS |
| 1 | EC | 256 | GLN |
| 1 | EC | 285 | GLN |
| 2 | ED | 100 | ASN |
| 2 | ED | 334 | GLN |
| 1 | EE | 101 | ASN |
| 1 | EE | 192 | HIS |
| 1 | EE | 256 | GLN |
| 1 | EE | 285 | GLN |
| 2 | EF | 100 | ASN |
| 2 | EF | 227 | HIS |
| 2 | EF | 334 | GLN |
| 1 | FA | 11 | GLN |
| 1 | FA | 101 | ASN |
| 1 | FA | 192 | HIS |
| 1 | FA | 283 | HIS |
| 1 | FA | 285 | GLN |
| 2 | FB | 100 | ASN |
| 2 | FB | 227 | HIS |
| 2 | FB | 334 | GLN |
| 1 | FC | 101 | ASN |
| 1 | FC | 192 | HIS |
| 1 | FC | 256 | GLN |
| 1 | FC | 283 | HIS |
| 2 | FD | 100 | ASN |
| 2 | FD | 227 | HIS |
| 2 | FD | 334 | GLN |
| 1 | FE | 101 | ASN |
| 1 | FE | 192 | HIS |
| 1 | FE | 256 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | FE | 283 | HIS |
| 2 | FF | 100 | ASN |
| 2 | FF | 227 | HIS |
| 2 | FF | 334 | GLN |
| 1 | GA | 101 | ASN |
| 1 | GA | 192 | HIS |
| 1 | GA | 283 | HIS |
| 2 | GB | 100 | ASN |
| 2 | GB | 227 | HIS |
| 2 | GB | 334 | GLN |
| 1 | GC | 101 | ASN |
| 1 | GC | 192 | HIS |
| 1 | GC | 256 | GLN |
| 1 | GC | 283 | HIS |
| 2 | GD | 100 | ASN |
| 2 | GD | 227 | HIS |
| 2 | GD | 334 | GLN |
| 1 | GE | 101 | ASN |
| 1 | GE | 192 | HIS |
| 1 | GE | 256 | GLN |
| 1 | GE | 283 | HIS |
| 2 | GF | 100 | ASN |
| 2 | GF | 227 | HIS |
| 2 | GF | 334 | GLN |
| 1 | HA | 101 | ASN |
| 1 | HA | 192 | HIS |
| 2 | HB | 100 | ASN |
| 2 | HB | 227 | HIS |
| 2 | HB | 334 | GLN |
| 1 | HC | 101 | ASN |
| 1 | HC | 192 | HIS |
| 1 | HC | 256 | GLN |
| 2 | HD | 100 | ASN |
| 2 | HD | 227 | HIS |
| 2 | HD | 334 | GLN |
| 1 | HE | 101 | ASN |
| 1 | HE | 192 | HIS |
| 1 | HE | 256 | GLN |
| 1 | HE | 285 | GLN |
| 2 | HF | 100 | ASN |
| 2 | HF | 227 | HIS |
| 2 | HF | 334 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | IA | 101 | ASN |
| 1 | IA | 192 | HIS |
| 2 | IB | 100 | ASN |
| 2 | IB | 227 | HIS |
| 2 | IB | 334 | GLN |
| 2 | IB | 424 | GLN |
| 1 | IC | 101 | ASN |
| 1 | IC | 192 | HIS |
| 1 | IC | 256 | GLN |
| 2 | ID | 100 | ASN |
| 2 | ID | 227 | HIS |
| 2 | ID | 334 | GLN |
| 2 | ID | 424 | GLN |
| 1 | IE | 101 | ASN |
| 1 | IE | 192 | HIS |
| 1 | IE | 256 | GLN |
| 2 | IF | 100 | ASN |
| 2 | IF | 227 | HIS |
| 2 | IF | 334 | GLN |
| 2 | IF | 424 | GLN |
| 1 | JA | 88 | HIS |
| 1 | JA | 101 | ASN |
| 1 | JA | 128 | ASN |
| 1 | JA | 192 | HIS |
| 1 | JA | 285 | GLN |
| 2 | JB | 100 | ASN |
| 2 | JB | 227 | HIS |
| 2 | JB | 334 | GLN |
| 1 | JC | 88 | HIS |
| 1 | JC | 101 | ASN |
| 1 | JC | 192 | HIS |
| 1 | JC | 256 | GLN |
| 1 | JC | 285 | GLN |
| 2 | JD | 100 | ASN |
| 2 | JD | 227 | HIS |
| 2 | JD | 334 | GLN |
| 1 | JE | 88 | HIS |
| 1 | JE | 101 | ASN |
| 1 | JE | 192 | HIS |
| 1 | JE | 256 | GLN |
| 1 | JE | 285 | GLN |
| 2 | JF | 100 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | JF | 227 | HIS |
| 2 | JF | 334 | GLN |
| 1 | KA | 101 | ASN |
| 1 | KA | 192 | HIS |
| 2 | KB | 83 | GLN |
| 2 | KB | 100 | ASN |
| 2 | KB | 227 | HIS |
| 2 | KB | 334 | GLN |
| 2 | KB | 335 | ASN |
| 1 | KC | 101 | ASN |
| 1 | KC | 192 | HIS |
| 1 | KC | 256 | GLN |
| 1 | KC | 285 | GLN |
| 2 | KD | 83 | GLN |
| 2 | KD | 100 | ASN |
| 2 | KD | 227 | HIS |
| 2 | KD | 334 | GLN |
| 2 | KD | 335 | ASN |
| 1 | KE | 101 | ASN |
| 1 | KE | 192 | HIS |
| 1 | KE | 256 | GLN |
| 1 | KE | 285 | GLN |
| 2 | KF | 100 | ASN |
| 2 | KF | 227 | HIS |
| 2 | KF | 334 | GLN |
| 2 | KF | 335 | ASN |
| 1 | LA | 35 | GLN |
| 1 | LA | 101 | ASN |
| 1 | LA | 192 | HIS |
| 2 | LB | 11 | GLN |
| 2 | LB | 15 | GLN |
| 2 | LB | 100 | ASN |
| 2 | LB | 334 | GLN |
| 2 | LB | 337 | ASN |
| 1 | LC | 35 | GLN |
| 1 | LC | 101 | ASN |
| 1 | LC | 192 | HIS |
| 1 | LC | 249 | ASN |
| 1 | LC | 256 | GLN |
| 2 | LD | 15 | GLN |
| 2 | LD | 100 | ASN |
| 2 | LD | 334 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | LD | 337 | ASN |
| 1 | LE | 35 | GLN |
| 1 | LE | 101 | ASN |
| 1 | LE | 192 | HIS |
| 1 | LE | 256 | GLN |
| 2 | LF | 15 | GLN |
| 2 | LF | 100 | ASN |
| 2 | LF | 334 | GLN |
| 2 | LF | 337 | ASN |
| 1 | MA | 11 | GLN |
| 1 | MA | 101 | ASN |
| 1 | MA | 192 | HIS |
| 2 | MB | 100 | ASN |
| 2 | MB | 334 | GLN |
| 1 | MC | 11 | GLN |
| 1 | MC | 101 | ASN |
| 1 | MC | 192 | HIS |
| 1 | MC | 256 | GLN |
| 2 | MD | 11 | GLN |
| 2 | MD | 100 | ASN |
| 2 | MD | 227 | HIS |
| 2 | MD | 334 | GLN |
| 1 | ME | 11 | GLN |
| 1 | ME | 101 | ASN |
| 1 | ME | 192 | HIS |
| 1 | ME | 256 | GLN |
| 2 | MF | 100 | ASN |
| 2 | MF | 227 | HIS |
| 2 | MF | 334 | GLN |
| 3 | 1A | 65 | GLN |
| 3 | 1A | 69 | ASN |
| 3 | 1B | 65 | GLN |
| 3 | 1B | 69 | ASN |
| 3 | 1C | 65 | GLN |
| 3 | 1C | 69 | ASN |
| 4 | 2A | 27 | ASN |
| 4 | 2A | 49 | GLN |
| 4 | 2A | 144 | ASN |
| 4 | 2A | 148 | ASN |
| 4 | 2A | 162 | GLN |
| 4 | 2B | 27 | ASN |
| 4 | 2B | 49 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2B | 148 | ASN |
| 4 | 2B | 162 | GLN |
| 4 | 2C | 27 | ASN |
| 4 | 2C | 49 | GLN |
| 4 | 2C | 144 | ASN |
| 4 | 2C | 162 | GLN |
| 5 | 3A | 3 | GLN |
| 5 | 3A | 108 | GLN |
| 5 | 3A | 192 | GLN |
| 5 | 3A | 211 | GLN |
| 5 | 3A | 290 | GLN |
| 5 | 3A | 331 | GLN |
| 5 | 3A | 381 | ASN |
| 5 | 3B | 3 | GLN |
| 5 | 3B | 108 | GLN |
| 5 | 3B | 192 | GLN |
| 5 | 3B | 290 | GLN |
| 5 | 3B | 331 | GLN |
| 5 | 3C | 3 | GLN |
| 5 | 3C | 108 | GLN |
| 5 | 3C | 192 | GLN |
| 5 | 3C | 211 | GLN |
| 5 | 3C | 290 | GLN |
| 5 | 3C | 331 | GLN |
| 5 | 3C | 381 | ASN |
| 6 | 4A | 97 | GLN |
| 6 | 4A | 136 | HIS |
| 6 | 4A | 195 | ASN |
| 6 | 4A | 196 | GLN |
| 6 | 4A | 198 | ASN |
| 6 | 4A | 256 | ASN |
| 6 | 4B | 97 | GLN |
| 6 | 4B | 195 | ASN |
| 6 | 4B | 196 | GLN |
| 6 | 4B | 198 | ASN |
| 6 | 4B | 256 | ASN |
| 6 | 4B | 262 | ASN |
| 6 | 4C | 97 | GLN |
| 6 | 4C | 136 | HIS |
| 6 | 4C | 195 | ASN |
| 6 | 4C | 198 | ASN |
| 6 | 4C | 219 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | 4C | 256 | ASN |
| 6 | 4C | 262 | ASN |
| 6 | 4D | 97 | GLN |
| 6 | 4D | 195 | ASN |
| 6 | 4D | 196 | GLN |
| 6 | 4D | 198 | ASN |
| 6 | 4D | 219 | ASN |
| 6 | 4D | 256 | ASN |
| 6 | 4D | 262 | ASN |
| 7 | 5A | 806 | GLN |
| 7 | 5A | 834 | ASN |
| 7 | 5A | 835 | GLN |
| 7 | 5A | 911 | ASN |
| 7 | 5A | 921 | HIS |
| 7 | 5A | 1057 | HIS |
| 7 | 5A | 1319 | HIS |
| 7 | 5A | 1332 | GLN |
| 7 | 5A | 1333 | ASN |
| 7 | 5A | 1339 | GLN |
| 7 | 5A | 1384 | GLN |
| 7 | 5A | 1391 | GLN |
| 7 | 5A | 1407 | GLN |
| 7 | 5A | 1424 | GLN |
| 7 | 5A | 1442 | GLN |
| 7 | 5A | 1452 | HIS |
| 7 | 5A | 1557 | HIS |
| 7 | 5B | 806 | GLN |
| 7 | 5B | 828 | GLN |
| 7 | 5B | 834 | ASN |
| 7 | 5B | 835 | GLN |
| 7 | 5B | 921 | HIS |
| 7 | 5B | 1057 | HIS |
| 7 | 5B | 1319 | HIS |
| 7 | 5B | 1332 | GLN |
| 7 | 5B | 1339 | GLN |
| 7 | 5B | 1384 | GLN |
| 7 | 5B | 1391 | GLN |
| 7 | 5B | 1407 | GLN |
| 7 | 5B | 1413 | GLN |
| 7 | 5B | 1424 | GLN |
| 7 | 5B | 1442 | GLN |
| 7 | 5B | 1452 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | 5B | 1557 | HIS |
| 7 | 5C | 806 | GLN |
| 7 | 5C | 834 | ASN |
| 7 | 5C | 835 | GLN |
| 7 | 5C | 911 | ASN |
| 7 | 5C | 921 | HIS |
| 7 | 5C | 1057 | HIS |
| 7 | 5C | 1319 | HIS |
| 7 | 5C | 1332 | GLN |
| 7 | 5C | 1339 | GLN |
| 7 | 5C | 1384 | GLN |
| 7 | 5C | 1391 | GLN |
| 7 | 5C | 1407 | GLN |
| 7 | 5C | 1424 | GLN |
| 7 | 5C | 1442 | GLN |
| 7 | 5C | 1452 | HIS |
| 7 | 5C | 1557 | HIS |
| 8 | 6A | 70 | ASN |
| 8 | 6A | 102 | ASN |
| 8 | 6B | 70 | ASN |
| 8 | 6B | 102 | ASN |
| 8 | 6C | 70 | ASN |
| 8 | 6C | 102 | ASN |
| 8 | 6C | 110 | ASN |

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 117 ligands modelled in this entry, 39 are monoatomic - leaving 78 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 | $\# Z > 2$ |
| 11 | GTP | AA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | LB | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | DC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | JB | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | MC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | KB | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | LE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | DD | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | LA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | BB | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | AB | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | BD | 501 | - | 25,30,30 | 1.01 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | FF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | BF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | GA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | KA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | CF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | JC | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | AC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | CC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | MA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | ME | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | KD | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | JD | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | BA | 501 | 12 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | HC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | CD | 501 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 11 | GTP | KE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | MF | 502 | - | 25,30,30 | 1.01 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 11 | GTP | IC | 501 | 12 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | EB | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | LD | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | FB | 502 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | ID | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | HD | 501 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.02 | 1 (3%) |
| 11 | GTP | DE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | HE | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | FD | 502 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | MD | 502 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | IF | 501 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 13 | GDP | AD | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 13 | GDP | CB | 501 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 13 | GDP | GD | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.02 | 2 (6%) |
| 13 | GDP | LF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | JE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | BE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | GE | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | AF | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 11 | GTP | GC | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | DF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | DB | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | GB | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | FC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | HA | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | EA | 501 | 12 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | IB | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | EF | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | LC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | BC | 501 | 12 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | KF | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | FE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | HB | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 11 | GTP | IE | 501 | 12 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | CE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | GDP | HF | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | JF | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 13 | GDP | GF | 501 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | CA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 13 | GDP | MB | 502 | - | 25,30,30 | 1.00 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | DA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 13 | GDP | ED | 502 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 11 | GTP | EC | 501 | 12 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | AE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 11 | GTP | JA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | IA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | EE | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | KC | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 11 | GTP | FA | 501 | 12 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 11 | GTP | AA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | LB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | DC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | JB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | MC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | KB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | LE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | DD | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | LA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | BB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | AB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | BD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | FF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | BF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | GA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | KA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | CF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 11 | GTP | JC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | AC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | CC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | MA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | ME | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | KD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | JD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | BA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | HC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | CD | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | KE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | MF | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | IC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | EB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | LD | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | FB | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | ID | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | HD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | DE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | HE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | FD | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | MD | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | IF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | AD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | CB | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | GD | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | LF | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | JE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | BE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | GE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | AF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | GC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | DF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | DB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | GB | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | FC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | HA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | EA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 13 | GDP | IB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | EF | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | LC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | BC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | KF | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | FE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | HB | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | IE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | CE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | HF | 501 | - | - | 0/12/32/32 | 0/3/3/3 |
| 13 | GDP | JF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 13 | GDP | GF | 501 | - | - | 1/12/32/32 | 0/3/3/3 |
| 11 | GTP | CA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | MB | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | DA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 13 | GDP | ED | 502 | - | - | 0/12/32/32 | 0/3/3/3 |
| 11 | GTP | EC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | AE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | JA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | IA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | EE | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | KC | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |
| 11 | GTP | FA | 501 | 12 | - | 8/18/38/38 | 0/3/3/3 |

All (117) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | CE | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 11 | CC | 501 | GTP | C5-C6 | -4.14 | 1.39 | 1.47 |
| 11 | JC | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 11 | GC | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 11 | HA | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 11 | LA | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 11 | KC | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 11 | CA | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 11 | LC | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 11 | LE | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 11 | DC | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 11 | GA | 501 | GTP | C5-C6 | -4.11 | 1.39 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11 | DE | 501 | GTP | C5-C6 | -4.11 | 1.39 | 1.47 |
| 11 | AA | 501 | GTP | C5-C6 | -4.10 | 1.39 | 1.47 |
| 11 | KA | 501 | GTP | C5-C6 | -4.10 | 1.39 | 1.47 |
| 11 | MA | 501 | GTP | C5-C6 | -4.10 | 1.39 | 1.47 |
| 11 | AC | 501 | GTP | C5-C6 | -4.10 | 1.39 | 1.47 |
| 11 | JA | 501 | GTP | C5-C6 | -4.09 | 1.39 | 1.47 |
| 11 | IA | 501 | GTP | C5-C6 | -4.09 | 1.39 | 1.47 |
| 11 | HE | 501 | GTP | C5-C6 | -4.09 | 1.39 | 1.47 |
| 11 | BE | 501 | GTP | C5-C6 | -4.09 | 1.39 | 1.47 |
| 11 | HC | 501 | GTP | C5-C6 | -4.08 | 1.39 | 1.47 |
| 11 | DA | 501 | GTP | C5-C6 | -4.08 | 1.39 | 1.47 |
| 11 | BA | 501 | GTP | C5-C6 | -4.08 | 1.39 | 1.47 |
| 11 | MC | 501 | GTP | C5-C6 | -4.08 | 1.39 | 1.47 |
| 11 | EE | 501 | GTP | C5-C6 | -4.07 | 1.39 | 1.47 |
| 11 | FC | 501 | GTP | C5-C6 | -4.07 | 1.39 | 1.47 |
| 11 | ME | 501 | GTP | C5-C6 | -4.07 | 1.39 | 1.47 |
| 11 | JE | 501 | GTP | C5-C6 | -4.07 | 1.39 | 1.47 |
| 11 | IC | 501 | GTP | C5-C6 | -4.07 | 1.39 | 1.47 |
| 11 | FA | 501 | GTP | C5-C6 | -4.06 | 1.39 | 1.47 |
| 11 | KE | 501 | GTP | C5-C6 | -4.06 | 1.39 | 1.47 |
| 11 | AE | 501 | GTP | C5-C6 | -4.06 | 1.39 | 1.47 |
| 11 | FE | 501 | GTP | C5-C6 | -4.06 | 1.39 | 1.47 |
| 11 | EC | 501 | GTP | C5-C6 | -4.05 | 1.39 | 1.47 |
| 11 | IE | 501 | GTP | C5-C6 | -4.05 | 1.39 | 1.47 |
| 11 | BC | 501 | GTP | C5-C6 | -4.04 | 1.39 | 1.47 |
| 11 | EA | 501 | GTP | C5-C6 | -4.04 | 1.39 | 1.47 |
| 11 | GE | 501 | GTP | C5-C6 | -4.04 | 1.39 | 1.47 |
| 13 | GD | 501 | GDP | C6-N1 | -2.56 | 1.33 | 1.37 |
| 13 | JD | 501 | GDP | C6-N1 | -2.55 | 1.33 | 1.37 |
| 13 | AD | 501 | GDP | C6-N1 | -2.54 | 1.33 | 1.37 |
| 13 | ID | 501 | GDP | C6-N1 | -2.53 | 1.33 | 1.37 |
| 13 | MF | 502 | GDP | C6-N1 | -2.52 | 1.33 | 1.37 |
| 13 | BD | 501 | GDP | C6-N1 | -2.52 | 1.33 | 1.37 |
| 13 | LD | 501 | GDP | C6-N1 | -2.52 | 1.33 | 1.37 |
| 13 | KD | 501 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 13 | EF | 501 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 13 | KF | 501 | GDP | C6-N1 | -2.51 | 1.34 | 1.37 |
| 13 | CF | 501 | GDP | C6-N1 | -2.50 | 1.34 | 1.37 |
| 13 | FB | 502 | GDP | C6-N1 | -2.50 | 1.34 | 1.37 |
| 13 | GB | 501 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |
| 13 | GF | 501 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |
| 13 | HF | 501 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 13 | DD | 501 | GDP | C6-N1 | -2.49 | 1.34 | 1.37 |
| 13 | MB | 502 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 13 | BB | 501 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 13 | MD | 502 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 13 | IF | 501 | GDP | C6-N1 | -2.48 | 1.34 | 1.37 |
| 13 | HD | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | AF | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | DB | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | ED | 502 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | AB | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | IB | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | HB | 501 | GDP | C6-N1 | -2.47 | 1.34 | 1.37 |
| 13 | LB | 501 | GDP | C6-N1 | -2.46 | 1.34 | 1.37 |
| 13 | LF | 501 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 13 | JB | 501 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 13 | JF | 501 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 13 | KB | 501 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 13 | FF | 501 | GDP | C6-N1 | -2.44 | 1.34 | 1.37 |
| 13 | CB | 501 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 13 | DF | 501 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 13 | CD | 501 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 13 | BF | 501 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 13 | EB | 501 | GDP | C6-N1 | -2.42 | 1.34 | 1.37 |
| 13 | FD | 502 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 11 | BC | 501 | GTP | C2-N3 | 2.20 | 1.38 | 1.33 |
| 11 | HE | 501 | GTP | C2-N3 | 2.19 | 1.38 | 1.33 |
| 11 | IE | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 11 | BE | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 11 | DC | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 11 | EE | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 11 | BA | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 11 | DA | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 11 | AE | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 11 | KC | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 11 | EC | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 11 | GE | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | JE | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | JC | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | KE | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | JA | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | HA | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 11 | MC | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 11 | GA | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | CA | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | HC | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | FE | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | EA | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | AC | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 11 | AA | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 11 | ME | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 11 | KA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | MA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | DE | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | CE | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | FA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | LA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | GC | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | LE | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 11 | IA | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 11 | CC | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 11 | IC | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 11 | FC | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 11 | LC | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |

All (229) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11 | LC | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 11 | CE | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 11 | BE | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 11 | LE | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 11 | MA | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 11 | BA | 501 | GTP | C8-N7-C5 | 3.56 | 108.62 | 102.55 |
| 11 | KC | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 11 | LA | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 11 | FC | 501 | GTP | C8-N7-C5 | 3.56 | 108.60 | 102.55 |
| 11 | GC | 501 | GTP | C8-N7-C5 | 3.56 | 108.60 | 102.55 |
| 11 | IA | 501 | GTP | C8-N7-C5 | 3.56 | 108.60 | 102.55 |
| 11 | KE | 501 | GTP | C8-N7-C5 | 3.55 | 108.60 | 102.55 |
| 11 | AC | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 11 | IC | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 11 | EA | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 11 | MC | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 11 | AE | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | GE | 501 | GTP | C8-N7-C5 | 3.55 | 108.59 | 102.55 |
| 11 | DC | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 11 | JC | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 11 | EE | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 11 | AA | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 11 | HE | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 11 | BC | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 11 | CA | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 11 | ME | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 11 | HC | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 11 | HA | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 11 | JA | 501 | GTP | C8-N7-C5 | 3.53 | 108.57 | 102.55 |
| 11 | CC | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 11 | JE | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 11 | DE | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 11 | GA | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 11 | KA | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 11 | FE | 501 | GTP | C8-N7-C5 | 3.52 | 108.55 | 102.55 |
| 11 | FA | 501 | GTP | C8-N7-C5 | 3.52 | 108.54 | 102.55 |
| 11 | DA | 501 | GTP | C8-N7-C5 | 3.52 | 108.53 | 102.55 |
| 11 | EC | 501 | GTP | C8-N7-C5 | 3.51 | 108.53 | 102.55 |
| 11 | IE | 501 | GTP | C8-N7-C5 | 3.51 | 108.53 | 102.55 |
| 11 | DE | 501 | GTP | C2-N1-C6 | -3.07 | 119.50 | 125.11 |
| 11 | CE | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 11 | CC | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 11 | BA | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 11 | MC | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 11 | GA | 501 | GTP | C5-C6-N1 | 3.05 | 119.90 | 114.07 |
| 11 | GC | 501 | GTP | C2-N1-C6 | -3.05 | 119.52 | 125.11 |
| 11 | JA | 501 | GTP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 11 | KA | 501 | GTP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 11 | CE | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 11 | MA | 501 | GTP | C5-C6-N1 | 3.04 | 119.88 | 114.07 |
| 11 | GC | 501 | GTP | C5-C6-N1 | 3.04 | 119.87 | 114.07 |
| 11 | DE | 501 | GTP | C5-C6-N1 | 3.04 | 119.87 | 114.07 |
| 11 | KA | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 11 | LC | 501 | GTP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 11 | AA | 501 | GTP | C5-C6-N1 | 3.04 | 119.86 | 114.07 |
| 11 | EE | 501 | GTP | C5-C6-N1 | 3.04 | 119.86 | 114.07 |
| 11 | BC | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 11 | CC | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 11 | KC | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | CA | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 11 | LE | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 11 | BE | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 11 | HC | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 11 | LC | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 11 | JC | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 11 | DC | 501 | GTP | C2-N1-C6 | -3.03 | 119.57 | 125.11 |
| 11 | EC | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 11 | MC | 501 | GTP | C2-N1-C6 | -3.03 | 119.57 | 125.11 |
| 11 | LA | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 11 | LE | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 11 | MA | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 11 | DC | 501 | GTP | C5-C6-N1 | 3.02 | 119.84 | 114.07 |
| 11 | HC | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 11 | KC | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 11 | LA | 501 | GTP | C2-N1-C6 | -3.02 | 119.58 | 125.11 |
| 11 | AC | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | HA | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | FA | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | IA | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | ME | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | FC | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | DA | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 11 | IC | 501 | GTP | C2-N1-C6 | -3.02 | 119.59 | 125.11 |
| 11 | AA | 501 | GTP | C2-N1-C6 | -3.01 | 119.59 | 125.11 |
| 11 | KE | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 11 | GA | 501 | GTP | C2-N1-C6 | -3.01 | 119.59 | 125.11 |
| 11 | AC | 501 | GTP | C2-N1-C6 | -3.01 | 119.60 | 125.11 |
| 11 | HE | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 11 | IC | 501 | GTP | C5-C6-N1 | 3.01 | 119.82 | 114.07 |
| 11 | DA | 501 | GTP | C2-N1-C6 | -3.01 | 119.60 | 125.11 |
| 11 | IA | 501 | GTP | C2-N1-C6 | -3.01 | 119.60 | 125.11 |
| 11 | AE | 501 | GTP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 11 | BA | 501 | GTP | C2-N1-C6 | -3.01 | 119.61 | 125.11 |
| 11 | EA | 501 | GTP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 11 | IE | 501 | GTP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 11 | JC | 501 | GTP | C2-N1-C6 | -3.00 | 119.61 | 125.11 |
| 11 | FE | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 11 | EE | 501 | GTP | C2-N1-C6 | -3.00 | 119.61 | 125.11 |
| 11 | CA | 501 | GTP | C2-N1-C6 | -3.00 | 119.62 | 125.11 |
| 11 | JE | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 11 | JA | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11 | HA | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 11 | FE | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 11 | GE | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 11 | EA | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 11 | FC | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 11 | ME | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 11 | FA | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 11 | BC | 501 | GTP | C2-N1-C6 | -2.96 | 119.68 | 125.11 |
| 11 | KE | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 11 | EC | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 11 | AE | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 11 | IE | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 11 | JE | 501 | GTP | C2-N1-C6 | -2.96 | 119.70 | 125.11 |
| 11 | BE | 501 | GTP | C2-N1-C6 | -2.95 | 119.70 | 125.11 |
| 11 | GE | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 11 | HE | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 13 | EF | 501 | GDP | C8-N7-C5 | 2.81 | 107.34 | 102.55 |
| 13 | DF | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 13 | JB | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 13 | GB | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 13 | HB | 501 | GDP | C8-N7-C5 | 2.79 | 107.29 | 102.55 |
| 13 | DB | 501 | GDP | C8-N7-C5 | 2.78 | 107.29 | 102.55 |
| 13 | ED | 502 | GDP | C8-N7-C5 | 2.78 | 107.29 | 102.55 |
| 13 | BD | 501 | GDP | C8-N7-C5 | 2.78 | 107.29 | 102.55 |
| 13 | CD | 501 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 13 | FB | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 13 | AB | 501 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 13 | HF | 501 | GDP | C8-N7-C5 | 2.77 | 107.26 | 102.55 |
| 13 | BF | 501 | GDP | C8-N7-C5 | 2.77 | 107.26 | 102.55 |
| 13 | FF | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 13 | KF | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 13 | AF | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 13 | IB | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 13 | KB | 501 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 13 | JF | 501 | GDP | C8-N7-C5 | 2.75 | 107.24 | 102.55 |
| 13 | LF | 501 | GDP | C8-N7-C5 | 2.75 | 107.24 | 102.55 |
| 13 | CF | 501 | GDP | C8-N7-C5 | 2.75 | 107.24 | 102.55 |
| 13 | JD | 501 | GDP | C8-N7-C5 | 2.75 | 107.24 | 102.55 |
| 13 | BB | 501 | GDP | C8-N7-C5 | 2.75 | 107.23 | 102.55 |
| 13 | LB | 501 | GDP | C8-N7-C5 | 2.75 | 107.23 | 102.55 |
| 13 | CB | 501 | GDP | C8-N7-C5 | 2.75 | 107.22 | 102.55 |
| 13 | GD | 501 | GDP | C8-N7-C5 | 2.75 | 107.22 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 13 | HD | 501 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 13 | LD | 501 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 13 | KD | 501 | GDP | C8-N7-C5 | 2.74 | 107.22 | 102.55 |
| 13 | AD | 501 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 13 | DD | 501 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 13 | FD | 502 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 13 | IF | 501 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 13 | EB | 501 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 13 | ID | 501 | GDP | C8-N7-C5 | 2.73 | 107.20 | 102.55 |
| 13 | GF | 501 | GDP | C8-N7-C5 | 2.73 | 107.19 | 102.55 |
| 13 | MB | 502 | GDP | C8-N7-C5 | 2.71 | 107.17 | 102.55 |
| 13 | MF | 502 | GDP | C8-N7-C5 | 2.71 | 107.16 | 102.55 |
| 13 | MD | 502 | GDP | C8-N7-C5 | 2.70 | 107.15 | 102.55 |
| 11 | BA | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 11 | BC | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 11 | MC | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 11 | ME | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 11 | MA | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 11 | JA | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 11 | EA | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 11 | BE | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 11 | FE | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 11 | CE | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 11 | KE | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 11 | JC | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 11 | FA | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 11 | KC | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 11 | IC | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 11 | CC | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 11 | FC | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 11 | GA | 501 | GTP | O6-C6-C5 | -2.07 | 120.21 | 124.32 |
| 11 | DA | 501 | GTP | O6-C6-C5 | -2.07 | 120.21 | 124.32 |
| 11 | CA | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 11 | AC | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 11 | EC | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 11 | IA | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 11 | AA | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 11 | HE | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 13 | FB | 502 | GDP | C5-C6-N1 | 2.07 | 118.01 | 114.07 |
| 11 | DE | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 11 | EE | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 11 | LC | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 13 | DB | 501 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 11 | IE | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 11 | GC | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 11 | DC | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 11 | LE | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 11 | AE | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 11 | HC | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 11 | JE | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 13 | BD | 501 | GDP | C5-C6-N1 | 2.05 | 117.99 | 114.07 |
| 11 | LA | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 11 | GE | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 11 | HA | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 13 | LF | 501 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 13 | DF | 501 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 11 | KA | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 13 | ED | 502 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 13 | IB | 501 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 13 | BB | 501 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 13 | GB | 501 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 13 | LB | 501 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 13 | KB | 501 | GDP | C5-C6-N1 | 2.04 | 117.95 | 114.07 |
| 13 | DD | 501 | GDP | C5-C6-N1 | 2.03 | 117.95 | 114.07 |
| 13 | JB | 501 | GDP | C5-C6-N1 | 2.03 | 117.95 | 114.07 |
| 13 | EF | 501 | GDP | C5-C6-N1 | 2.03 | 117.95 | 114.07 |
| 13 | KD | 501 | GDP | C5-C6-N1 | 2.03 | 117.95 | 114.07 |
| 13 | JD | 501 | GDP | C5-C6-N1 | 2.03 | 117.95 | 114.07 |
| 13 | AB | 501 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 13 | MD | 502 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 13 | MF | 502 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 13 | GD | 501 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 13 | FF | 501 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 13 | HB | 501 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 13 | LD | 501 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 13 | EB | 501 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 13 | AD | 501 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 13 | FD | 502 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 13 | KF | 501 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 13 | MB | 502 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 13 | ID | 501 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 13 | JF | 501 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 13 | GF | 501 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |
| 13 | BF | 501 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 13 | CF | 501 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |
| 13 | HF | 501 | GDP | C5-C6-N1 | 2.00 | 117.89 | 114.07 |

There are no chirality outliers.

All (327) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 11 | AA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | AA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | AA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | AC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | AC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | AC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | AE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | AE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | AE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | BA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | BA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | BA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | BC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | BC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | BC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | BE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | BE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | BE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | CA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | CA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | CA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | CC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | CC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | CC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | CE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | CE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | CE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | DA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | DA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | DA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | DC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | DC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | DC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | DE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | DE | 501 | GTP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 11 | DE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | EA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | EA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | EA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | EC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | EC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | EC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | EE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | EE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | EE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | FA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | FA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | FA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | FC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | FC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | FC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | FE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | FE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | FE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | GA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | GA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | GA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | GC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | GC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | GC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | GE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | GE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | GE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | HA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | HA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | HA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | HC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | HC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | HC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | HE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | HE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | HE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | IA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | IA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | IA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | IC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | IC | 501 | GTP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | IC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | IE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | IE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | IE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | JA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | JA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | JA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | JC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | JC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | JC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | JE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | JE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | JE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | KA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | KA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | KA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | KC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | KC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | KC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | KE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | KE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | KE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | LA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | LA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | LA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | LC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | LC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | LC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | LE | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | LE | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | LE | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | MA | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | MA | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | MA | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | MC | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | MC | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | MC | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | ME | 501 | GTP | C5'-O5'-PA-O3A |
| 11 | ME | 501 | GTP | C5'-O5'-PA-O1A |
| 11 | ME | 501 | GTP | C5'-O5'-PA-O2A |
| 11 | AE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | CE | 501 | GTP | O4'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | DA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | DE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | EA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | EC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | EE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | FA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | FC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | FE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | GC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | GE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | HE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | IA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | IE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | JE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | KE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | LE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | MA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | MC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | AA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | AA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | AC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | AC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | AE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | BA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | BA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | BC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | BC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | BE | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | BE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | CA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | CA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | CC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | CC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | CE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | DA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | DC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | DC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | DE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | EA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | EC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | EE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | FA | 501 | GTP | C3'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 11 | FC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | FE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | GA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | GA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | GC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | GE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | HA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | HA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | HC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | HC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | HE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | IA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | IC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | IC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | IE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | JA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | JA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | JC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | JC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | JE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | KA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | KA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | KC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | KC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | KE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | LA | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | LA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | LC | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | LC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | LE | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | MA | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | MC | 501 | GTP | C3'-C4'-C5'-O5' |
| 11 | ME | 501 | GTP | O4'-C4'-C5'-O5' |
| 11 | ME | 501 | GTP | C3'-C4'-C5'-O5' |
| 13 | AF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | BF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | CB | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | CD | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | CF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | DD | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | DF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | FB | 502 | GDP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 13 | FF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | GB | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | GF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | IF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | JF | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | LD | 501 | GDP | C5'-O5'-PA-O1A |
| 13 | MD | 502 | GDP | C5'-O5'-PA-O1A |
| 11 | AA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | AC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | AE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | BA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | BC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | BE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | CA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | CC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | CE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | DA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | DC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | DE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | EA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | EC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | EE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | FA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | FC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | FE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | GA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | GC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | GE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | HA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | HC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | HE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | IA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | IC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | IE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | JA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | JC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | JE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | KA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | KC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | KE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | LA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | LC | 501 | GTP | C4'-C5'-O5'-PA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 11 | LE | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | MA | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | MC | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | ME | 501 | GTP | C4'-C5'-O5'-PA |
| 11 | AA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | AC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | AE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | BA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | BC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | BE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | CA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | CC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | CE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | DA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | DC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | DE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | EA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | EC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | EE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | FA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | FC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | FE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | GA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | GC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | GE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | HA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | HC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | HE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | IA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | IC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | IE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | JA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | JC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | JE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | KA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | KC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | KE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | LA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | LC | 501 | GTP | PA-O3A-PB-O2B |
| 11 | LE | 501 | GTP | PA-O3A-PB-O2B |
| 11 | MA | 501 | GTP | PA-O3A-PB-O2B |
| 11 | MC | 501 | GTP | PA-O3A-PB-O2B |

Continued on next page...

Continued from previous page...

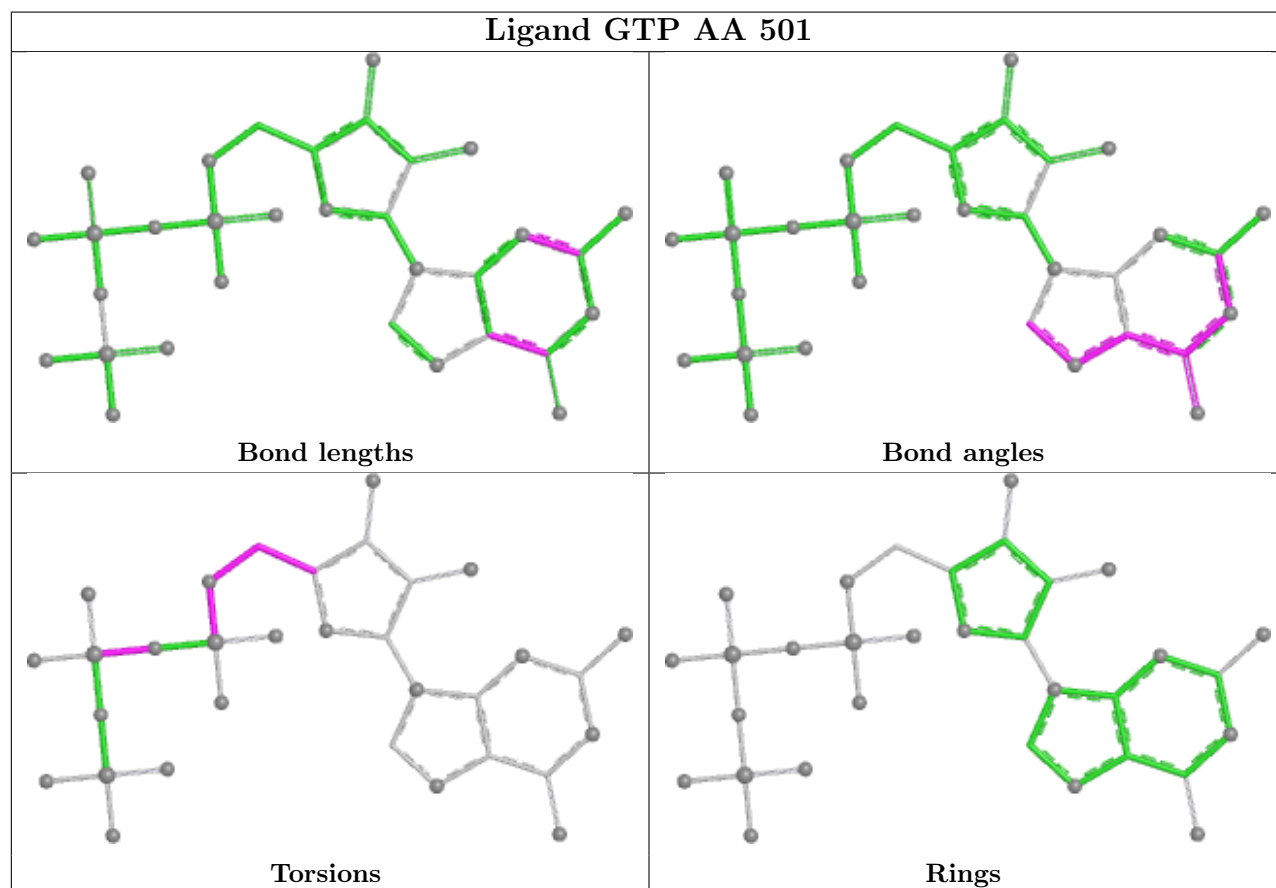
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 11 | ME | 501 | GTP | PA-O3A-PB-O2B |
| 11 | AA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | AC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | AE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | BA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | BC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | BE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | CA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | CC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | CE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | DA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | DC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | DE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | EA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | EC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | EE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | FA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | FC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | FE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | GA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | GC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | GE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | HA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | HC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | HE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | IA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | IC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | IE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | JA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | JC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | JE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | KA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | KC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | KE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | LA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | LC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | LE | 501 | GTP | PA-O3A-PB-O1B |
| 11 | MA | 501 | GTP | PA-O3A-PB-O1B |
| 11 | MC | 501 | GTP | PA-O3A-PB-O1B |
| 11 | ME | 501 | GTP | PA-O3A-PB-O1B |

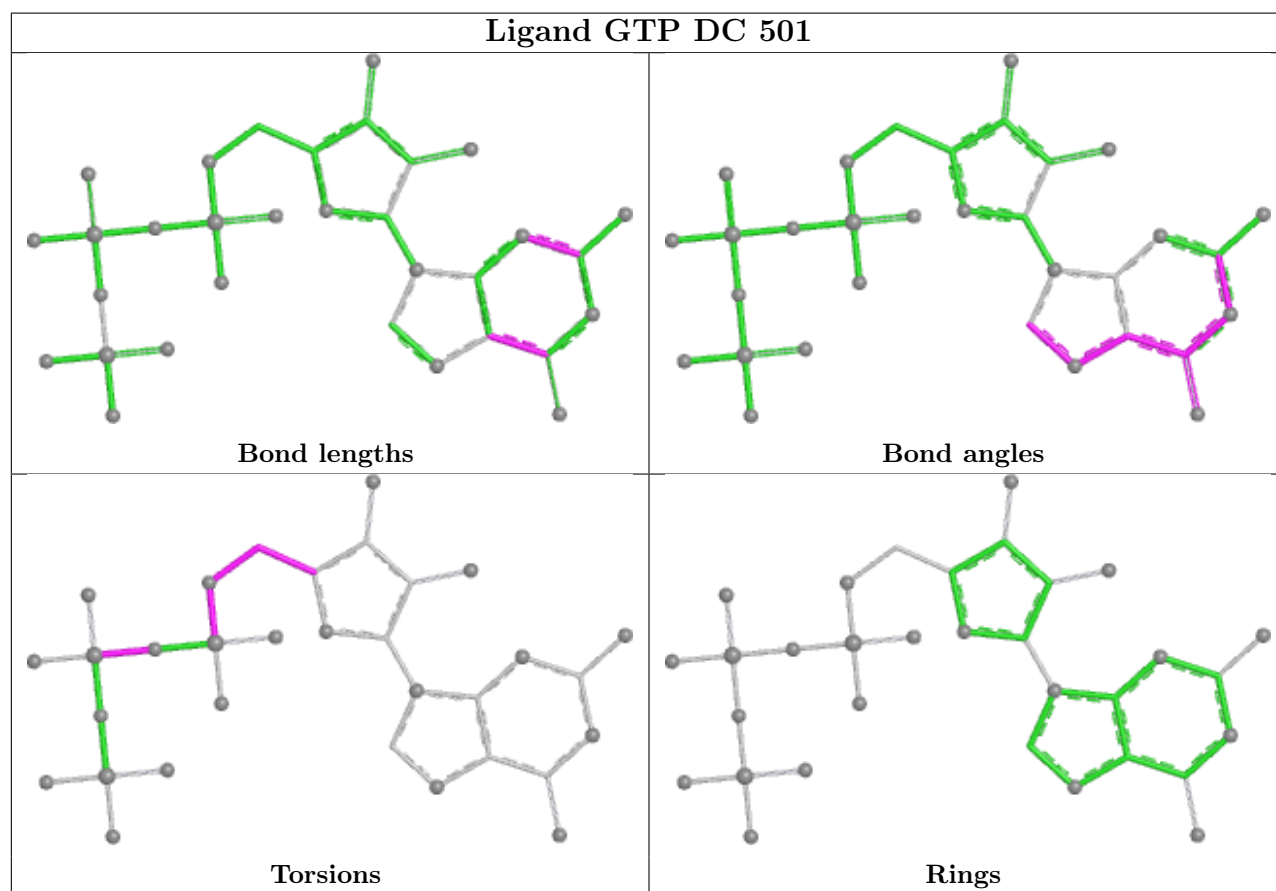
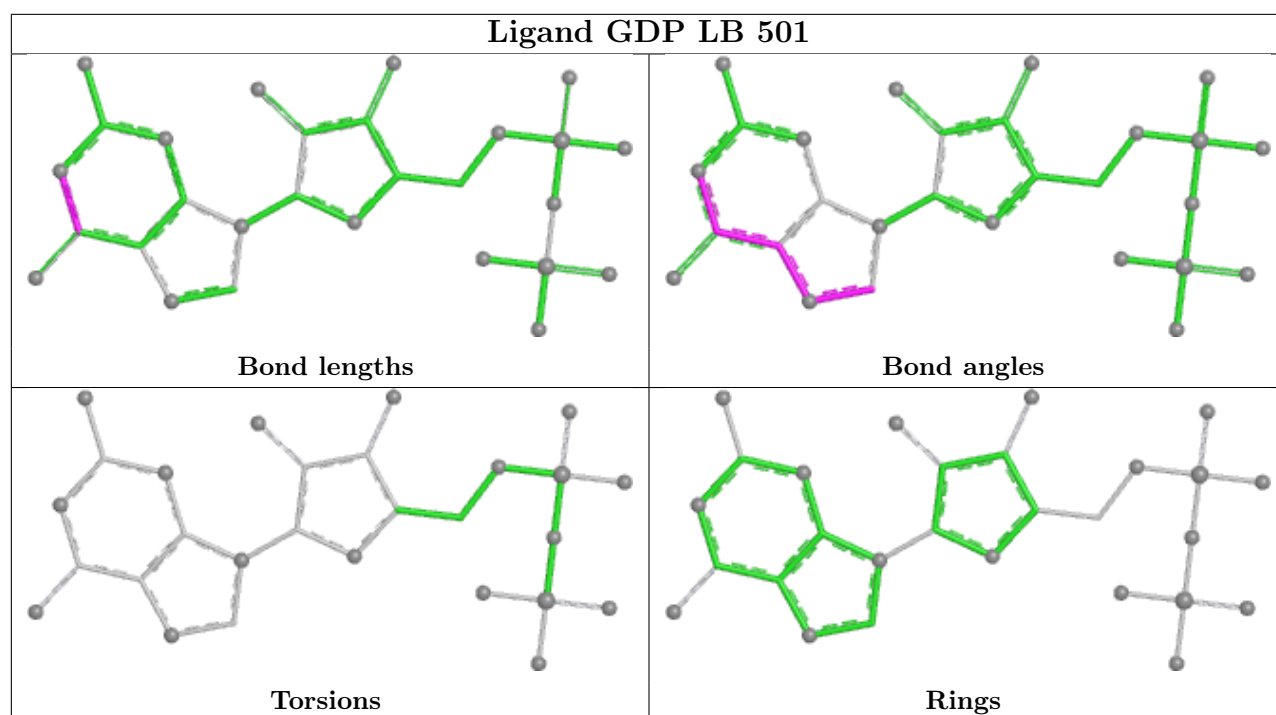
There are no ring outliers.

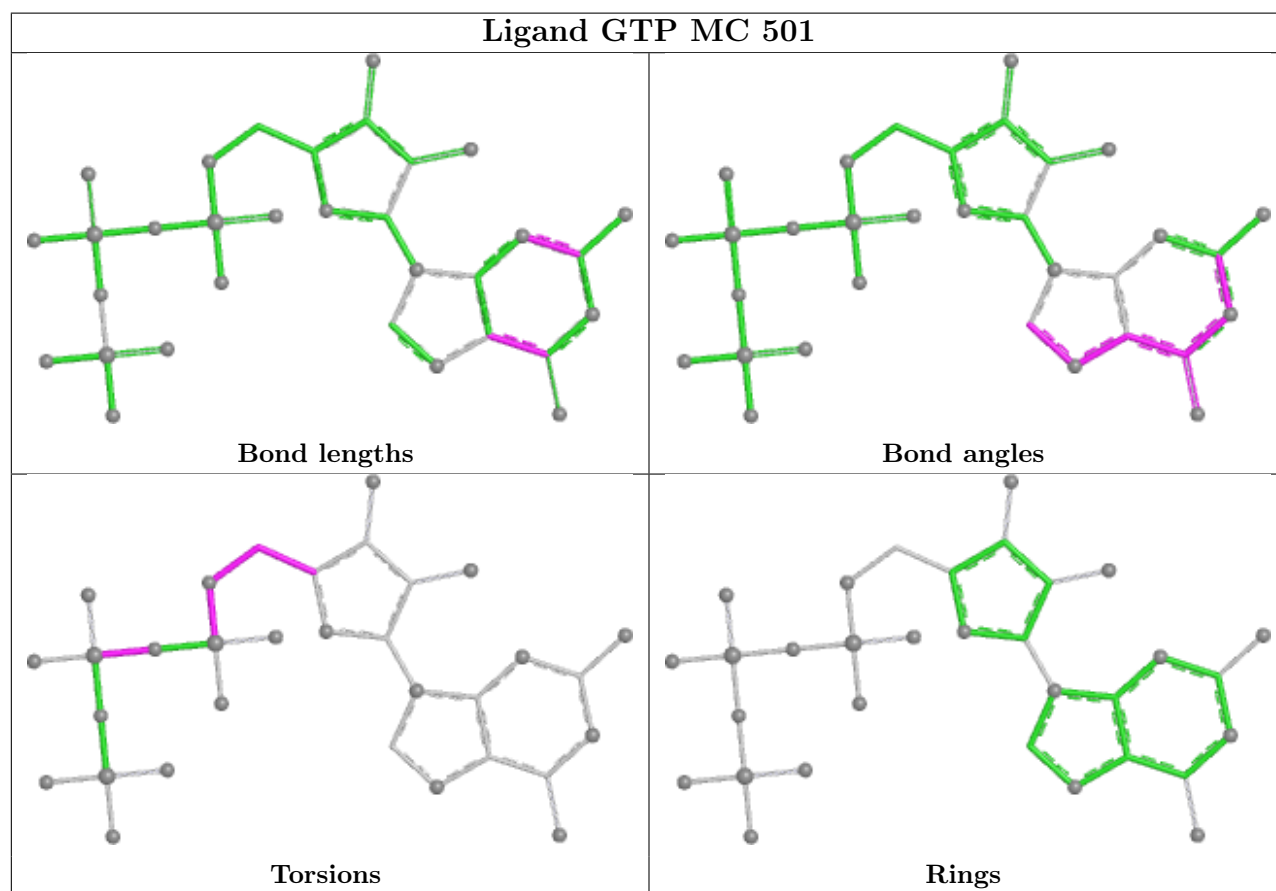
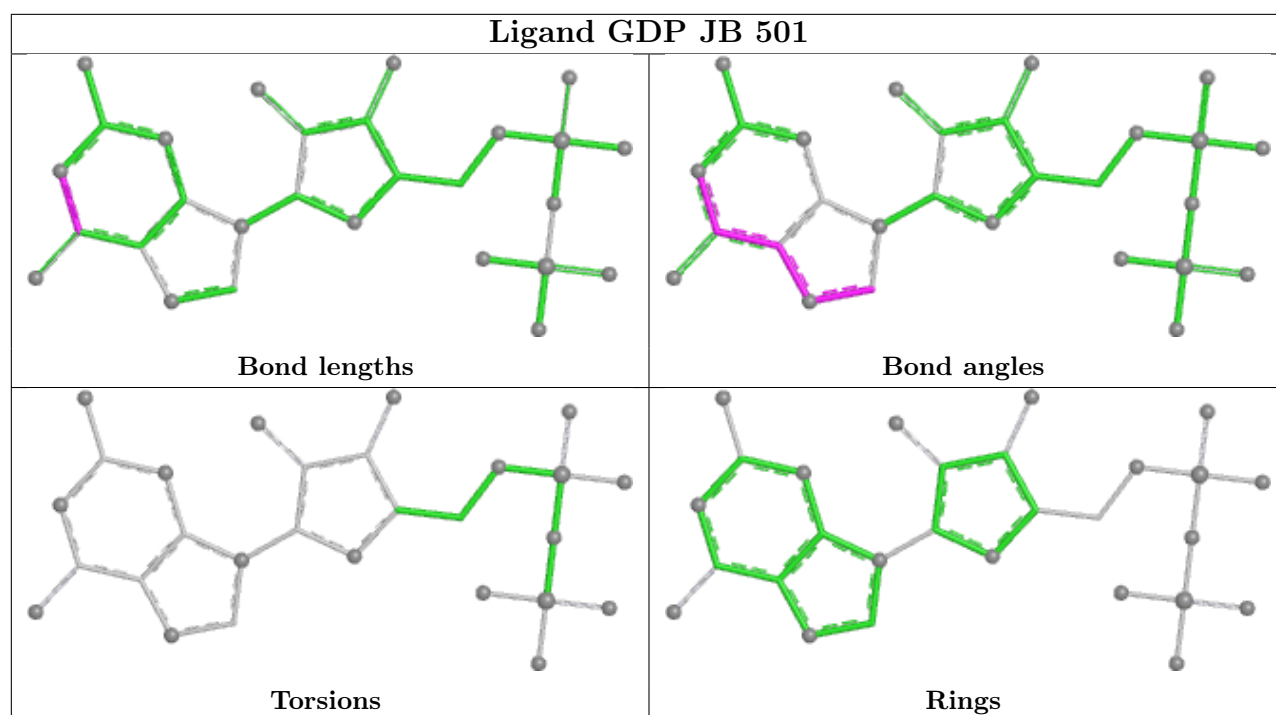
41 monomers are involved in 103 short contacts:

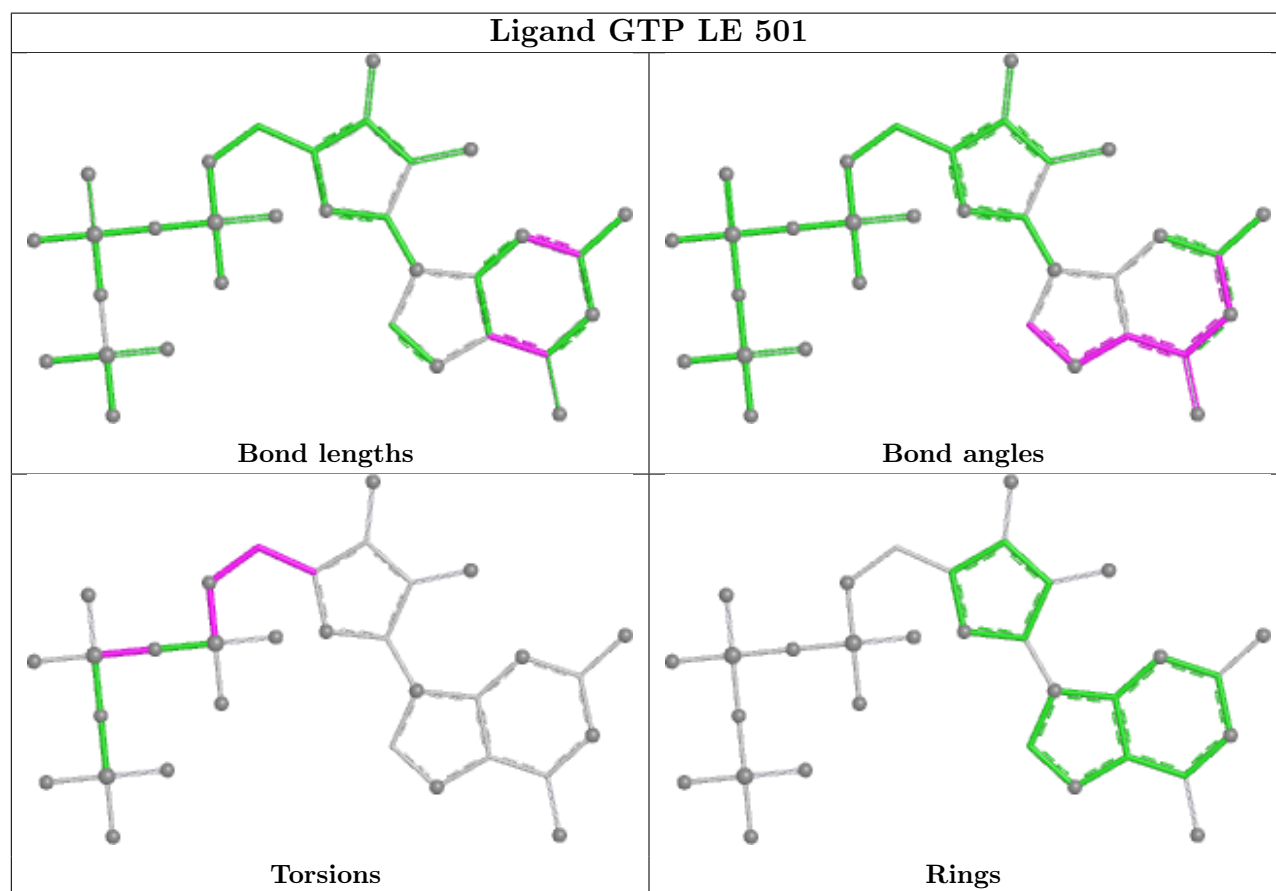
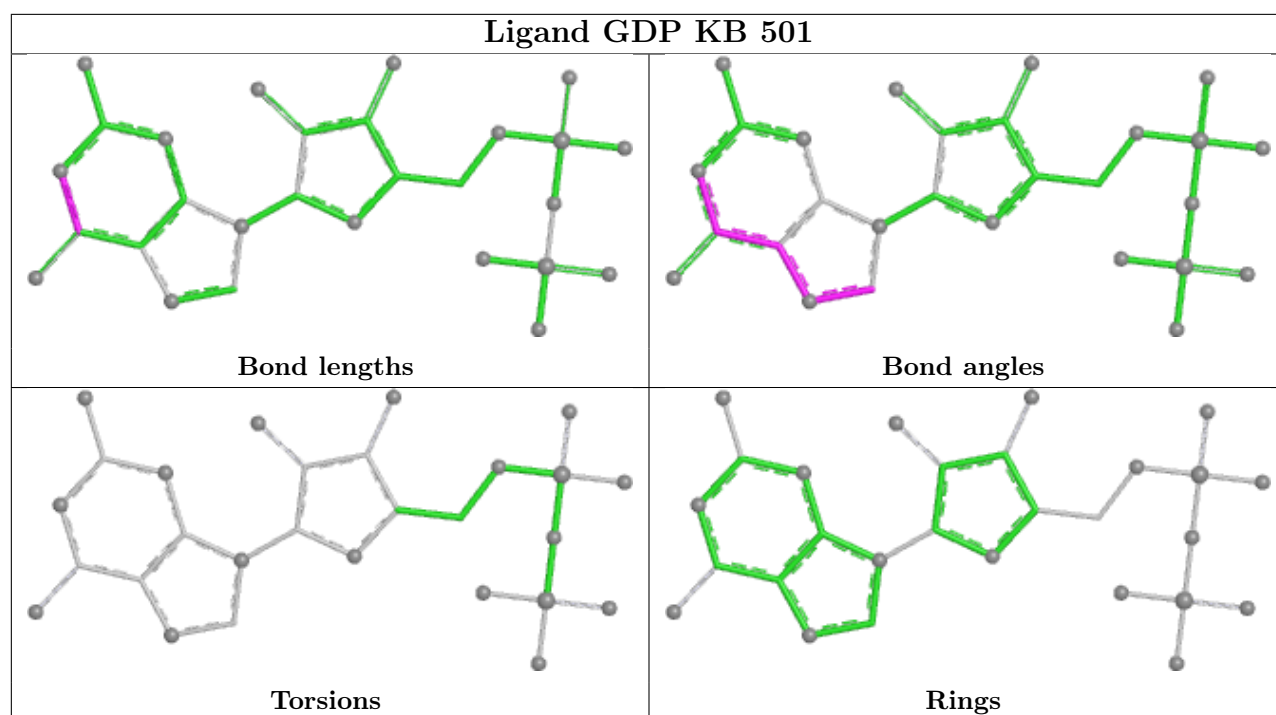
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13 | LB | 501 | GDP | 2 | 0 |
| 13 | JB | 501 | GDP | 3 | 0 |
| 11 | MC | 501 | GTP | 1 | 0 |
| 13 | KB | 501 | GDP | 3 | 0 |
| 13 | DD | 501 | GDP | 3 | 0 |
| 13 | BB | 501 | GDP | 3 | 0 |
| 13 | AB | 501 | GDP | 2 | 0 |
| 13 | BD | 501 | GDP | 3 | 0 |
| 13 | FF | 501 | GDP | 2 | 0 |
| 13 | BF | 501 | GDP | 2 | 0 |
| 13 | CF | 501 | GDP | 2 | 0 |
| 11 | MA | 501 | GTP | 1 | 0 |
| 13 | KD | 501 | GDP | 3 | 0 |
| 13 | JD | 501 | GDP | 3 | 0 |
| 13 | CD | 501 | GDP | 3 | 0 |
| 13 | MF | 502 | GDP | 2 | 0 |
| 13 | EB | 501 | GDP | 4 | 0 |
| 13 | LD | 501 | GDP | 2 | 0 |
| 13 | FB | 502 | GDP | 4 | 0 |
| 13 | ID | 501 | GDP | 3 | 0 |
| 13 | HD | 501 | GDP | 3 | 0 |
| 13 | FD | 502 | GDP | 4 | 0 |
| 13 | MD | 502 | GDP | 2 | 0 |
| 13 | IF | 501 | GDP | 2 | 0 |
| 13 | AD | 501 | GDP | 2 | 0 |
| 13 | CB | 501 | GDP | 3 | 0 |
| 13 | GD | 501 | GDP | 3 | 0 |
| 13 | LF | 501 | GDP | 2 | 0 |
| 13 | AF | 501 | GDP | 1 | 0 |
| 13 | DF | 501 | GDP | 2 | 0 |
| 13 | DB | 501 | GDP | 3 | 0 |
| 13 | GB | 501 | GDP | 3 | 0 |
| 13 | IB | 501 | GDP | 3 | 0 |
| 13 | EF | 501 | GDP | 2 | 0 |
| 13 | KF | 501 | GDP | 2 | 0 |
| 13 | HB | 501 | GDP | 3 | 0 |
| 13 | HF | 501 | GDP | 2 | 0 |
| 13 | JF | 501 | GDP | 2 | 0 |
| 13 | GF | 501 | GDP | 2 | 0 |
| 13 | MB | 502 | GDP | 2 | 0 |
| 13 | ED | 502 | GDP | 4 | 0 |

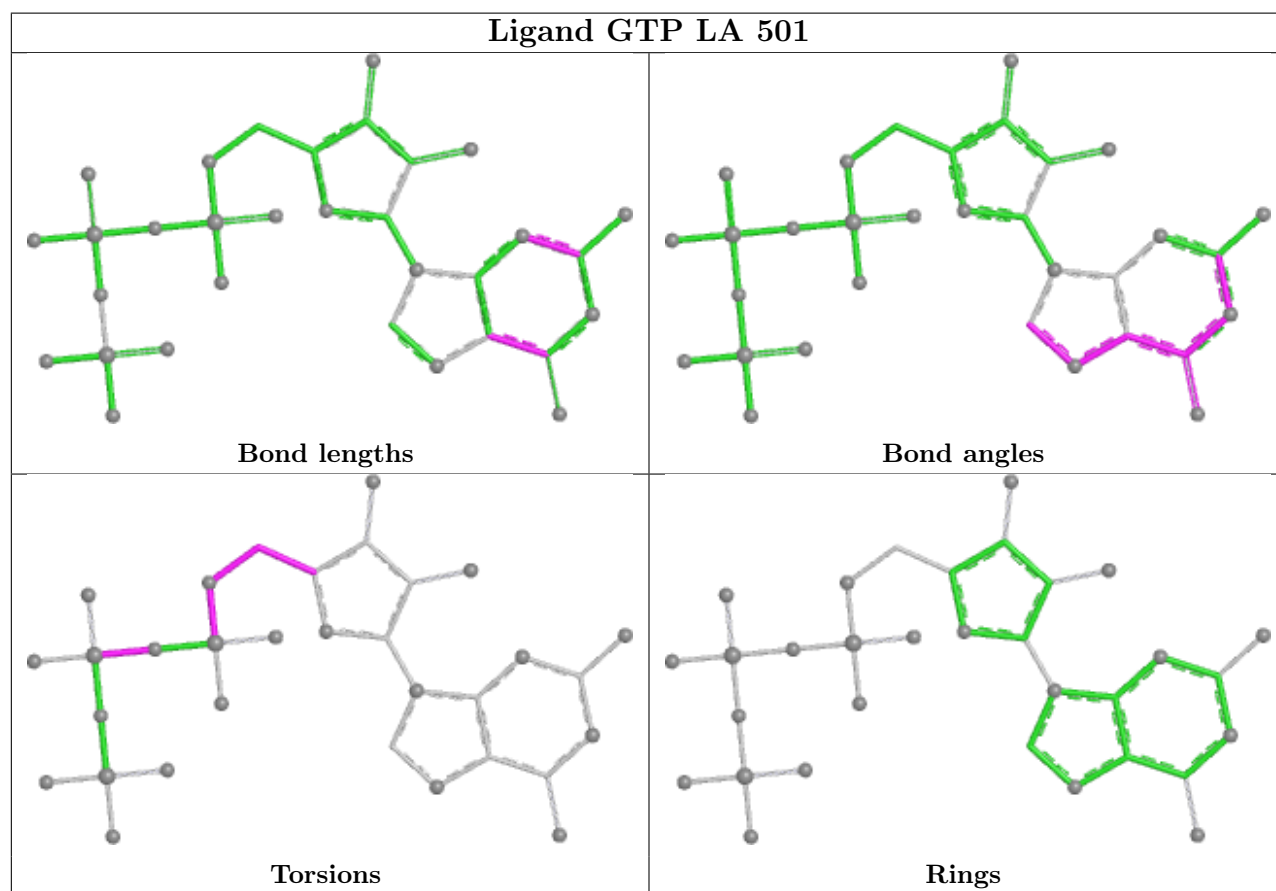
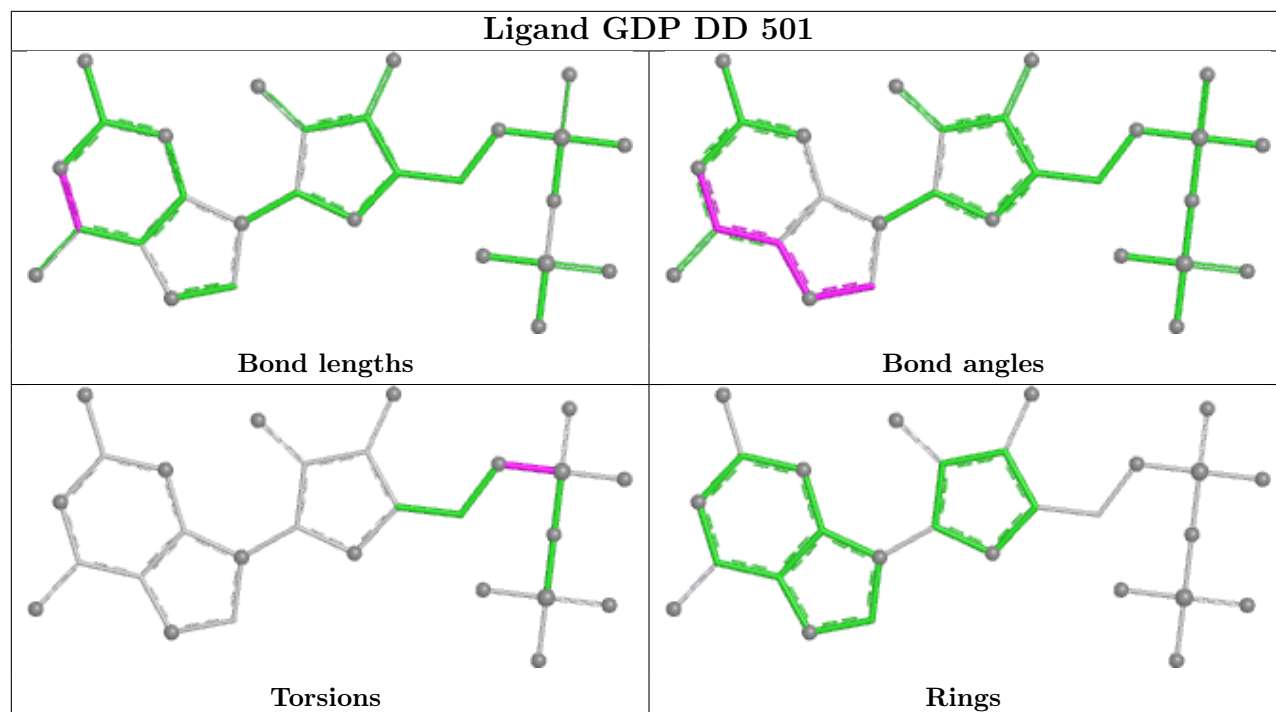
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

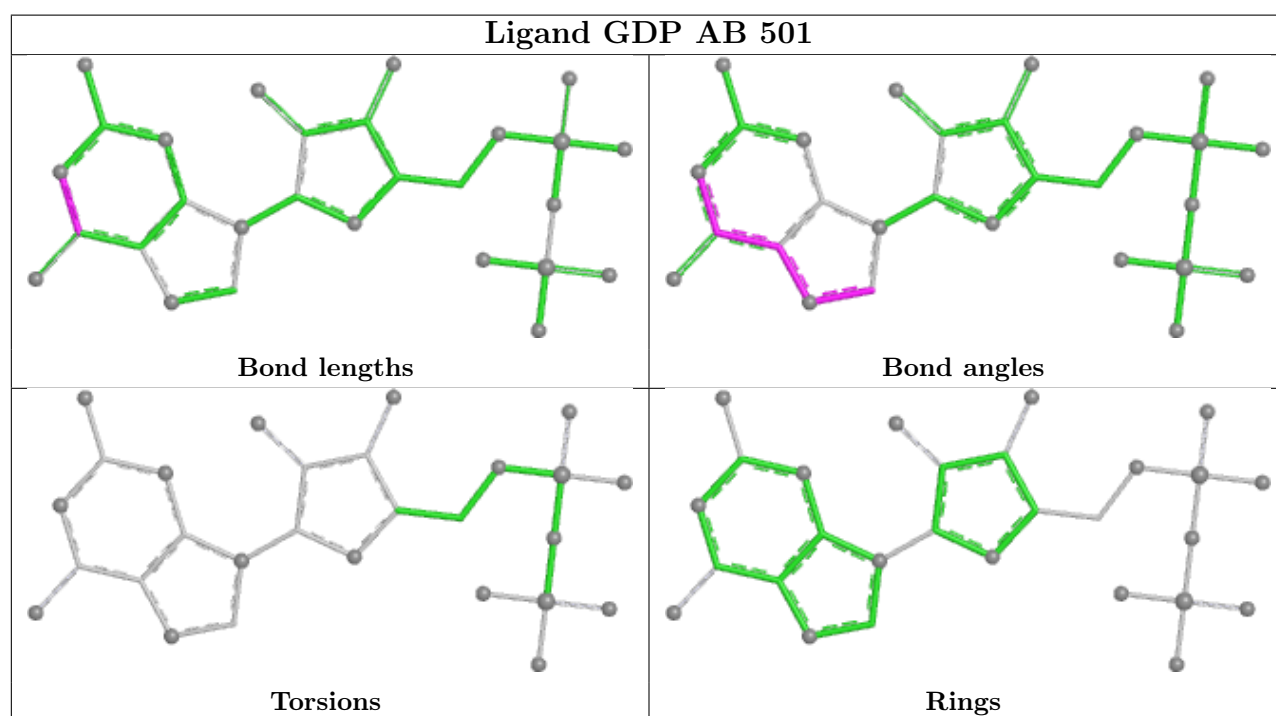
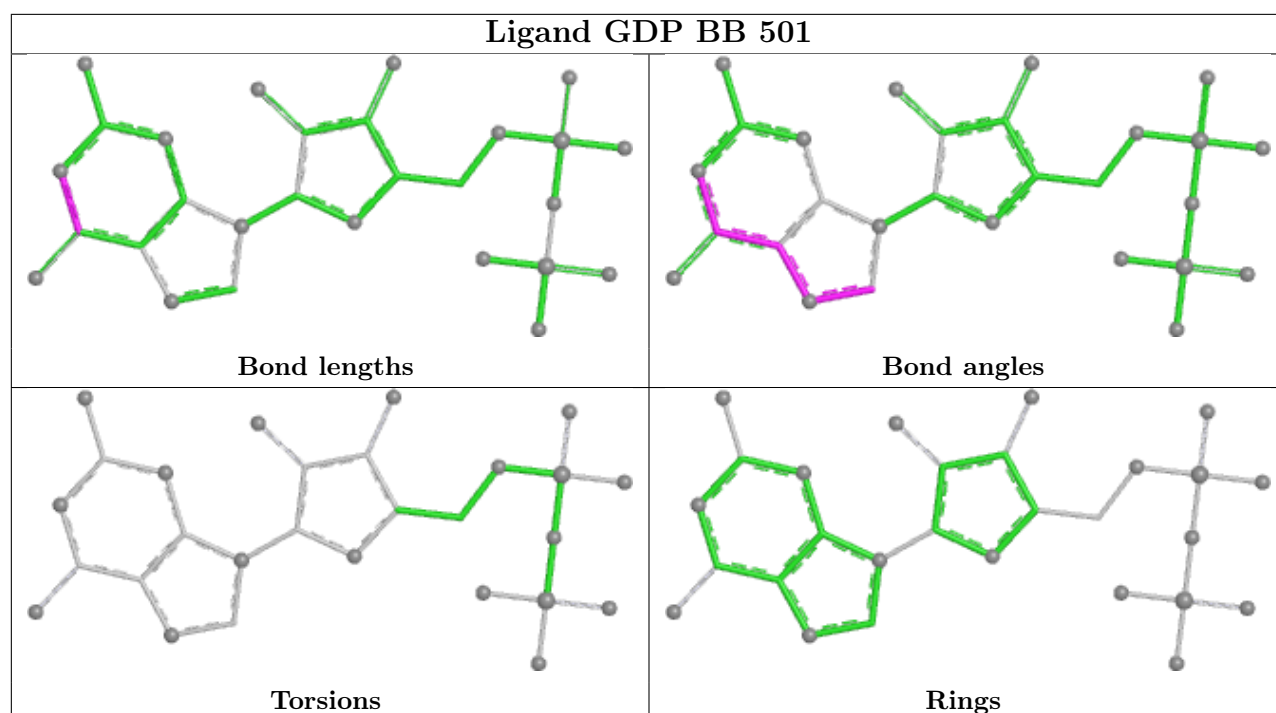


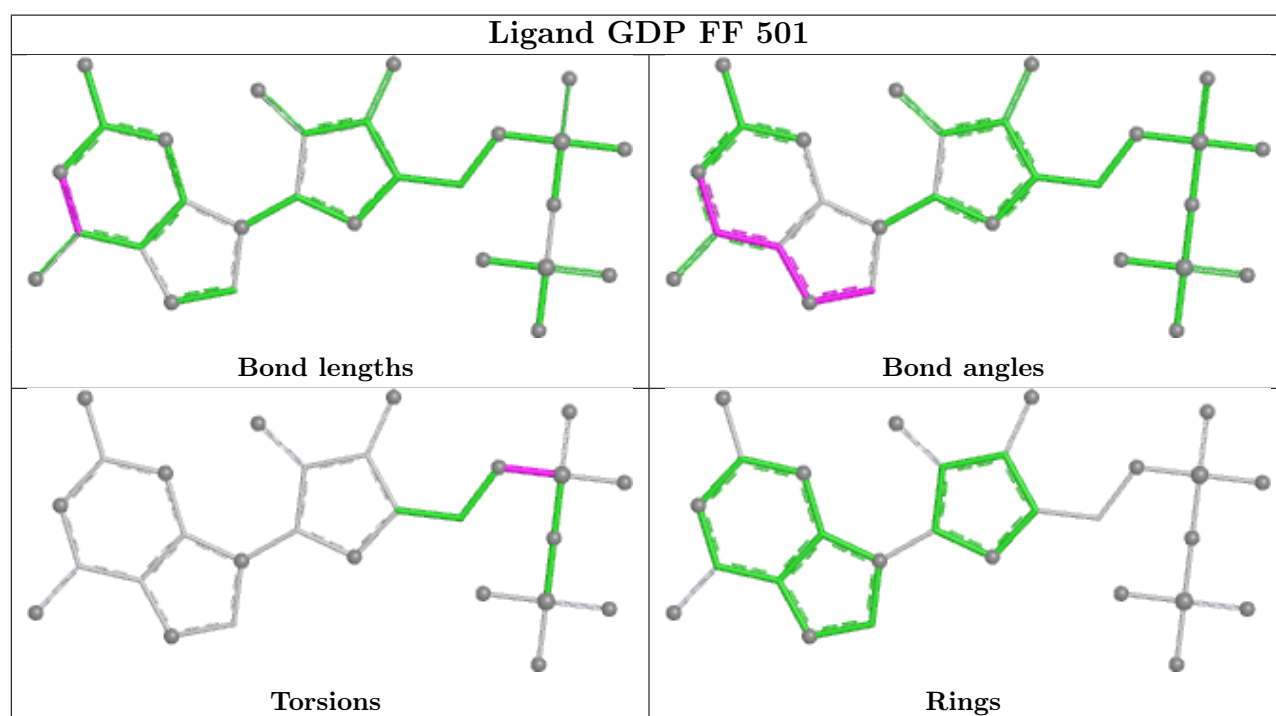
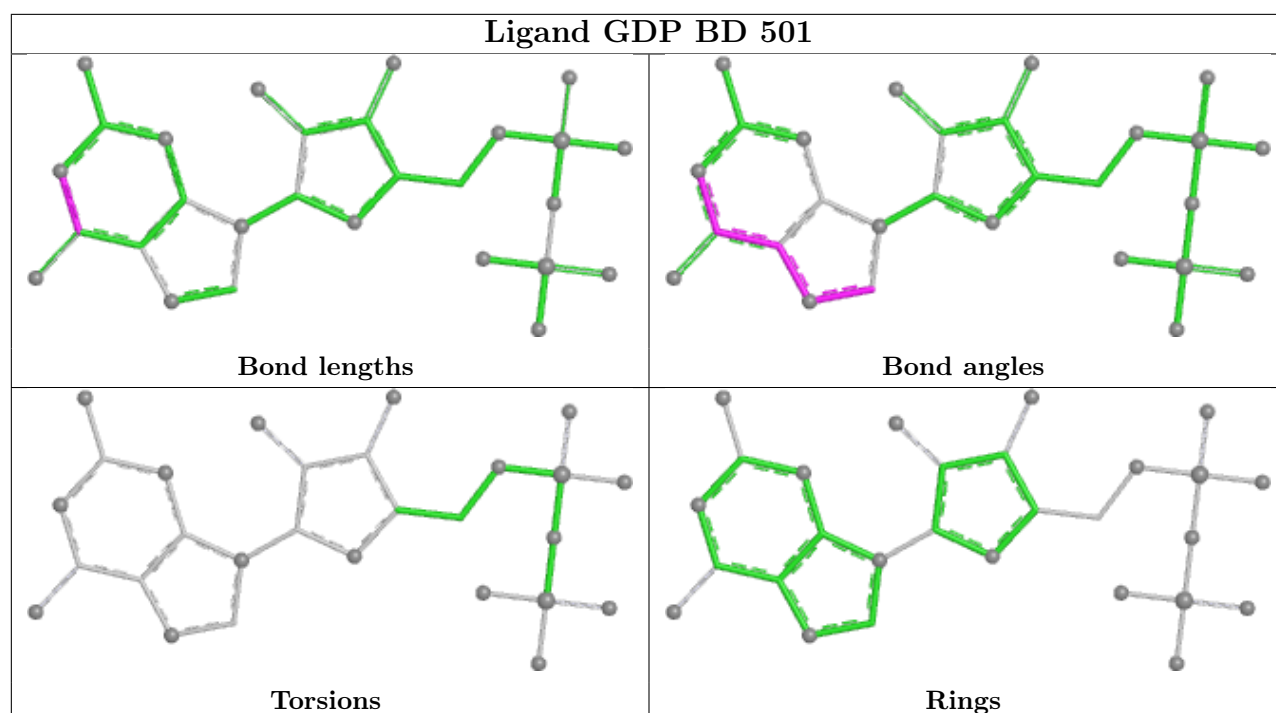




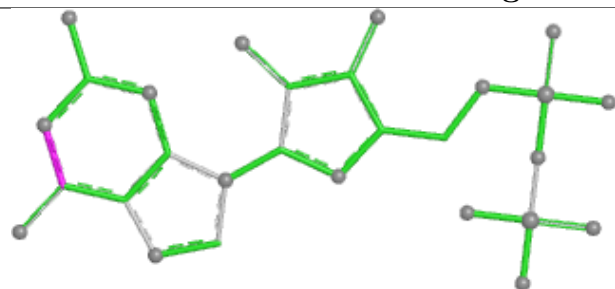




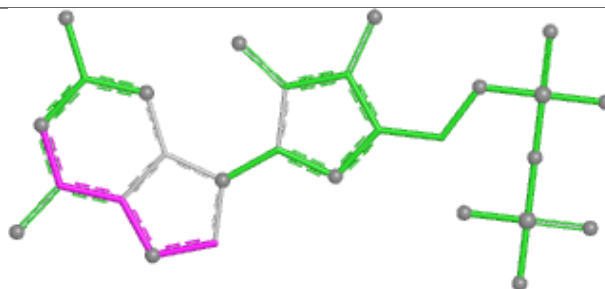




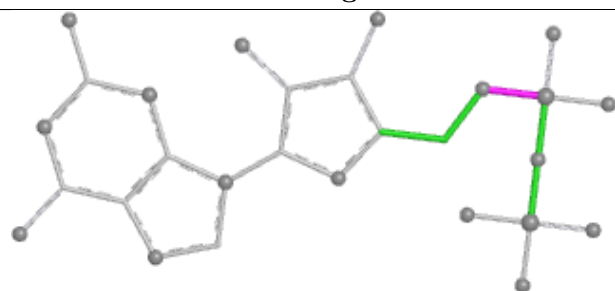
Ligand GDP BF 501



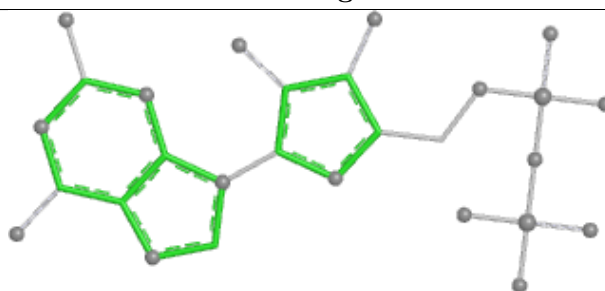
Bond lengths



Bond angles

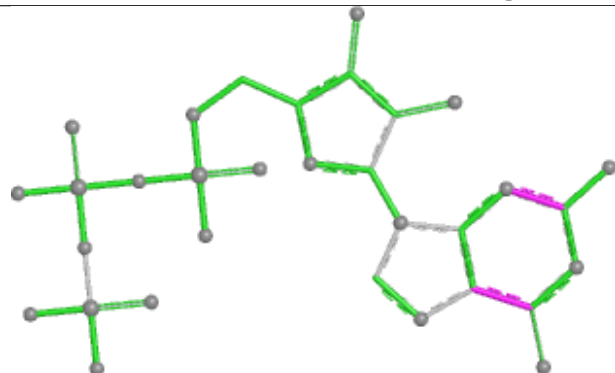


Torsions

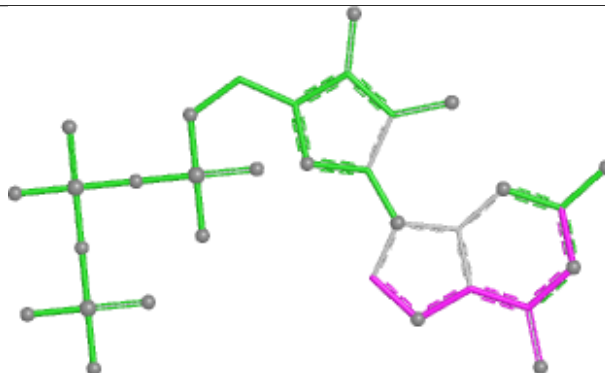


Rings

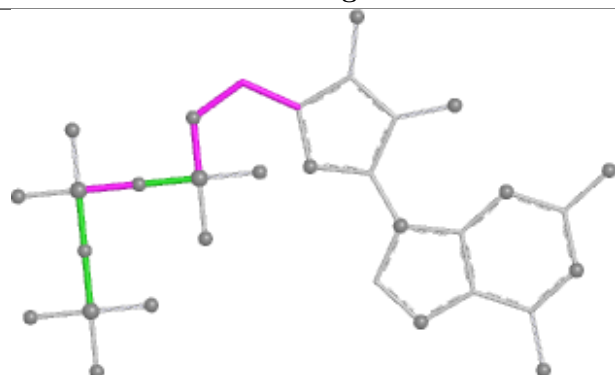
Ligand GTP GA 501



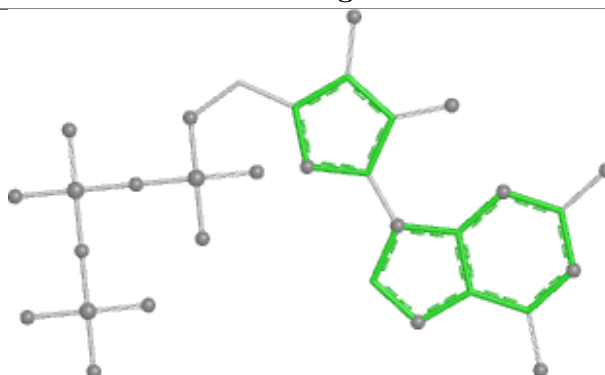
Bond lengths



Bond angles

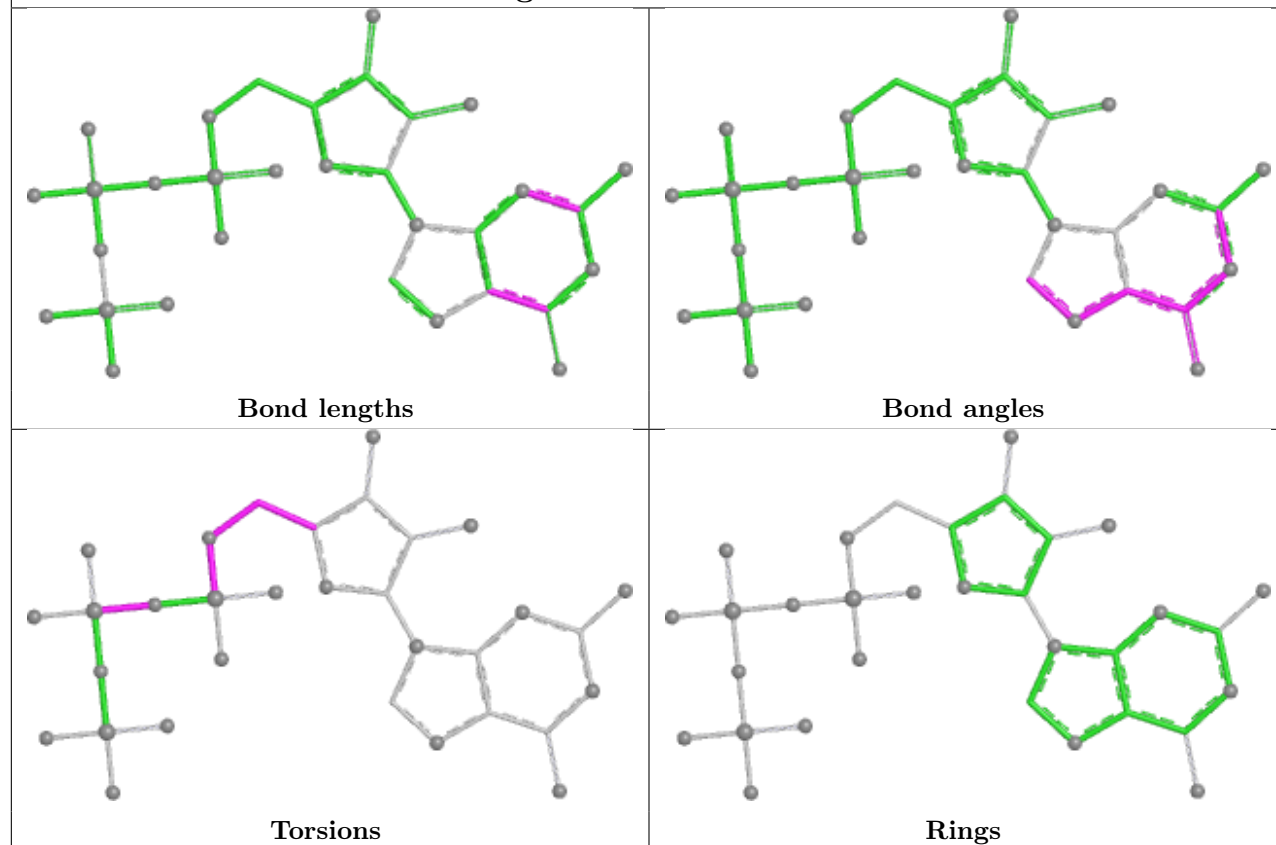


Torsions

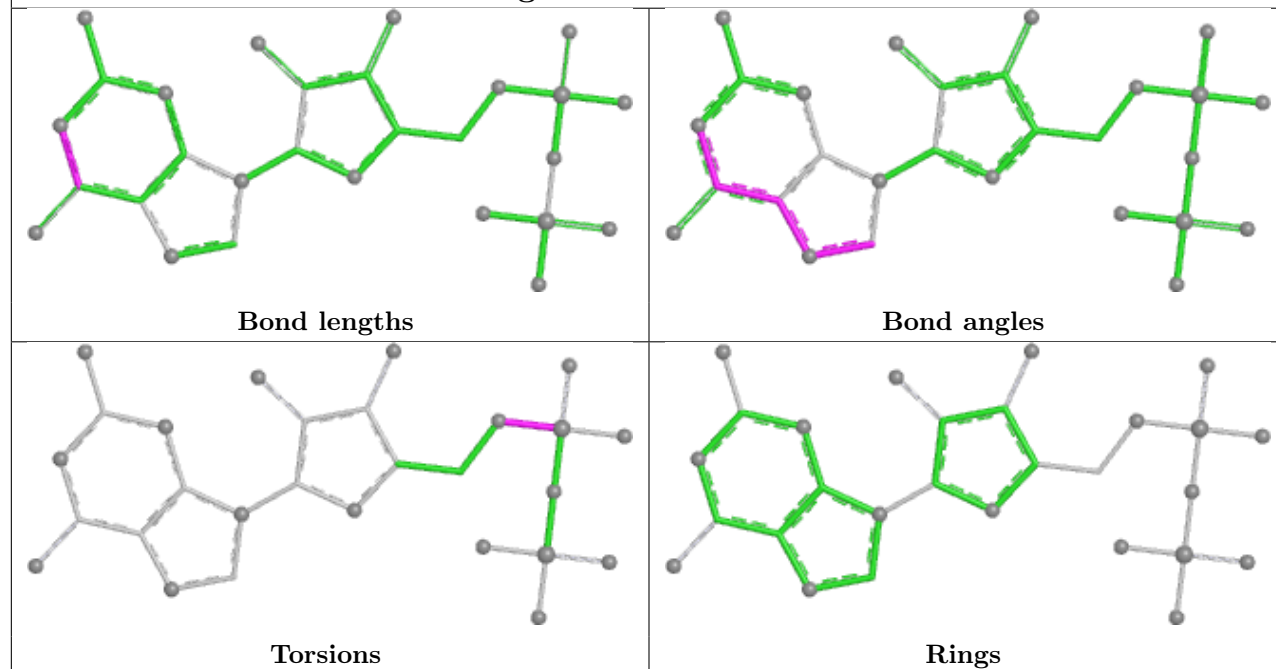


Rings

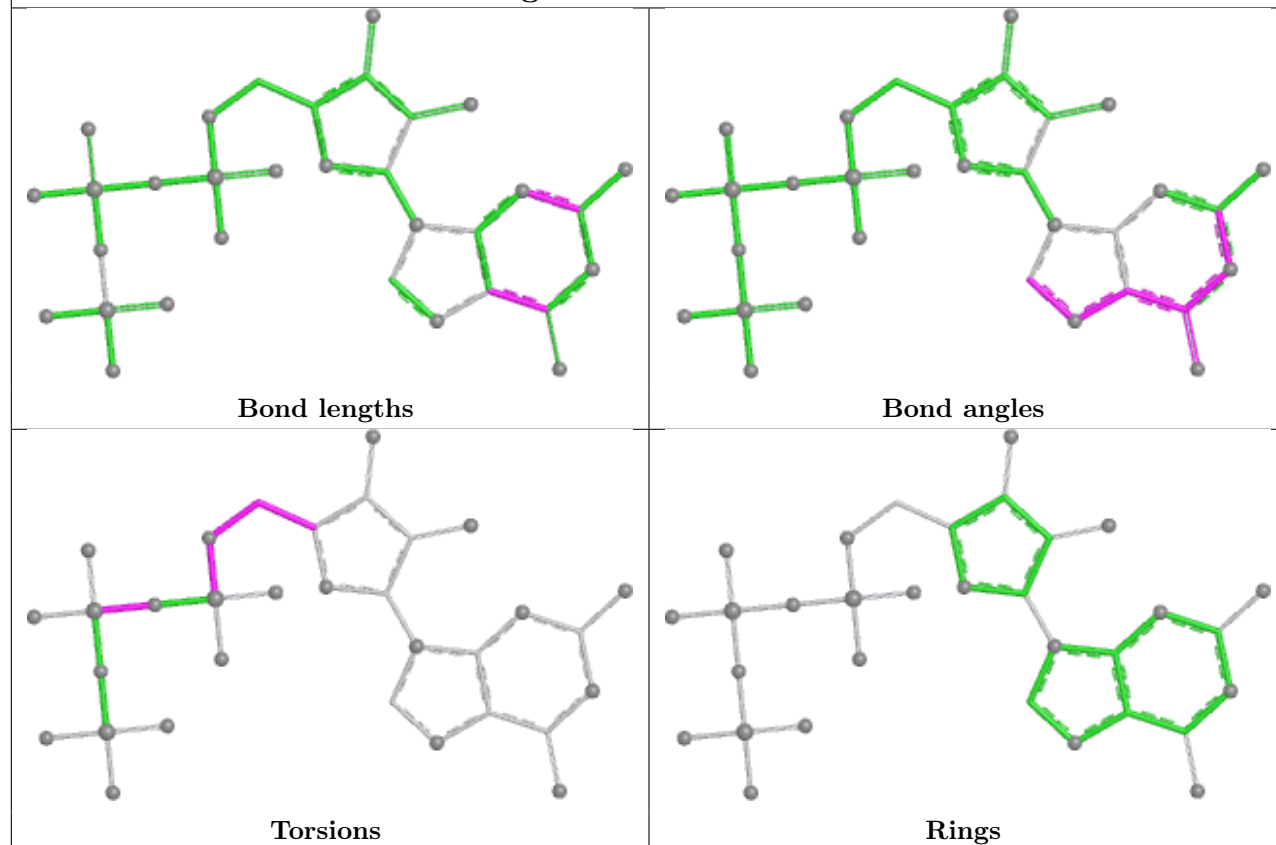
Ligand GTP KA 501



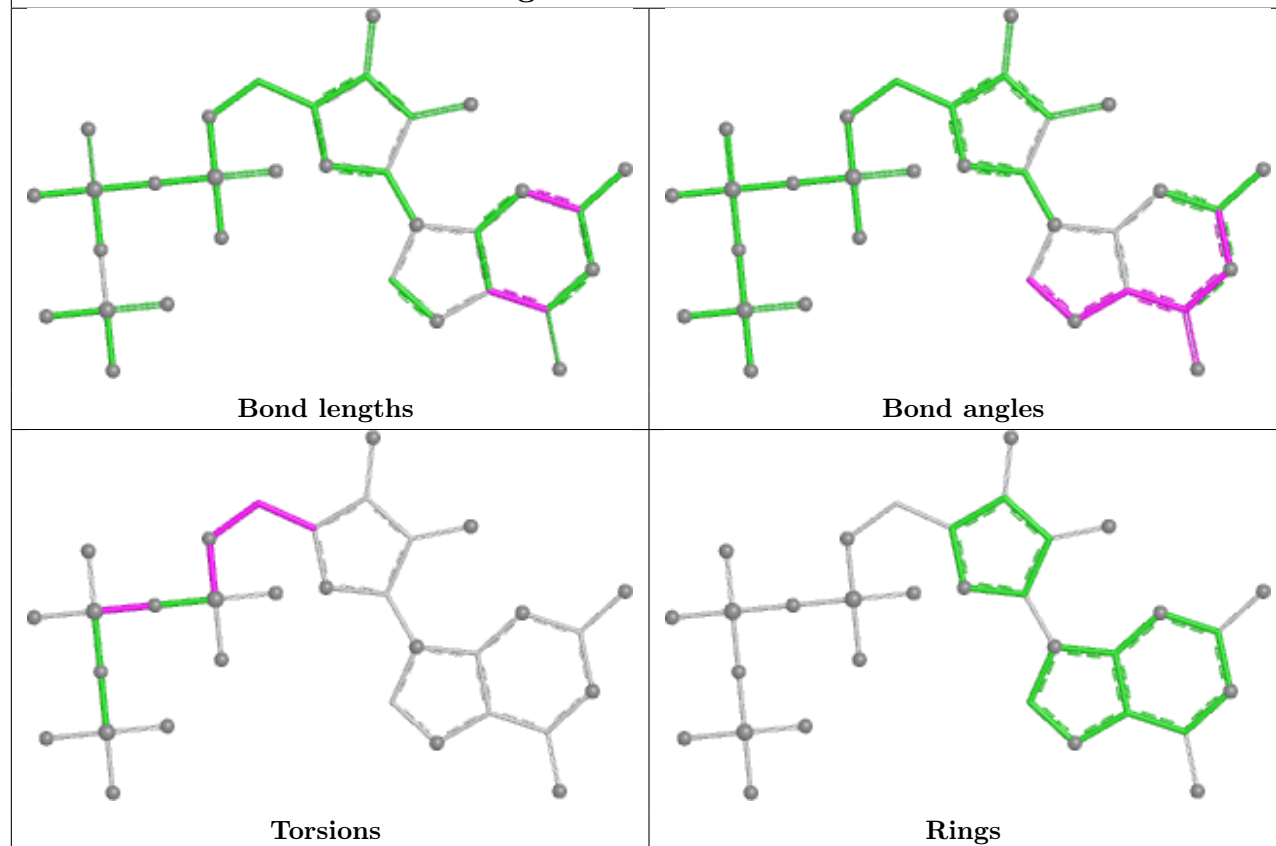
Ligand GDP CF 501



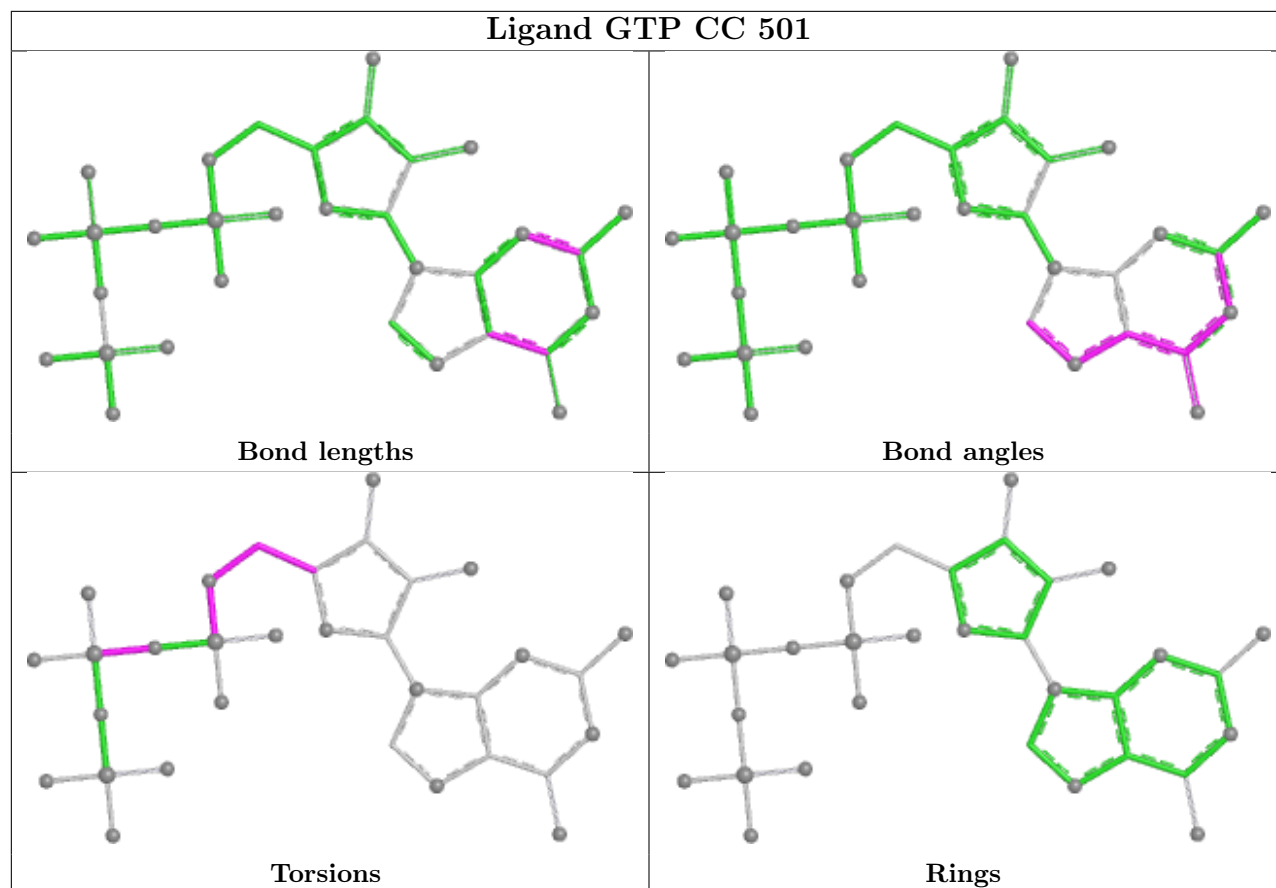
Ligand GTP JC 501



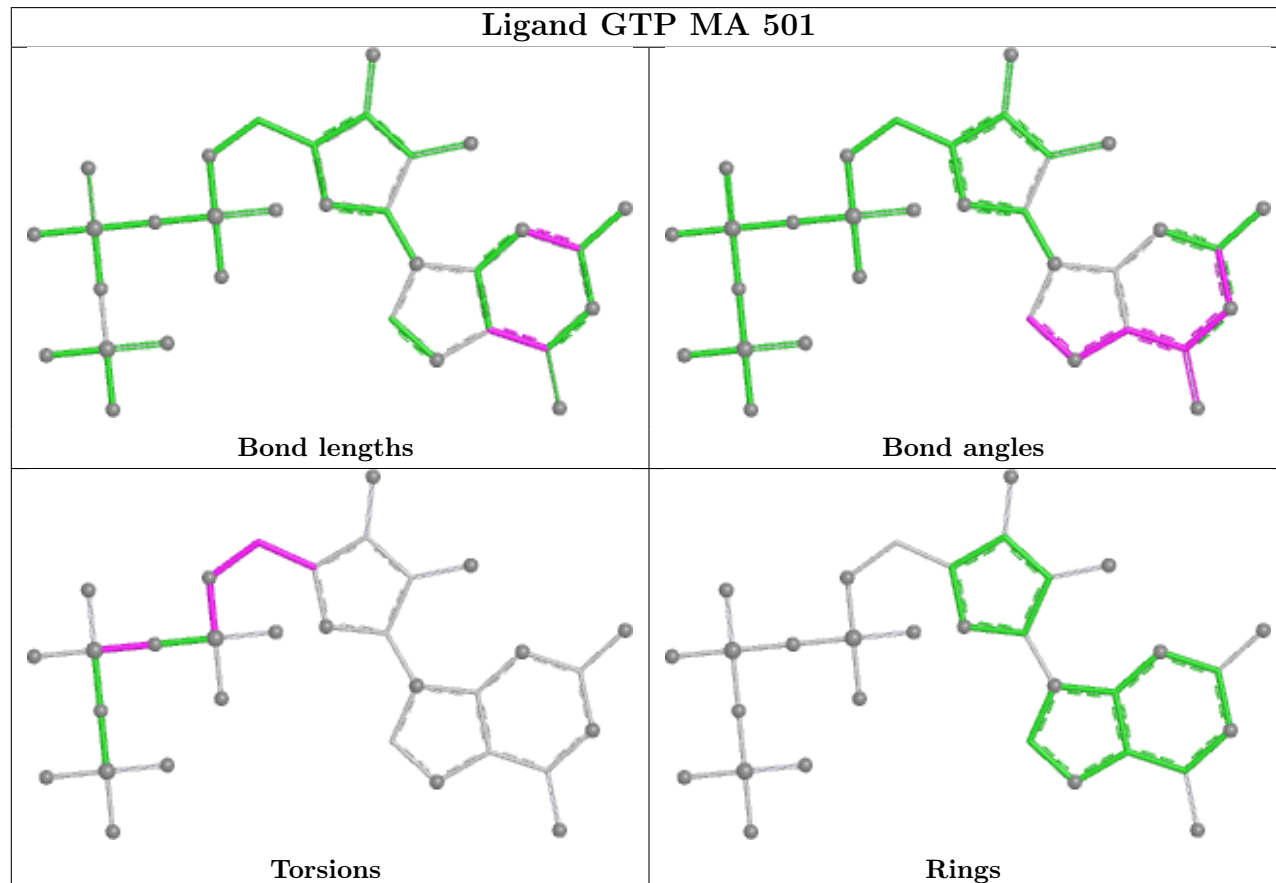
Ligand GTP AC 501



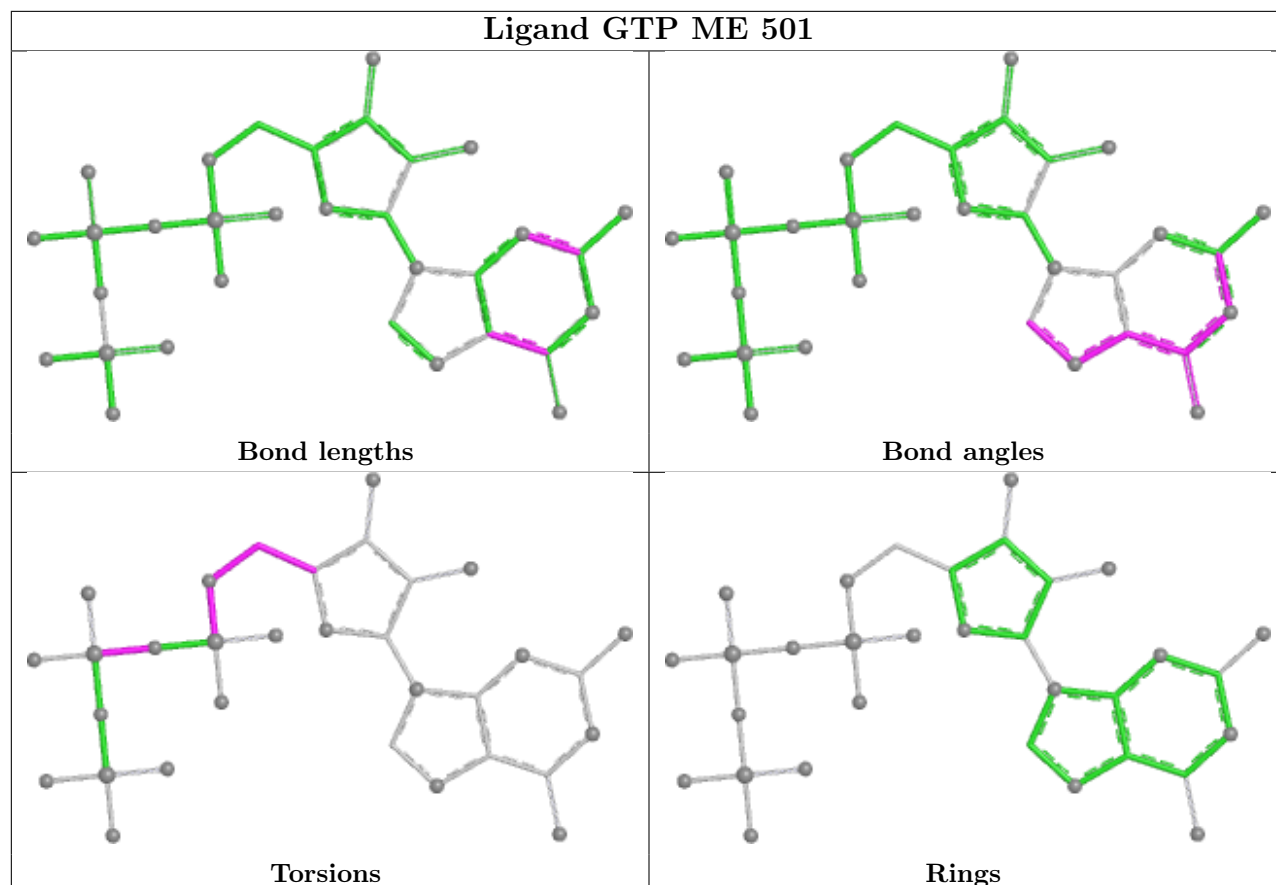
Ligand GTP CC 501



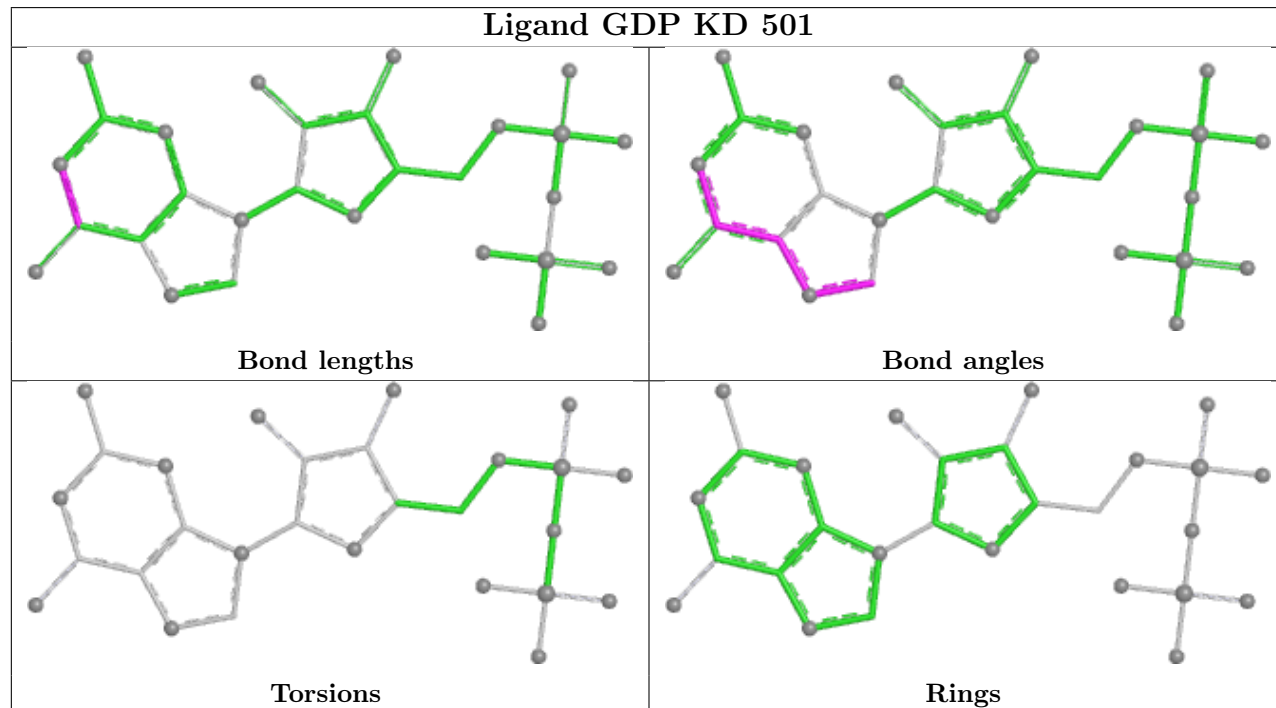
Ligand GTP MA 501

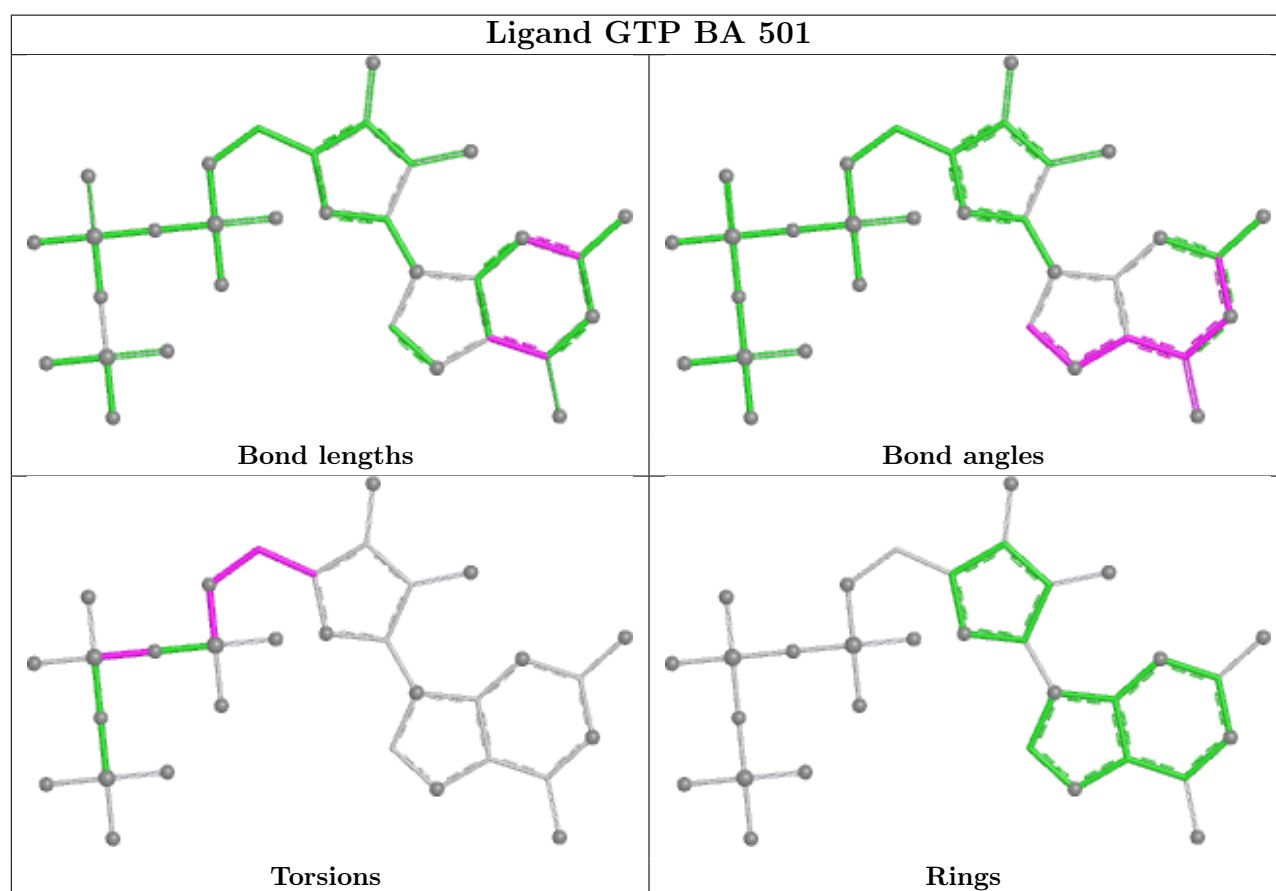
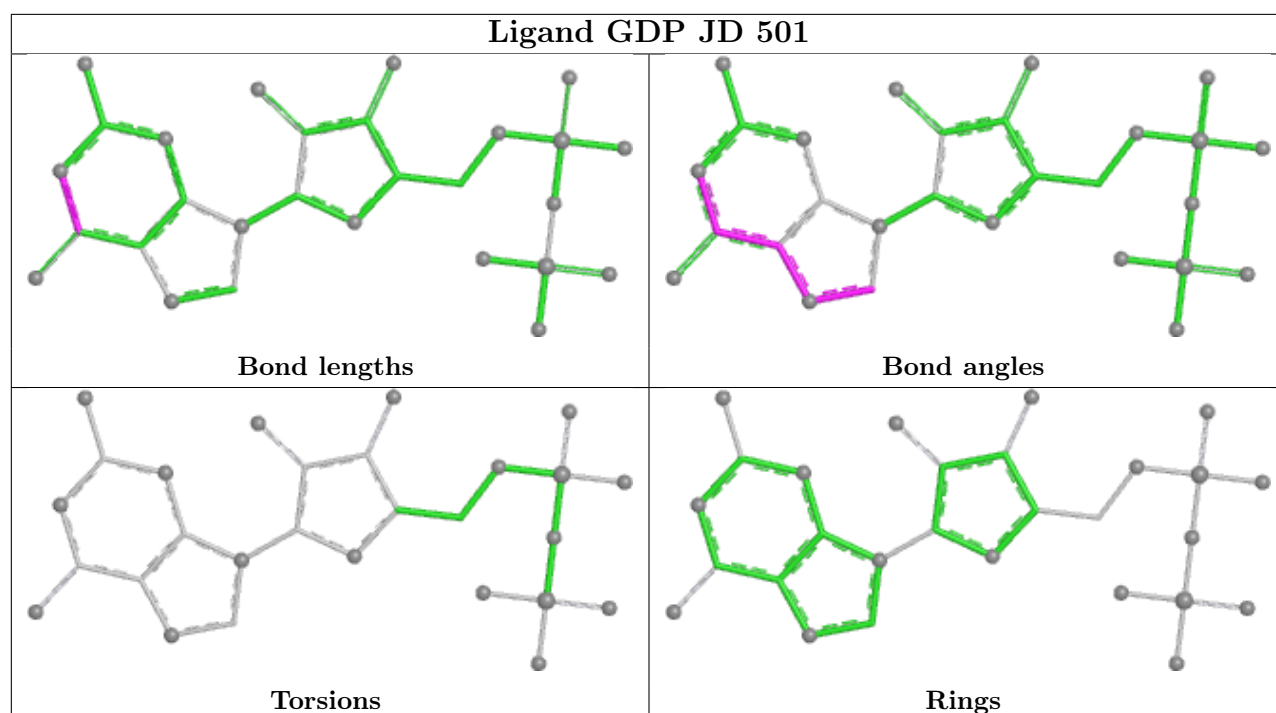


Ligand GTP ME 501

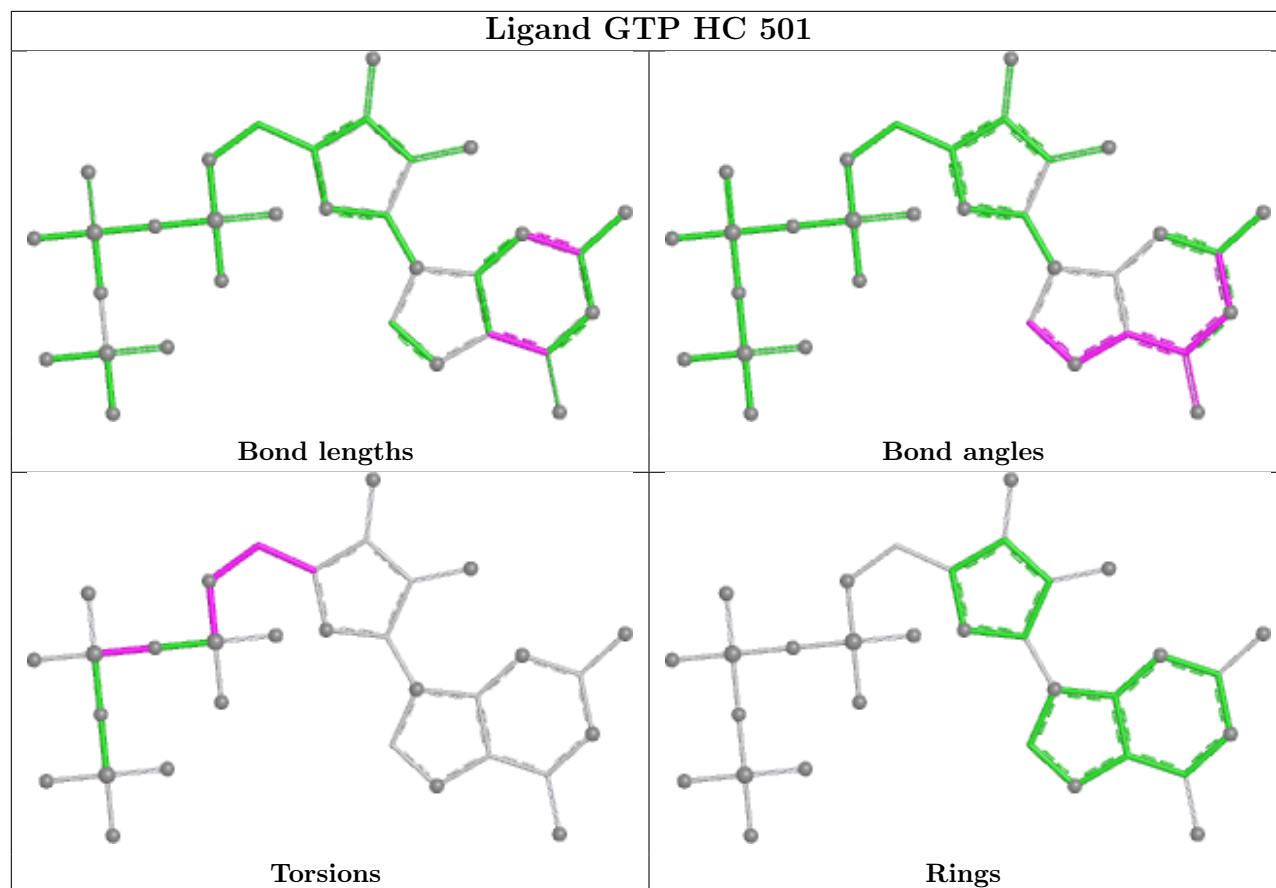


Ligand GDP KD 501

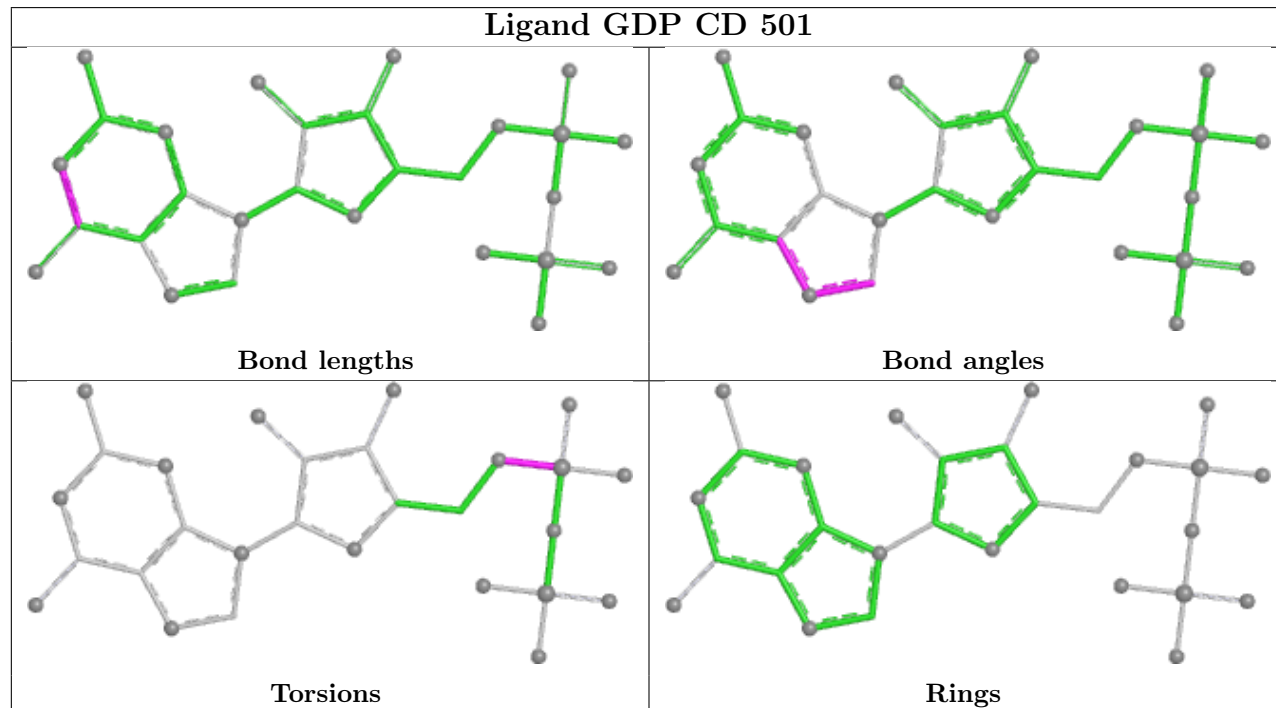




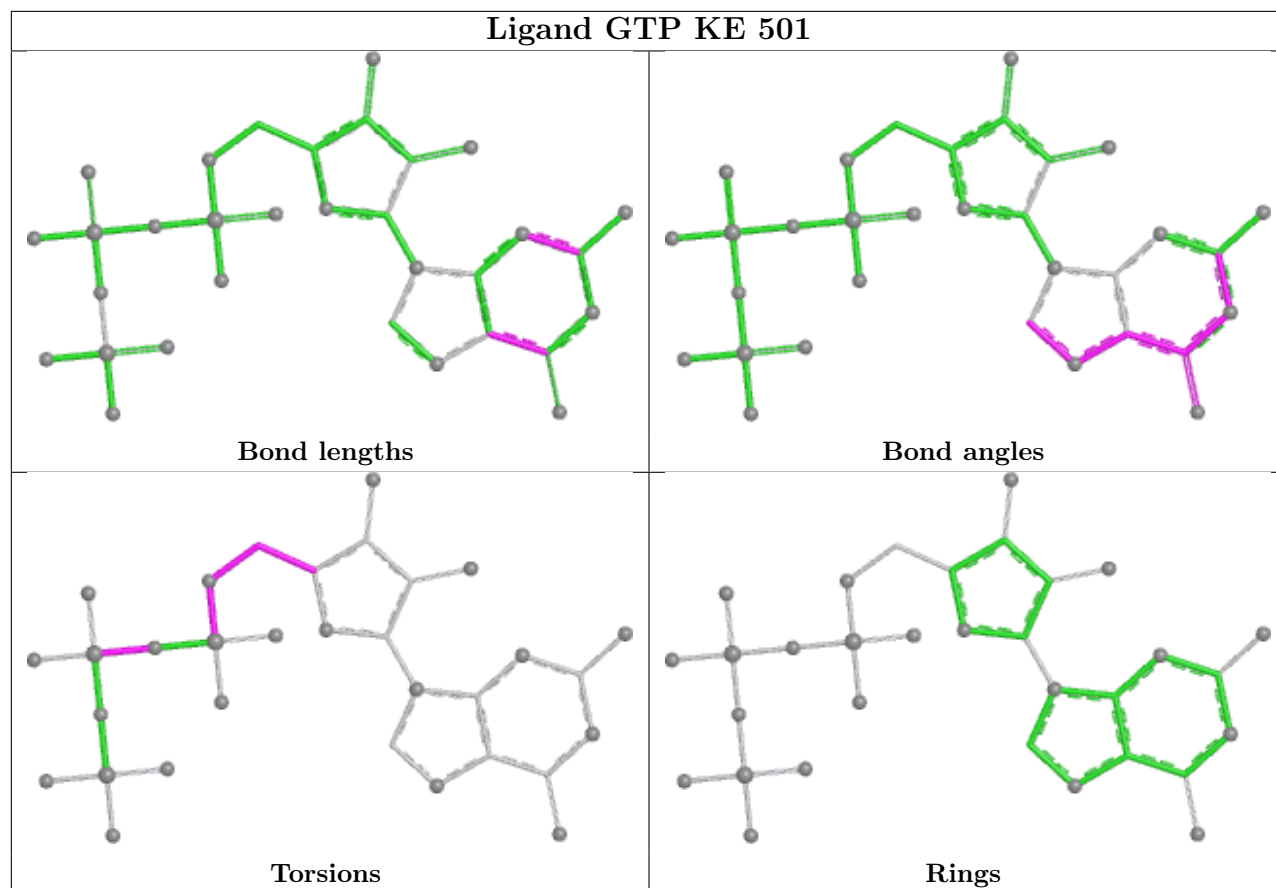
Ligand GTP HC 501



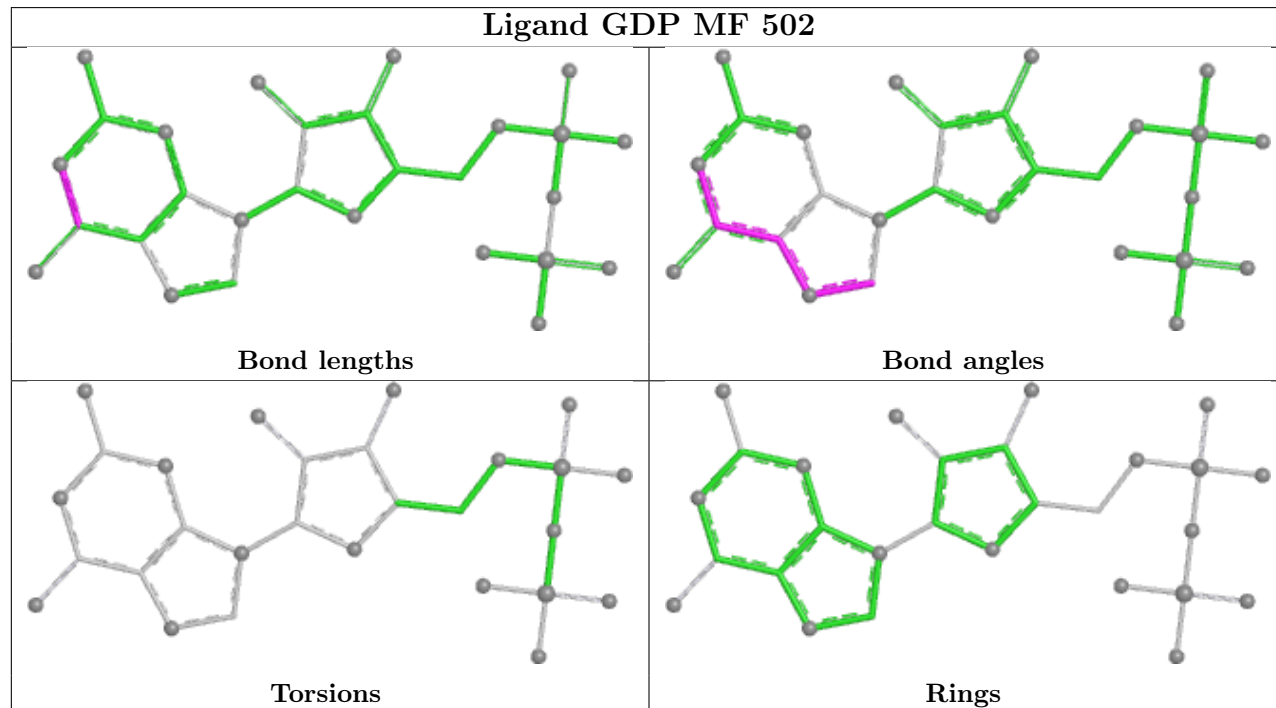
Ligand GDP CD 501

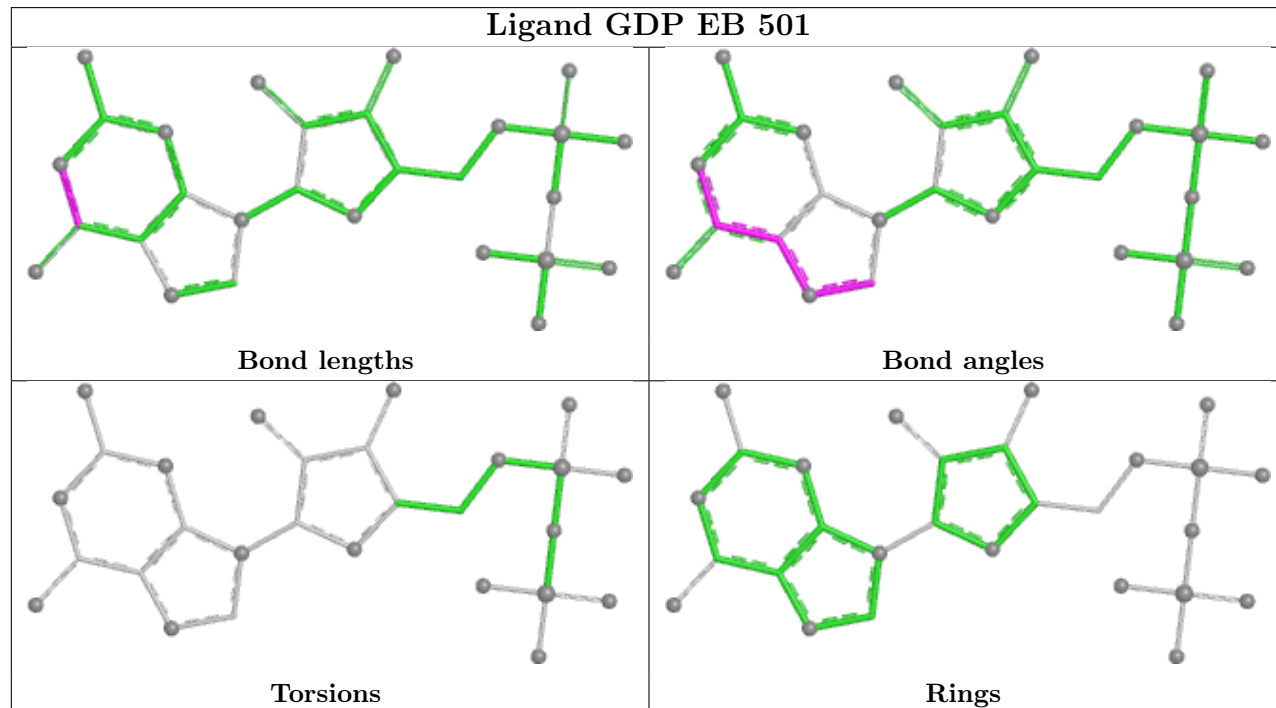
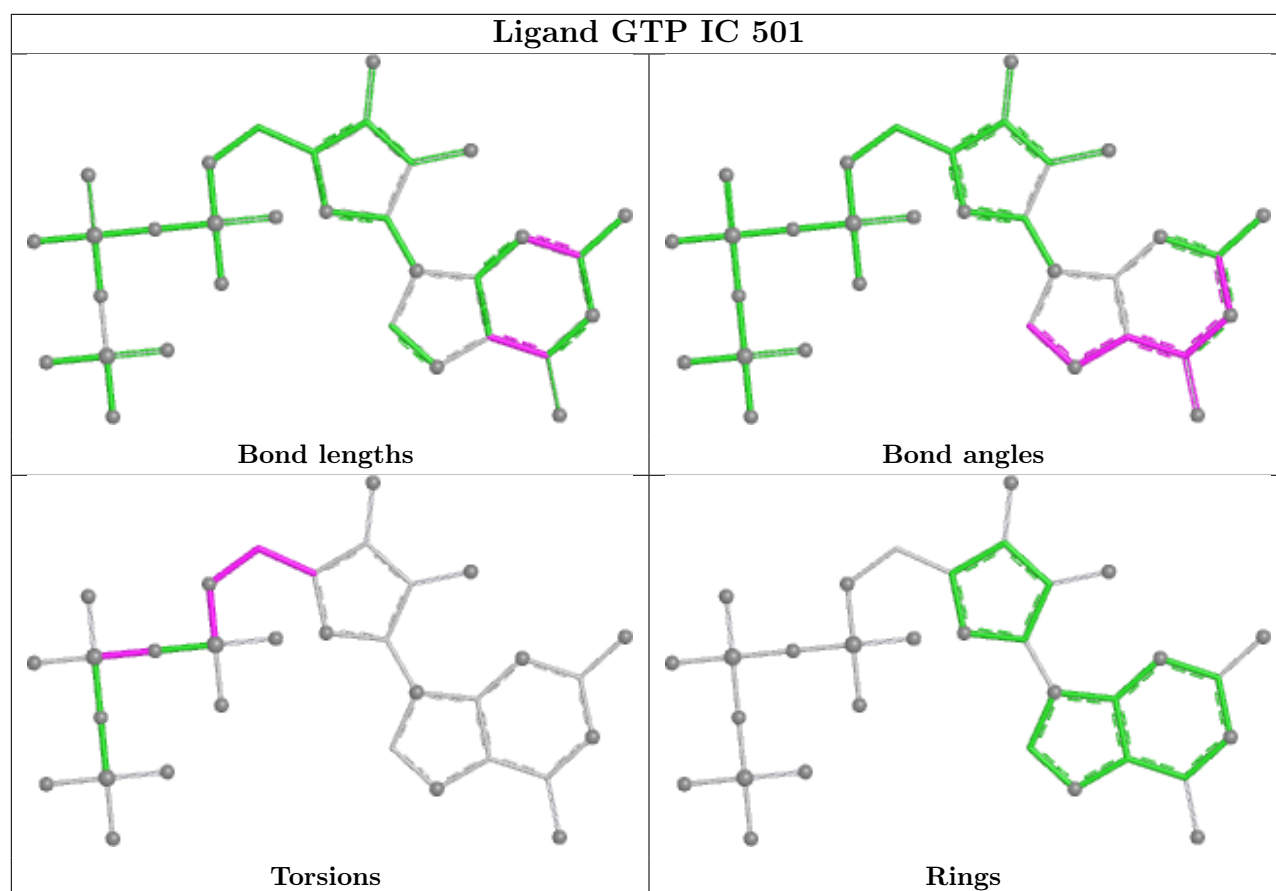


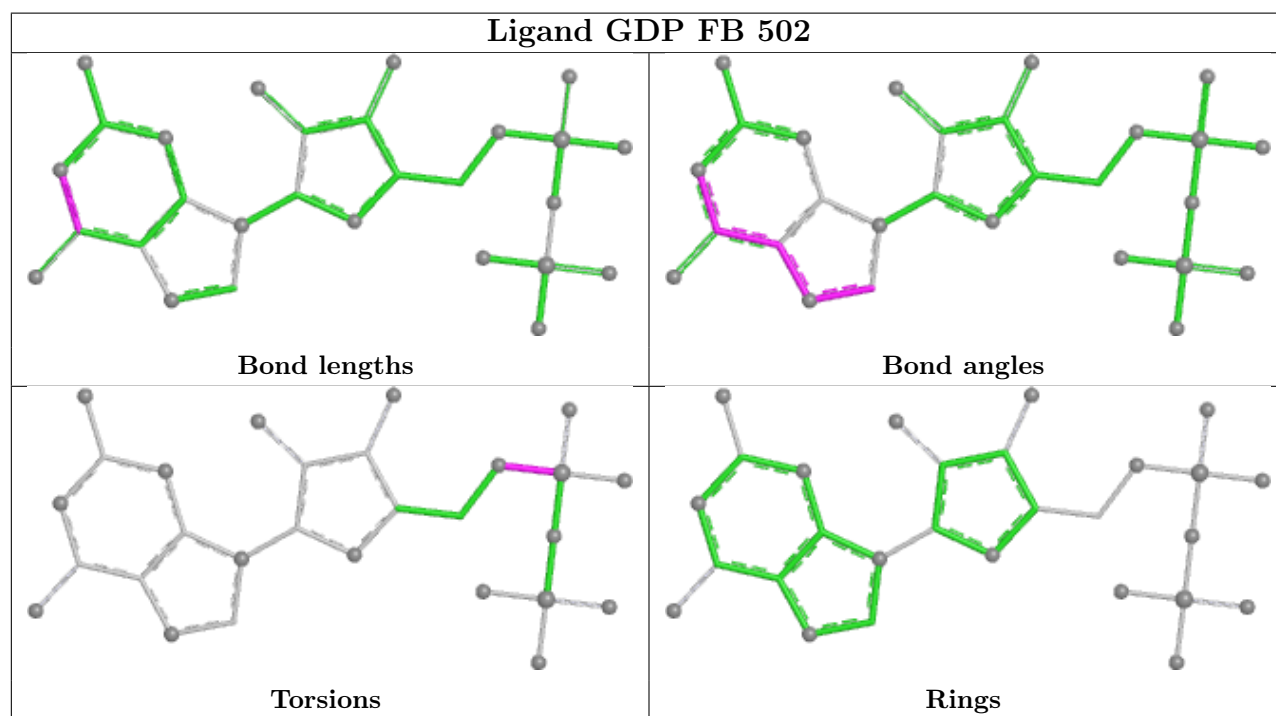
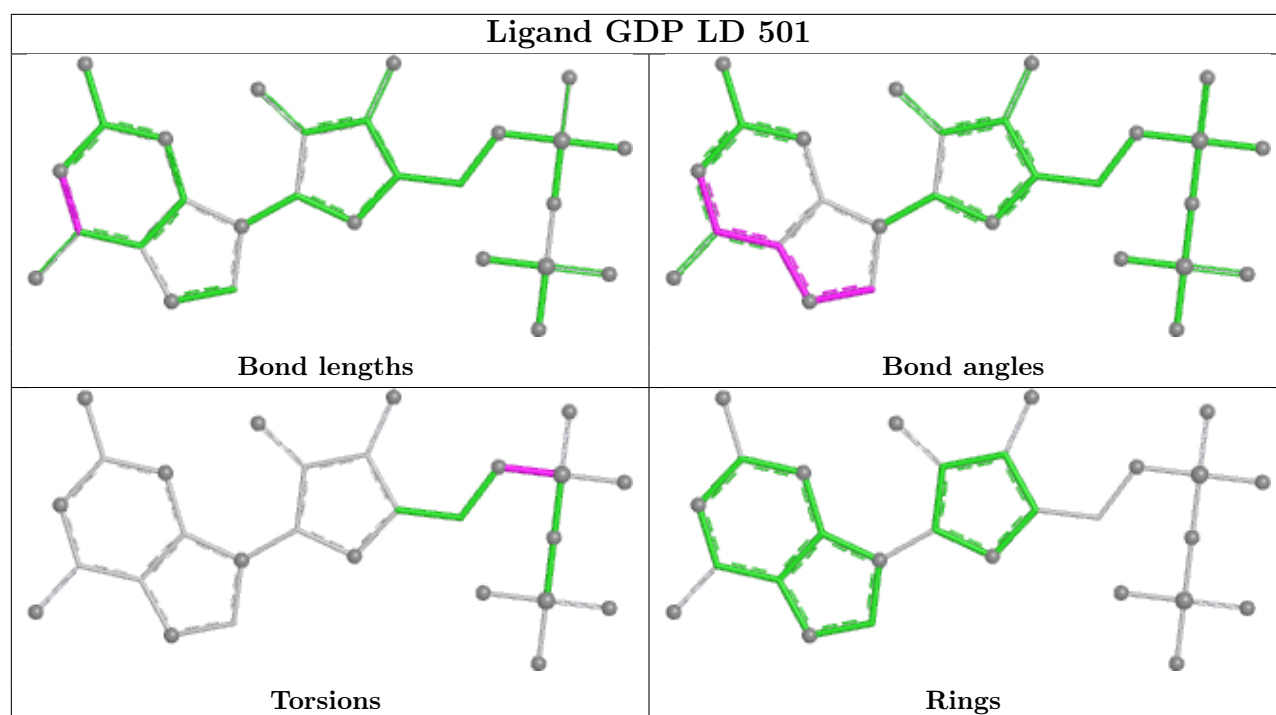
Ligand GTP KE 501

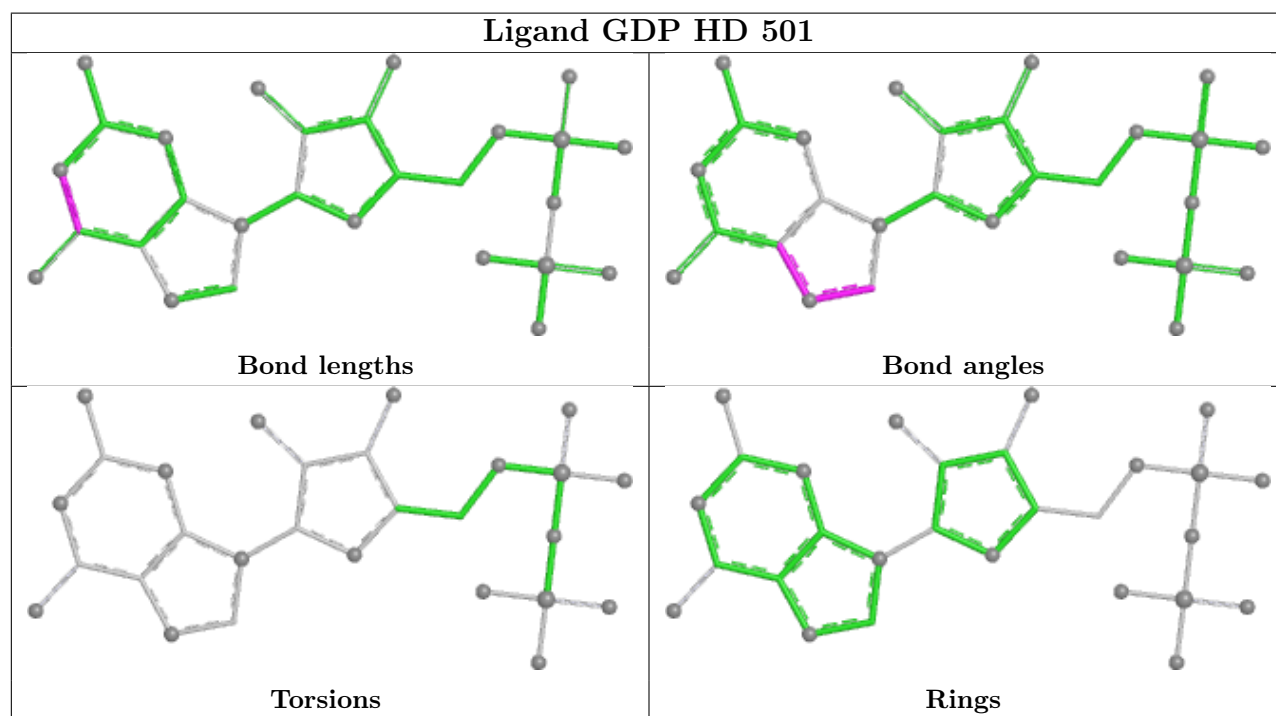
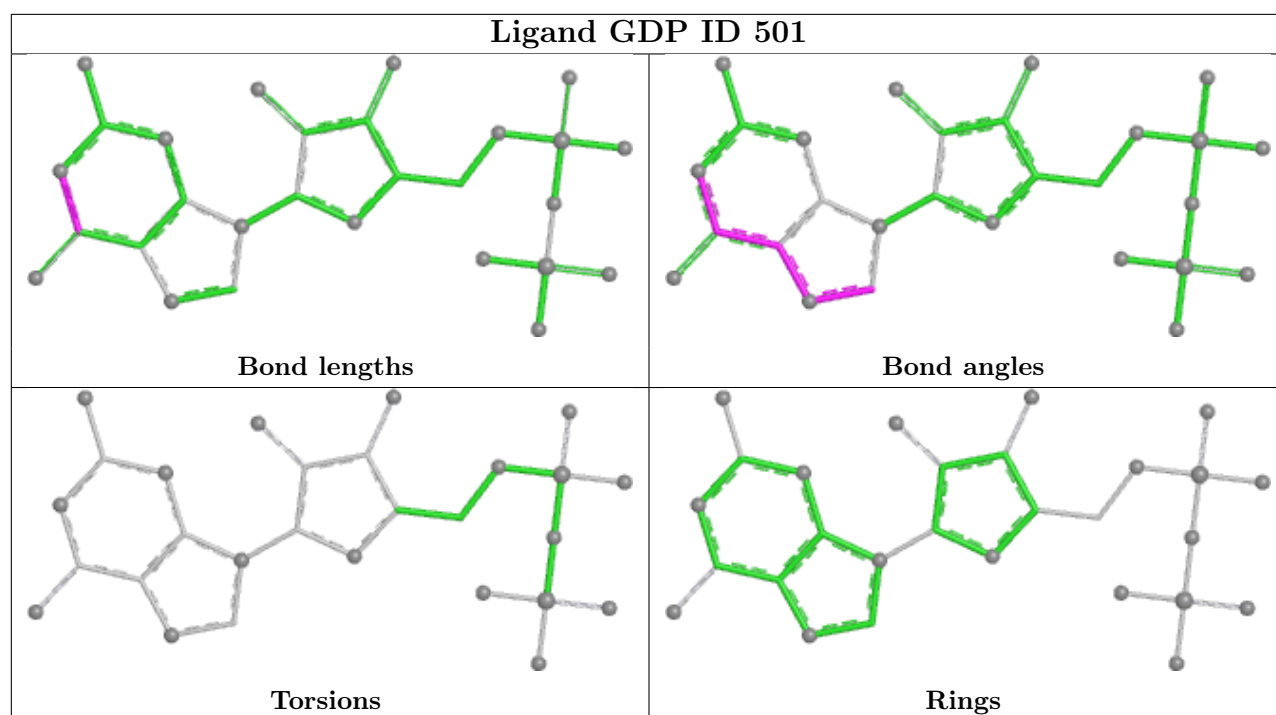


Ligand GDP MF 502

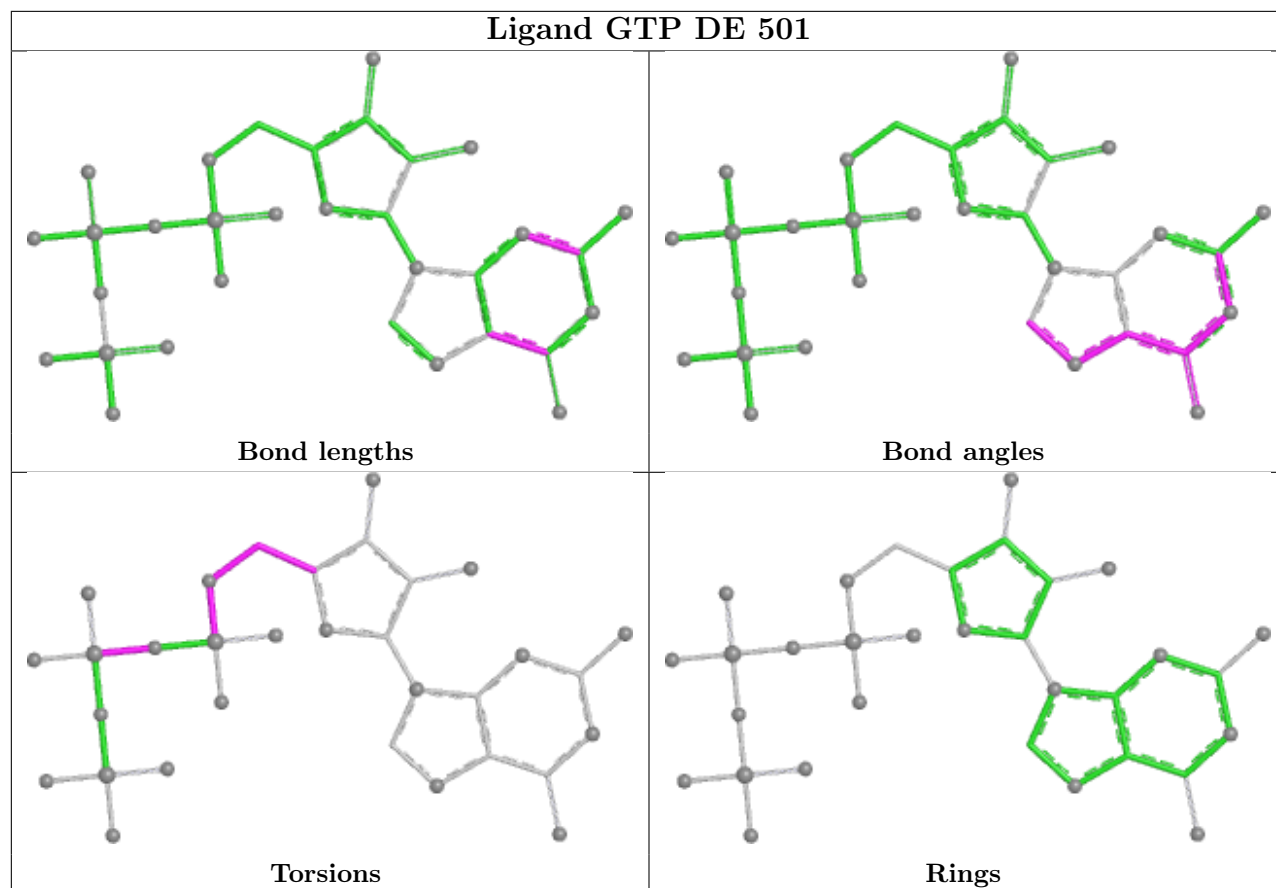




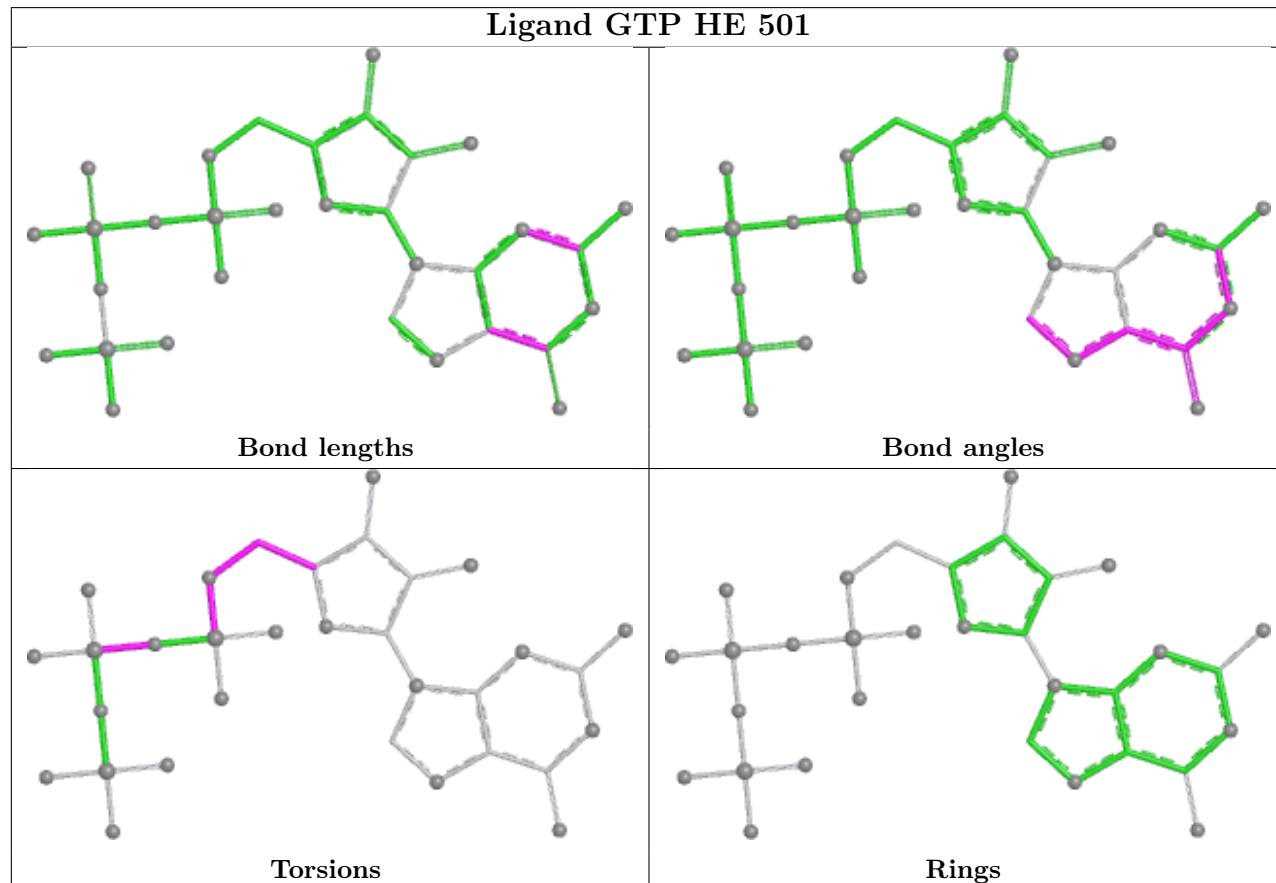


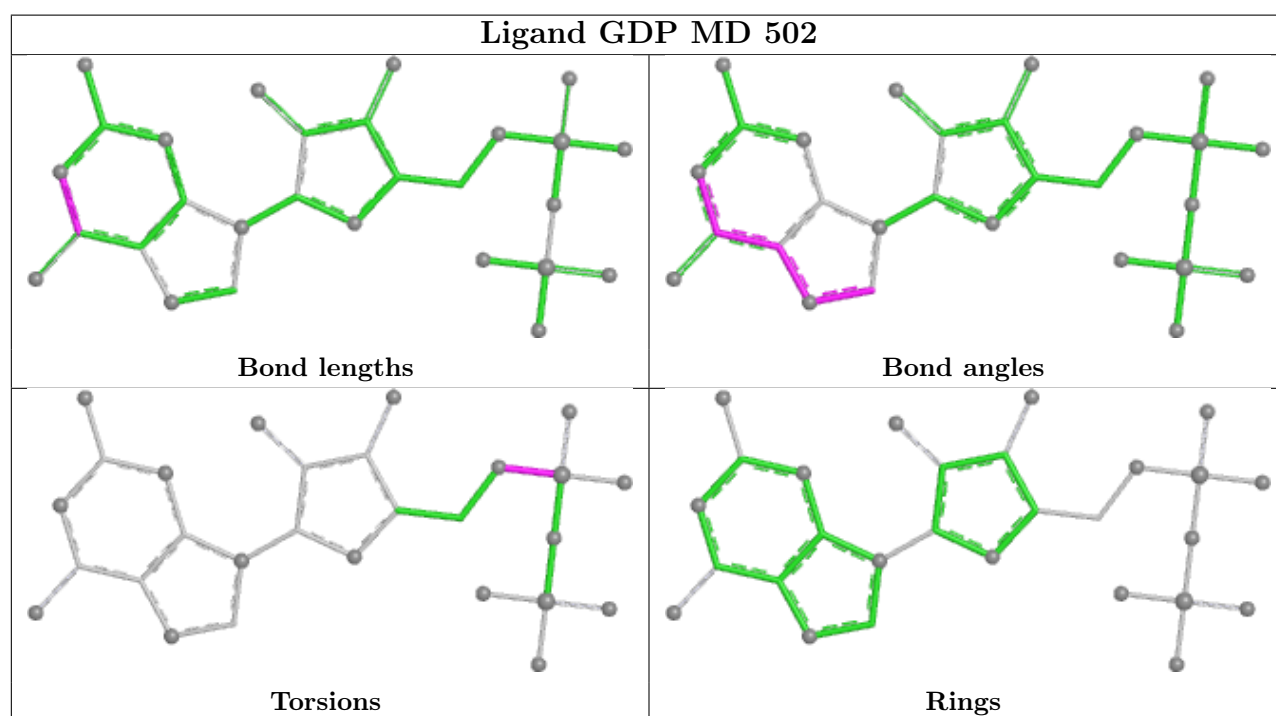
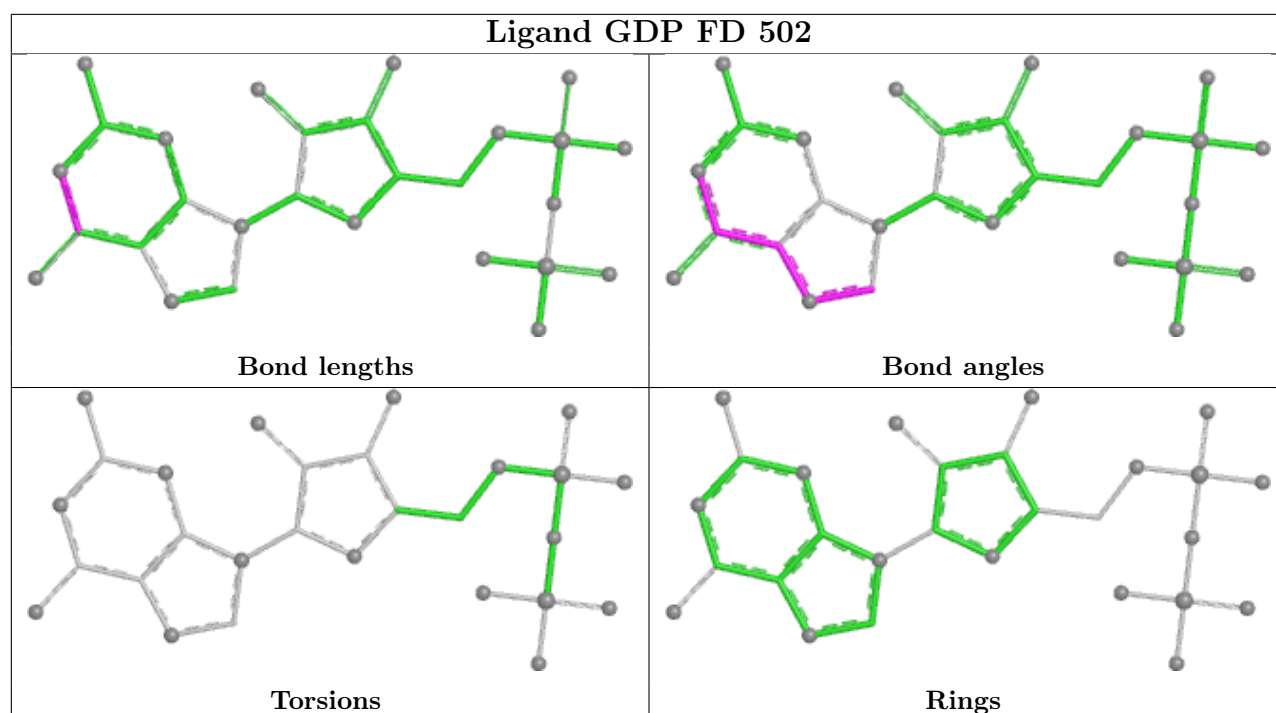


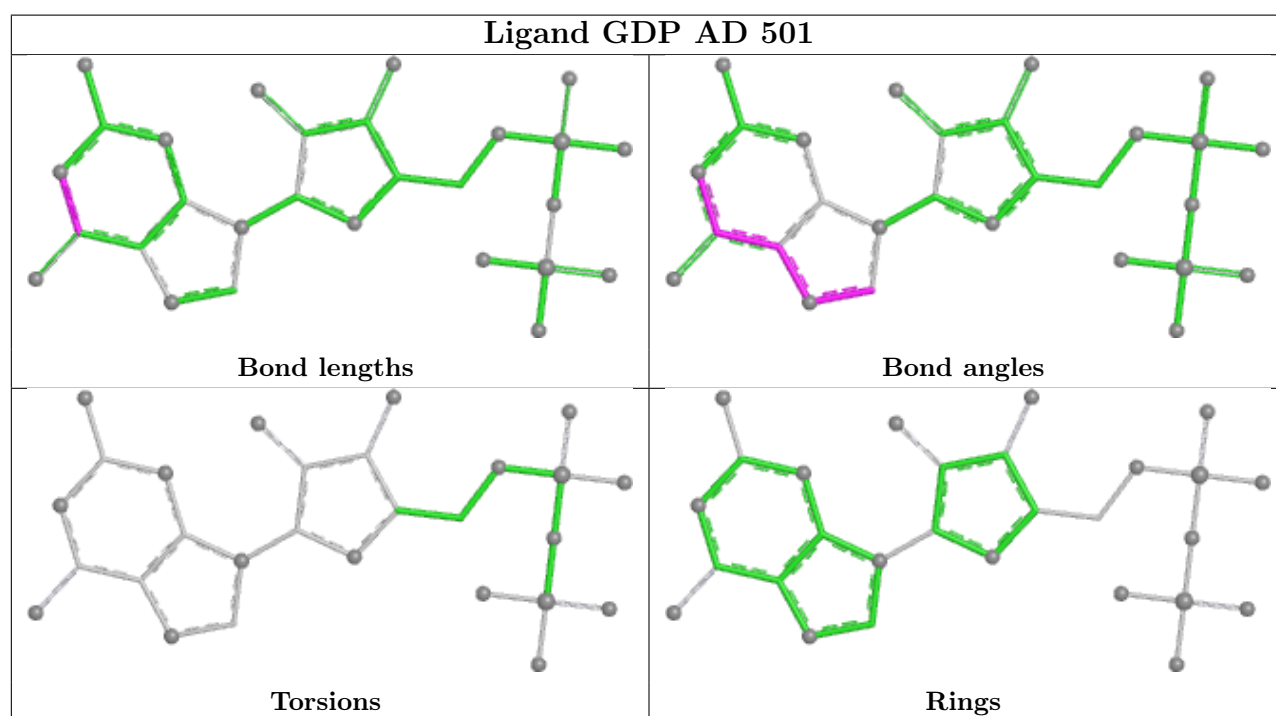
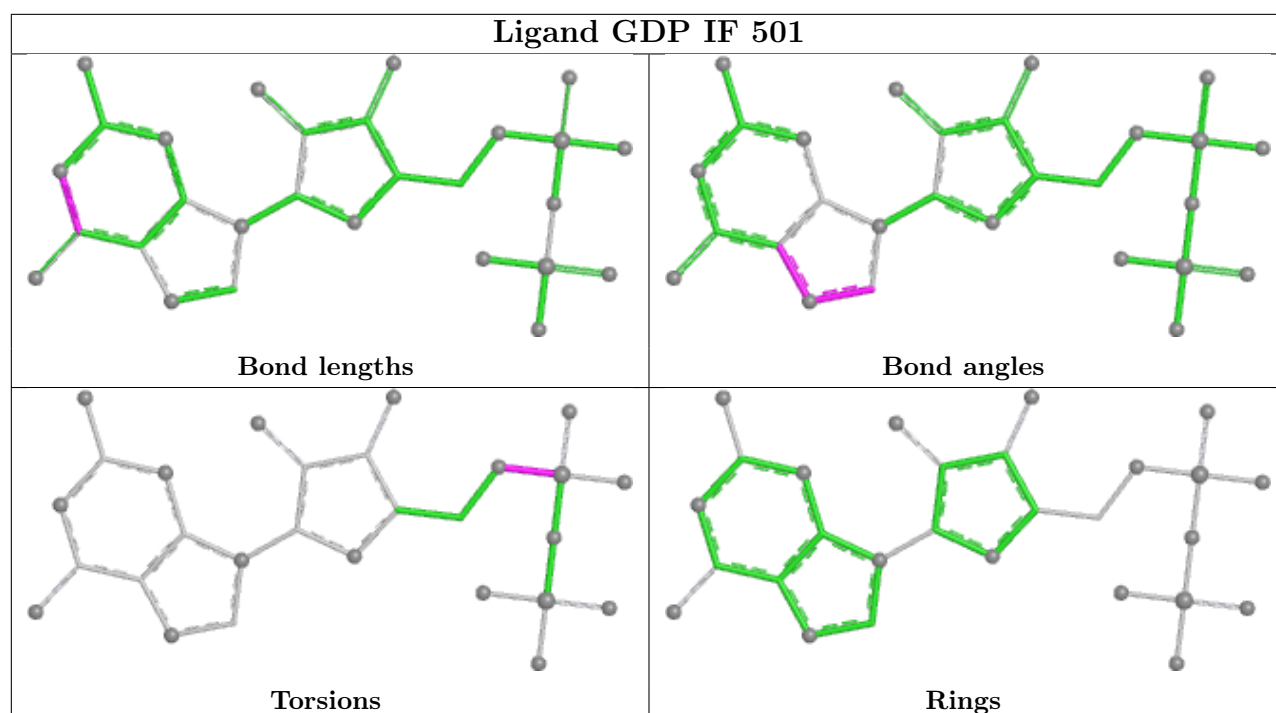
Ligand GTP DE 501

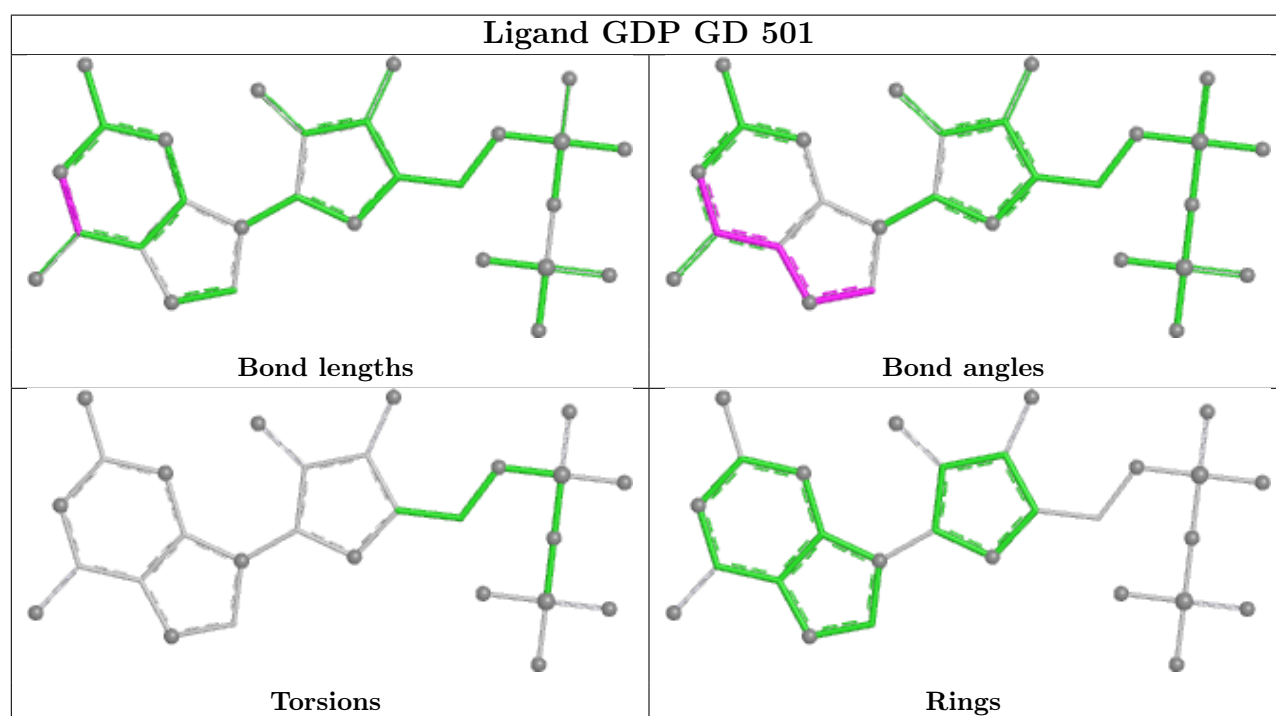
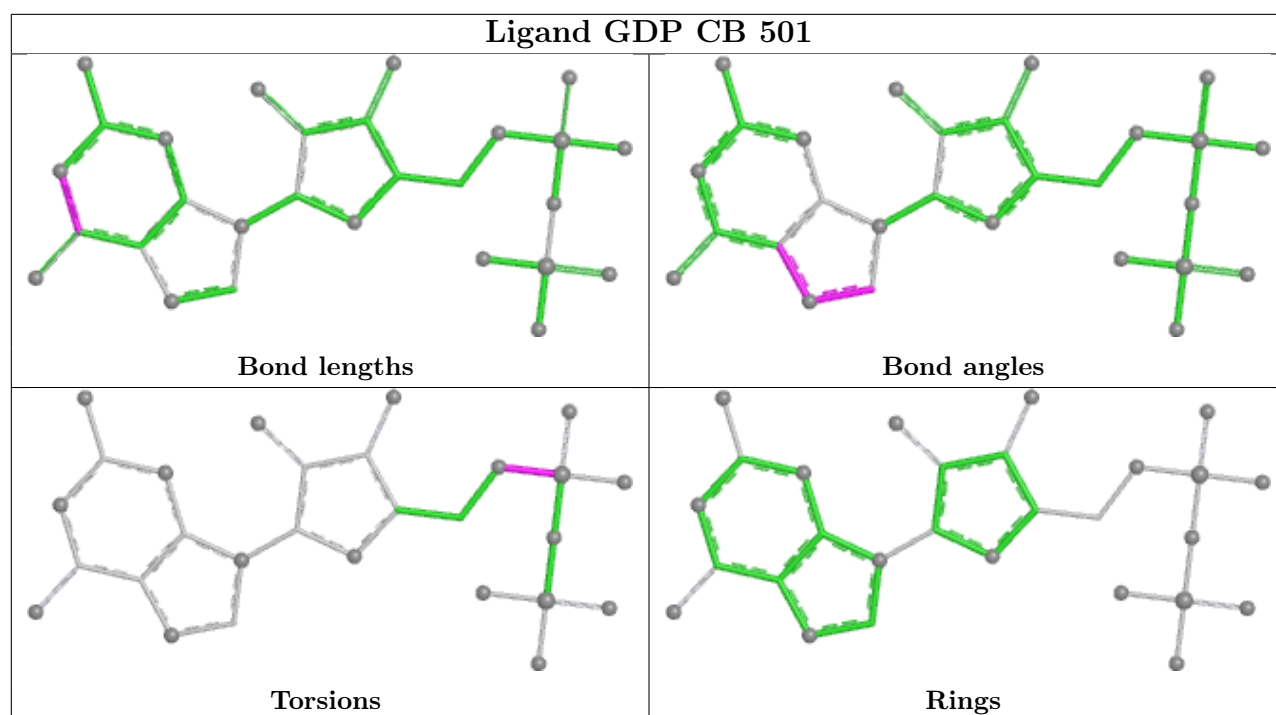


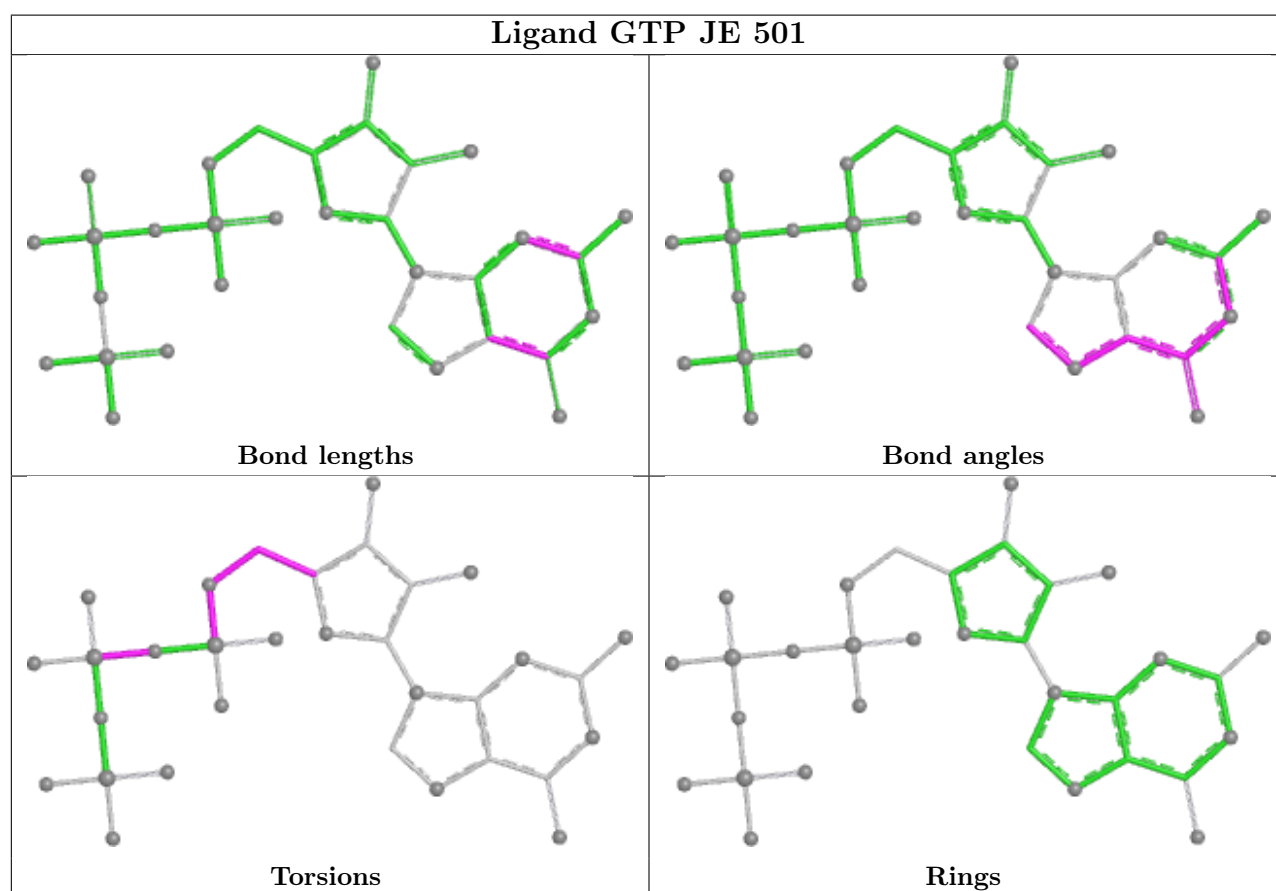
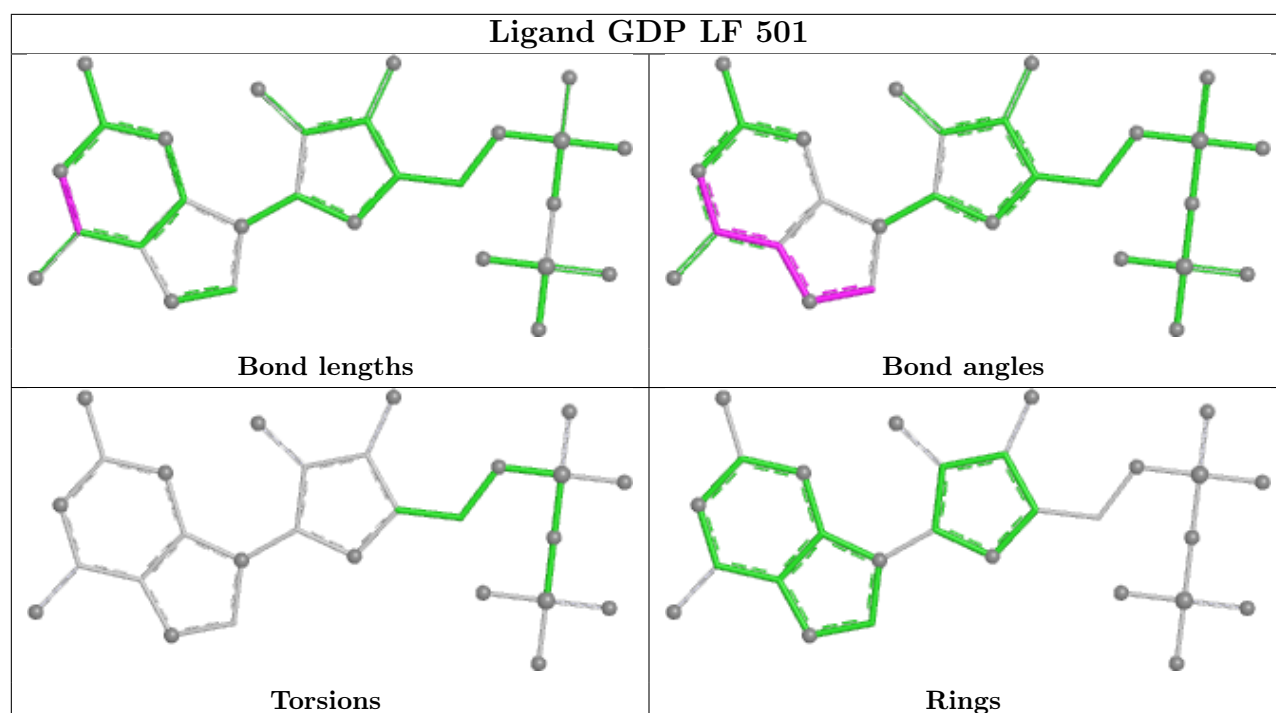
Ligand GTP HE 501



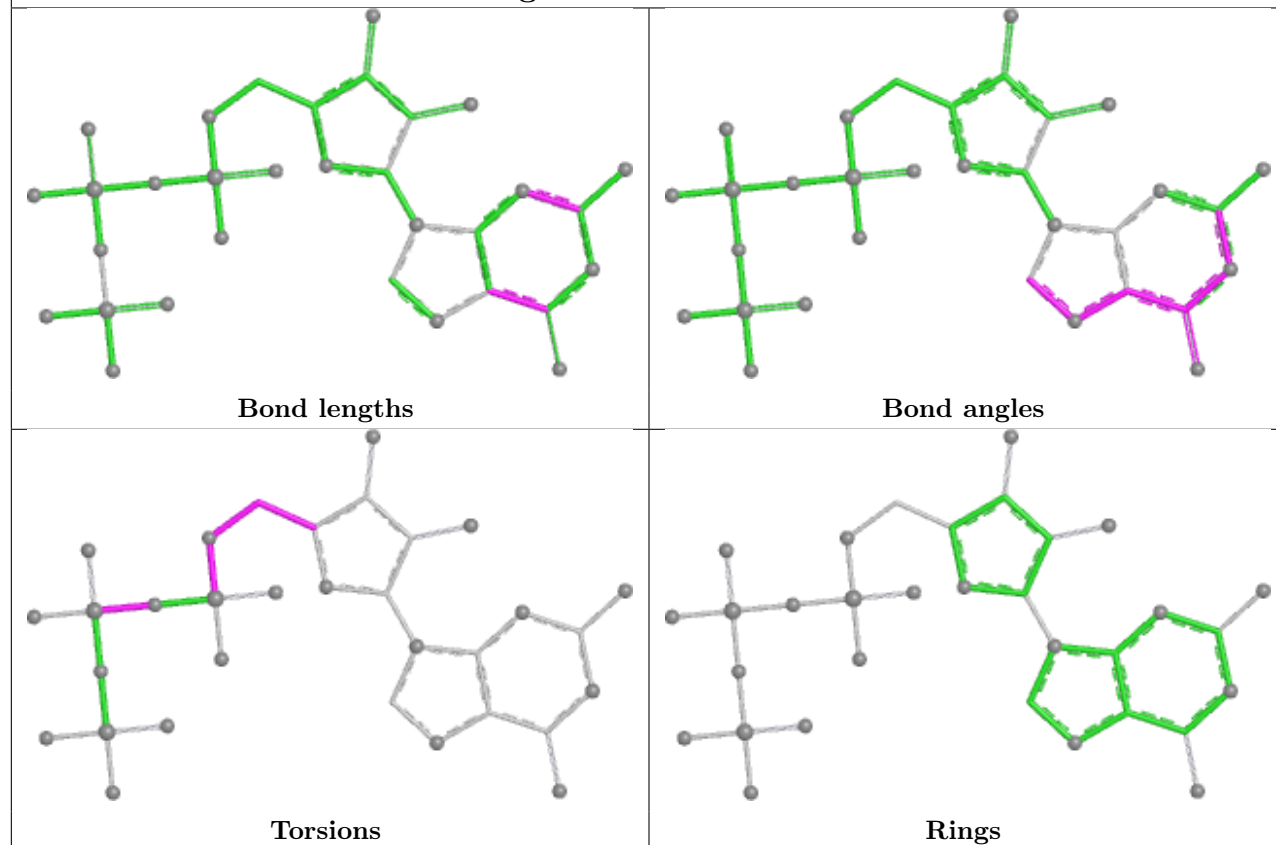




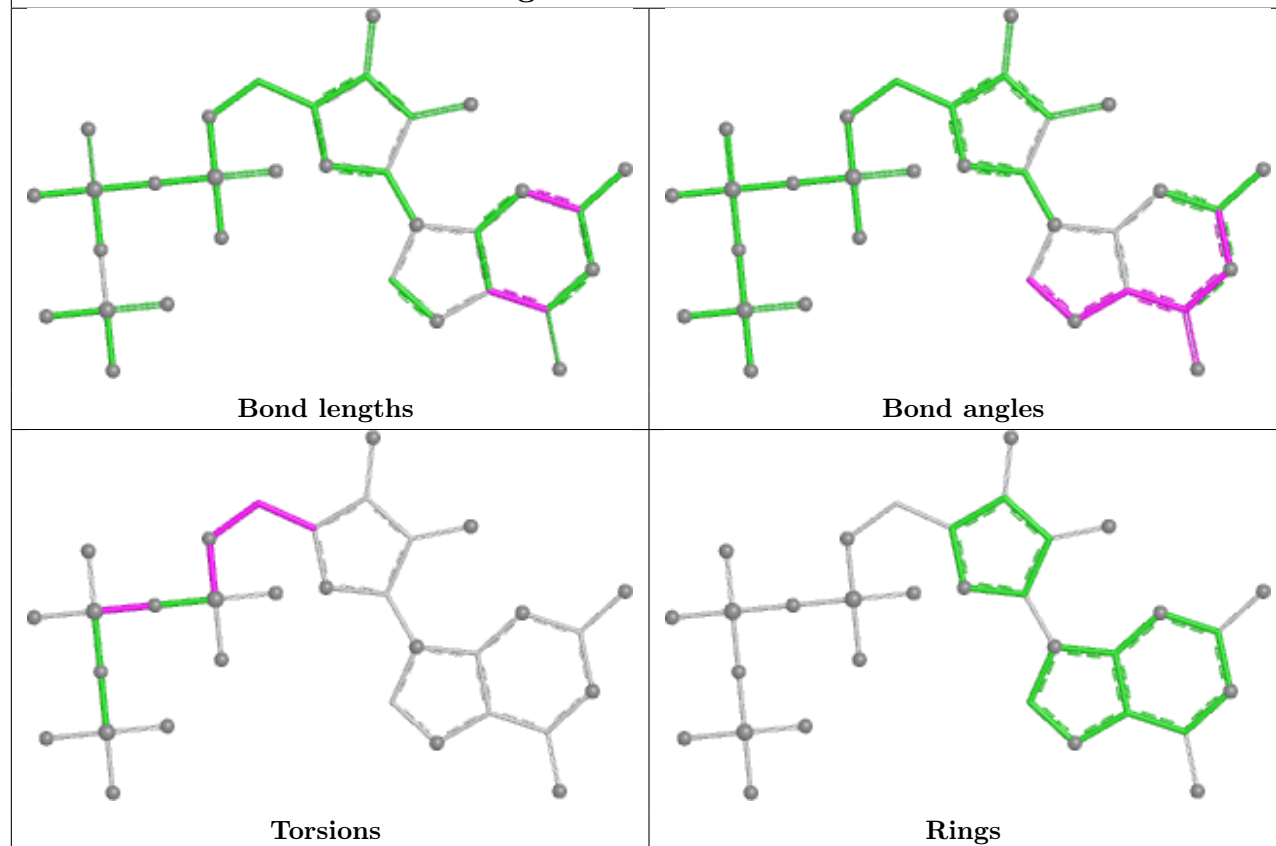


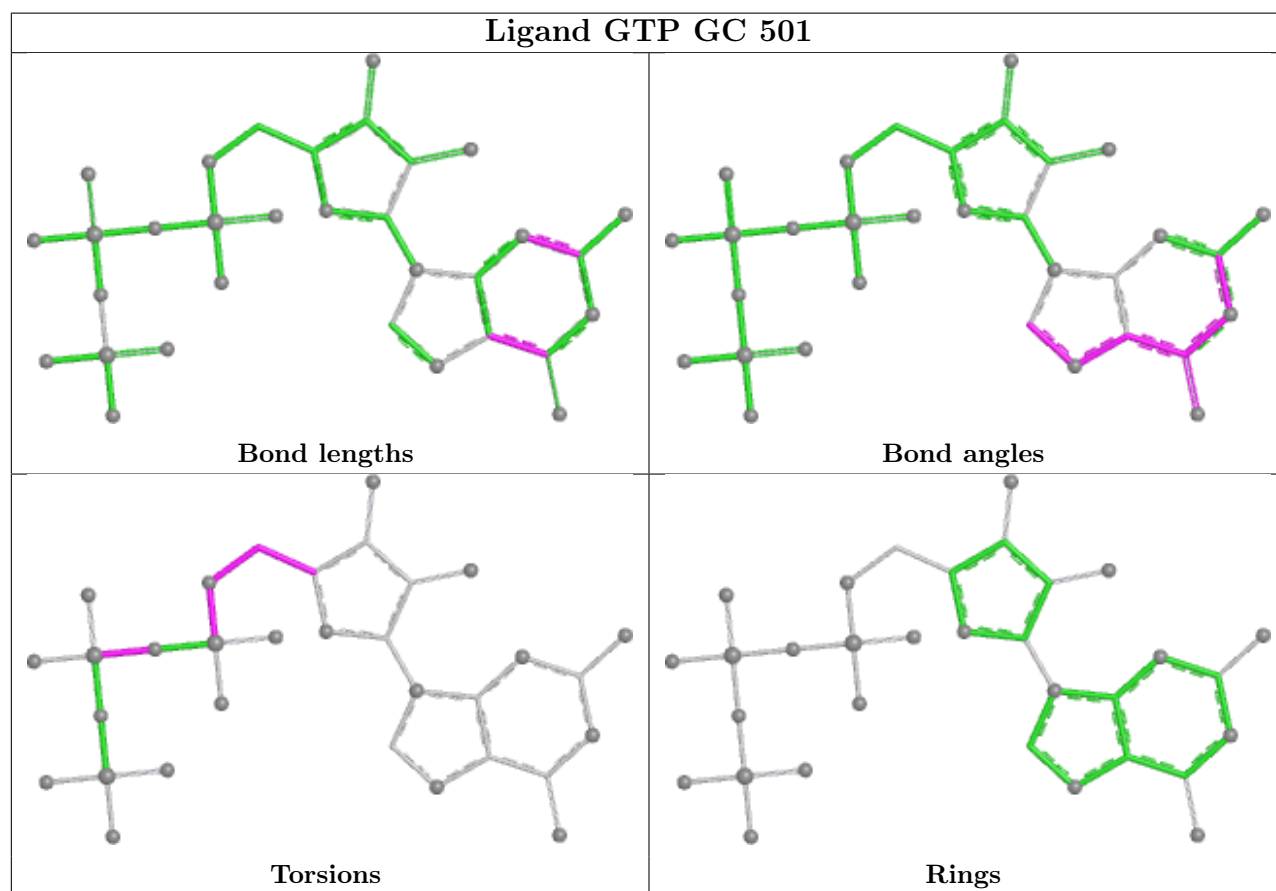
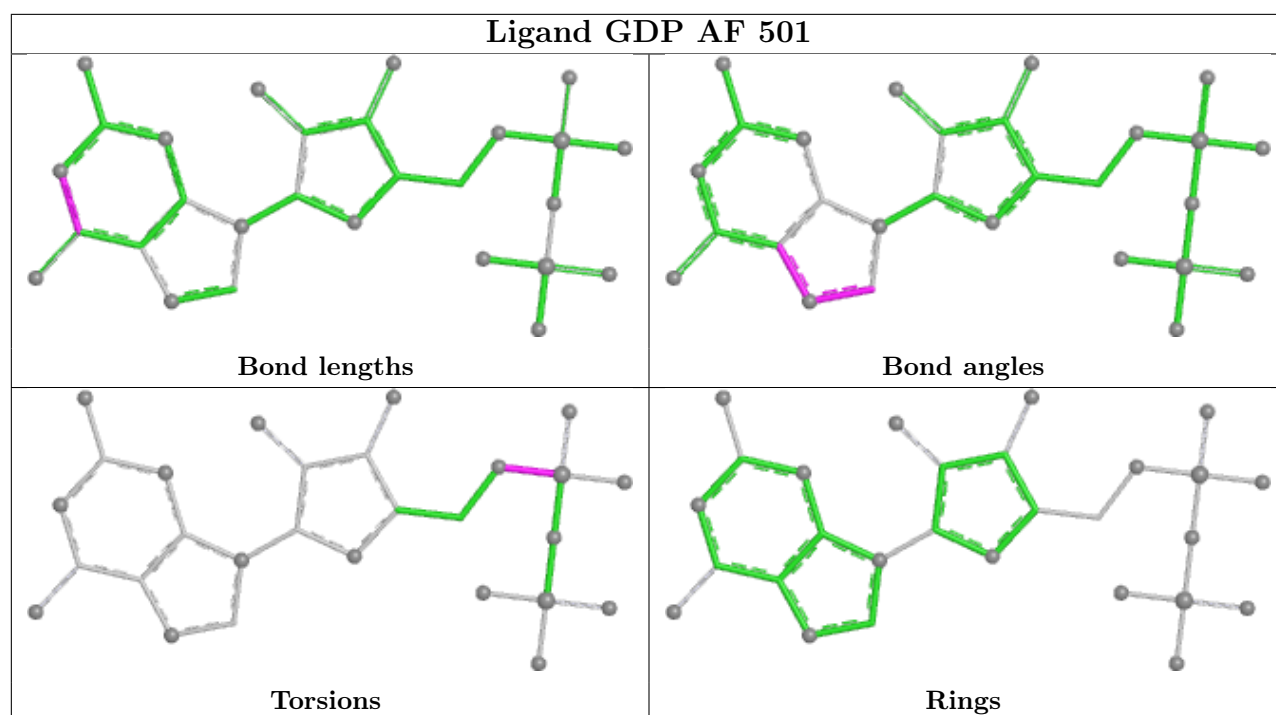


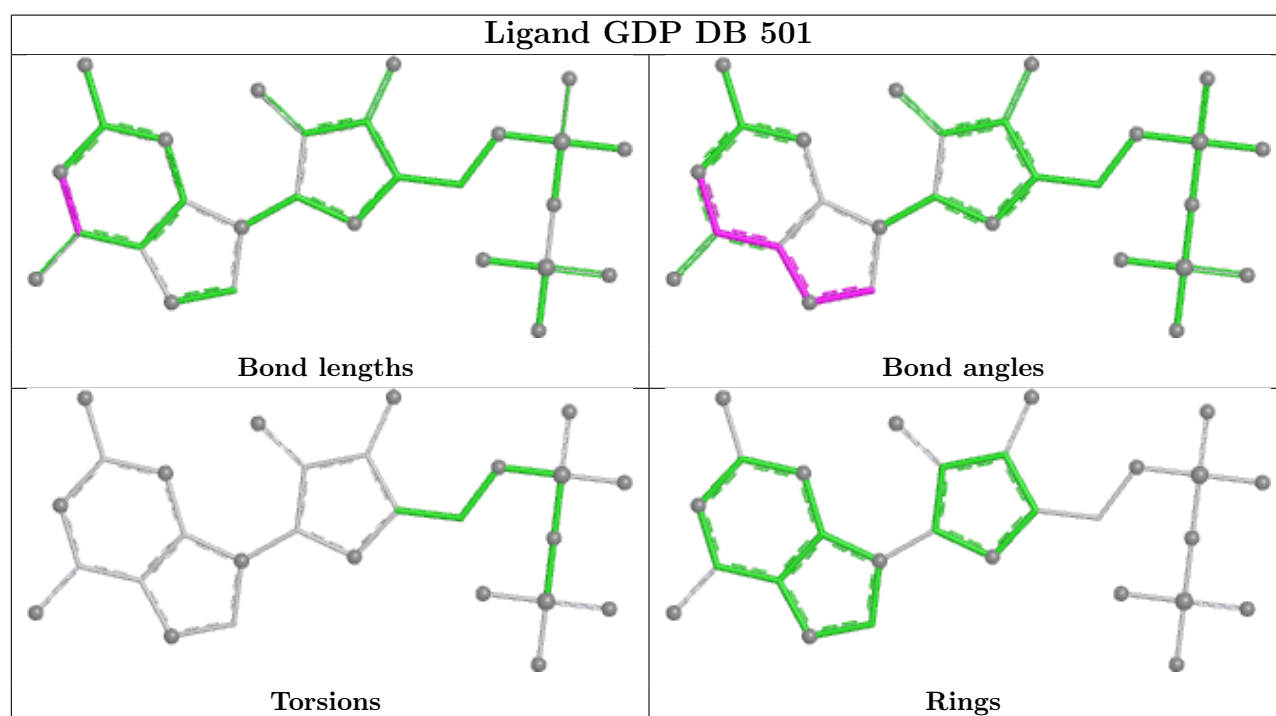
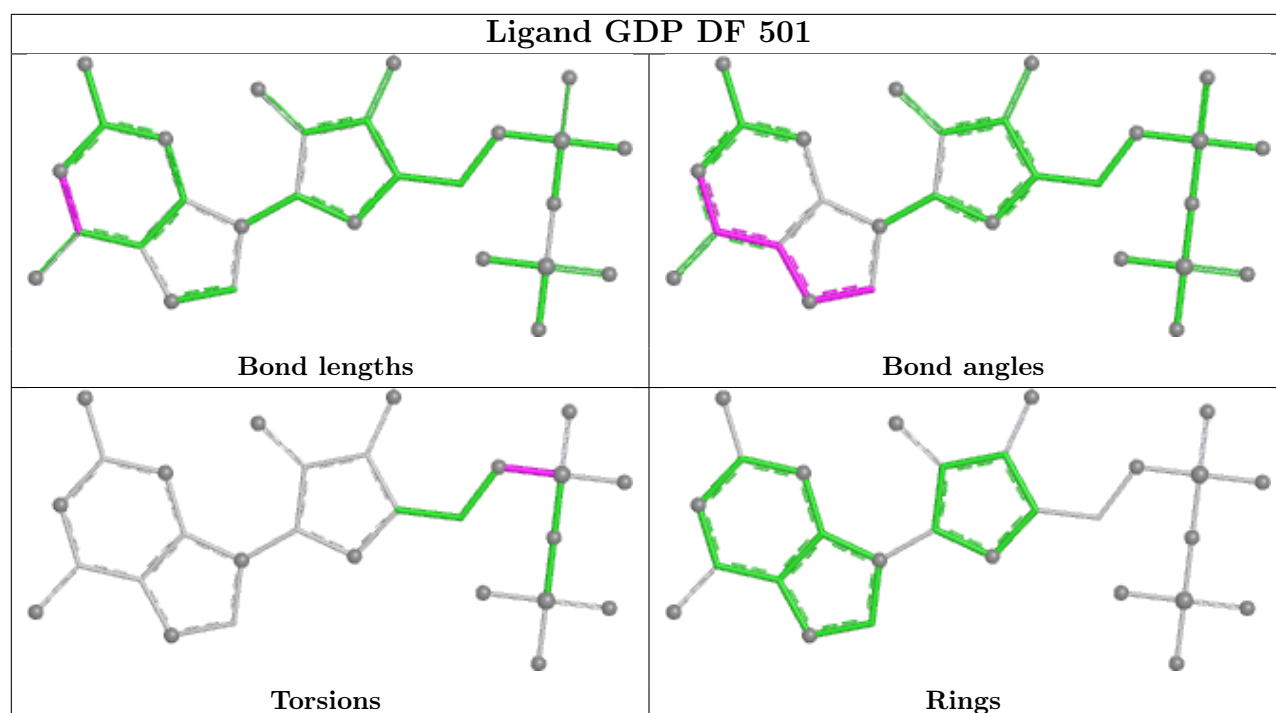
Ligand GTP BE 501

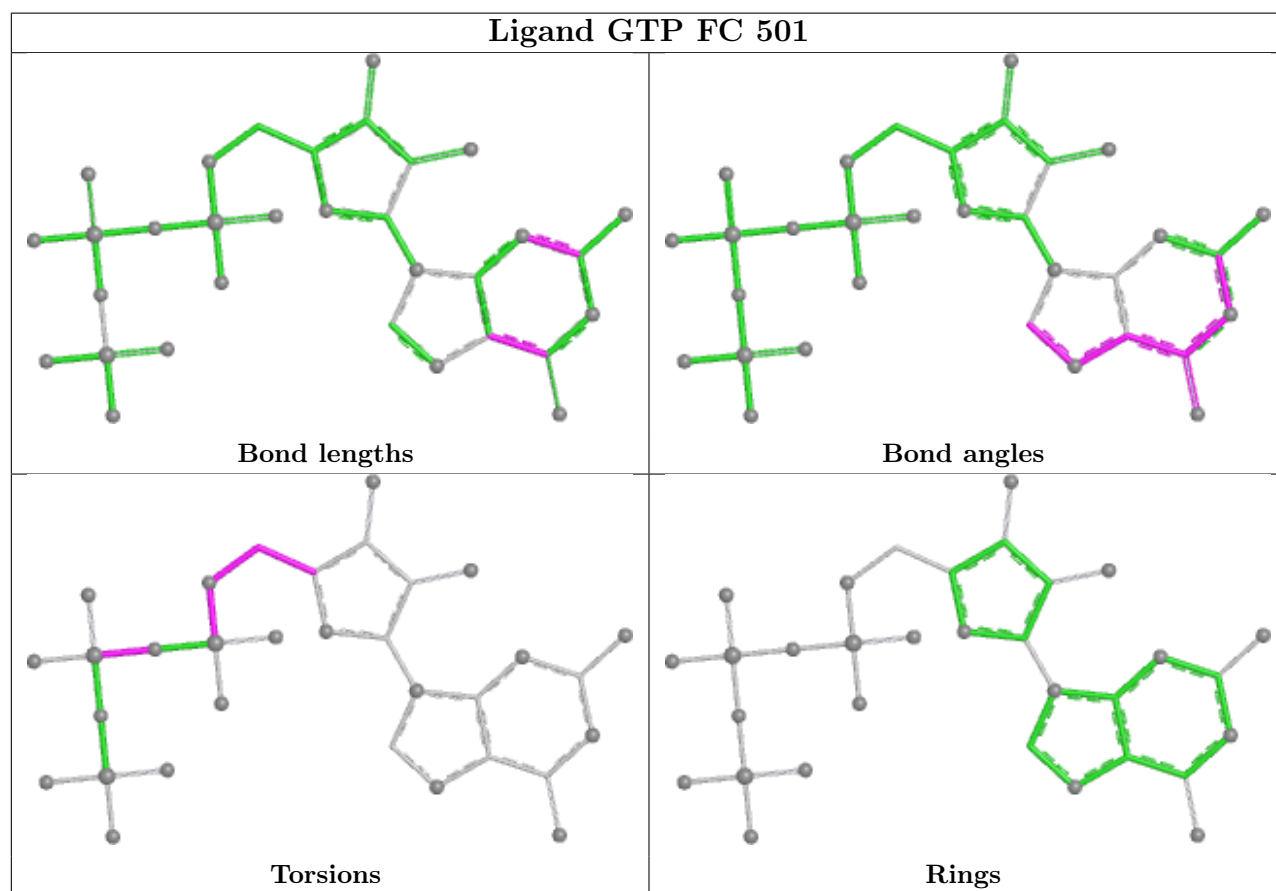
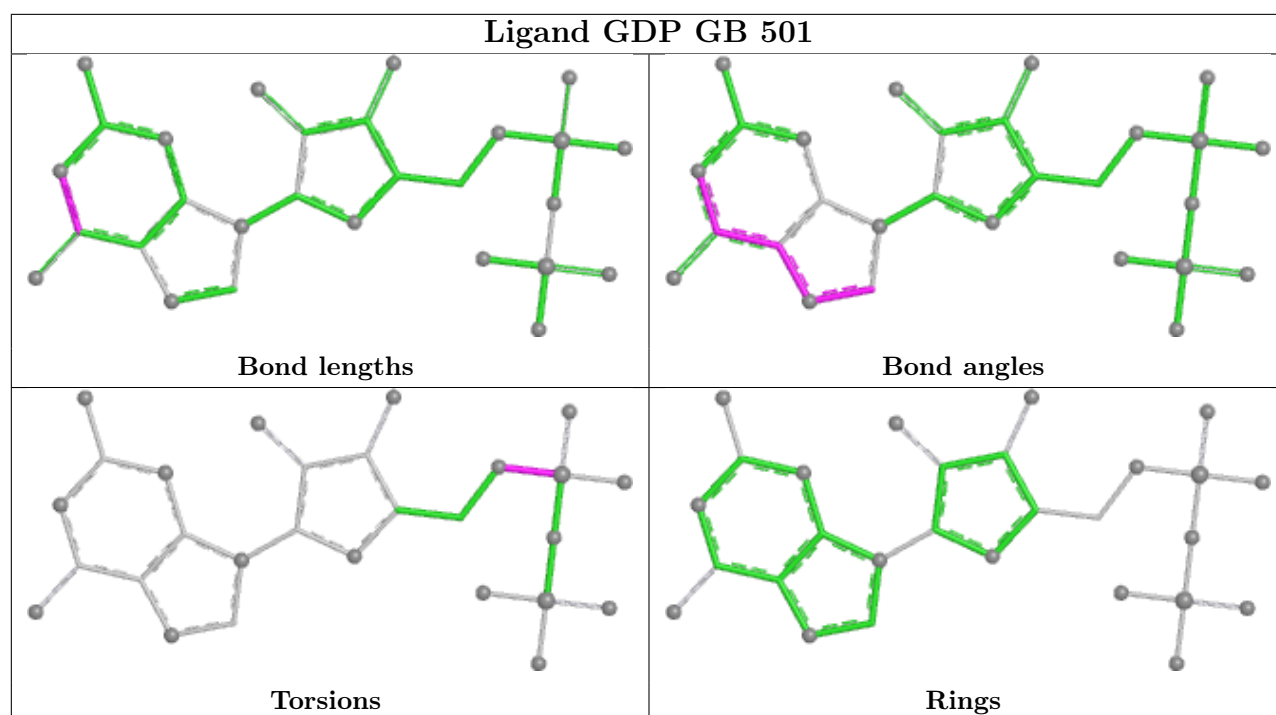


Ligand GTP GE 501

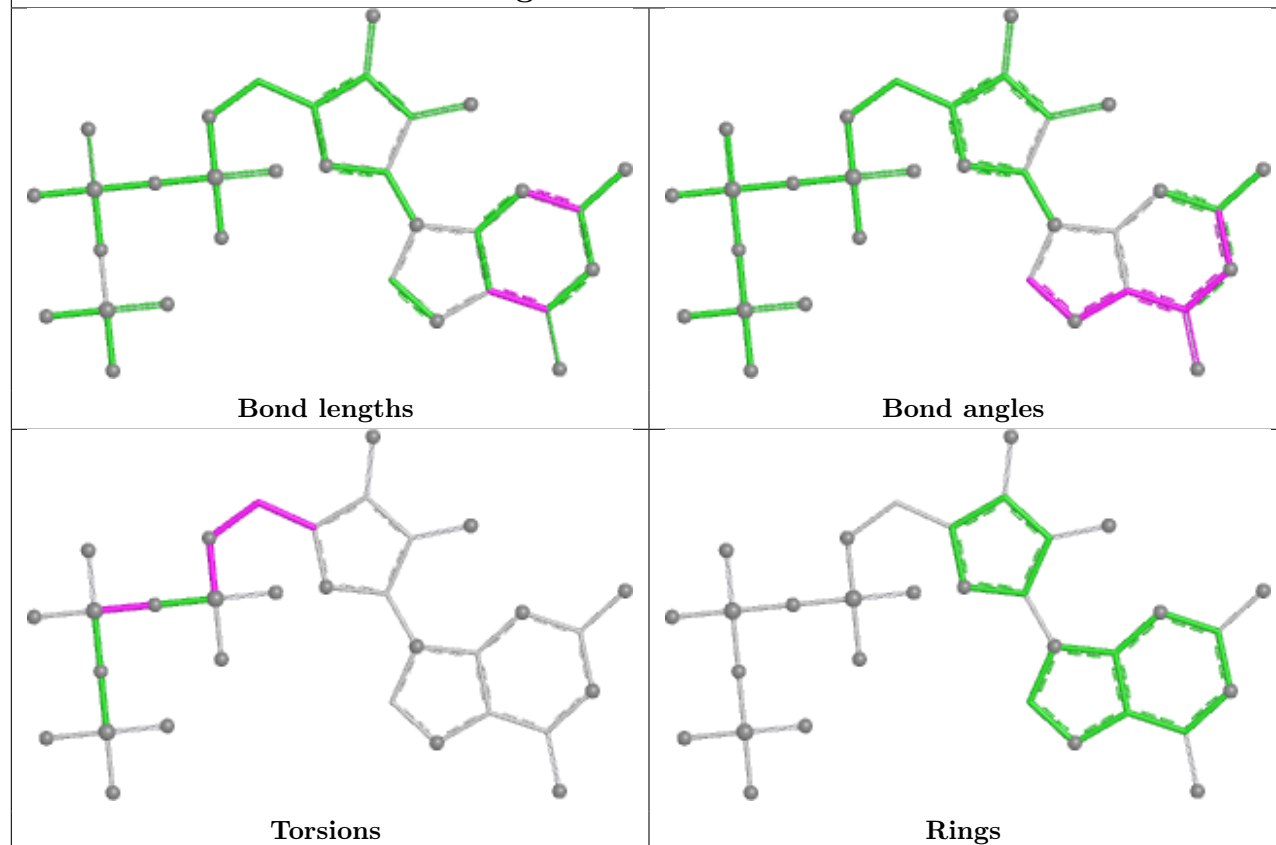




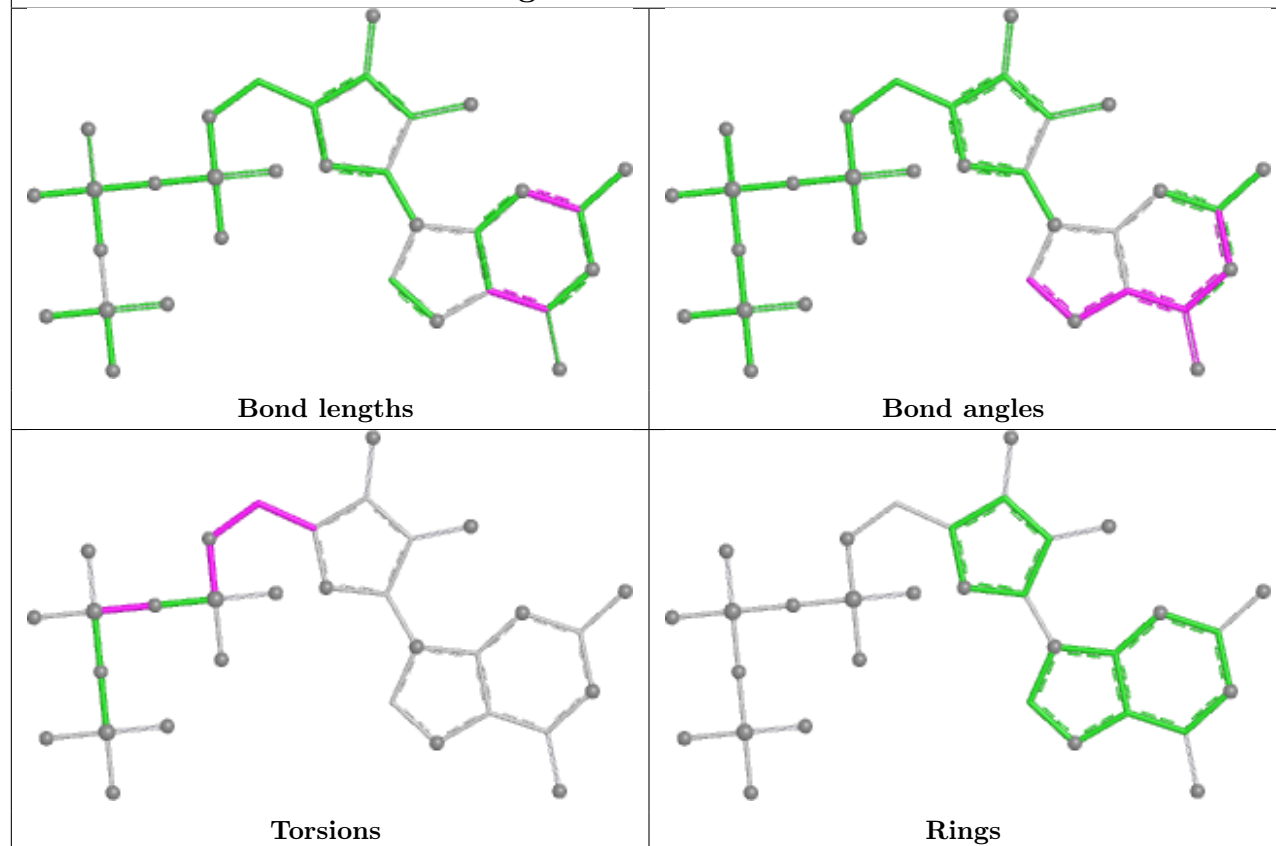


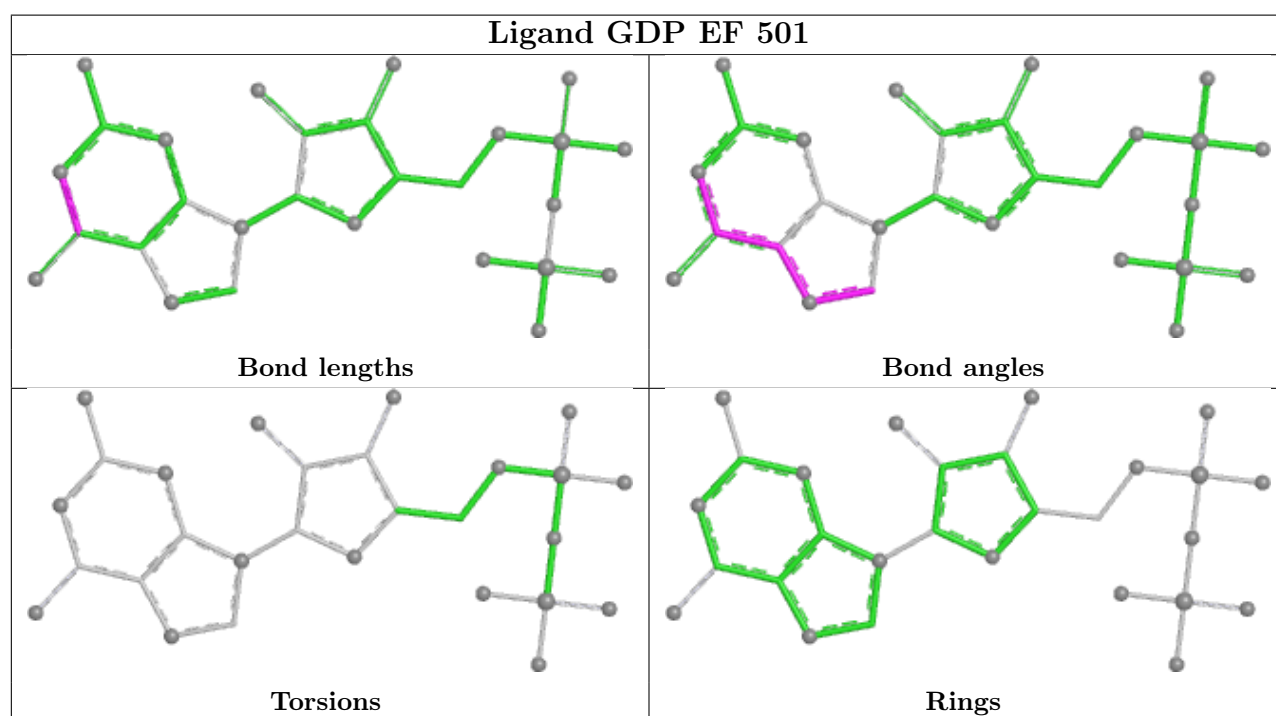
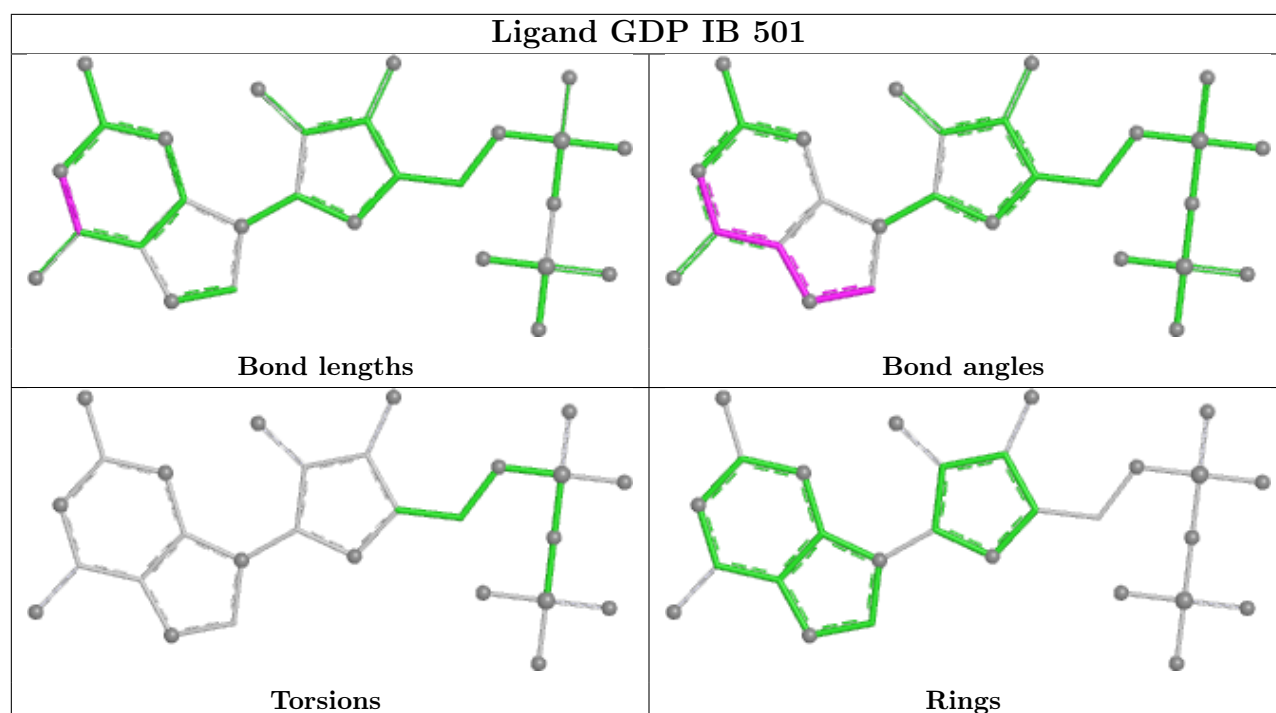


Ligand GTP HA 501

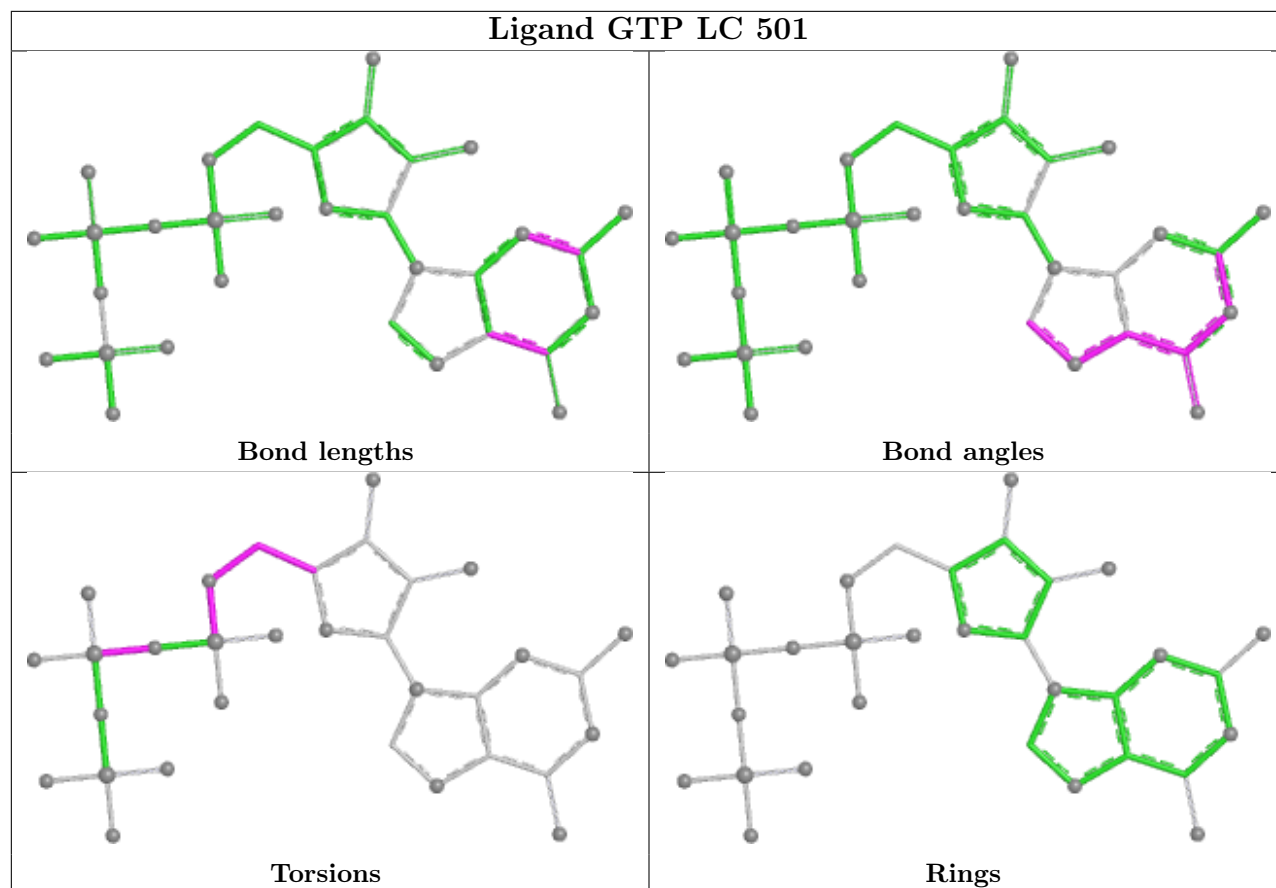


Ligand GTP EA 501

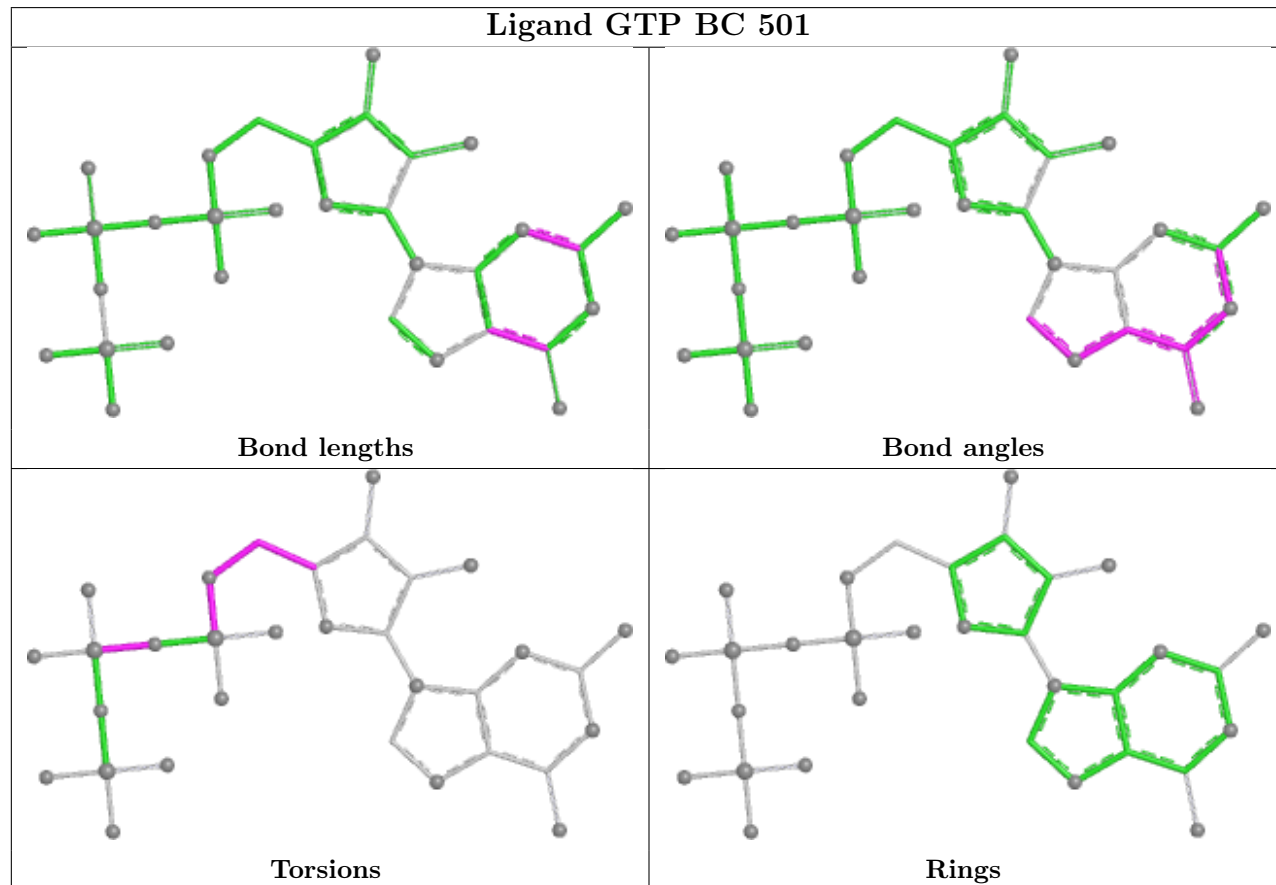


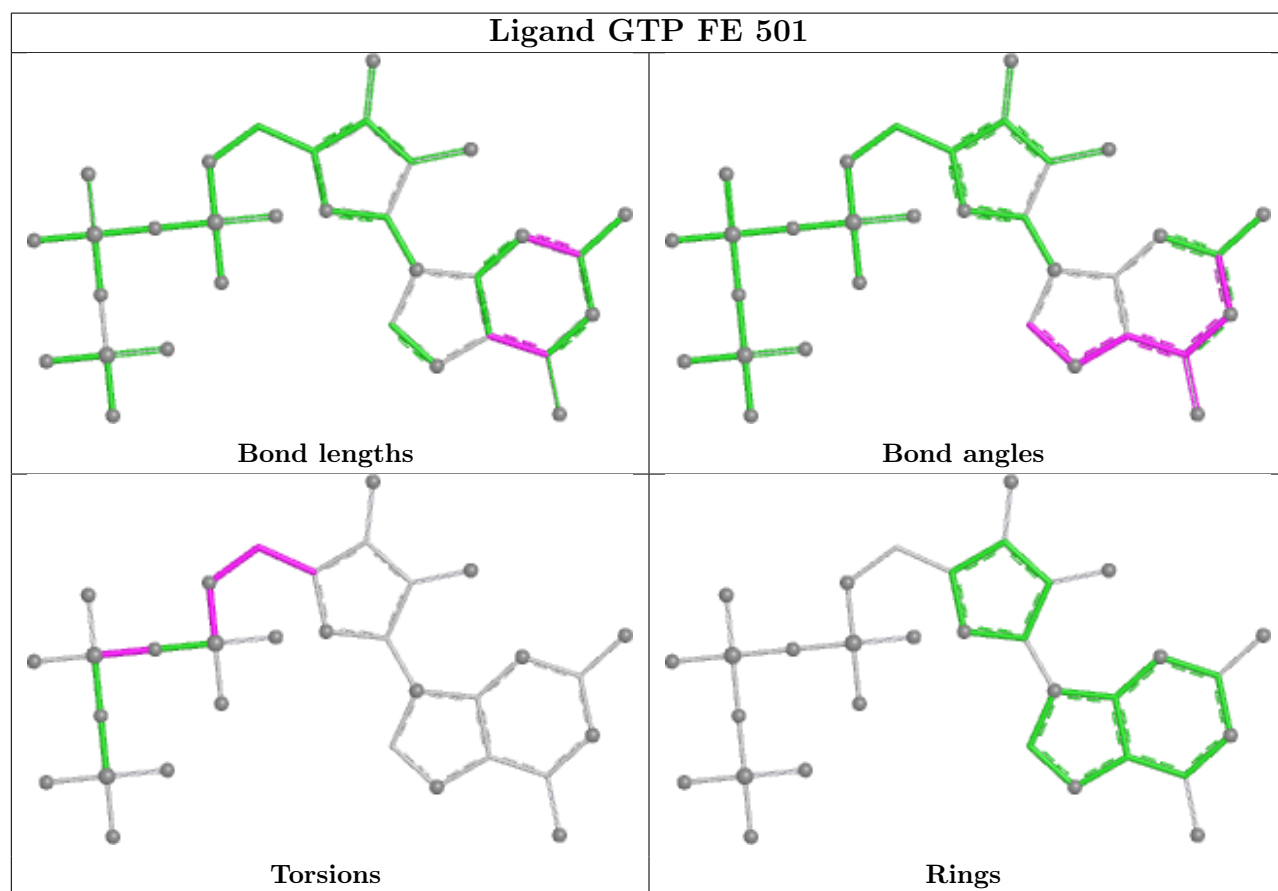
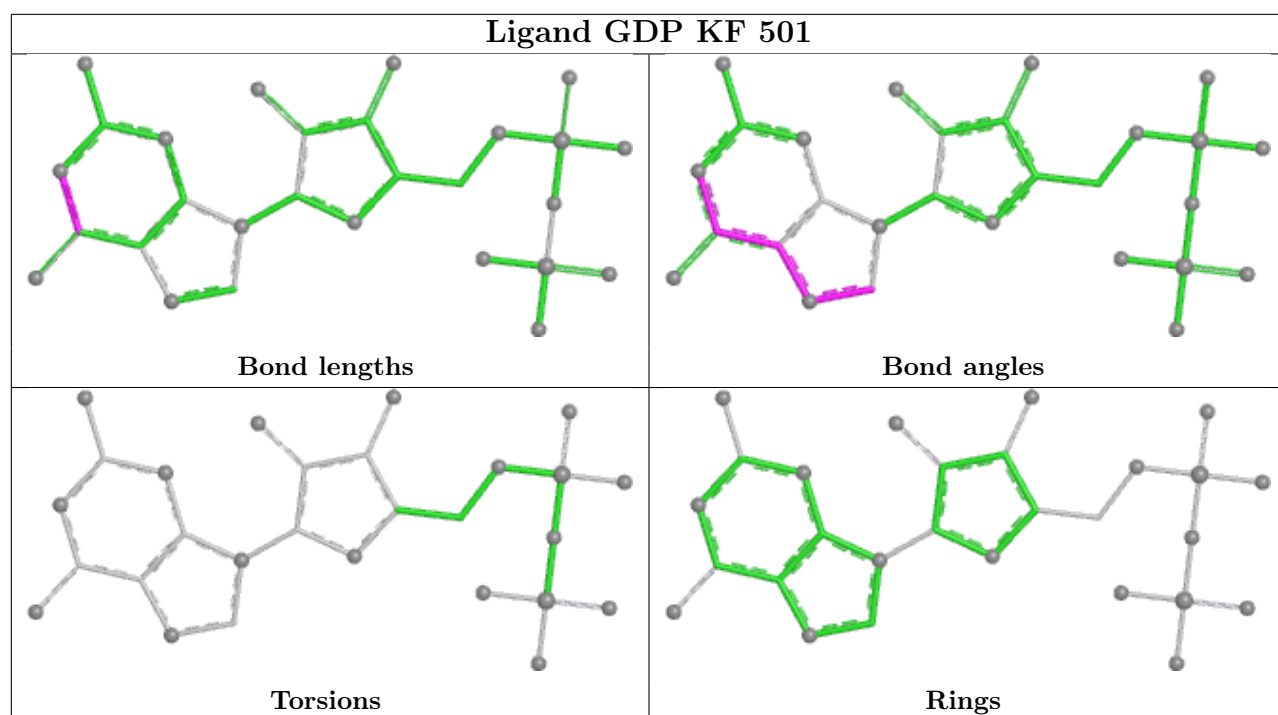


Ligand GTP LC 501

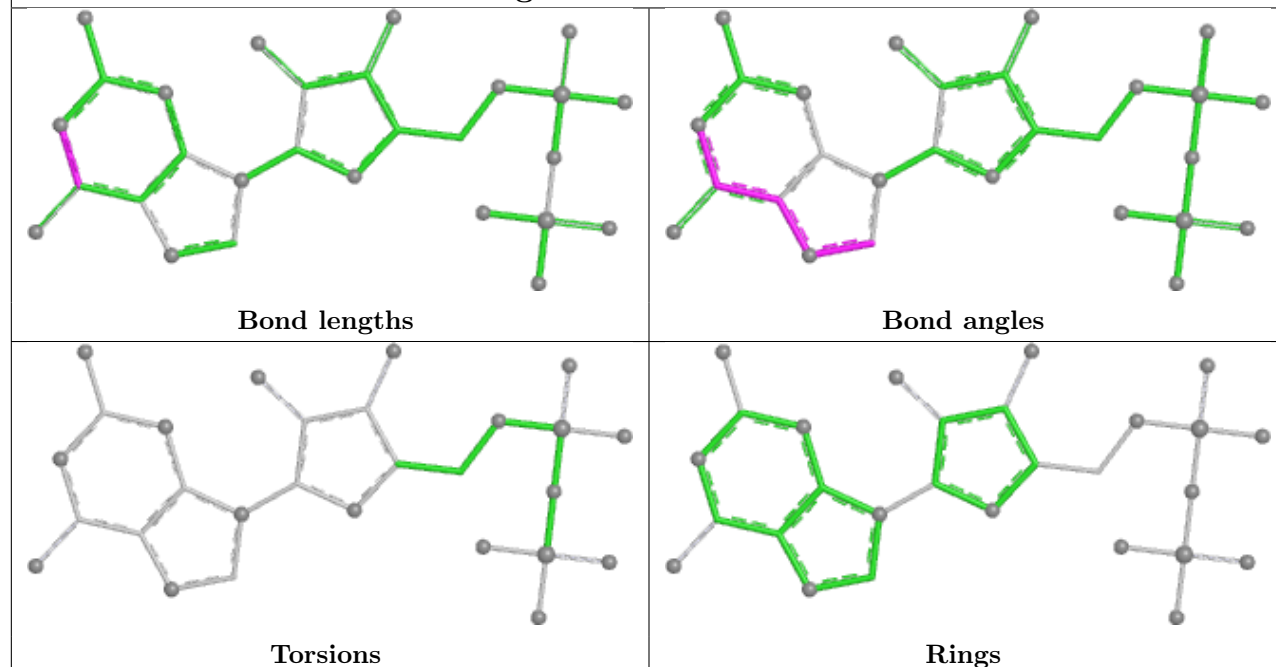


Ligand GTP BC 501

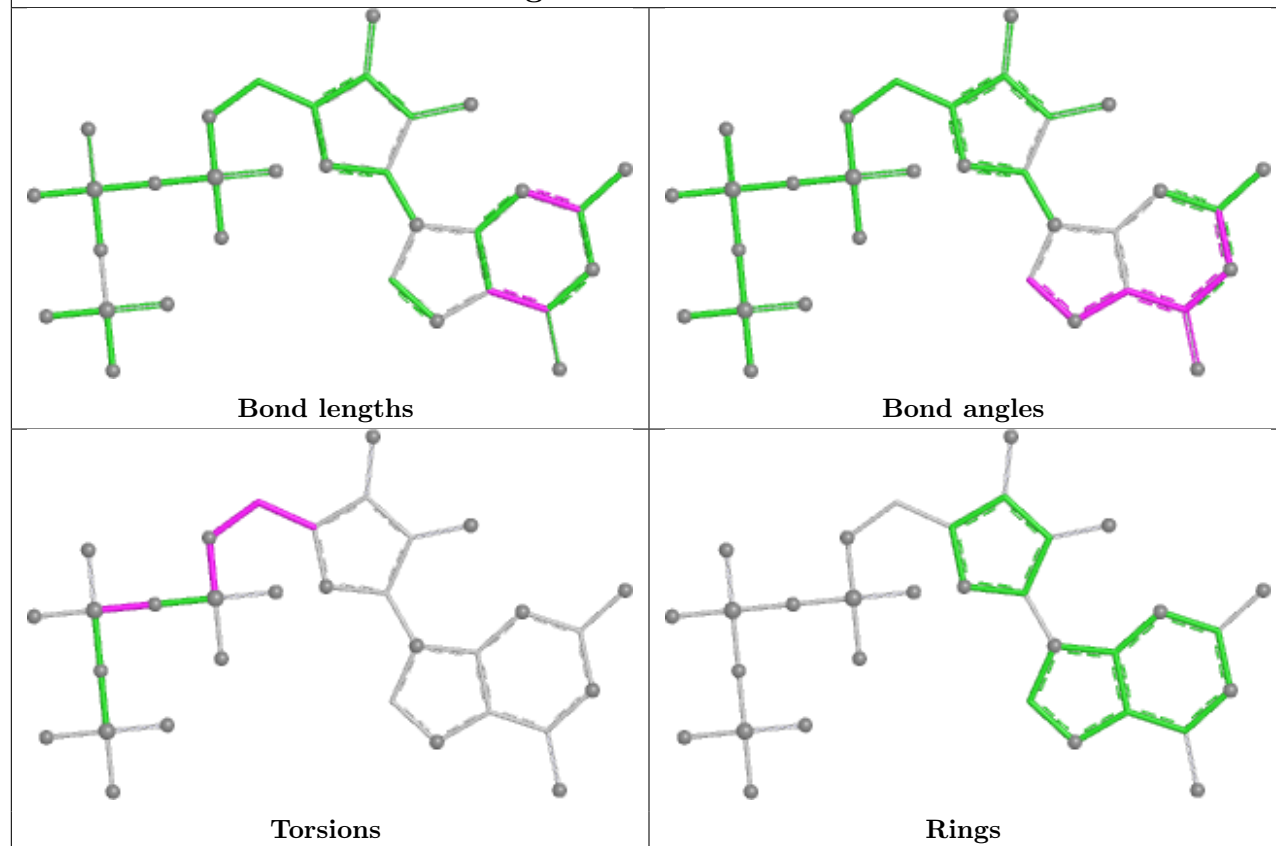




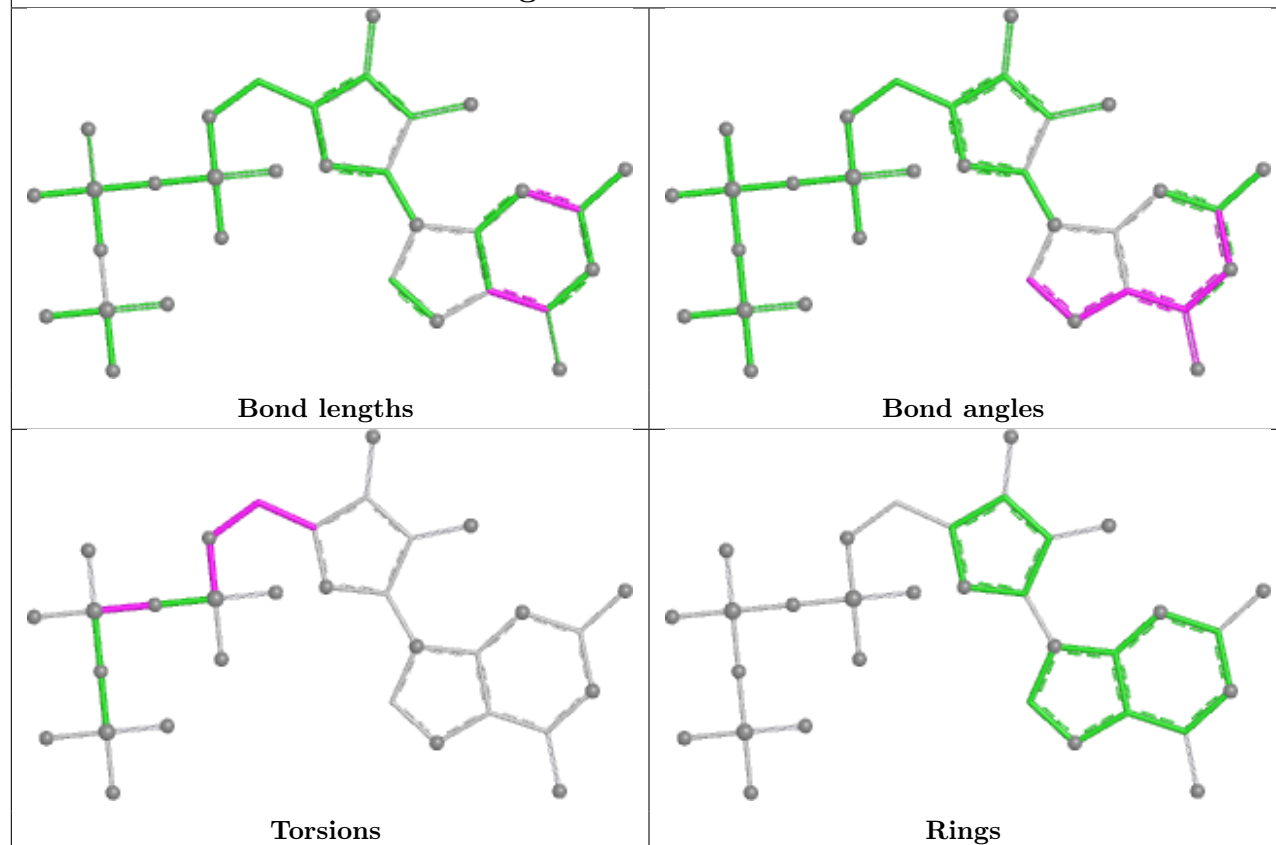
Ligand GDP HB 501



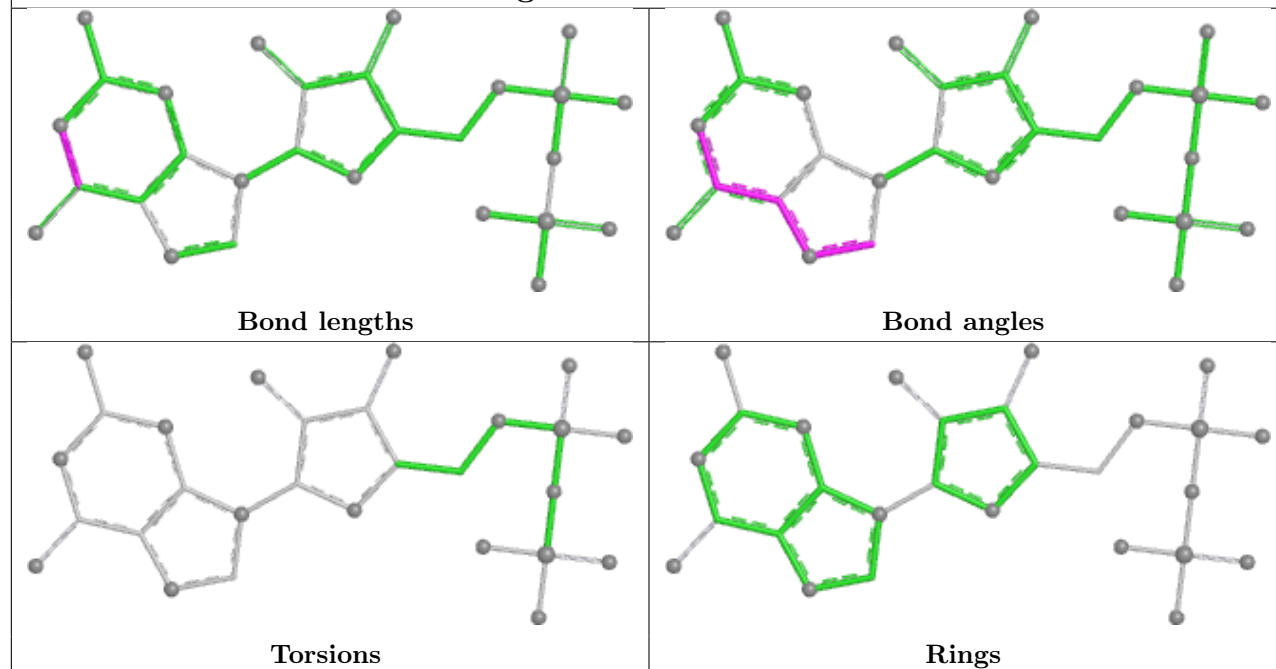
Ligand GTP IE 501

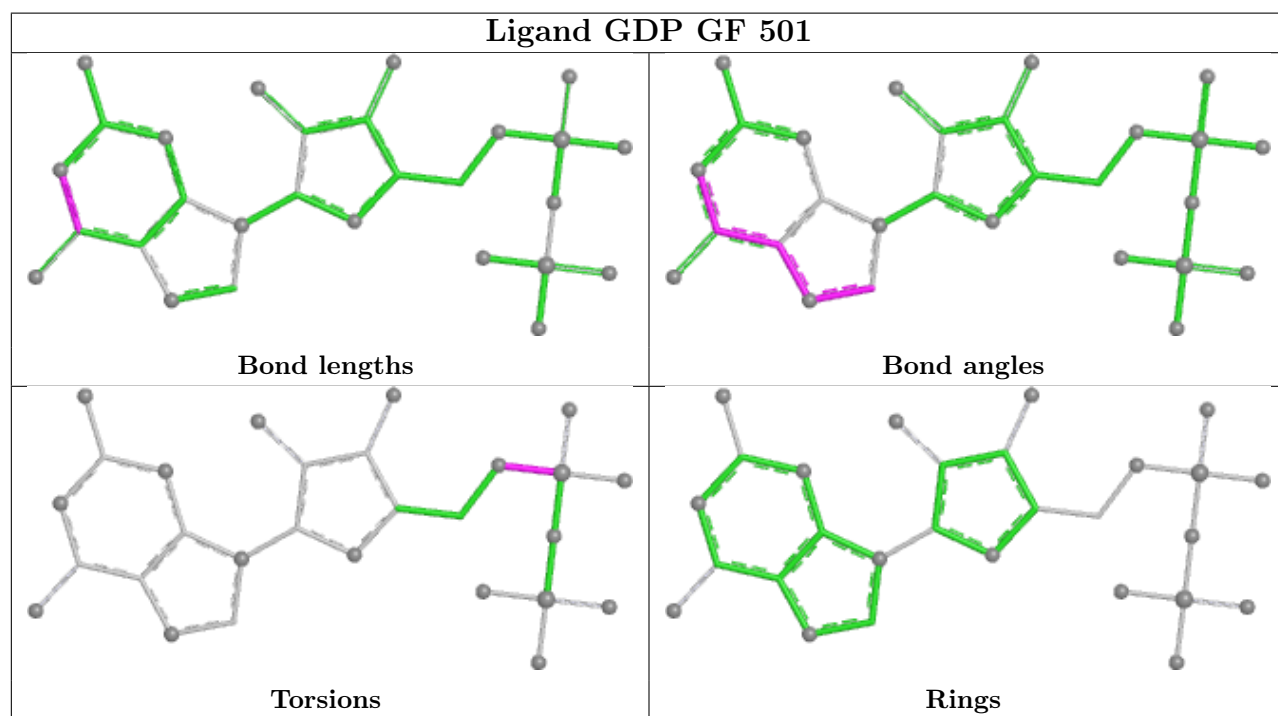
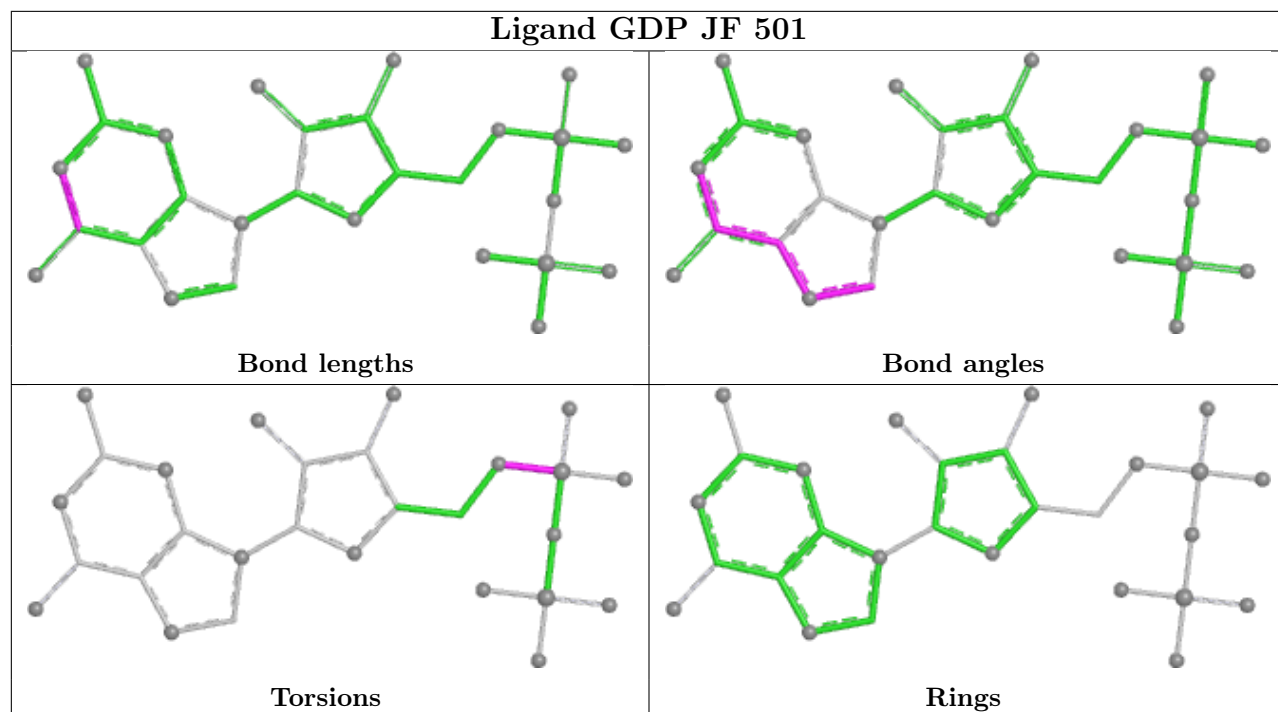


Ligand GTP CE 501

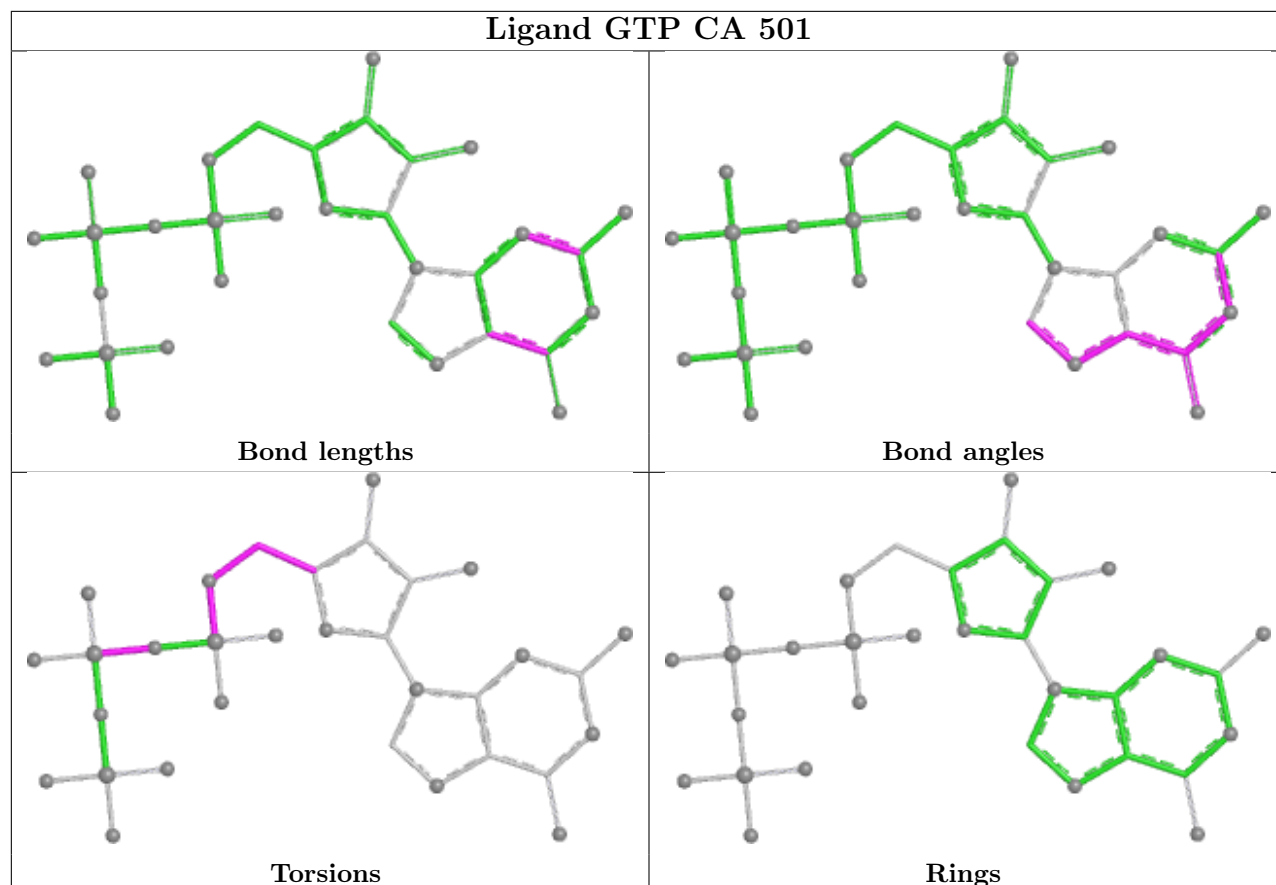


Ligand GDP HF 501

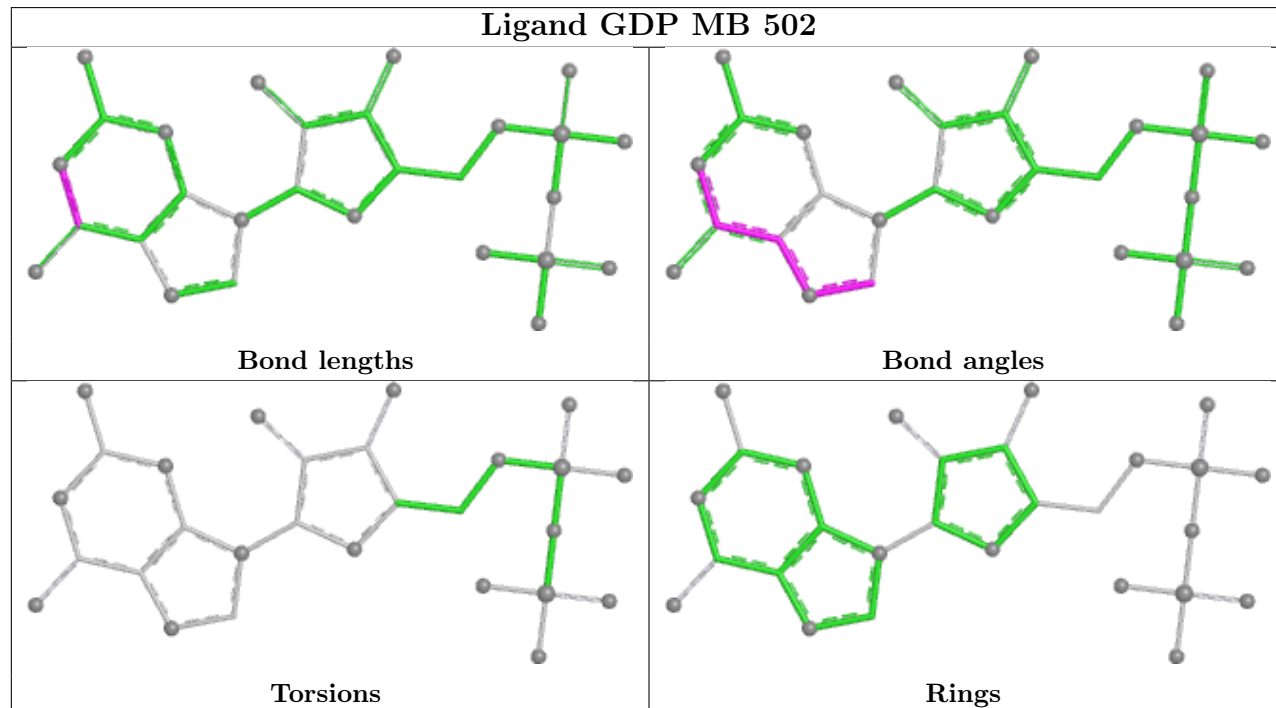




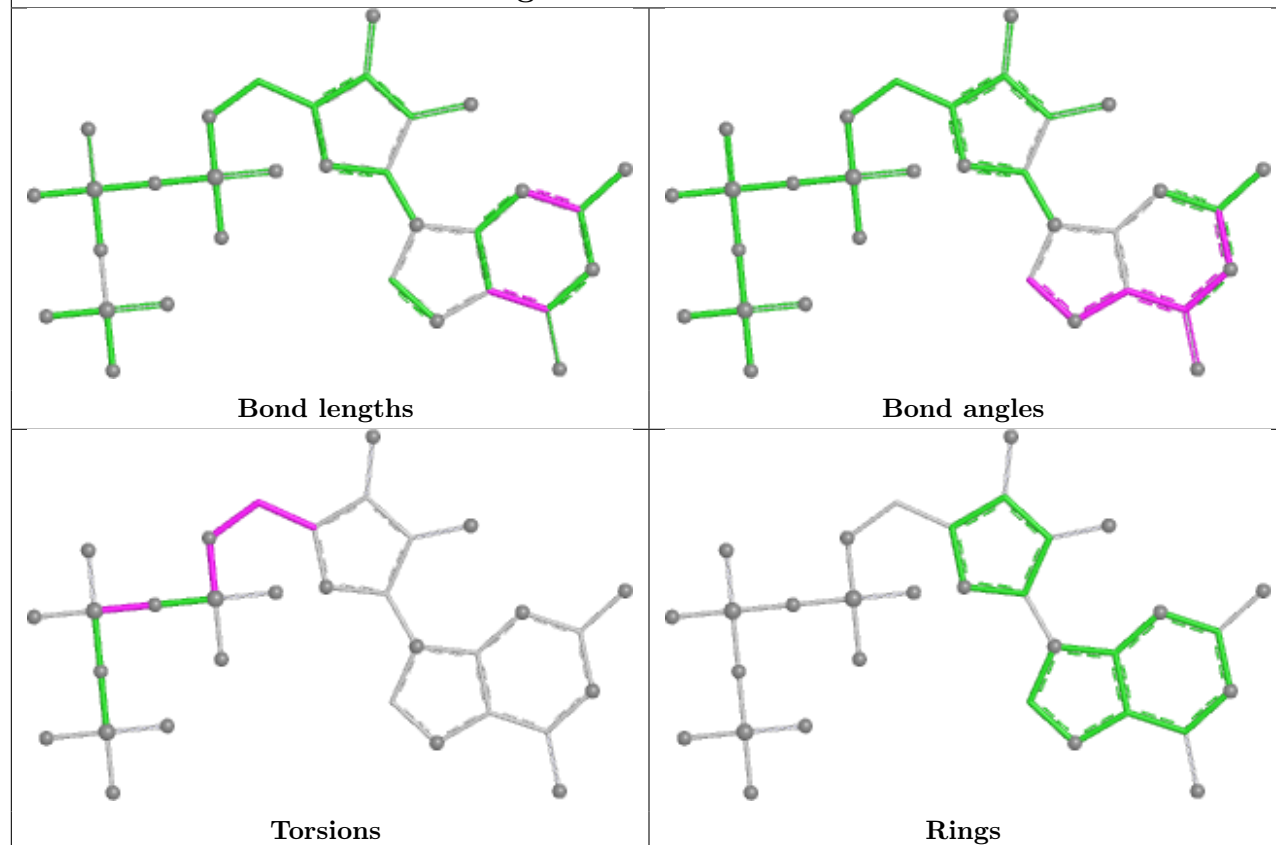
Ligand GTP CA 501



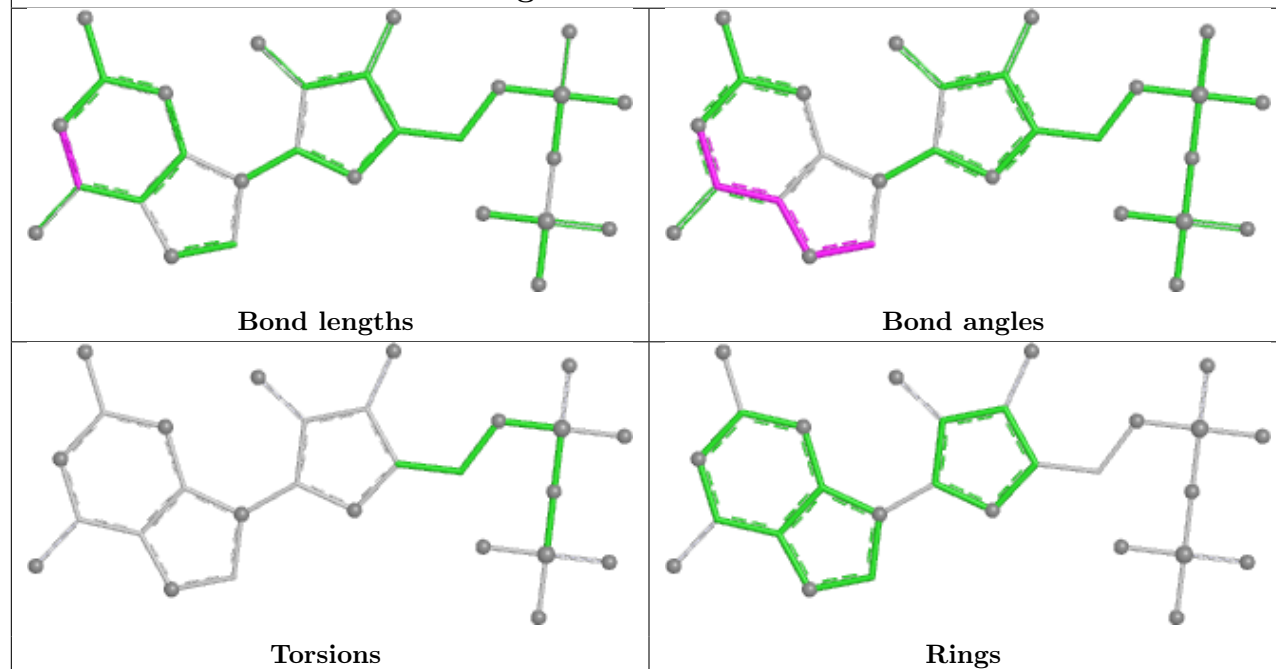
Ligand GDP MB 502



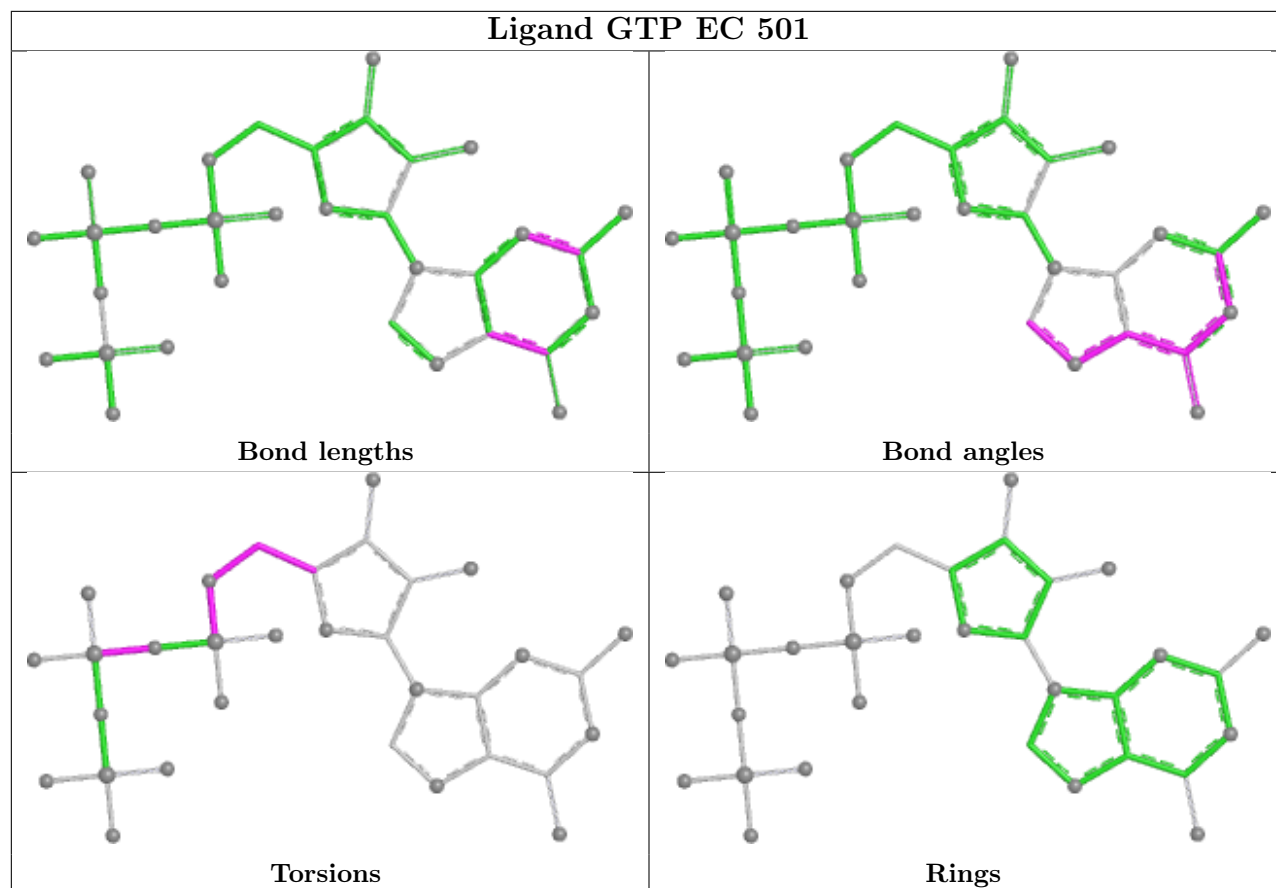
Ligand GTP DA 501



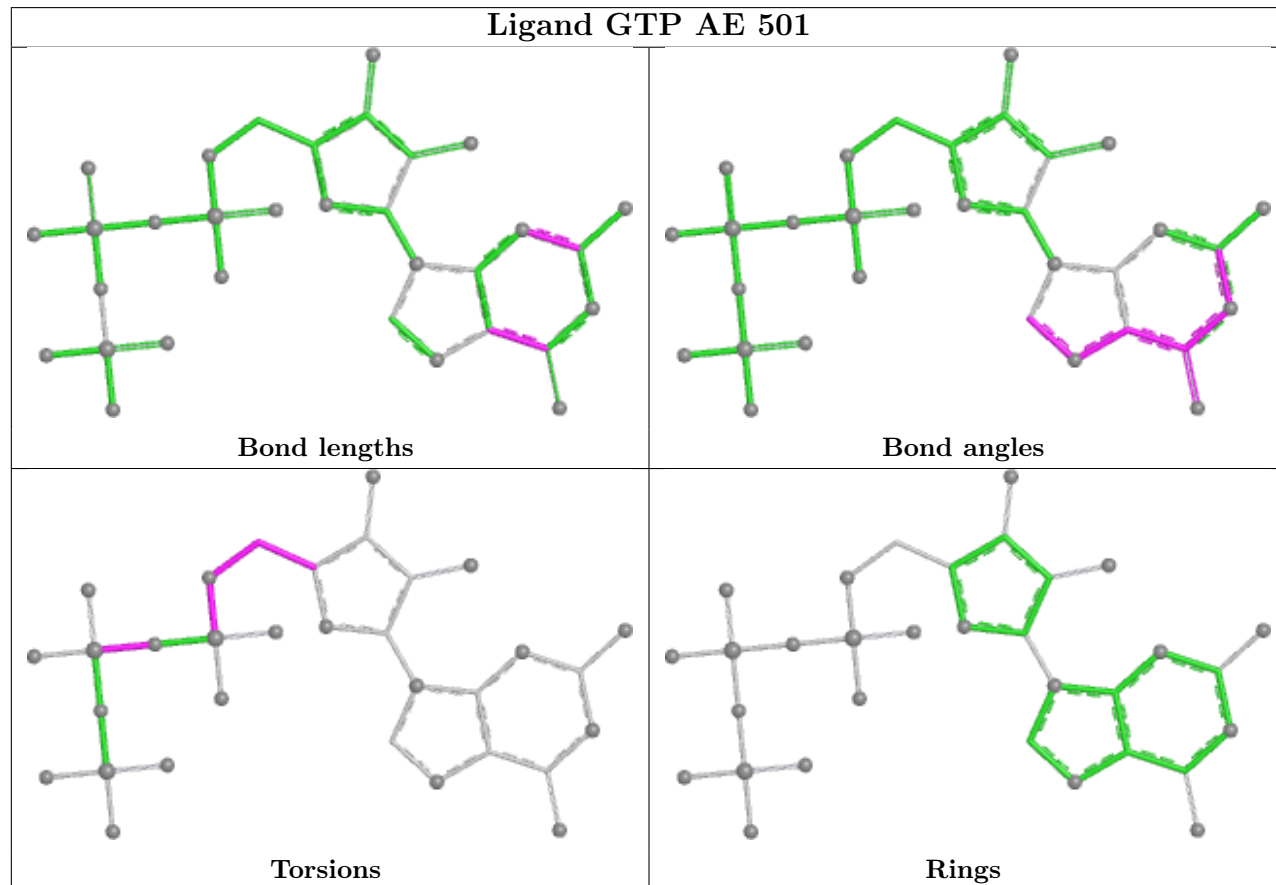
Ligand GDP ED 502



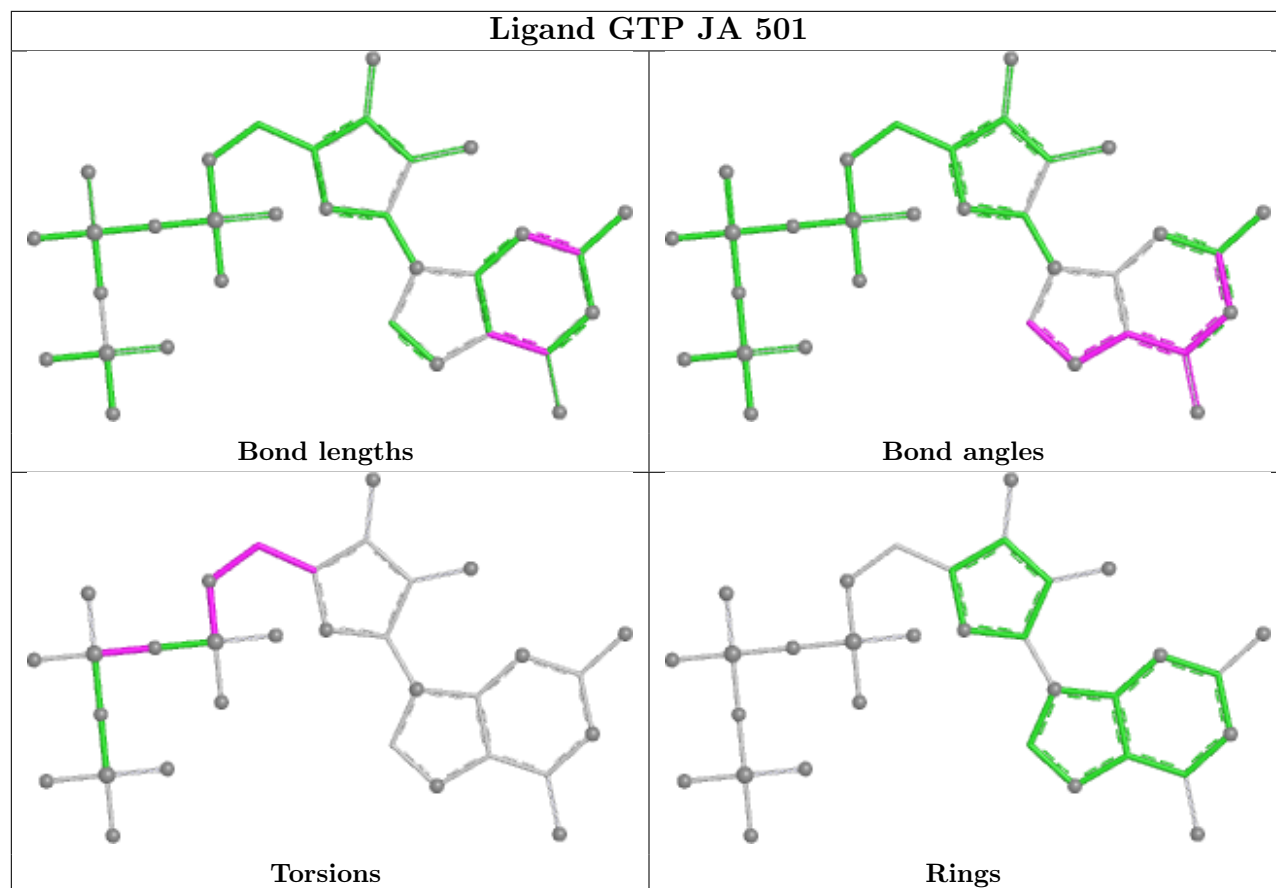
Ligand GTP EC 501



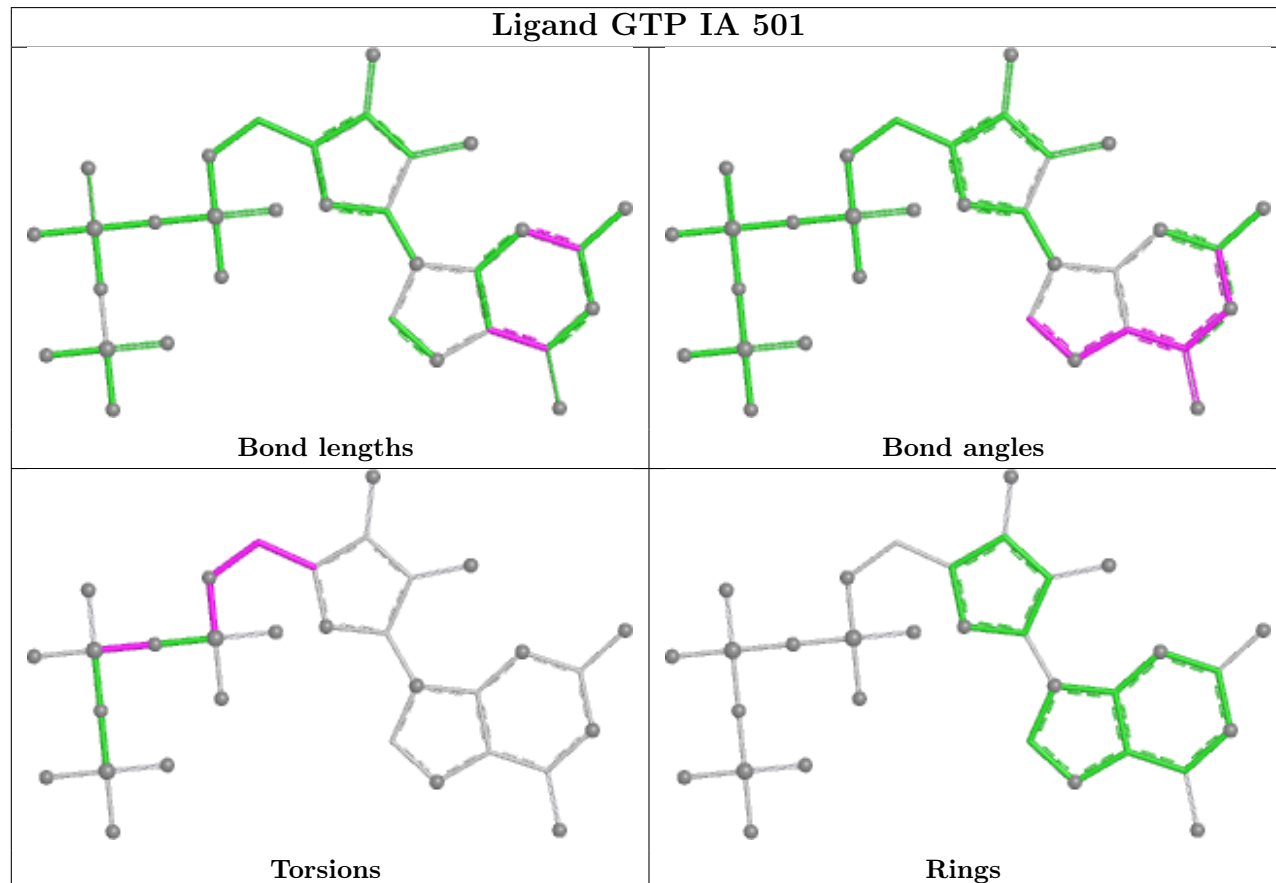
Ligand GTP AE 501



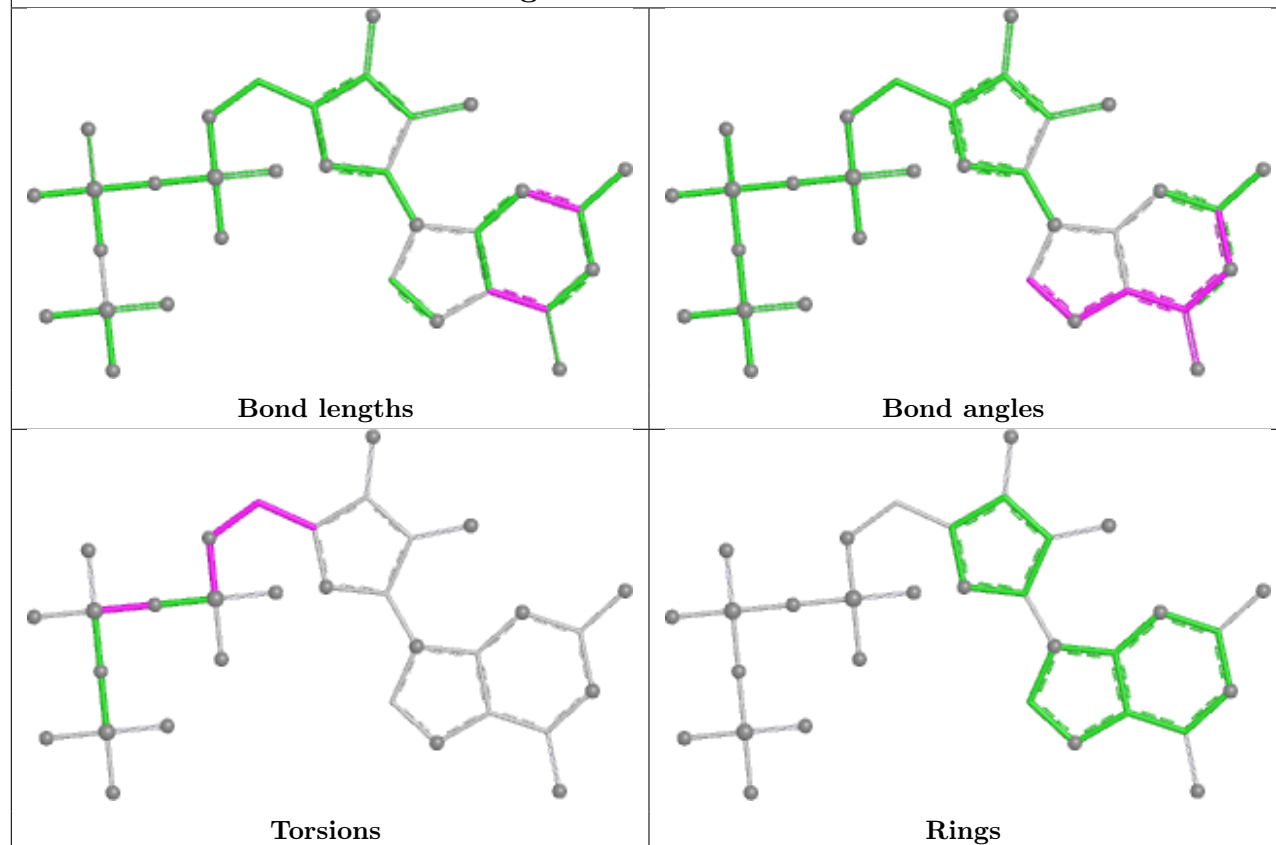
Ligand GTP JA 501



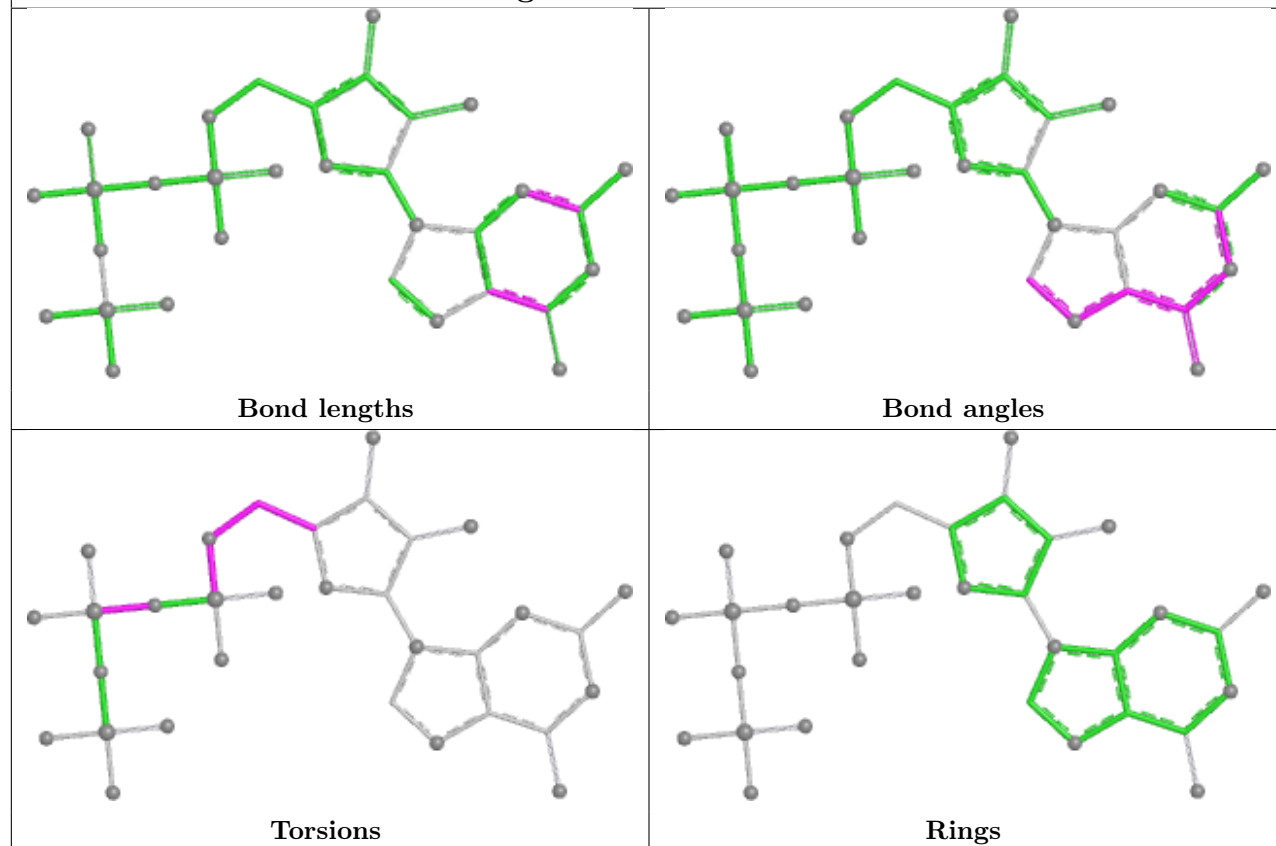
Ligand GTP IA 501

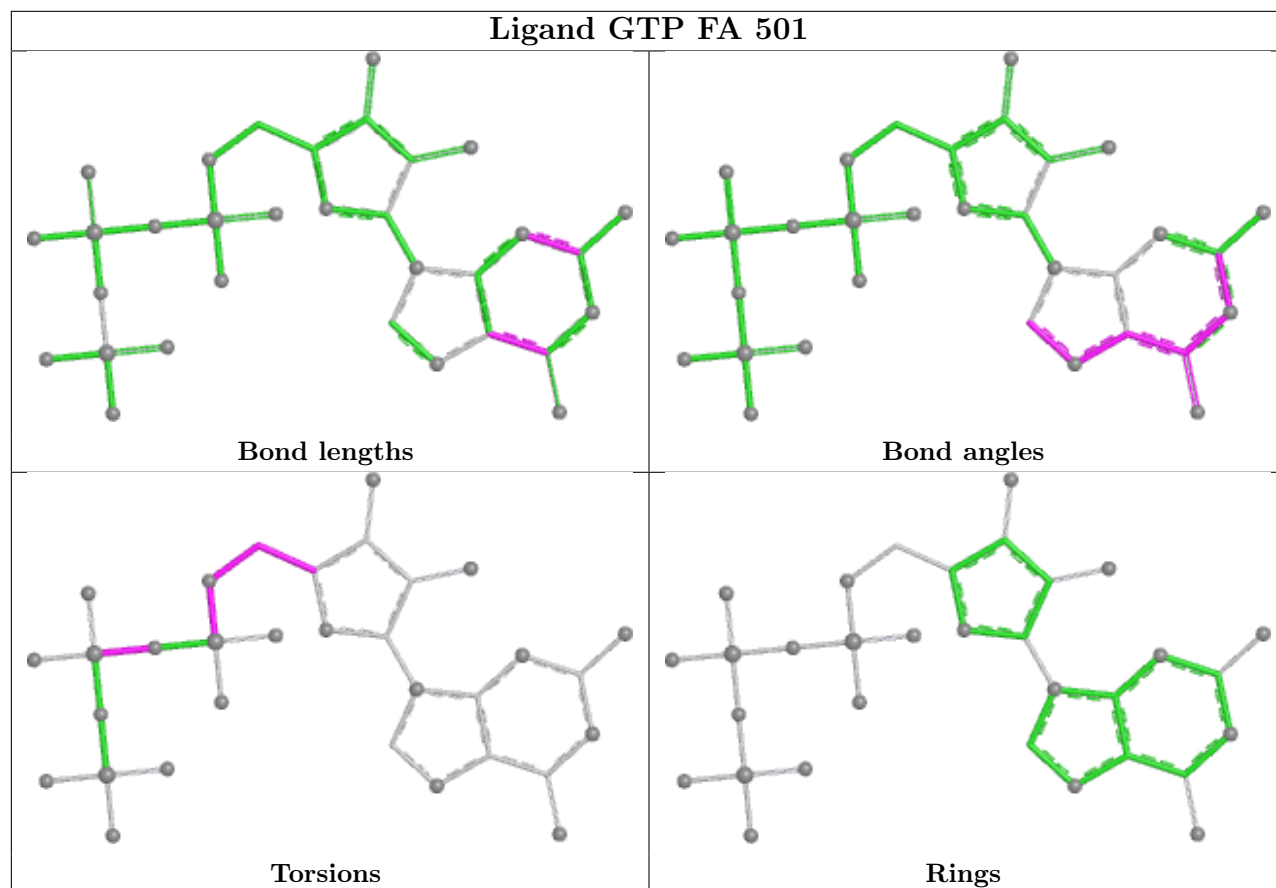


Ligand GTP EE 501



Ligand GTP KC 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.

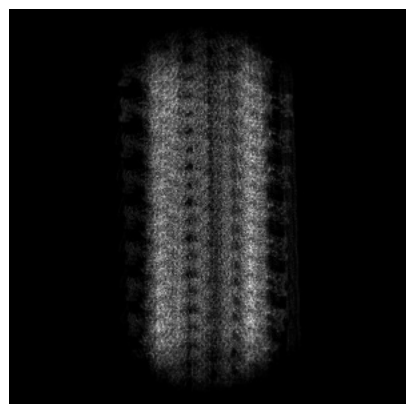
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49872. These allow visual inspection of the internal detail of the map and identification of artifacts.

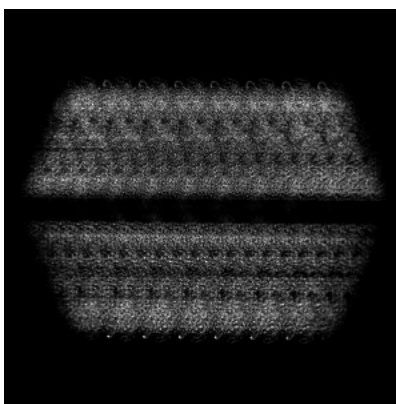
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

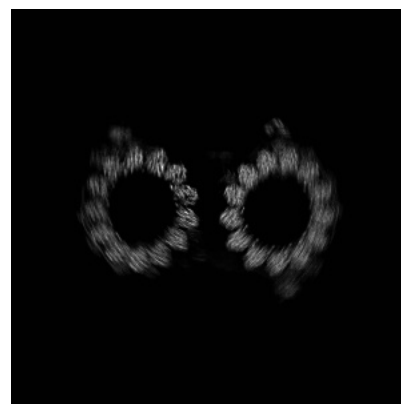
6.1.1 Primary map



X

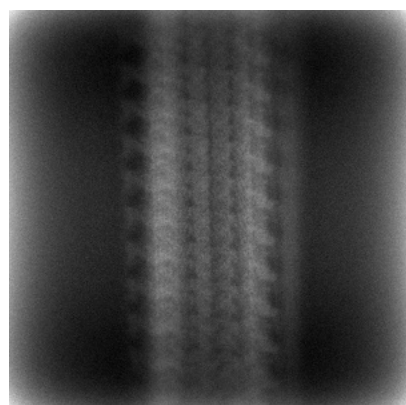


Y

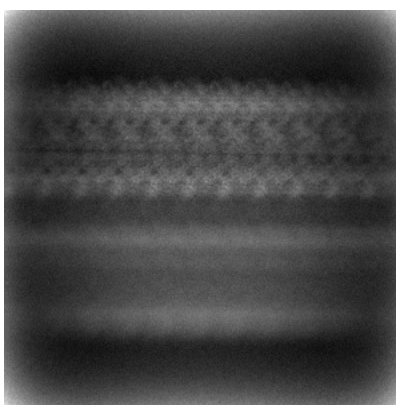


Z

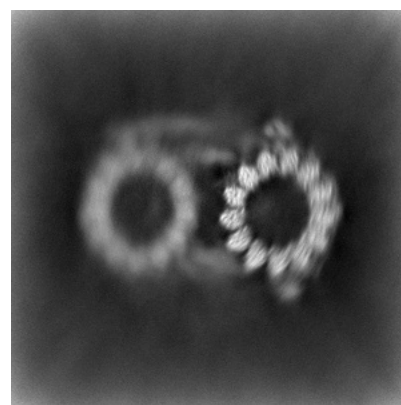
6.1.2 Raw map



X



Y

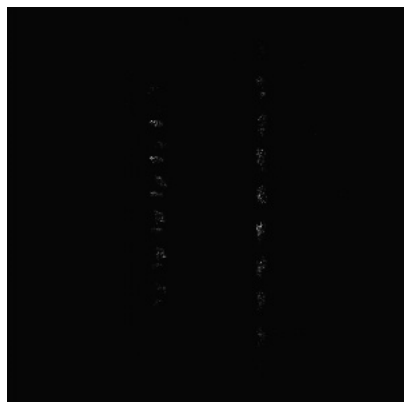


Z

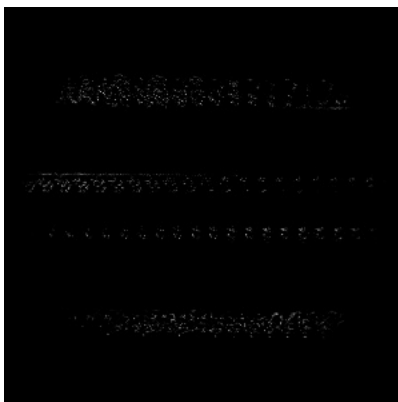
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 340

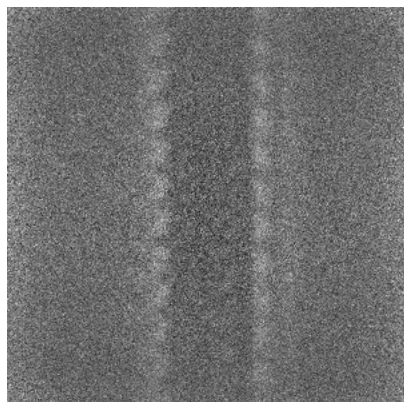


Y Index: 340

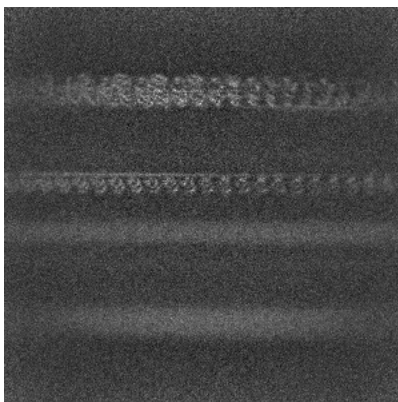


Z Index: 340

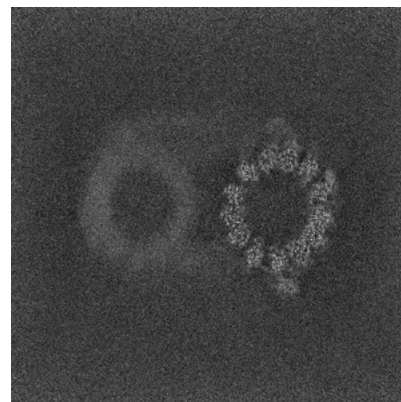
6.2.2 Raw map



X Index: 340



Y Index: 340

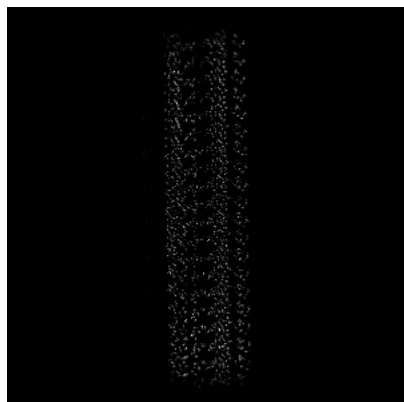


Z Index: 340

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

6.3 Largest variance slices [i](#)

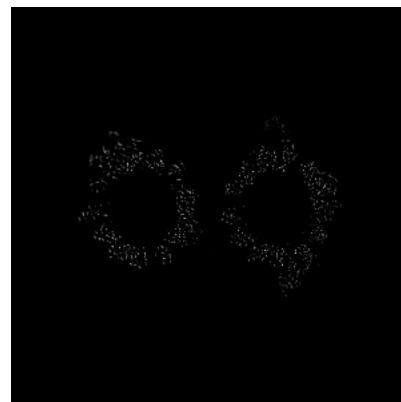
6.3.1 Primary map



X Index: 388

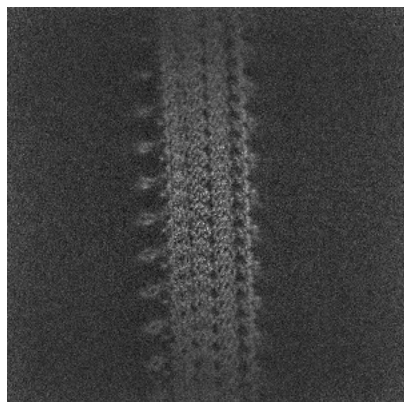


Y Index: 410

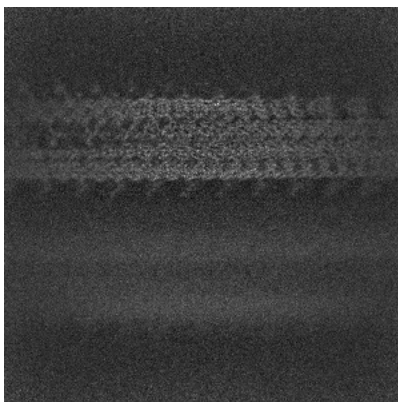


Z Index: 207

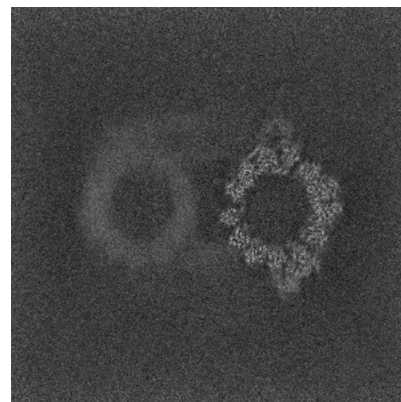
6.3.2 Raw map



X Index: 520



Y Index: 408

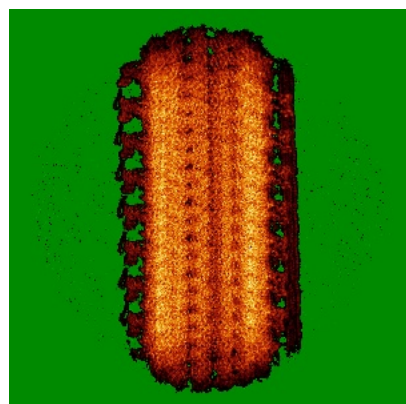


Z Index: 327

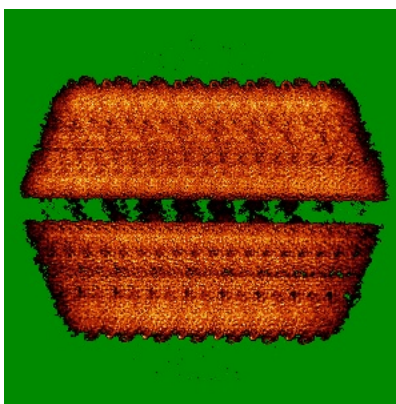
The images above show the largest variance slices of the map in three orthogonal directions.

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

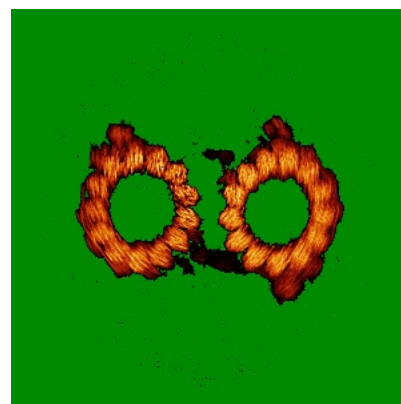
6.4.1 Primary map



X

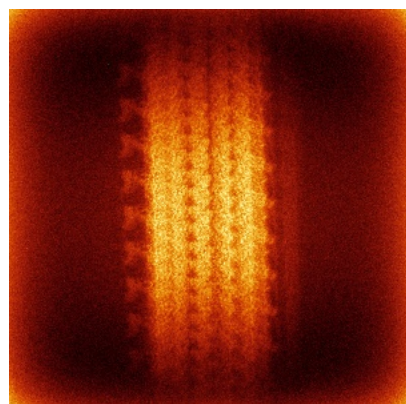


Y

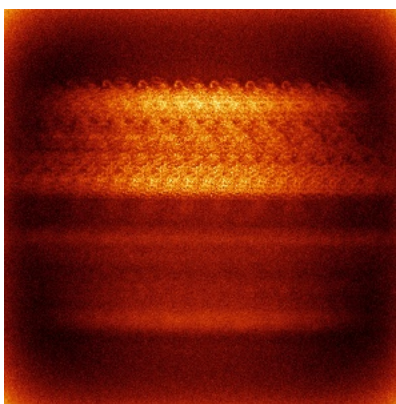


Z

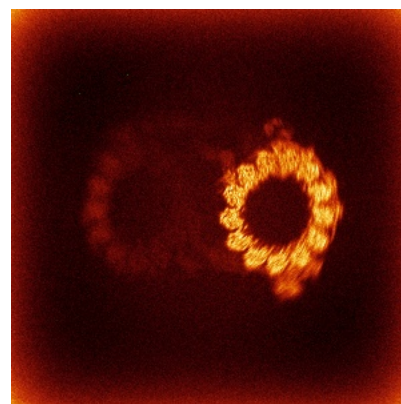
6.4.2 Raw map



X



Y

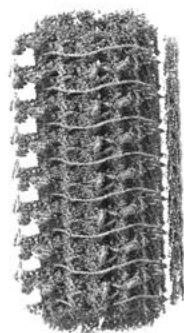


Z

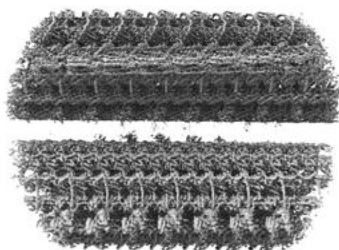
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

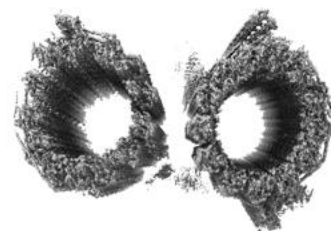
6.5.1 Primary map



X



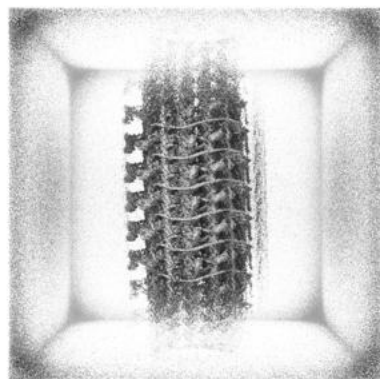
Y



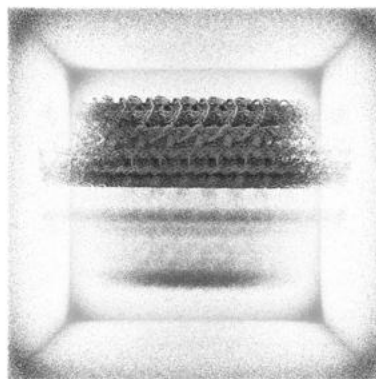
Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

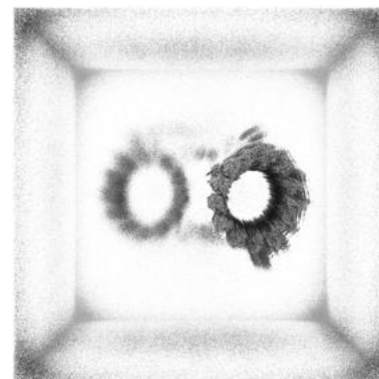
6.5.2 Raw map



X



Y



Z

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.

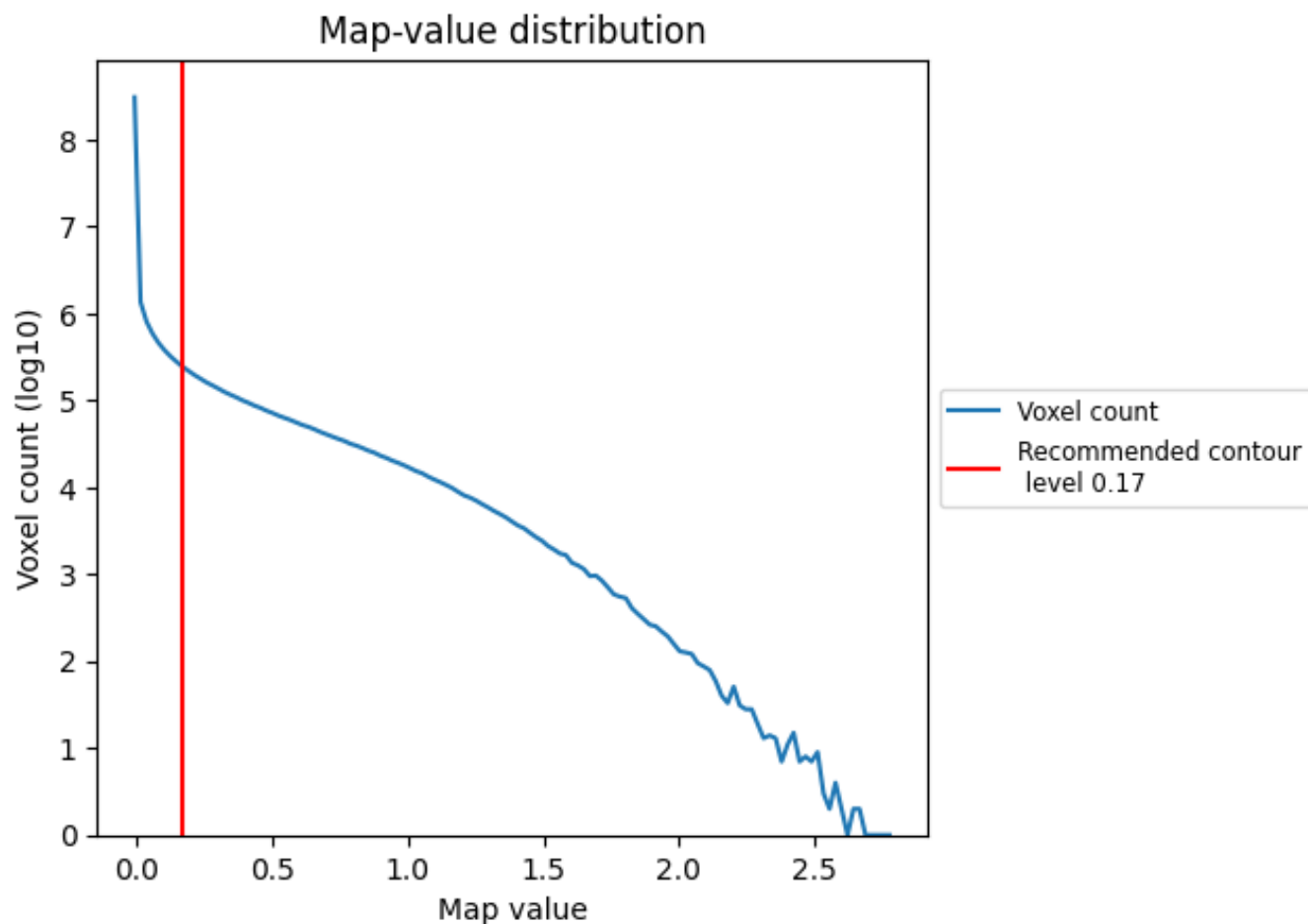
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

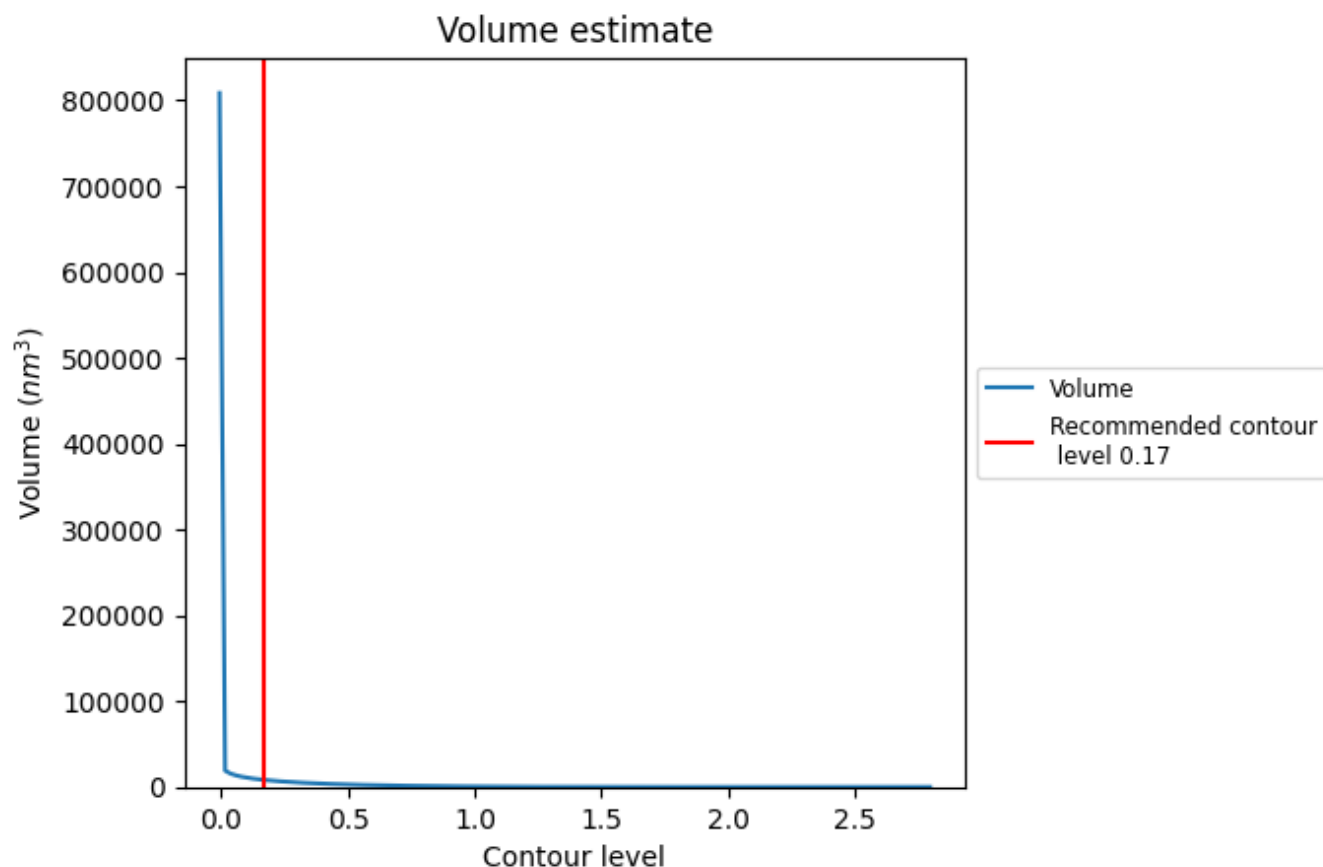
This section contains the results of statistical analysis of the map.

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.

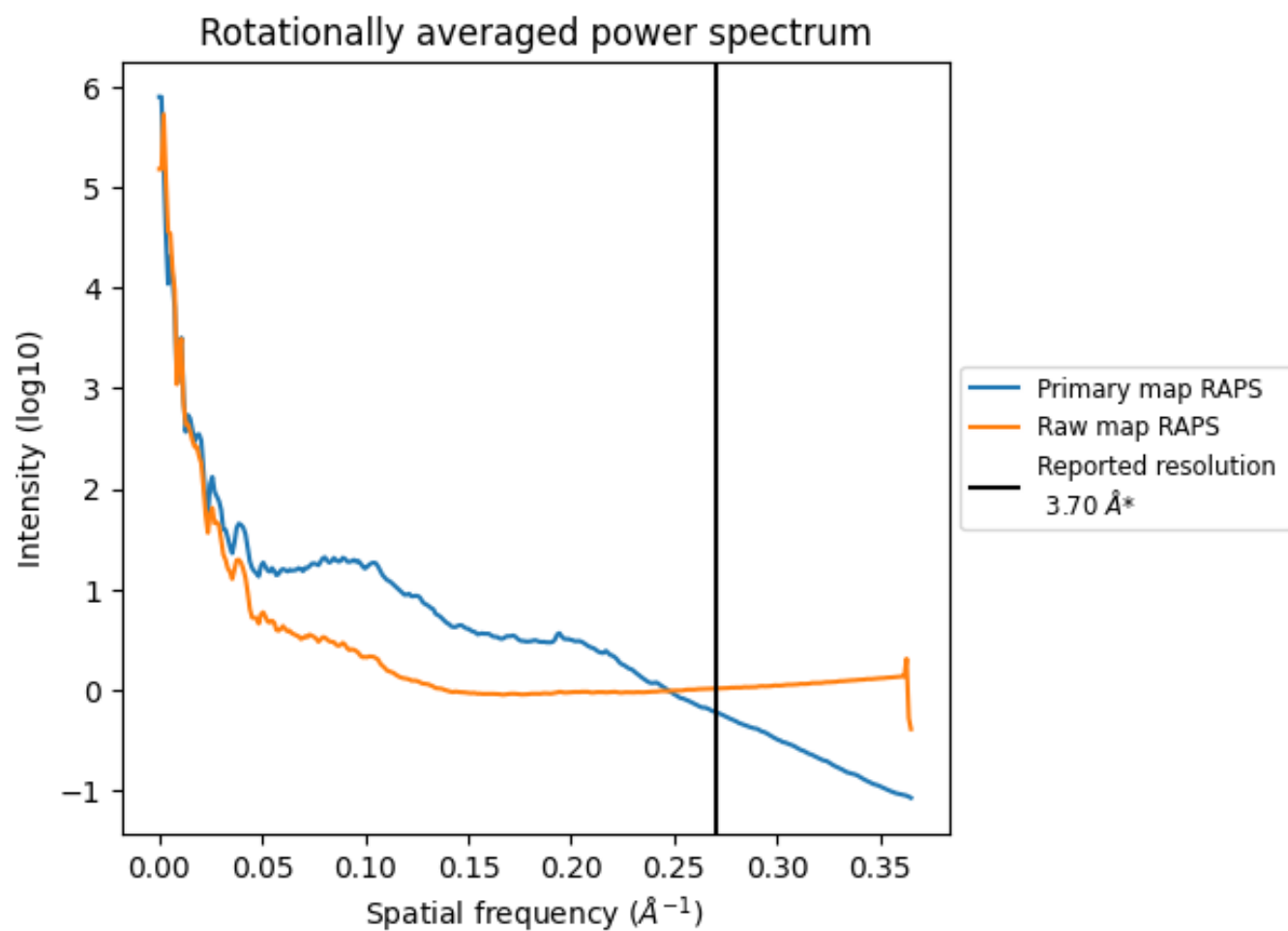
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8171 nm^3 ; this corresponds to an approximate mass of 7381 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 ⓘ

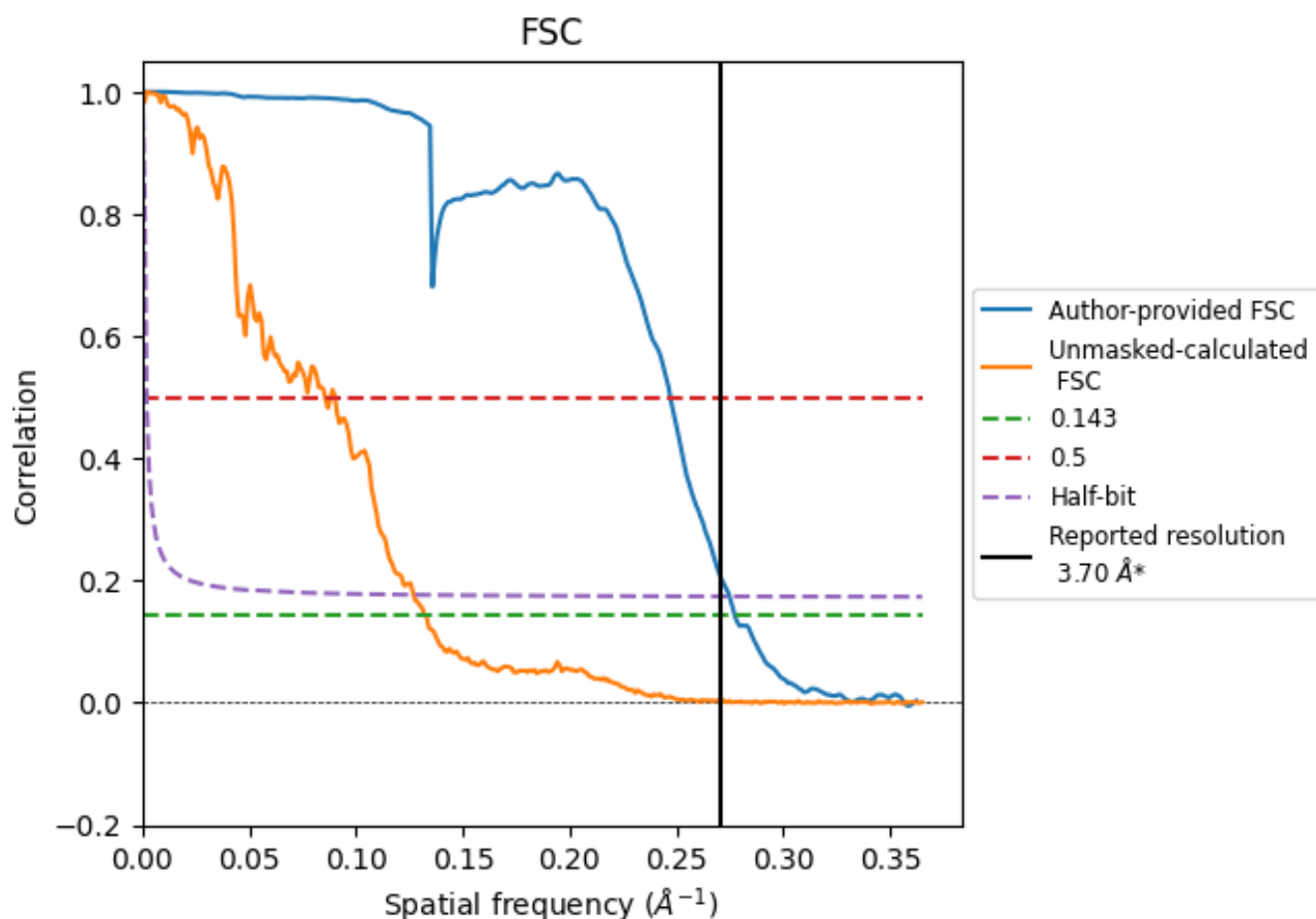


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

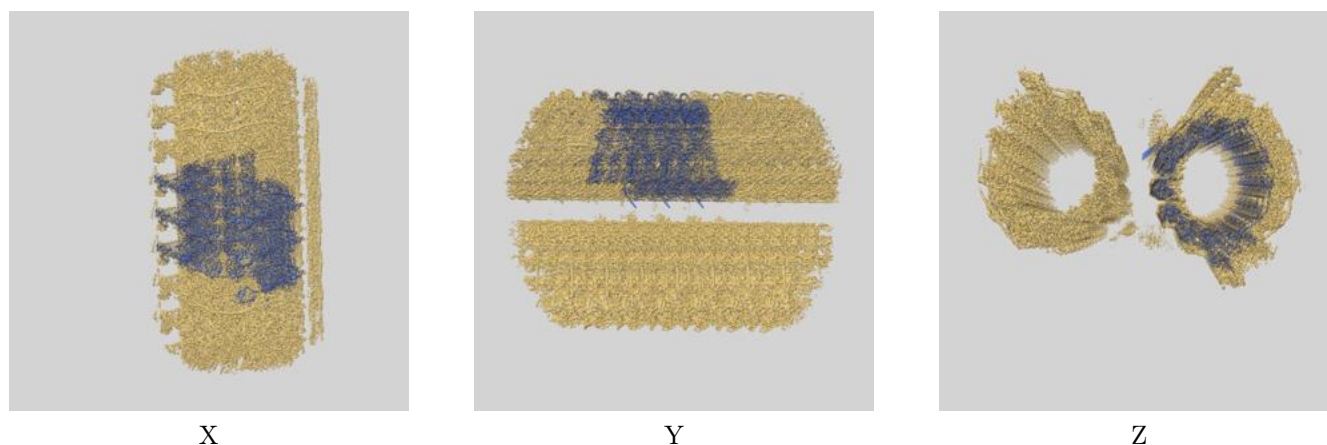
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.70 | - | - |
| Author-provided FSC curve | 3.61 | 4.05 | 3.64 |
| Unmasked-calculated* | 7.56 | 11.68 | 7.87 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.56 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

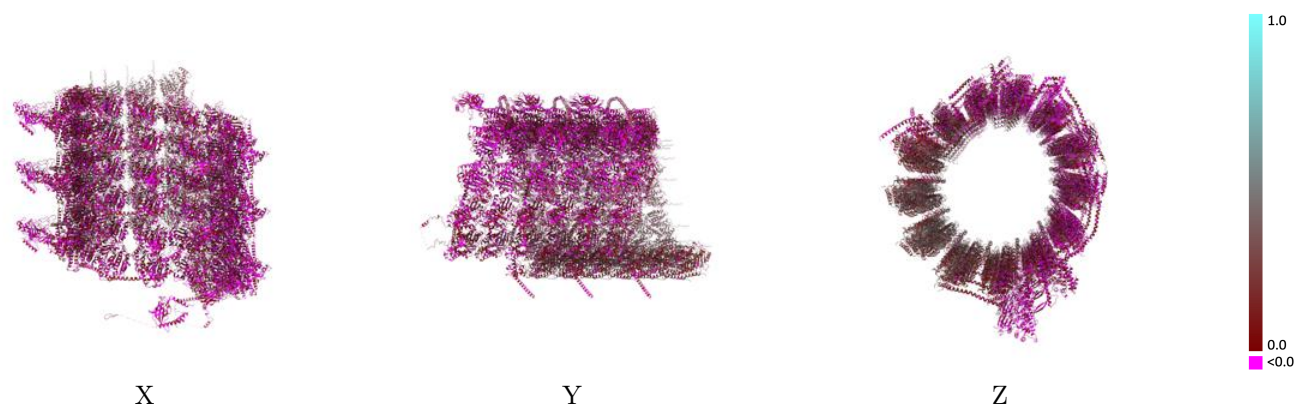
This section contains information regarding the fit between EMDB map EMD-49872 and PDB model 9NW3. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)



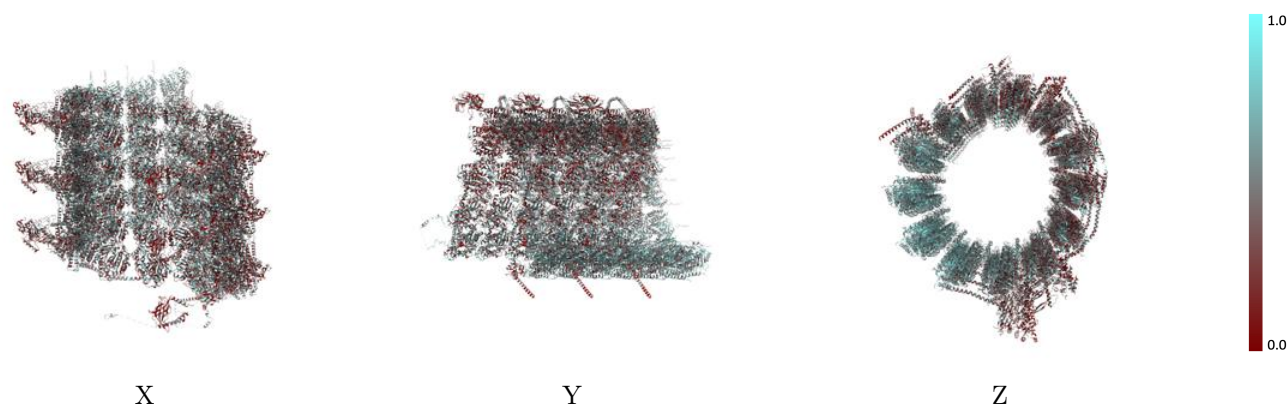
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



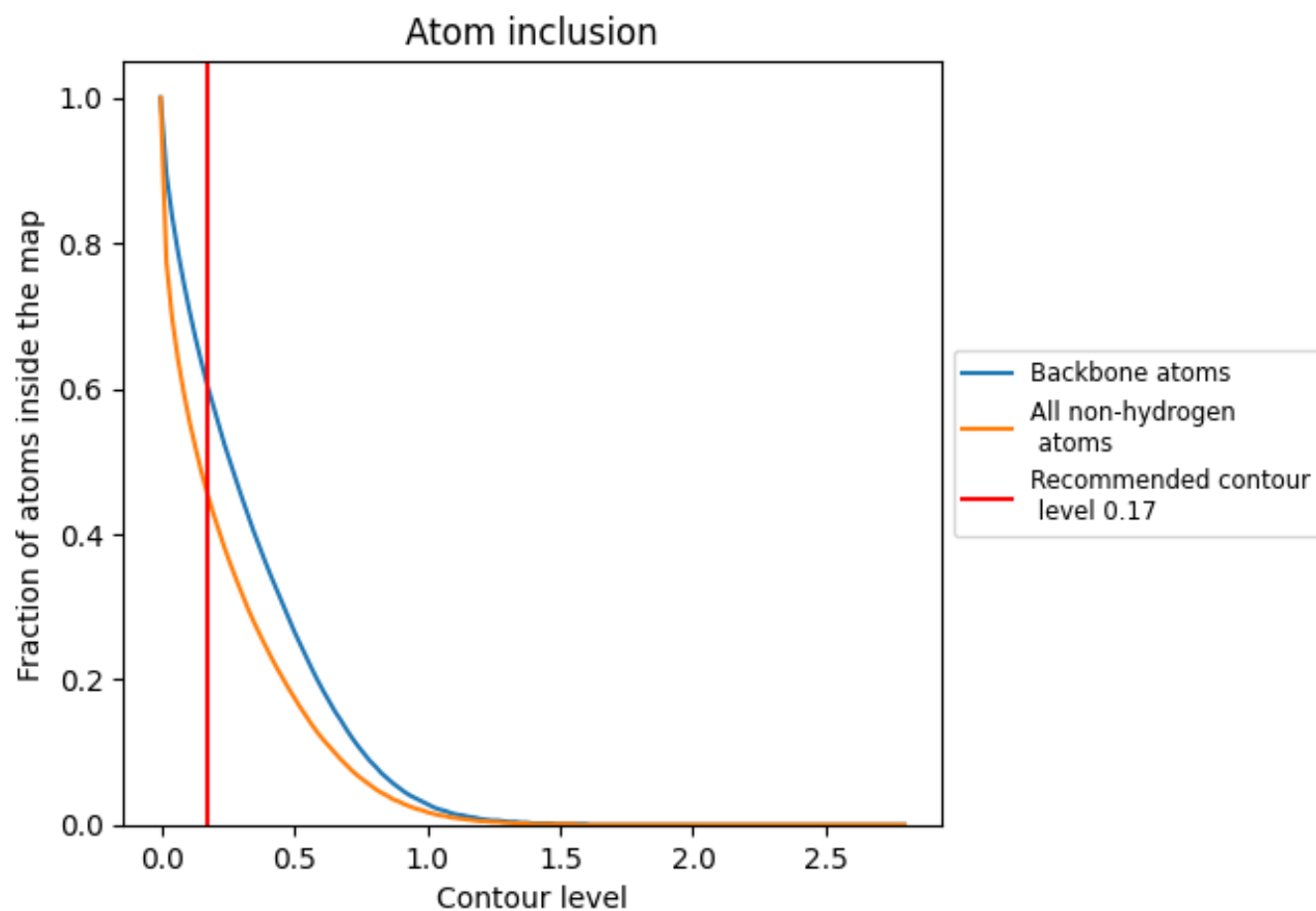
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|---|
| All |  0.4550 |  0.1370 |
| 1A |  0.2930 |  0.0820 |
| 1B |  0.2820 |  0.0750 |
| 1C |  0.3090 |  0.0770 |
| 2A |  0.3760 |  0.0670 |
| 2B |  0.3770 |  0.0590 |
| 2C |  0.3700 |  0.0770 |
| 3A |  0.2760 |  0.0160 |
| 3B |  0.2780 |  0.0100 |
| 3C |  0.2670 |  0.0100 |
| 4A |  0.5490 |  0.2790 |
| 4B |  0.5460 |  0.2330 |
| 4C |  0.5210 |  0.2260 |
| 4D |  0.5490 |  0.1840 |
| 5A |  0.3430 |  0.0690 |
| 5B |  0.3440 |  0.0600 |
| 5C |  0.3330 |  0.0520 |
| 6A |  0.2950 |  0.0020 |
| 6B |  0.3240 |  0.0110 |
| 6C |  0.2940 |  -0.0160 |
| 7A |  0.3110 |  0.0210 |
| 7B |  0.3240 |  0.0160 |
| 7C |  0.3320 |  0.0460 |
| 7D |  0.2980 |  0.0160 |
| 7E |  0.3240 |  0.0440 |
| 7F |  0.3060 |  0.0270 |
| 8A |  0.5560 |  0.2440 |
| 8B |  0.4600 |  0.2670 |
| 8C |  0.5180 |  0.2650 |
| 8D |  0.5820 |  0.3310 |
| 8E |  0.6300 |  0.3780 |
| 8F |  0.6090 |  0.3700 |
| 8G |  0.5770 |  0.3190 |
| 8H |  0.5820 |  0.3340 |
| 8I |  0.5820 |  0.3400 |























































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 8J |  0.6140 |  0.2900 |
| 8K |  0.5930 |  0.2960 |
| 8L |  0.5560 |  0.2870 |
| 8M |  0.6190 |  0.2670 |
| 8N |  0.6450 |  0.2700 |
| 8O |  0.5980 |  0.2560 |
| 8P |  0.6090 |  0.2170 |
| 8Q |  0.6090 |  0.2400 |
| 8R |  0.6140 |  0.2470 |
| 8S |  0.4390 |  0.1840 |
| 8T |  0.4920 |  0.2080 |
| 8U |  0.4920 |  0.2010 |
| 8V |  0.4020 |  0.1670 |
| 8W |  0.3230 |  0.1630 |
| 8X |  0.3180 |  0.1780 |
| 8Y |  0.2590 |  0.0830 |
| 8Z |  0.4340 |  0.1630 |
| 9A |  0.4340 |  0.1580 |
| AA |  0.5470 |  0.2130 |
| AB |  0.5180 |  0.1970 |
| AC |  0.5490 |  0.2330 |
| AD |  0.5180 |  0.2090 |
| AE |  0.5410 |  0.2300 |
| AF |  0.5170 |  0.2090 |
| BA |  0.5930 |  0.2920 |
| BB |  0.6010 |  0.3000 |
| BC |  0.6040 |  0.3080 |
| BD |  0.5960 |  0.2990 |
| BE |  0.6010 |  0.3070 |
| BF |  0.5950 |  0.3010 |
| CA |  0.6260 |  0.3110 |
| CB |  0.6220 |  0.3150 |
| CC |  0.6320 |  0.3320 |
| CD |  0.6150 |  0.3200 |
| CE |  0.6300 |  0.3330 |
| CF |  0.6100 |  0.3180 |
| DA |  0.5770 |  0.2440 |
| DB |  0.5780 |  0.2570 |
| DC |  0.5930 |  0.2760 |
| DD |  0.5840 |  0.2740 |
| DE |  0.6070 |  0.2910 |
| DF |  0.5910 |  0.2810 |

























Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| EA |  0.4910 |  0.1470 |
| EB |  0.4920 |  0.1590 |
| EC |  0.5110 |  0.1740 |
| ED |  0.5160 |  0.1840 |
| EE |  0.5280 |  0.1930 |
| EF |  0.5370 |  0.1920 |
| FA |  0.4420 |  0.0830 |
| FB |  0.4360 |  0.0790 |
| FC |  0.4550 |  0.1020 |
| FD |  0.4540 |  0.0930 |
| FE |  0.4710 |  0.1180 |
| FF |  0.4690 |  0.1070 |
| GA |  0.4110 |  0.0660 |
| GB |  0.3980 |  0.0560 |
| GC |  0.3960 |  0.0590 |
| GD |  0.4050 |  0.0600 |
| GE |  0.3990 |  0.0610 |
| GF |  0.4020 |  0.0600 |
| HA |  0.4130 |  0.0920 |
| HB |  0.4100 |  0.0860 |
| HC |  0.4060 |  0.0940 |
| HD |  0.4010 |  0.0810 |
| HE |  0.3880 |  0.0820 |
| HF |  0.3920 |  0.0700 |
| IA |  0.4020 |  0.0900 |
| IB |  0.4040 |  0.1020 |
| IC |  0.4120 |  0.0990 |
| ID |  0.4030 |  0.0910 |
| IE |  0.3970 |  0.0860 |
| IF |  0.3970 |  0.0790 |
| JA |  0.3890 |  0.0790 |
| JB |  0.3830 |  0.0710 |
| JC |  0.3810 |  0.0730 |
| JD |  0.3620 |  0.0510 |
| JE |  0.3660 |  0.0600 |
| JF |  0.3490 |  0.0390 |
| KA |  0.3580 |  0.0460 |
| KB |  0.3710 |  0.0480 |
| KC |  0.3560 |  0.0400 |
| KD |  0.3740 |  0.0360 |
| KE |  0.3550 |  0.0260 |
| KF |  0.3780 |  0.0200 |

Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| LA |  0.4220 |  0.0710 |
| LB |  0.4300 |  0.0830 |
| LC |  0.4260 |  0.0750 |
| LD |  0.4330 |  0.0810 |
| LE |  0.4340 |  0.0670 |
| LF |  0.4380 |  0.0680 |
| MA |  0.4860 |  0.1590 |
| MB |  0.4740 |  0.1390 |
| MC |  0.4840 |  0.1490 |
| MD |  0.4750 |  0.1330 |
| ME |  0.4740 |  0.1310 |
| MF |  0.4850 |  0.1170 |