



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 PM GMT

PDB ID : 4V41
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-MONOCLINIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 2000-06-07
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

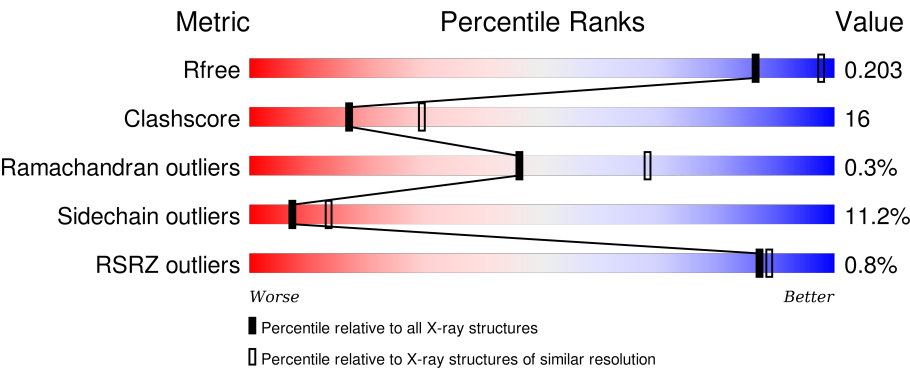
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 91344 | 3553 (2.50-2.50) |
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |
| RSRZ outliers | 91569 | 3562 (2.50-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1023 | <div><div>59%</div><div>30%</div><div>9%</div><div>.</div></div> |
| 1 | B | 1023 | <div><div>58%</div><div>31%</div><div>9%</div><div>.</div></div> |
| 1 | C | 1023 | <div><div>58%</div><div>32%</div><div>9%</div><div>.</div></div> |
| 1 | D | 1023 | <div><div>58%</div><div>30%</div><div>9%</div><div>.</div></div> |
| 1 | E | 1023 | <div><div>59%</div><div>30%</div><div>9%</div><div>.</div></div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | F | 1023 |  58% 31% 9% • |
| 1 | G | 1023 |  58% 31% 9% • |
| 1 | H | 1023 |  58% 31% 9% • |
| 1 | I | 1023 |  58% 31% 9% • |
| 1 | J | 1023 |  58% 31% 9% • |
| 1 | K | 1023 |  58% 31% 9% • |
| 1 | L | 1023 |  58% 31% 9% • |
| 1 | M | 1023 |  59% 30% 9% • |
| 1 | N | 1023 |  59% 30% 9% • |
| 1 | O | 1023 |  58% 31% 9% • |
| 1 | P | 1023 |  58% 32% 9% • |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 138704 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called BETA-GALACTOSIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | B | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | C | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | D | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | E | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | F | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | G | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | H | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | I | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | J | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | K | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | L | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | M | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | N | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | O | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |
| 1 | P | 1021 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 8232 | 5201 | 1462 | 1528 | 41 | | | |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| A | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| A | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| B | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| B | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| B | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| C | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| C | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| C | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| D | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| D | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| D | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| E | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| E | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| E | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| F | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| F | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| F | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| G | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| G | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| G | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| H | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| H | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| H | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| I | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| I | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| I | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| J | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| J | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| J | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| K | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| K | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| K | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| L | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| L | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| L | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| M | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| M | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| M | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| N | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| N | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| N | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| O | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| O | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| O | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| P | 748 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| P | 914 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |
| P | 1021 | CME | CYS | MODIFIED RESIDUE | UNP P00722 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

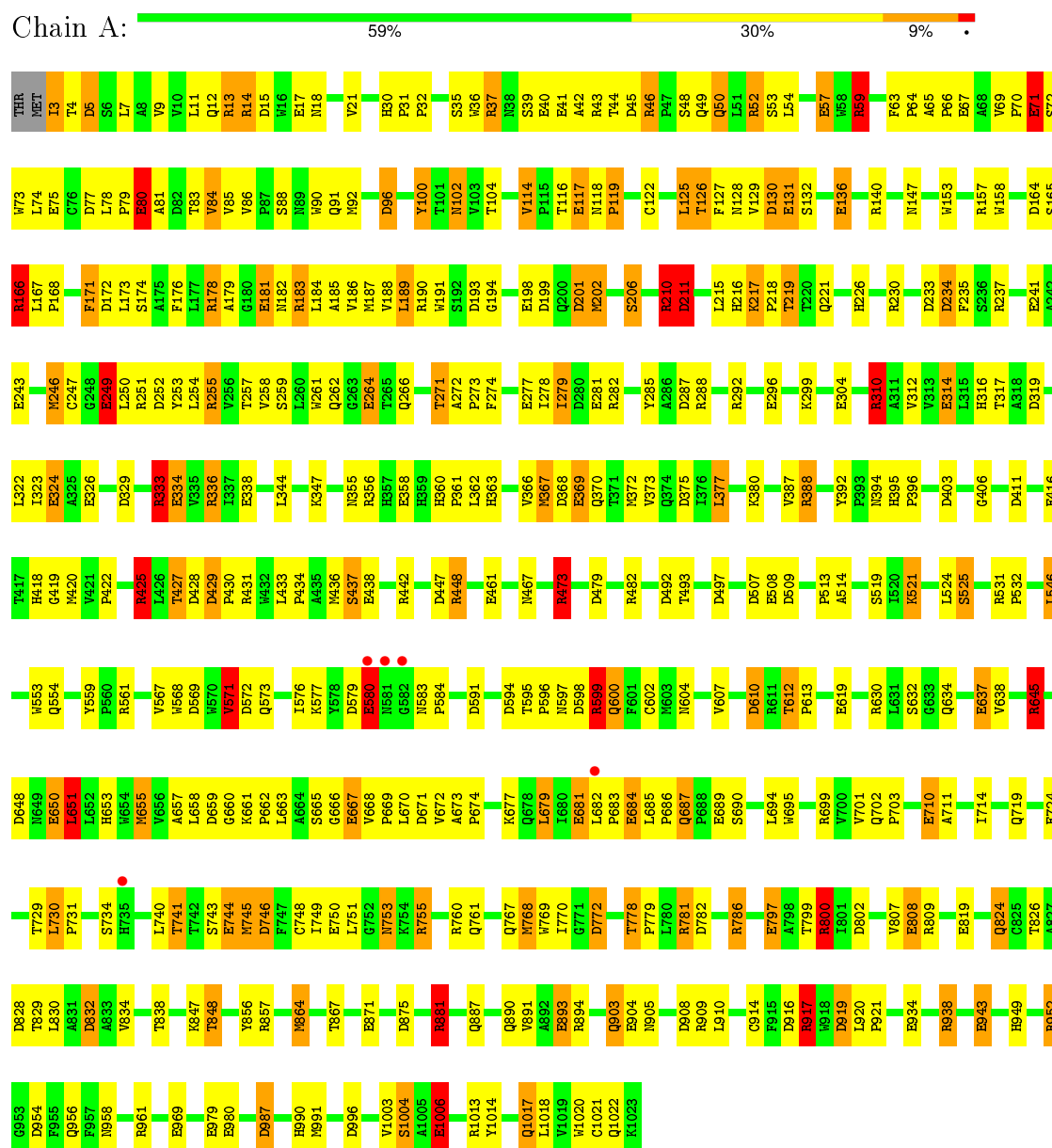
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3 | A | 434 | Total O 434 434 | 0 | 0 |
| 3 | B | 436 | Total O 436 436 | 0 | 0 |
| 3 | C | 433 | Total O 433 433 | 0 | 0 |
| 3 | D | 437 | Total O 437 437 | 0 | 0 |
| 3 | E | 435 | Total O 435 435 | 0 | 0 |
| 3 | F | 436 | Total O 436 436 | 0 | 0 |
| 3 | G | 434 | Total O 434 434 | 0 | 0 |
| 3 | H | 435 | Total O 435 435 | 0 | 0 |
| 3 | I | 434 | Total O 434 434 | 0 | 0 |
| 3 | J | 436 | Total O 436 436 | 0 | 0 |
| 3 | K | 435 | Total O 435 435 | 0 | 0 |
| 3 | L | 435 | Total O 435 435 | 0 | 0 |
| 3 | M | 434 | Total O 434 434 | 0 | 0 |
| 3 | N | 436 | Total O 436 436 | 0 | 0 |
| 3 | O | 433 | Total O 433 433 | 0 | 0 |
| 3 | P | 437 | Total O 437 437 | 0 | 0 |

3 Residue-property plots

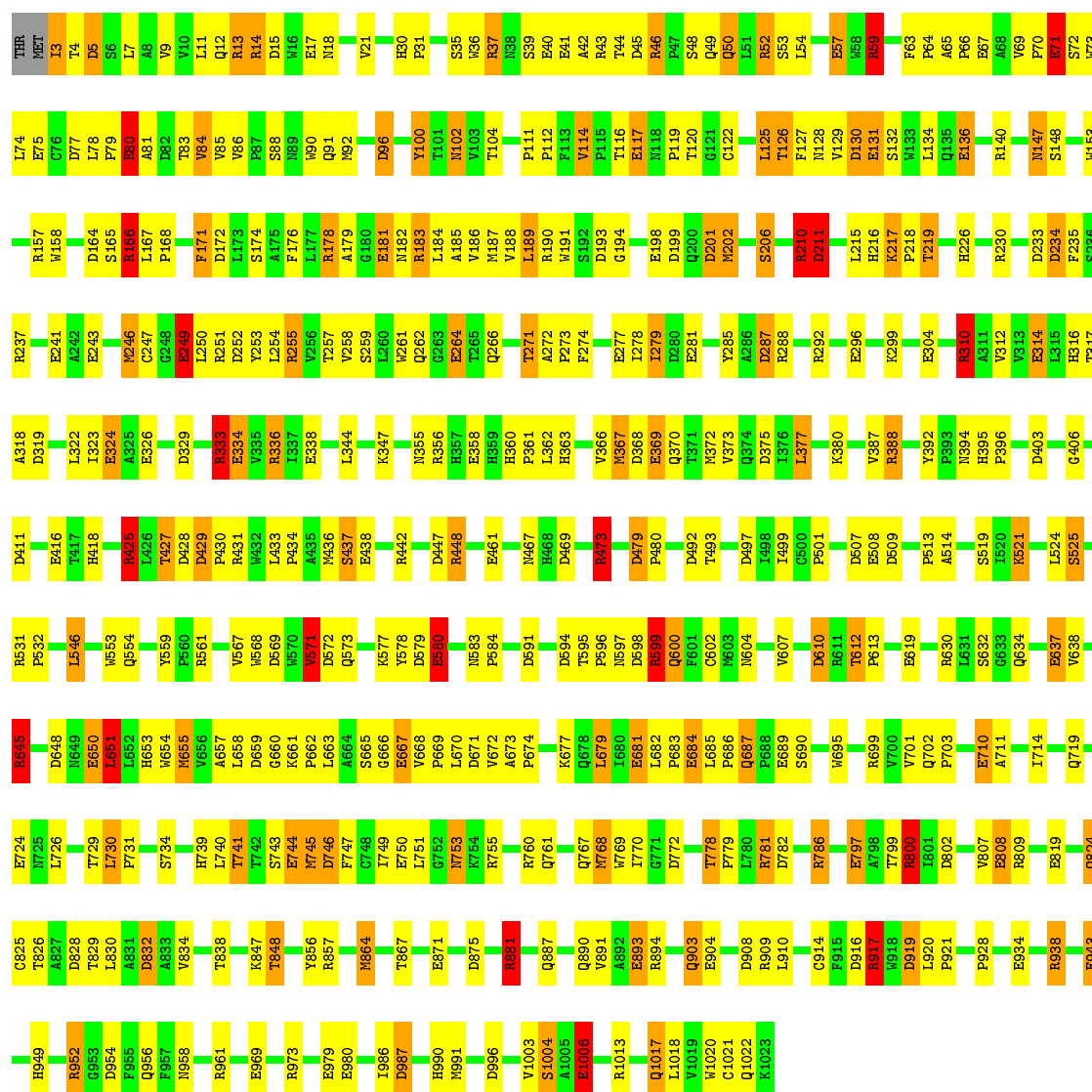
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: BETA-GALACTOSIDASE



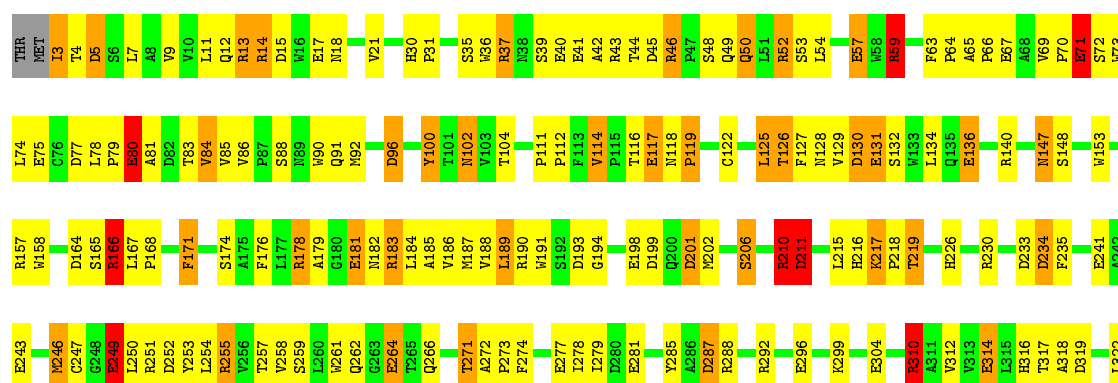
• Molecule 1: BETA-GALACTOSIDASE

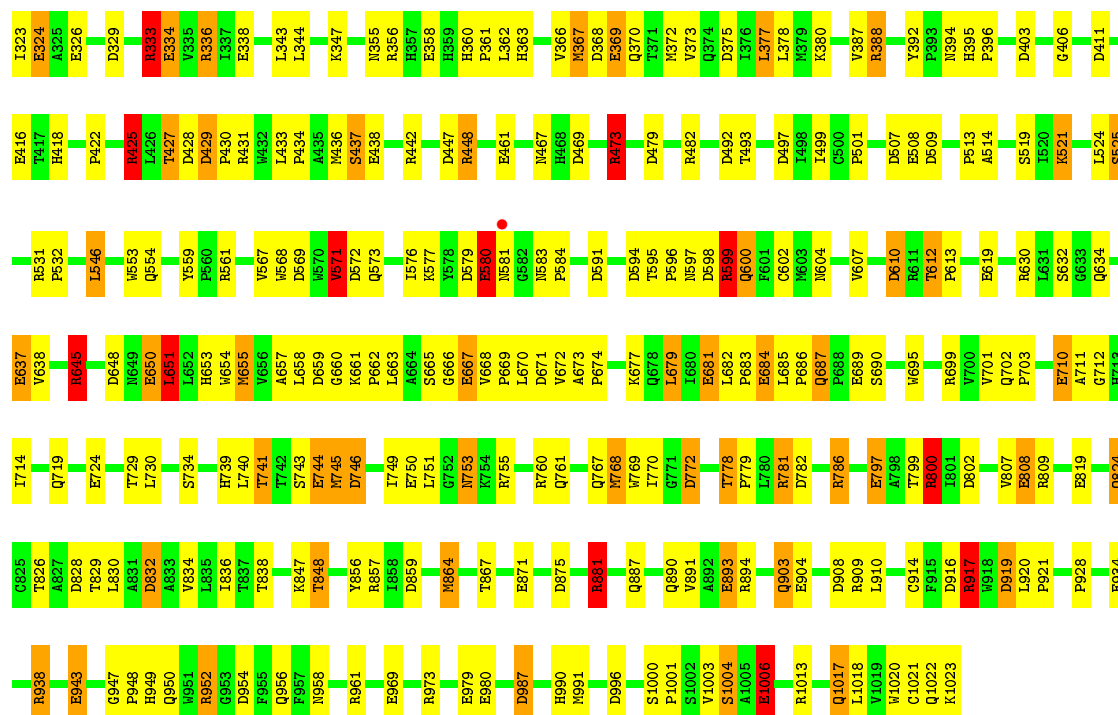
Chain B: 



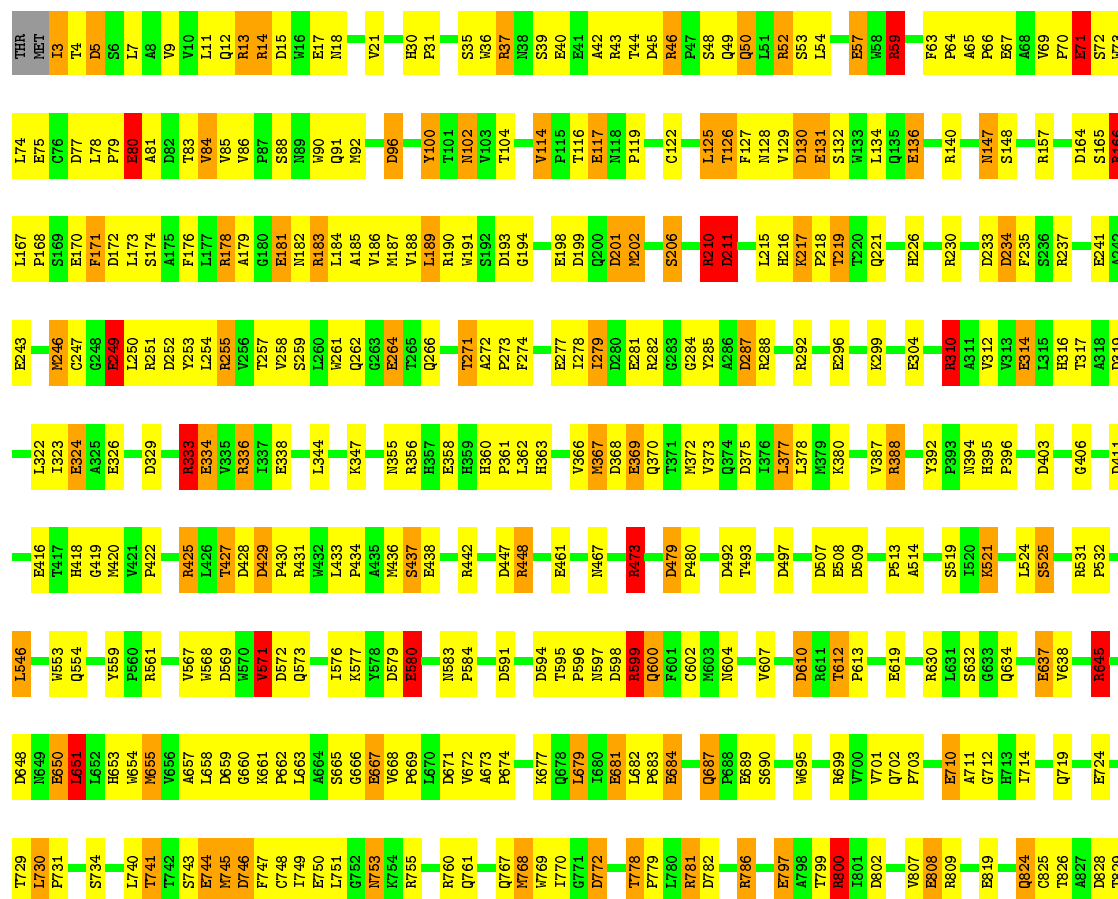
• Molecule 1: BETA-GALACTOSIDASE

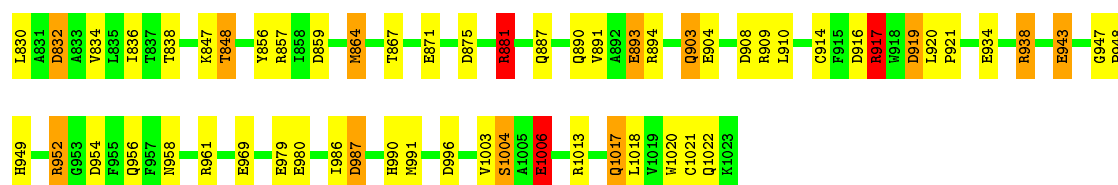
Chain C: 



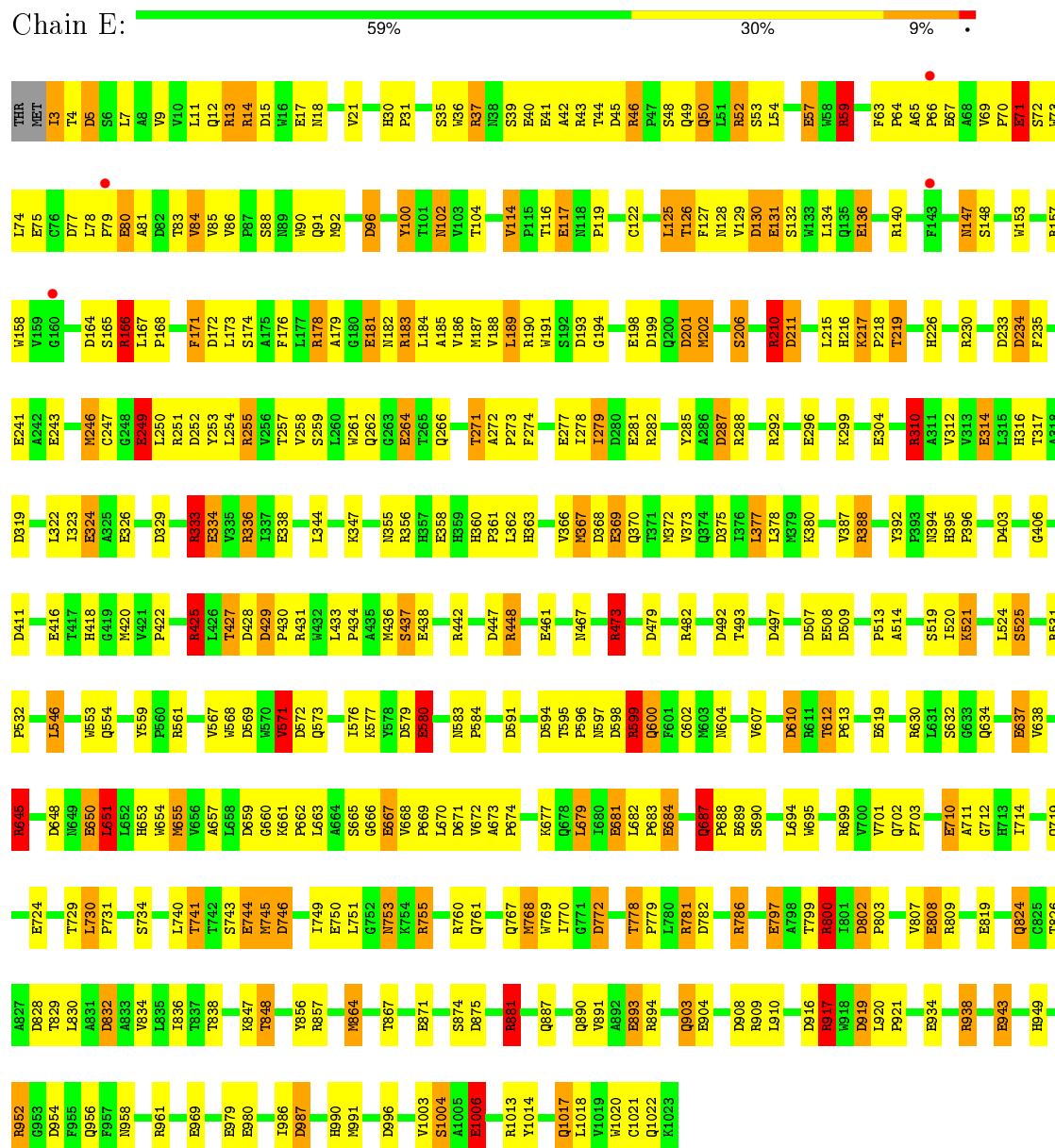


- Molecule 1: BETA-GALACTOSIDASE

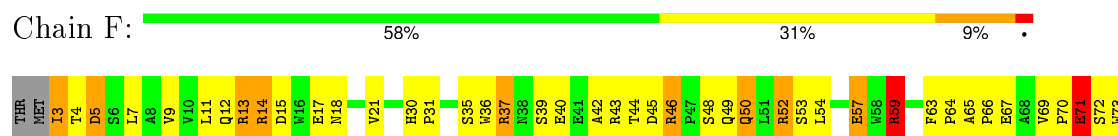




• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





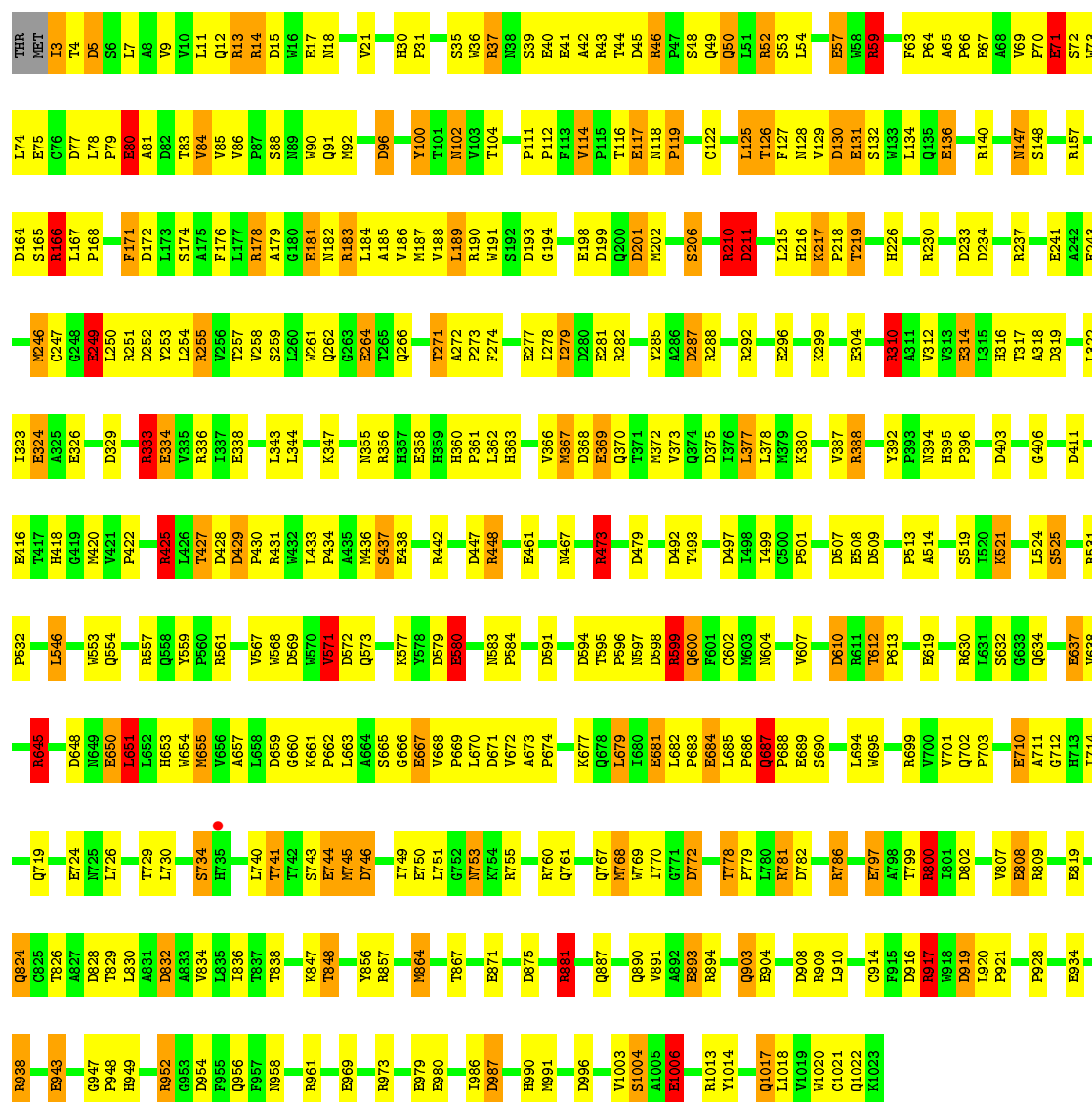
| Response | Percentage |
|------------------|------------|
| Yes | 58% |
| No | 31% |
| Don't know | 9% |
| Refuse to answer | 2% |





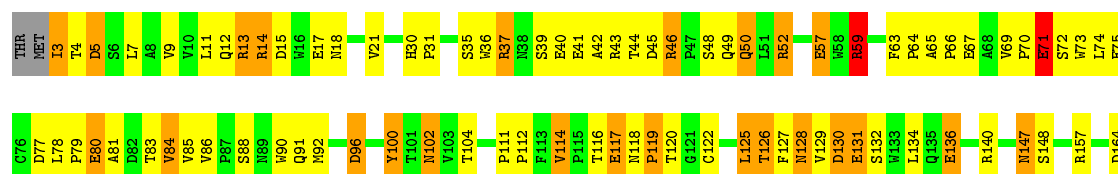
• Molecule 1: BETA-GALACTOSIDASE

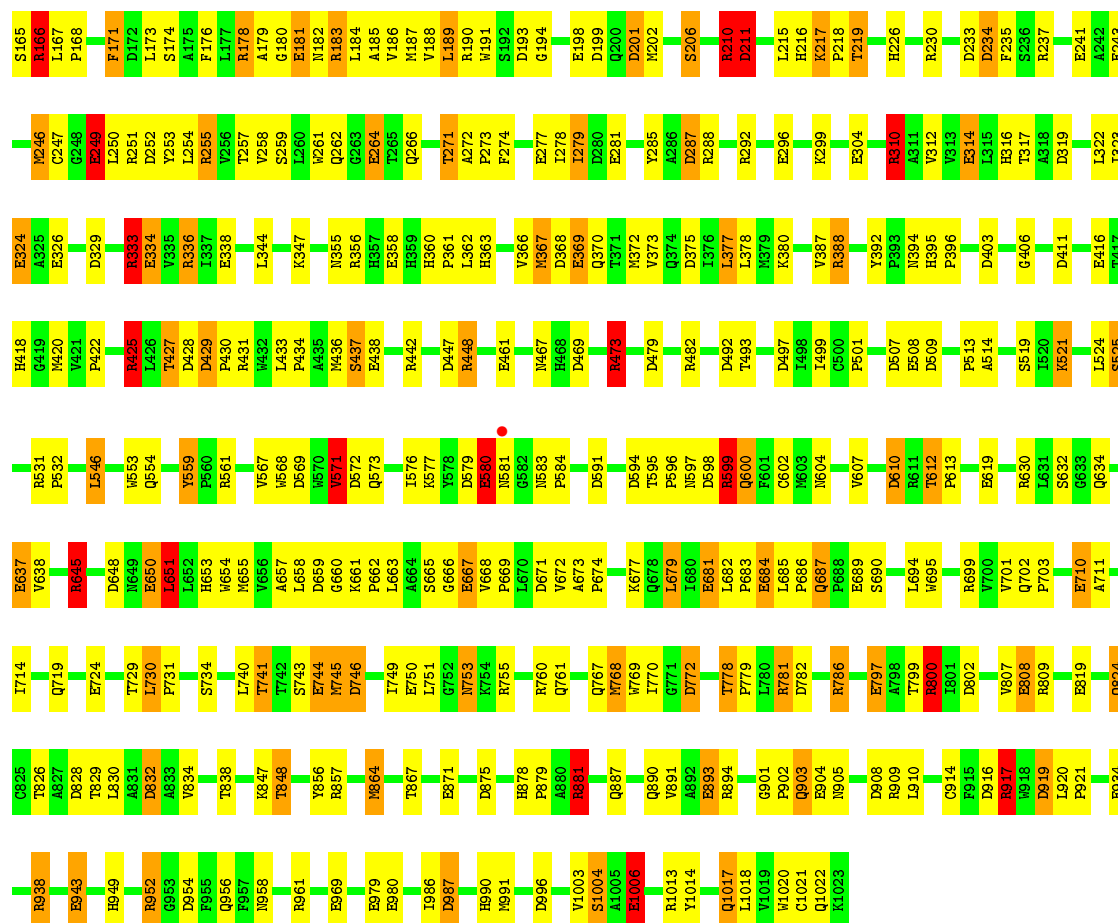
Chain I: 58% 31% 9%

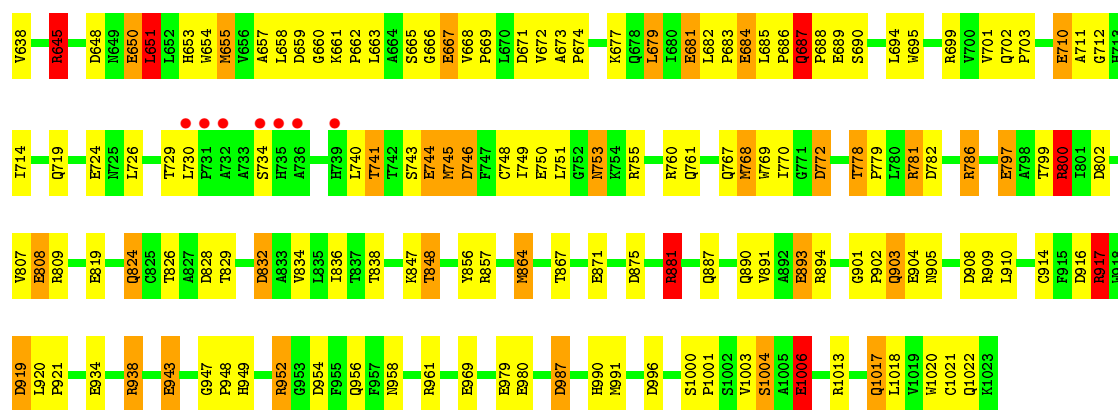


• Molecule 1: BETA-GALACTOSIDASE

Chain J: 58% 31% 9%

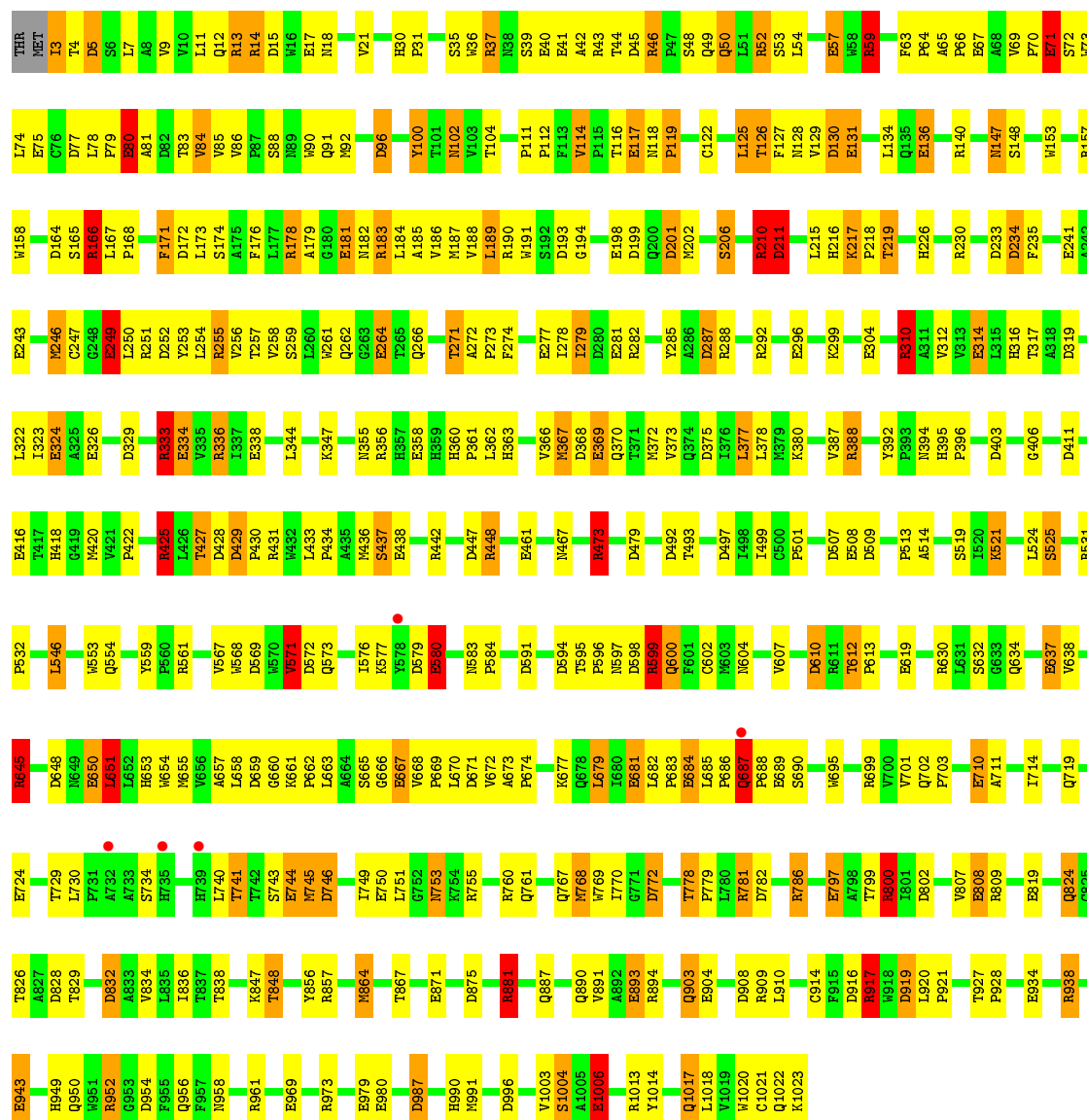






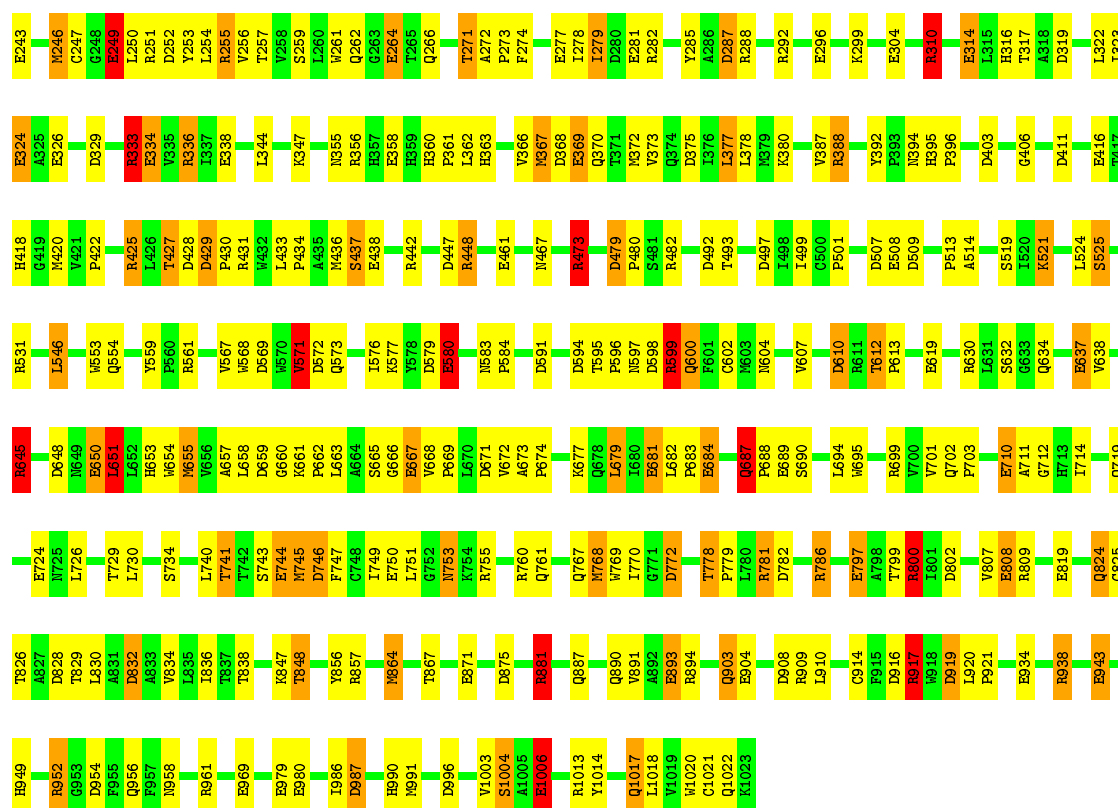
• Molecule 1: BETA-GALACTOSIDASE

Chain L:  58%  31% 9% •



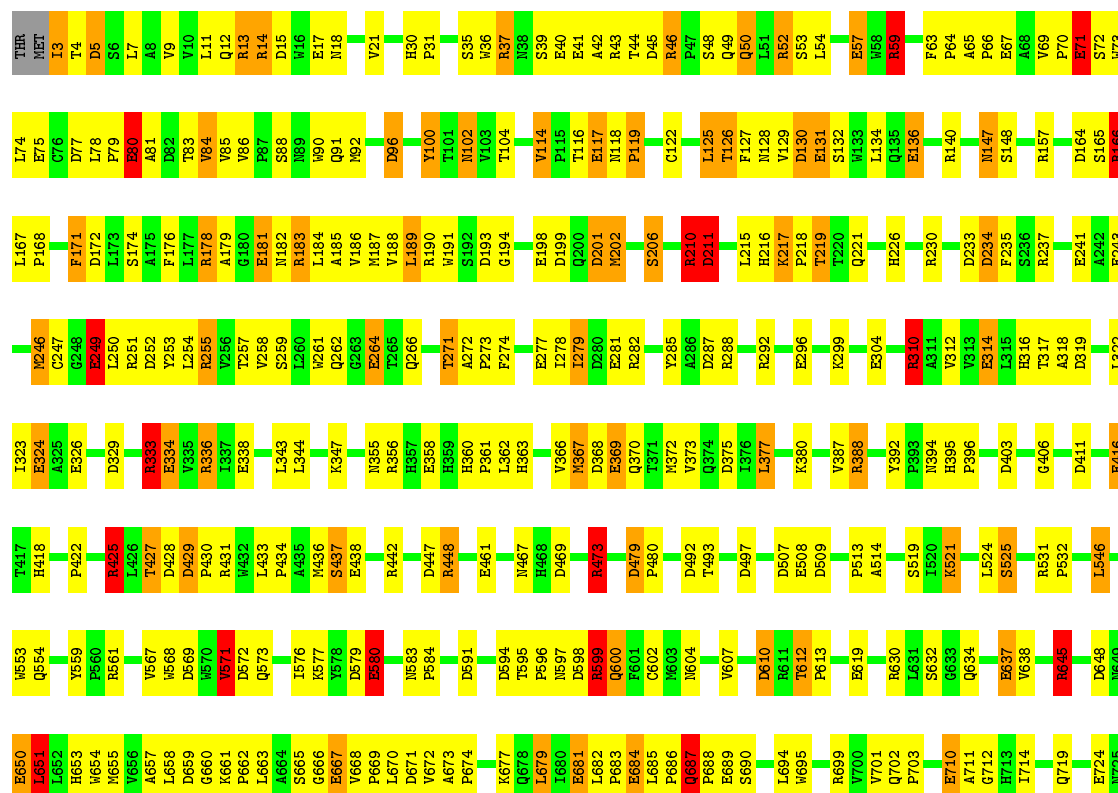
• Molecule 1: BETA-GALACTOSIDASE

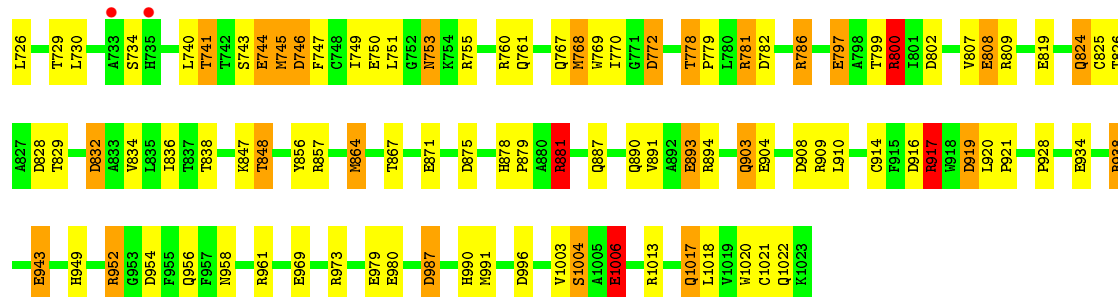




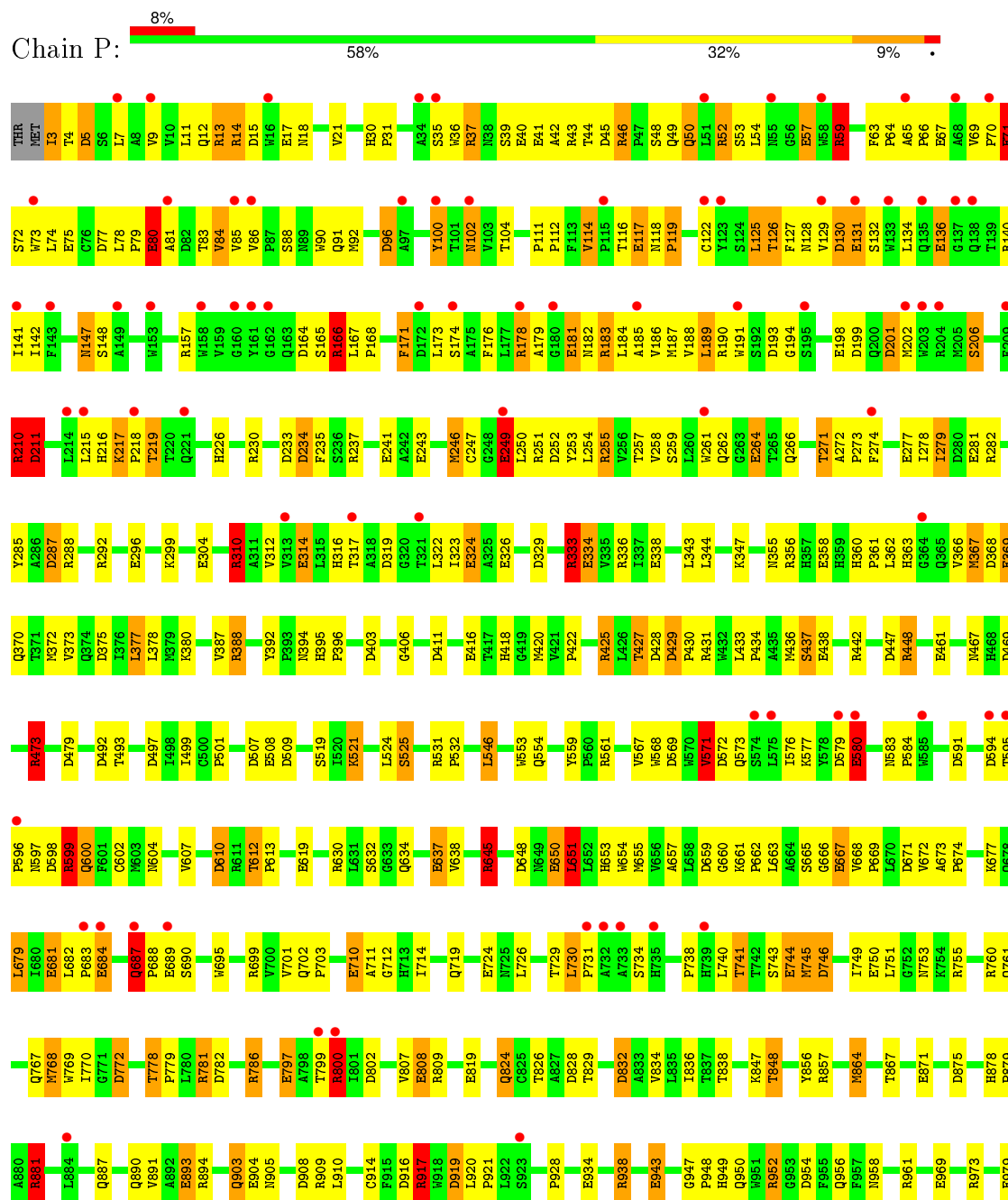
Molecule 1: BETA-GALACTOSIDASE

Chain O: 58% 31% 9%





• Molecule 1: BETA-GALACTOSIDASE



| | |
|-------|--|
| E980 | |
| I986 | |
| D987 | |
| H990 | |
| M991 | |
| D996 | |
| V1003 | |
| S1004 | |
| A1005 | |
| E1006 | |
| R1013 | |
| Y1014 | |
| Q1017 | |
| L1018 | |
| V1019 | |
| W1020 | |
| C1021 | |
| Q1022 | |
| K1023 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00° | Depositor |
| Resolution (Å) | (Not available) – 2.50 92.62 – 2.00 | Depositor EDS |
| % Data completeness (in resolution range) | 71.0 ((Not available)-2.50) 39.3 (92.62-2.00) | Depositor EDS |
| R_{merge} | 0.07 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.07 (at 2.00Å) | Xtriage |
| Refinement program | TNT | Depositor |
| R, R_{free} | 0.199 , 0.207 0.190 , 0.203 | Depositor DCC |
| R_{free} test set | 1680 reflections (0.29%) | DCC |
| Wilson B-factor (Å ²) | 27.6 | Xtriage |
| Anisotropy | 0.197 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 99.9 | EDS |
| Estimated twinning fraction | 0.009 for h,-k,-h-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 590207 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 138704 | wwPDB-VP |
| Average B, all atoms (Å ²) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | B | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | C | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | D | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | E | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | F | 1.23 | 55/8472 (0.6%) | 1.69 | 186/11553 (1.6%) |
| 1 | G | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | H | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | I | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | J | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | K | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | L | 1.23 | 56/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | M | 1.23 | 56/8472 (0.7%) | 1.69 | 189/11553 (1.6%) |
| 1 | N | 1.23 | 56/8472 (0.7%) | 1.69 | 187/11553 (1.6%) |
| 1 | O | 1.23 | 57/8472 (0.7%) | 1.69 | 188/11553 (1.6%) |
| 1 | P | 1.23 | 56/8472 (0.7%) | 1.69 | 187/11553 (1.6%) |
| All | All | 1.23 | 896/135552 (0.7%) | 1.69 | 3010/184848 (1.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 2 | 0 |
| 1 | B | 2 | 0 |
| 1 | C | 2 | 0 |
| 1 | D | 2 | 0 |
| 1 | E | 2 | 0 |
| 1 | F | 2 | 0 |
| 1 | G | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | H | 2 | 0 |
| 1 | I | 2 | 0 |
| 1 | J | 2 | 0 |
| 1 | K | 2 | 0 |
| 1 | L | 2 | 0 |
| 1 | M | 2 | 0 |
| 1 | N | 2 | 0 |
| 1 | O | 2 | 0 |
| 1 | P | 2 | 0 |
| All | All | 32 | 0 |

All (896) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 249 | GLU | CD-OE2 | 12.04 | 1.38 | 1.25 |
| 1 | O | 249 | GLU | CD-OE2 | 12.03 | 1.38 | 1.25 |
| 1 | H | 249 | GLU | CD-OE2 | 12.01 | 1.38 | 1.25 |
| 1 | J | 249 | GLU | CD-OE2 | 12.01 | 1.38 | 1.25 |
| 1 | P | 249 | GLU | CD-OE2 | 12.01 | 1.38 | 1.25 |
| 1 | I | 249 | GLU | CD-OE2 | 12.00 | 1.38 | 1.25 |
| 1 | B | 249 | GLU | CD-OE2 | 11.99 | 1.38 | 1.25 |
| 1 | F | 249 | GLU | CD-OE2 | 11.99 | 1.38 | 1.25 |
| 1 | D | 249 | GLU | CD-OE2 | 11.98 | 1.38 | 1.25 |
| 1 | A | 249 | GLU | CD-OE2 | 11.97 | 1.38 | 1.25 |
| 1 | N | 249 | GLU | CD-OE2 | 11.96 | 1.38 | 1.25 |
| 1 | K | 249 | GLU | CD-OE2 | 11.95 | 1.38 | 1.25 |
| 1 | E | 249 | GLU | CD-OE2 | 11.93 | 1.38 | 1.25 |
| 1 | M | 249 | GLU | CD-OE2 | 11.93 | 1.38 | 1.25 |
| 1 | L | 249 | GLU | CD-OE2 | 11.92 | 1.38 | 1.25 |
| 1 | G | 249 | GLU | CD-OE2 | 11.92 | 1.38 | 1.25 |
| 1 | M | 744 | GLU | CD-OE2 | 11.53 | 1.38 | 1.25 |
| 1 | L | 744 | GLU | CD-OE2 | 11.52 | 1.38 | 1.25 |
| 1 | K | 744 | GLU | CD-OE2 | 11.50 | 1.38 | 1.25 |
| 1 | H | 744 | GLU | CD-OE2 | 11.48 | 1.38 | 1.25 |
| 1 | J | 744 | GLU | CD-OE2 | 11.47 | 1.38 | 1.25 |
| 1 | C | 744 | GLU | CD-OE2 | 11.47 | 1.38 | 1.25 |
| 1 | B | 744 | GLU | CD-OE2 | 11.46 | 1.38 | 1.25 |
| 1 | G | 744 | GLU | CD-OE2 | 11.46 | 1.38 | 1.25 |
| 1 | D | 744 | GLU | CD-OE2 | 11.45 | 1.38 | 1.25 |
| 1 | A | 744 | GLU | CD-OE2 | 11.45 | 1.38 | 1.25 |
| 1 | E | 744 | GLU | CD-OE2 | 11.45 | 1.38 | 1.25 |
| 1 | P | 744 | GLU | CD-OE2 | 11.43 | 1.38 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | F | 744 | GLU | CD-OE2 | 11.43 | 1.38 | 1.25 |
| 1 | O | 744 | GLU | CD-OE2 | 11.40 | 1.38 | 1.25 |
| 1 | N | 744 | GLU | CD-OE2 | 11.38 | 1.38 | 1.25 |
| 1 | I | 744 | GLU | CD-OE2 | 11.37 | 1.38 | 1.25 |
| 1 | N | 689 | GLU | CD-OE2 | 10.61 | 1.37 | 1.25 |
| 1 | F | 689 | GLU | CD-OE2 | 10.59 | 1.37 | 1.25 |
| 1 | C | 689 | GLU | CD-OE2 | 10.58 | 1.37 | 1.25 |
| 1 | B | 689 | GLU | CD-OE2 | 10.54 | 1.37 | 1.25 |
| 1 | A | 689 | GLU | CD-OE2 | 10.53 | 1.37 | 1.25 |
| 1 | P | 689 | GLU | CD-OE2 | 10.53 | 1.37 | 1.25 |
| 1 | E | 689 | GLU | CD-OE2 | 10.52 | 1.37 | 1.25 |
| 1 | D | 689 | GLU | CD-OE2 | 10.52 | 1.37 | 1.25 |
| 1 | L | 689 | GLU | CD-OE2 | 10.51 | 1.37 | 1.25 |
| 1 | J | 689 | GLU | CD-OE2 | 10.50 | 1.37 | 1.25 |
| 1 | O | 689 | GLU | CD-OE2 | 10.50 | 1.37 | 1.25 |
| 1 | M | 689 | GLU | CD-OE2 | 10.50 | 1.37 | 1.25 |
| 1 | I | 689 | GLU | CD-OE2 | 10.49 | 1.37 | 1.25 |
| 1 | H | 689 | GLU | CD-OE2 | 10.49 | 1.37 | 1.25 |
| 1 | K | 689 | GLU | CD-OE2 | 10.49 | 1.37 | 1.25 |
| 1 | G | 689 | GLU | CD-OE2 | 10.48 | 1.37 | 1.25 |
| 1 | I | 819 | GLU | CD-OE2 | 10.44 | 1.37 | 1.25 |
| 1 | G | 819 | GLU | CD-OE2 | 10.42 | 1.37 | 1.25 |
| 1 | H | 819 | GLU | CD-OE2 | 10.41 | 1.37 | 1.25 |
| 1 | M | 819 | GLU | CD-OE2 | 10.41 | 1.37 | 1.25 |
| 1 | E | 819 | GLU | CD-OE2 | 10.41 | 1.37 | 1.25 |
| 1 | C | 819 | GLU | CD-OE2 | 10.40 | 1.37 | 1.25 |
| 1 | L | 819 | GLU | CD-OE2 | 10.39 | 1.37 | 1.25 |
| 1 | O | 819 | GLU | CD-OE2 | 10.39 | 1.37 | 1.25 |
| 1 | A | 819 | GLU | CD-OE2 | 10.39 | 1.37 | 1.25 |
| 1 | K | 819 | GLU | CD-OE2 | 10.38 | 1.37 | 1.25 |
| 1 | N | 819 | GLU | CD-OE2 | 10.38 | 1.37 | 1.25 |
| 1 | D | 819 | GLU | CD-OE2 | 10.37 | 1.37 | 1.25 |
| 1 | B | 819 | GLU | CD-OE2 | 10.37 | 1.37 | 1.25 |
| 1 | F | 819 | GLU | CD-OE2 | 10.34 | 1.37 | 1.25 |
| 1 | P | 819 | GLU | CD-OE2 | 10.33 | 1.37 | 1.25 |
| 1 | J | 819 | GLU | CD-OE2 | 10.32 | 1.37 | 1.25 |
| 1 | G | 75 | GLU | CD-OE2 | 10.18 | 1.36 | 1.25 |
| 1 | L | 75 | GLU | CD-OE2 | 10.18 | 1.36 | 1.25 |
| 1 | J | 75 | GLU | CD-OE2 | 10.18 | 1.36 | 1.25 |
| 1 | O | 75 | GLU | CD-OE2 | 10.18 | 1.36 | 1.25 |
| 1 | M | 75 | GLU | CD-OE2 | 10.17 | 1.36 | 1.25 |
| 1 | I | 75 | GLU | CD-OE2 | 10.15 | 1.36 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 75 | GLU | CD-OE2 | 10.15 | 1.36 | 1.25 |
| 1 | C | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | E | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | A | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | F | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | N | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | D | 75 | GLU | CD-OE2 | 10.14 | 1.36 | 1.25 |
| 1 | H | 75 | GLU | CD-OE2 | 10.10 | 1.36 | 1.25 |
| 1 | P | 75 | GLU | CD-OE2 | 10.10 | 1.36 | 1.25 |
| 1 | K | 75 | GLU | CD-OE2 | 10.09 | 1.36 | 1.25 |
| 1 | F | 580 | GLU | CD-OE2 | 9.81 | 1.36 | 1.25 |
| 1 | D | 580 | GLU | CD-OE2 | 9.79 | 1.36 | 1.25 |
| 1 | C | 580 | GLU | CD-OE2 | 9.78 | 1.36 | 1.25 |
| 1 | I | 580 | GLU | CD-OE2 | 9.76 | 1.36 | 1.25 |
| 1 | B | 580 | GLU | CD-OE2 | 9.75 | 1.36 | 1.25 |
| 1 | M | 580 | GLU | CD-OE2 | 9.75 | 1.36 | 1.25 |
| 1 | L | 580 | GLU | CD-OE2 | 9.74 | 1.36 | 1.25 |
| 1 | E | 580 | GLU | CD-OE2 | 9.74 | 1.36 | 1.25 |
| 1 | A | 580 | GLU | CD-OE2 | 9.73 | 1.36 | 1.25 |
| 1 | N | 580 | GLU | CD-OE2 | 9.72 | 1.36 | 1.25 |
| 1 | G | 580 | GLU | CD-OE2 | 9.72 | 1.36 | 1.25 |
| 1 | O | 580 | GLU | CD-OE2 | 9.71 | 1.36 | 1.25 |
| 1 | K | 580 | GLU | CD-OE2 | 9.71 | 1.36 | 1.25 |
| 1 | H | 580 | GLU | CD-OE2 | 9.70 | 1.36 | 1.25 |
| 1 | J | 580 | GLU | CD-OE2 | 9.70 | 1.36 | 1.25 |
| 1 | P | 580 | GLU | CD-OE2 | 9.70 | 1.36 | 1.25 |
| 1 | I | 131 | GLU | CD-OE2 | 9.58 | 1.36 | 1.25 |
| 1 | C | 131 | GLU | CD-OE2 | 9.58 | 1.36 | 1.25 |
| 1 | H | 131 | GLU | CD-OE2 | 9.57 | 1.36 | 1.25 |
| 1 | E | 131 | GLU | CD-OE2 | 9.54 | 1.36 | 1.25 |
| 1 | P | 131 | GLU | CD-OE2 | 9.54 | 1.36 | 1.25 |
| 1 | G | 131 | GLU | CD-OE2 | 9.53 | 1.36 | 1.25 |
| 1 | A | 131 | GLU | CD-OE2 | 9.52 | 1.36 | 1.25 |
| 1 | F | 131 | GLU | CD-OE2 | 9.50 | 1.36 | 1.25 |
| 1 | B | 131 | GLU | CD-OE2 | 9.50 | 1.36 | 1.25 |
| 1 | J | 131 | GLU | CD-OE2 | 9.50 | 1.36 | 1.25 |
| 1 | K | 131 | GLU | CD-OE2 | 9.50 | 1.36 | 1.25 |
| 1 | D | 131 | GLU | CD-OE2 | 9.49 | 1.36 | 1.25 |
| 1 | O | 131 | GLU | CD-OE2 | 9.48 | 1.36 | 1.25 |
| 1 | M | 131 | GLU | CD-OE2 | 9.48 | 1.36 | 1.25 |
| 1 | N | 131 | GLU | CD-OE2 | 9.47 | 1.36 | 1.25 |
| 1 | L | 131 | GLU | CD-OE2 | 9.46 | 1.36 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | N | 980 | GLU | CD-OE2 | 9.37 | 1.35 | 1.25 |
| 1 | G | 980 | GLU | CD-OE2 | 9.37 | 1.35 | 1.25 |
| 1 | M | 980 | GLU | CD-OE2 | 9.36 | 1.35 | 1.25 |
| 1 | B | 980 | GLU | CD-OE2 | 9.35 | 1.35 | 1.25 |
| 1 | E | 980 | GLU | CD-OE2 | 9.32 | 1.35 | 1.25 |
| 1 | D | 980 | GLU | CD-OE2 | 9.32 | 1.35 | 1.25 |
| 1 | F | 980 | GLU | CD-OE2 | 9.31 | 1.35 | 1.25 |
| 1 | A | 980 | GLU | CD-OE2 | 9.31 | 1.35 | 1.25 |
| 1 | O | 980 | GLU | CD-OE2 | 9.29 | 1.35 | 1.25 |
| 1 | H | 980 | GLU | CD-OE2 | 9.28 | 1.35 | 1.25 |
| 1 | L | 980 | GLU | CD-OE2 | 9.27 | 1.35 | 1.25 |
| 1 | I | 980 | GLU | CD-OE2 | 9.27 | 1.35 | 1.25 |
| 1 | J | 980 | GLU | CD-OE2 | 9.27 | 1.35 | 1.25 |
| 1 | D | 684 | GLU | CD-OE2 | 9.26 | 1.35 | 1.25 |
| 1 | C | 980 | GLU | CD-OE2 | 9.25 | 1.35 | 1.25 |
| 1 | K | 980 | GLU | CD-OE2 | 9.24 | 1.35 | 1.25 |
| 1 | P | 980 | GLU | CD-OE2 | 9.22 | 1.35 | 1.25 |
| 1 | G | 684 | GLU | CD-OE2 | 9.20 | 1.35 | 1.25 |
| 1 | O | 684 | GLU | CD-OE2 | 9.20 | 1.35 | 1.25 |
| 1 | K | 684 | GLU | CD-OE2 | 9.19 | 1.35 | 1.25 |
| 1 | M | 684 | GLU | CD-OE2 | 9.19 | 1.35 | 1.25 |
| 1 | P | 684 | GLU | CD-OE2 | 9.19 | 1.35 | 1.25 |
| 1 | F | 684 | GLU | CD-OE2 | 9.19 | 1.35 | 1.25 |
| 1 | A | 684 | GLU | CD-OE2 | 9.19 | 1.35 | 1.25 |
| 1 | N | 684 | GLU | CD-OE2 | 9.18 | 1.35 | 1.25 |
| 1 | L | 684 | GLU | CD-OE2 | 9.17 | 1.35 | 1.25 |
| 1 | C | 684 | GLU | CD-OE2 | 9.16 | 1.35 | 1.25 |
| 1 | B | 684 | GLU | CD-OE2 | 9.16 | 1.35 | 1.25 |
| 1 | I | 684 | GLU | CD-OE2 | 9.15 | 1.35 | 1.25 |
| 1 | H | 684 | GLU | CD-OE2 | 9.15 | 1.35 | 1.25 |
| 1 | E | 684 | GLU | CD-OE2 | 9.13 | 1.35 | 1.25 |
| 1 | J | 684 | GLU | CD-OE2 | 9.12 | 1.35 | 1.25 |
| 1 | M | 296 | GLU | CD-OE2 | 9.06 | 1.35 | 1.25 |
| 1 | N | 296 | GLU | CD-OE2 | 9.04 | 1.35 | 1.25 |
| 1 | H | 296 | GLU | CD-OE2 | 9.03 | 1.35 | 1.25 |
| 1 | O | 296 | GLU | CD-OE2 | 9.03 | 1.35 | 1.25 |
| 1 | B | 296 | GLU | CD-OE2 | 9.02 | 1.35 | 1.25 |
| 1 | G | 296 | GLU | CD-OE2 | 9.02 | 1.35 | 1.25 |
| 1 | A | 296 | GLU | CD-OE2 | 9.02 | 1.35 | 1.25 |
| 1 | E | 296 | GLU | CD-OE2 | 9.02 | 1.35 | 1.25 |
| 1 | C | 296 | GLU | CD-OE2 | 9.02 | 1.35 | 1.25 |
| 1 | F | 296 | GLU | CD-OE2 | 9.01 | 1.35 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | C | 181 | GLU | CD-OE2 | 9.01 | 1.35 | 1.25 |
| 1 | L | 296 | GLU | CD-OE2 | 9.01 | 1.35 | 1.25 |
| 1 | D | 181 | GLU | CD-OE2 | 9.00 | 1.35 | 1.25 |
| 1 | J | 296 | GLU | CD-OE2 | 9.00 | 1.35 | 1.25 |
| 1 | K | 296 | GLU | CD-OE2 | 9.00 | 1.35 | 1.25 |
| 1 | I | 296 | GLU | CD-OE2 | 8.99 | 1.35 | 1.25 |
| 1 | H | 181 | GLU | CD-OE2 | 8.99 | 1.35 | 1.25 |
| 1 | D | 296 | GLU | CD-OE2 | 8.99 | 1.35 | 1.25 |
| 1 | I | 181 | GLU | CD-OE2 | 8.98 | 1.35 | 1.25 |
| 1 | N | 181 | GLU | CD-OE2 | 8.98 | 1.35 | 1.25 |
| 1 | P | 296 | GLU | CD-OE2 | 8.98 | 1.35 | 1.25 |
| 1 | J | 181 | GLU | CD-OE2 | 8.97 | 1.35 | 1.25 |
| 1 | A | 181 | GLU | CD-OE2 | 8.96 | 1.35 | 1.25 |
| 1 | K | 181 | GLU | CD-OE2 | 8.95 | 1.35 | 1.25 |
| 1 | G | 181 | GLU | CD-OE2 | 8.94 | 1.35 | 1.25 |
| 1 | B | 181 | GLU | CD-OE2 | 8.93 | 1.35 | 1.25 |
| 1 | M | 181 | GLU | CD-OE2 | 8.93 | 1.35 | 1.25 |
| 1 | O | 181 | GLU | CD-OE2 | 8.93 | 1.35 | 1.25 |
| 1 | E | 181 | GLU | CD-OE2 | 8.92 | 1.35 | 1.25 |
| 1 | F | 181 | GLU | CD-OE2 | 8.92 | 1.35 | 1.25 |
| 1 | L | 181 | GLU | CD-OE2 | 8.92 | 1.35 | 1.25 |
| 1 | G | 136 | GLU | CD-OE2 | 8.91 | 1.35 | 1.25 |
| 1 | L | 136 | GLU | CD-OE2 | 8.90 | 1.35 | 1.25 |
| 1 | O | 136 | GLU | CD-OE2 | 8.89 | 1.35 | 1.25 |
| 1 | P | 181 | GLU | CD-OE2 | 8.88 | 1.35 | 1.25 |
| 1 | K | 136 | GLU | CD-OE2 | 8.87 | 1.35 | 1.25 |
| 1 | B | 136 | GLU | CD-OE2 | 8.85 | 1.35 | 1.25 |
| 1 | E | 136 | GLU | CD-OE2 | 8.85 | 1.35 | 1.25 |
| 1 | D | 136 | GLU | CD-OE2 | 8.85 | 1.35 | 1.25 |
| 1 | F | 136 | GLU | CD-OE2 | 8.83 | 1.35 | 1.25 |
| 1 | A | 136 | GLU | CD-OE2 | 8.83 | 1.35 | 1.25 |
| 1 | C | 136 | GLU | CD-OE2 | 8.82 | 1.35 | 1.25 |
| 1 | P | 136 | GLU | CD-OE2 | 8.81 | 1.35 | 1.25 |
| 1 | J | 136 | GLU | CD-OE2 | 8.81 | 1.35 | 1.25 |
| 1 | I | 136 | GLU | CD-OE2 | 8.80 | 1.35 | 1.25 |
| 1 | H | 136 | GLU | CD-OE2 | 8.79 | 1.35 | 1.25 |
| 1 | N | 136 | GLU | CD-OE2 | 8.78 | 1.35 | 1.25 |
| 1 | E | 710 | GLU | CD-OE2 | 8.75 | 1.35 | 1.25 |
| 1 | N | 710 | GLU | CD-OE2 | 8.74 | 1.35 | 1.25 |
| 1 | M | 136 | GLU | CD-OE2 | 8.74 | 1.35 | 1.25 |
| 1 | P | 710 | GLU | CD-OE2 | 8.73 | 1.35 | 1.25 |
| 1 | F | 710 | GLU | CD-OE2 | 8.72 | 1.35 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | H | 710 | GLU | CD-OE2 | 8.71 | 1.35 | 1.25 |
| 1 | O | 710 | GLU | CD-OE2 | 8.70 | 1.35 | 1.25 |
| 1 | L | 710 | GLU | CD-OE2 | 8.70 | 1.35 | 1.25 |
| 1 | J | 710 | GLU | CD-OE2 | 8.70 | 1.35 | 1.25 |
| 1 | M | 710 | GLU | CD-OE2 | 8.70 | 1.35 | 1.25 |
| 1 | G | 710 | GLU | CD-OE2 | 8.69 | 1.35 | 1.25 |
| 1 | I | 710 | GLU | CD-OE2 | 8.69 | 1.35 | 1.25 |
| 1 | A | 710 | GLU | CD-OE2 | 8.68 | 1.35 | 1.25 |
| 1 | K | 710 | GLU | CD-OE2 | 8.66 | 1.35 | 1.25 |
| 1 | D | 710 | GLU | CD-OE2 | 8.66 | 1.35 | 1.25 |
| 1 | C | 710 | GLU | CD-OE2 | 8.65 | 1.35 | 1.25 |
| 1 | B | 710 | GLU | CD-OE2 | 8.62 | 1.35 | 1.25 |
| 1 | H | 264 | GLU | CD-OE2 | 8.60 | 1.35 | 1.25 |
| 1 | N | 264 | GLU | CD-OE2 | 8.58 | 1.35 | 1.25 |
| 1 | K | 264 | GLU | CD-OE2 | 8.57 | 1.35 | 1.25 |
| 1 | G | 264 | GLU | CD-OE2 | 8.57 | 1.35 | 1.25 |
| 1 | C | 264 | GLU | CD-OE2 | 8.57 | 1.35 | 1.25 |
| 1 | O | 264 | GLU | CD-OE2 | 8.57 | 1.35 | 1.25 |
| 1 | J | 264 | GLU | CD-OE2 | 8.56 | 1.35 | 1.25 |
| 1 | D | 264 | GLU | CD-OE2 | 8.55 | 1.35 | 1.25 |
| 1 | P | 264 | GLU | CD-OE2 | 8.54 | 1.35 | 1.25 |
| 1 | M | 264 | GLU | CD-OE2 | 8.53 | 1.35 | 1.25 |
| 1 | B | 264 | GLU | CD-OE2 | 8.52 | 1.35 | 1.25 |
| 1 | A | 264 | GLU | CD-OE2 | 8.52 | 1.35 | 1.25 |
| 1 | L | 264 | GLU | CD-OE2 | 8.51 | 1.35 | 1.25 |
| 1 | I | 264 | GLU | CD-OE2 | 8.50 | 1.34 | 1.25 |
| 1 | E | 264 | GLU | CD-OE2 | 8.50 | 1.34 | 1.25 |
| 1 | F | 264 | GLU | CD-OE2 | 8.49 | 1.34 | 1.25 |
| 1 | M | 797 | GLU | CD-OE2 | 8.44 | 1.34 | 1.25 |
| 1 | J | 797 | GLU | CD-OE2 | 8.44 | 1.34 | 1.25 |
| 1 | N | 797 | GLU | CD-OE2 | 8.42 | 1.34 | 1.25 |
| 1 | C | 277 | GLU | CD-OE2 | 8.42 | 1.34 | 1.25 |
| 1 | F | 797 | GLU | CD-OE2 | 8.41 | 1.34 | 1.25 |
| 1 | G | 797 | GLU | CD-OE2 | 8.41 | 1.34 | 1.25 |
| 1 | I | 277 | GLU | CD-OE2 | 8.41 | 1.34 | 1.25 |
| 1 | A | 797 | GLU | CD-OE2 | 8.40 | 1.34 | 1.25 |
| 1 | O | 797 | GLU | CD-OE2 | 8.40 | 1.34 | 1.25 |
| 1 | H | 797 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |
| 1 | B | 797 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |
| 1 | I | 797 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |
| 1 | O | 508 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |
| 1 | P | 797 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | K | 797 | GLU | CD-OE2 | 8.38 | 1.34 | 1.25 |
| 1 | E | 797 | GLU | CD-OE2 | 8.38 | 1.34 | 1.25 |
| 1 | F | 277 | GLU | CD-OE2 | 8.36 | 1.34 | 1.25 |
| 1 | A | 277 | GLU | CD-OE2 | 8.36 | 1.34 | 1.25 |
| 1 | E | 508 | GLU | CD-OE2 | 8.36 | 1.34 | 1.25 |
| 1 | M | 277 | GLU | CD-OE2 | 8.35 | 1.34 | 1.25 |
| 1 | O | 277 | GLU | CD-OE2 | 8.35 | 1.34 | 1.25 |
| 1 | L | 797 | GLU | CD-OE2 | 8.34 | 1.34 | 1.25 |
| 1 | J | 277 | GLU | CD-OE2 | 8.34 | 1.34 | 1.25 |
| 1 | C | 508 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | I | 508 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | D | 797 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | C | 797 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | E | 277 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | G | 508 | GLU | CD-OE2 | 8.33 | 1.34 | 1.25 |
| 1 | H | 508 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | B | 508 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | D | 508 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | N | 277 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | D | 277 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | J | 508 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | M | 508 | GLU | CD-OE2 | 8.32 | 1.34 | 1.25 |
| 1 | L | 508 | GLU | CD-OE2 | 8.31 | 1.34 | 1.25 |
| 1 | P | 277 | GLU | CD-OE2 | 8.31 | 1.34 | 1.25 |
| 1 | K | 277 | GLU | CD-OE2 | 8.31 | 1.34 | 1.25 |
| 1 | G | 277 | GLU | CD-OE2 | 8.31 | 1.34 | 1.25 |
| 1 | K | 508 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | F | 508 | GLU | CD-OE2 | 8.29 | 1.34 | 1.25 |
| 1 | H | 277 | GLU | CD-OE2 | 8.30 | 1.34 | 1.25 |
| 1 | L | 277 | GLU | CD-OE2 | 8.29 | 1.34 | 1.25 |
| 1 | N | 508 | GLU | CD-OE2 | 8.29 | 1.34 | 1.25 |
| 1 | B | 277 | GLU | CD-OE2 | 8.27 | 1.34 | 1.25 |
| 1 | A | 508 | GLU | CD-OE2 | 8.26 | 1.34 | 1.25 |
| 1 | P | 508 | GLU | CD-OE2 | 8.24 | 1.34 | 1.25 |
| 1 | G | 724 | GLU | CD-OE2 | 8.02 | 1.34 | 1.25 |
| 1 | I | 724 | GLU | CD-OE2 | 7.99 | 1.34 | 1.25 |
| 1 | J | 724 | GLU | CD-OE2 | 7.98 | 1.34 | 1.25 |
| 1 | K | 724 | GLU | CD-OE2 | 7.98 | 1.34 | 1.25 |
| 1 | M | 724 | GLU | CD-OE2 | 7.98 | 1.34 | 1.25 |
| 1 | E | 724 | GLU | CD-OE2 | 7.97 | 1.34 | 1.25 |
| 1 | O | 724 | GLU | CD-OE2 | 7.96 | 1.34 | 1.25 |
| 1 | C | 724 | GLU | CD-OE2 | 7.96 | 1.34 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | F | 724 | GLU | CD-OE2 | 7.95 | 1.34 | 1.25 |
| 1 | A | 724 | GLU | CD-OE2 | 7.95 | 1.34 | 1.25 |
| 1 | N | 724 | GLU | CD-OE2 | 7.94 | 1.34 | 1.25 |
| 1 | D | 893 | GLU | CD-OE2 | 7.94 | 1.34 | 1.25 |
| 1 | B | 724 | GLU | CD-OE2 | 7.93 | 1.34 | 1.25 |
| 1 | L | 724 | GLU | CD-OE2 | 7.93 | 1.34 | 1.25 |
| 1 | H | 724 | GLU | CD-OE2 | 7.92 | 1.34 | 1.25 |
| 1 | P | 724 | GLU | CD-OE2 | 7.91 | 1.34 | 1.25 |
| 1 | D | 724 | GLU | CD-OE2 | 7.91 | 1.34 | 1.25 |
| 1 | C | 893 | GLU | CD-OE2 | 7.89 | 1.34 | 1.25 |
| 1 | E | 893 | GLU | CD-OE2 | 7.88 | 1.34 | 1.25 |
| 1 | I | 893 | GLU | CD-OE2 | 7.88 | 1.34 | 1.25 |
| 1 | N | 893 | GLU | CD-OE2 | 7.88 | 1.34 | 1.25 |
| 1 | J | 893 | GLU | CD-OE2 | 7.87 | 1.34 | 1.25 |
| 1 | P | 893 | GLU | CD-OE2 | 7.87 | 1.34 | 1.25 |
| 1 | G | 893 | GLU | CD-OE2 | 7.87 | 1.34 | 1.25 |
| 1 | A | 893 | GLU | CD-OE2 | 7.83 | 1.34 | 1.25 |
| 1 | B | 893 | GLU | CD-OE2 | 7.82 | 1.34 | 1.25 |
| 1 | H | 893 | GLU | CD-OE2 | 7.82 | 1.34 | 1.25 |
| 1 | F | 893 | GLU | CD-OE2 | 7.79 | 1.34 | 1.25 |
| 1 | M | 893 | GLU | CD-OE2 | 7.78 | 1.34 | 1.25 |
| 1 | K | 893 | GLU | CD-OE2 | 7.78 | 1.34 | 1.25 |
| 1 | L | 893 | GLU | CD-OE2 | 7.77 | 1.34 | 1.25 |
| 1 | O | 893 | GLU | CD-OE2 | 7.76 | 1.34 | 1.25 |
| 1 | L | 438 | GLU | CD-OE2 | 7.58 | 1.33 | 1.25 |
| 1 | O | 438 | GLU | CD-OE2 | 7.58 | 1.33 | 1.25 |
| 1 | N | 438 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | H | 438 | GLU | CD-OE2 | 7.55 | 1.33 | 1.25 |
| 1 | I | 438 | GLU | CD-OE2 | 7.54 | 1.33 | 1.25 |
| 1 | J | 438 | GLU | CD-OE2 | 7.53 | 1.33 | 1.25 |
| 1 | C | 438 | GLU | CD-OE2 | 7.53 | 1.33 | 1.25 |
| 1 | A | 438 | GLU | CD-OE2 | 7.52 | 1.33 | 1.25 |
| 1 | F | 438 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | E | 438 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | G | 438 | GLU | CD-OE2 | 7.51 | 1.33 | 1.25 |
| 1 | D | 438 | GLU | CD-OE2 | 7.50 | 1.33 | 1.25 |
| 1 | K | 438 | GLU | CD-OE2 | 7.49 | 1.33 | 1.25 |
| 1 | M | 438 | GLU | CD-OE2 | 7.49 | 1.33 | 1.25 |
| 1 | B | 438 | GLU | CD-OE2 | 7.48 | 1.33 | 1.25 |
| 1 | O | 80 | GLU | CD-OE2 | 7.47 | 1.33 | 1.25 |
| 1 | H | 80 | GLU | CD-OE2 | 7.46 | 1.33 | 1.25 |
| 1 | K | 40 | GLU | CD-OE2 | 7.46 | 1.33 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | P | 438 | GLU | CD-OE2 | 7.46 | 1.33 | 1.25 |
| 1 | I | 40 | GLU | CD-OE2 | 7.45 | 1.33 | 1.25 |
| 1 | C | 80 | GLU | CD-OE2 | 7.45 | 1.33 | 1.25 |
| 1 | J | 80 | GLU | CD-OE2 | 7.45 | 1.33 | 1.25 |
| 1 | B | 80 | GLU | CD-OE2 | 7.45 | 1.33 | 1.25 |
| 1 | M | 80 | GLU | CD-OE2 | 7.45 | 1.33 | 1.25 |
| 1 | C | 40 | GLU | CD-OE2 | 7.44 | 1.33 | 1.25 |
| 1 | D | 40 | GLU | CD-OE2 | 7.43 | 1.33 | 1.25 |
| 1 | B | 40 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | E | 80 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | J | 40 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | A | 80 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | M | 40 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | F | 40 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | N | 80 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | I | 80 | GLU | CD-OE2 | 7.41 | 1.33 | 1.25 |
| 1 | L | 80 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | P | 40 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | P | 80 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | A | 40 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | G | 40 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | H | 40 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | K | 80 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | N | 40 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | O | 40 | GLU | CD-OE2 | 7.39 | 1.33 | 1.25 |
| 1 | L | 40 | GLU | CD-OE2 | 7.38 | 1.33 | 1.25 |
| 1 | G | 80 | GLU | CD-OE2 | 7.36 | 1.33 | 1.25 |
| 1 | E | 40 | GLU | CD-OE2 | 7.35 | 1.33 | 1.25 |
| 1 | D | 80 | GLU | CD-OE2 | 7.35 | 1.33 | 1.25 |
| 1 | B | 808 | GLU | CD-OE2 | 7.34 | 1.33 | 1.25 |
| 1 | F | 808 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | F | 80 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | E | 117 | GLU | CD-OE2 | 7.32 | 1.33 | 1.25 |
| 1 | D | 117 | GLU | CD-OE2 | 7.32 | 1.33 | 1.25 |
| 1 | D | 969 | GLU | CD-OE2 | 7.32 | 1.33 | 1.25 |
| 1 | C | 969 | GLU | CD-OE2 | 7.31 | 1.33 | 1.25 |
| 1 | M | 808 | GLU | CD-OE2 | 7.31 | 1.33 | 1.25 |
| 1 | I | 969 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | L | 808 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | P | 969 | GLU | CD-OE2 | 7.30 | 1.33 | 1.25 |
| 1 | N | 808 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |
| 1 | J | 808 | GLU | CD-OE2 | 7.29 | 1.33 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | F | 117 | GLU | CD-OE2 | 7.28 | 1.33 | 1.25 |
| 1 | G | 969 | GLU | CD-OE2 | 7.28 | 1.33 | 1.25 |
| 1 | A | 969 | GLU | CD-OE2 | 7.28 | 1.33 | 1.25 |
| 1 | J | 117 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | A | 808 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | K | 969 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | H | 808 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | O | 808 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | E | 808 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | J | 969 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | K | 808 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | L | 969 | GLU | CD-OE2 | 7.26 | 1.33 | 1.25 |
| 1 | H | 117 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | O | 969 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | H | 969 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | M | 969 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | I | 808 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | N | 969 | GLU | CD-OE2 | 7.25 | 1.33 | 1.25 |
| 1 | F | 969 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | B | 969 | GLU | CD-OE2 | 7.24 | 1.33 | 1.25 |
| 1 | M | 117 | GLU | CD-OE2 | 7.23 | 1.33 | 1.25 |
| 1 | D | 808 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | E | 969 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | I | 117 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | A | 117 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | N | 117 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | B | 117 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | C | 117 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 1 | C | 808 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 1 | K | 117 | GLU | CD-OE2 | 7.21 | 1.33 | 1.25 |
| 1 | P | 808 | GLU | CD-OE2 | 7.20 | 1.33 | 1.25 |
| 1 | G | 808 | GLU | CD-OE2 | 7.19 | 1.33 | 1.25 |
| 1 | P | 117 | GLU | CD-OE2 | 7.19 | 1.33 | 1.25 |
| 1 | O | 117 | GLU | CD-OE2 | 7.19 | 1.33 | 1.25 |
| 1 | L | 117 | GLU | CD-OE2 | 7.18 | 1.33 | 1.25 |
| 1 | G | 117 | GLU | CD-OE2 | 7.18 | 1.33 | 1.25 |
| 1 | K | 57 | GLU | CD-OE2 | 7.16 | 1.33 | 1.25 |
| 1 | D | 57 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | E | 57 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | I | 57 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | F | 57 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |
| 1 | G | 57 | GLU | CD-OE2 | 7.10 | 1.33 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | P | 57 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | M | 57 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | O | 57 | GLU | CD-OE2 | 7.09 | 1.33 | 1.25 |
| 1 | J | 57 | GLU | CD-OE2 | 7.08 | 1.33 | 1.25 |
| 1 | C | 57 | GLU | CD-OE2 | 7.08 | 1.33 | 1.25 |
| 1 | N | 57 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | B | 57 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | L | 57 | GLU | CD-OE2 | 7.03 | 1.33 | 1.25 |
| 1 | N | 637 | GLU | CD-OE2 | 7.01 | 1.33 | 1.25 |
| 1 | H | 57 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | A | 57 | GLU | CD-OE2 | 7.00 | 1.33 | 1.25 |
| 1 | H | 637 | GLU | CD-OE2 | 6.99 | 1.33 | 1.25 |
| 1 | O | 637 | GLU | CD-OE2 | 6.99 | 1.33 | 1.25 |
| 1 | F | 637 | GLU | CD-OE2 | 6.99 | 1.33 | 1.25 |
| 1 | G | 637 | GLU | CD-OE2 | 6.98 | 1.33 | 1.25 |
| 1 | I | 637 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | P | 637 | GLU | CD-OE2 | 6.97 | 1.33 | 1.25 |
| 1 | M | 637 | GLU | CD-OE2 | 6.96 | 1.33 | 1.25 |
| 1 | C | 369 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | A | 637 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | J | 637 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | B | 314 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | D | 637 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | G | 314 | GLU | CD-OE2 | 6.95 | 1.33 | 1.25 |
| 1 | K | 314 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | B | 637 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | K | 637 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | C | 637 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | J | 369 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | L | 637 | GLU | CD-OE2 | 6.94 | 1.33 | 1.25 |
| 1 | D | 369 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | E | 369 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | D | 314 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | F | 369 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | C | 314 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | I | 314 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | L | 314 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | O | 369 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | P | 369 | GLU | CD-OE2 | 6.92 | 1.33 | 1.25 |
| 1 | A | 314 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | A | 369 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | E | 637 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | F | 314 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | H | 369 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | H | 650 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | N | 369 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | E | 650 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | O | 314 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | G | 369 | GLU | CD-OE2 | 6.90 | 1.33 | 1.25 |
| 1 | I | 369 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | N | 314 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | P | 314 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | J | 650 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | D | 650 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | E | 314 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | P | 650 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | M | 681 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | C | 650 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | I | 681 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | P | 681 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | K | 369 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | M | 369 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | B | 650 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | C | 681 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | K | 650 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | M | 314 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | B | 369 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | L | 369 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |
| 1 | H | 314 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | J | 314 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | J | 681 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | O | 681 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | E | 241 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | E | 681 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | G | 650 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | F | 650 | GLU | CD-OE2 | 6.85 | 1.33 | 1.25 |
| 1 | A | 650 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | N | 650 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | G | 241 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | N | 681 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | B | 681 | GLU | CD-OE2 | 6.84 | 1.33 | 1.25 |
| 1 | G | 681 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | L | 650 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | O | 650 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | F | 681 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | M | 650 | GLU | CD-OE2 | 6.83 | 1.33 | 1.25 |
| 1 | A | 681 | GLU | CD-OE2 | 6.82 | 1.33 | 1.25 |
| 1 | I | 650 | GLU | CD-OE2 | 6.82 | 1.33 | 1.25 |
| 1 | D | 681 | GLU | CD-OE2 | 6.81 | 1.33 | 1.25 |
| 1 | O | 241 | GLU | CD-OE2 | 6.81 | 1.33 | 1.25 |
| 1 | K | 241 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | H | 241 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | H | 681 | GLU | CD-OE2 | 6.80 | 1.33 | 1.25 |
| 1 | L | 241 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 1 | A | 241 | GLU | CD-OE2 | 6.79 | 1.33 | 1.25 |
| 1 | I | 241 | GLU | CD-OE2 | 6.78 | 1.33 | 1.25 |
| 1 | D | 241 | GLU | CD-OE2 | 6.78 | 1.33 | 1.25 |
| 1 | F | 241 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | L | 681 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | B | 67 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | P | 241 | GLU | CD-OE2 | 6.77 | 1.33 | 1.25 |
| 1 | K | 681 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | M | 241 | GLU | CD-OE2 | 6.75 | 1.33 | 1.25 |
| 1 | M | 67 | GLU | CD-OE2 | 6.75 | 1.33 | 1.25 |
| 1 | N | 241 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | P | 67 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | I | 67 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | J | 241 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | B | 241 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | E | 67 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | C | 241 | GLU | CD-OE2 | 6.72 | 1.33 | 1.25 |
| 1 | G | 67 | GLU | CD-OE2 | 6.71 | 1.33 | 1.25 |
| 1 | A | 67 | GLU | CD-OE2 | 6.71 | 1.33 | 1.25 |
| 1 | F | 67 | GLU | CD-OE2 | 6.70 | 1.33 | 1.25 |
| 1 | O | 67 | GLU | CD-OE2 | 6.69 | 1.33 | 1.25 |
| 1 | C | 67 | GLU | CD-OE2 | 6.68 | 1.33 | 1.25 |
| 1 | H | 67 | GLU | CD-OE2 | 6.68 | 1.32 | 1.25 |
| 1 | L | 67 | GLU | CD-OE2 | 6.68 | 1.33 | 1.25 |
| 1 | D | 67 | GLU | CD-OE2 | 6.67 | 1.32 | 1.25 |
| 1 | N | 67 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | K | 67 | GLU | CD-OE2 | 6.66 | 1.32 | 1.25 |
| 1 | J | 67 | GLU | CD-OE2 | 6.64 | 1.32 | 1.25 |
| 1 | O | 243 | GLU | CD-OE2 | 6.62 | 1.32 | 1.25 |
| 1 | P | 243 | GLU | CD-OE2 | 6.59 | 1.32 | 1.25 |
| 1 | G | 667 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | K | 667 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | L | 667 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | N | 243 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | D | 943 | GLU | CD-OE2 | 6.58 | 1.32 | 1.25 |
| 1 | M | 243 | GLU | CD-OE2 | 6.57 | 1.32 | 1.25 |
| 1 | N | 943 | GLU | CD-OE2 | 6.56 | 1.32 | 1.25 |
| 1 | A | 667 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | B | 943 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | K | 943 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | B | 243 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | F | 667 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | C | 667 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | A | 243 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | C | 243 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | I | 243 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | D | 243 | GLU | CD-OE2 | 6.52 | 1.32 | 1.25 |
| 1 | J | 243 | GLU | CD-OE2 | 6.52 | 1.32 | 1.25 |
| 1 | H | 243 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | K | 243 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | J | 943 | GLU | CD-OE2 | 6.51 | 1.32 | 1.25 |
| 1 | P | 667 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | C | 943 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | O | 943 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | A | 943 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | H | 667 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | H | 943 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | L | 243 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | L | 943 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | F | 943 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | P | 943 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | J | 667 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | E | 943 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | M | 667 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | N | 667 | GLU | CD-OE2 | 6.49 | 1.32 | 1.25 |
| 1 | M | 943 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | E | 243 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | F | 243 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | O | 667 | GLU | CD-OE2 | 6.47 | 1.32 | 1.25 |
| 1 | D | 667 | GLU | CD-OE2 | 6.47 | 1.32 | 1.25 |
| 1 | G | 243 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 1 | B | 667 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | E | 667 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | I | 943 | GLU | CD-OE2 | 6.44 | 1.32 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | I | 667 | GLU | CD-OE2 | 6.43 | 1.32 | 1.25 |
| 1 | G | 943 | GLU | CD-OE2 | 6.43 | 1.32 | 1.25 |
| 1 | K | 358 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | C | 358 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | O | 358 | GLU | CD-OE2 | 6.40 | 1.32 | 1.25 |
| 1 | B | 358 | GLU | CD-OE2 | 6.40 | 1.32 | 1.25 |
| 1 | G | 358 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | J | 358 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | F | 358 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 1 | N | 358 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | H | 358 | GLU | CD-OE2 | 6.37 | 1.32 | 1.25 |
| 1 | L | 358 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | D | 358 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | A | 358 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | E | 358 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | I | 358 | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 1 | M | 358 | GLU | CD-OE2 | 6.34 | 1.32 | 1.25 |
| 1 | P | 358 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | B | 904 | GLU | CD-OE2 | 6.09 | 1.32 | 1.25 |
| 1 | F | 904 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | H | 904 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 |
| 1 | E | 904 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | J | 904 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | K | 904 | GLU | CD-OE2 | 6.06 | 1.32 | 1.25 |
| 1 | C | 904 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | N | 904 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | L | 281 | GLU | CD-OE2 | 6.05 | 1.32 | 1.25 |
| 1 | I | 281 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | O | 904 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | G | 281 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | L | 338 | GLU | CD-OE2 | 6.04 | 1.32 | 1.25 |
| 1 | I | 904 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | O | 281 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | C | 338 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | L | 904 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | E | 281 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | K | 338 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | M | 904 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | N | 338 | GLU | CD-OE2 | 6.03 | 1.32 | 1.25 |
| 1 | D | 281 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | A | 281 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |
| 1 | P | 904 | GLU | CD-OE2 | 6.02 | 1.32 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1 | D | 904 | GLU | CD-OE2 | 6.01 | 1.32 | 1.25 |
| 1 | H | 281 | GLU | CD-OE2 | 6.01 | 1.32 | 1.25 |
| 1 | P | 281 | GLU | CD-OE2 | 6.01 | 1.32 | 1.25 |
| 1 | C | 281 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | J | 281 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | E | 1006 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | B | 338 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | M | 338 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | F | 338 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | B | 1006 | GLU | CD-OE2 | 5.99 | 1.32 | 1.25 |
| 1 | K | 281 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | F | 281 | GLU | CD-OE2 | 5.98 | 1.32 | 1.25 |
| 1 | A | 338 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | A | 904 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | H | 338 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | O | 338 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | D | 338 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | G | 904 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | O | 1006 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | G | 338 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |
| 1 | M | 281 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | P | 1006 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | F | 1006 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | N | 281 | GLU | CD-OE2 | 5.96 | 1.32 | 1.25 |
| 1 | B | 281 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | I | 338 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | P | 338 | GLU | CD-OE2 | 5.95 | 1.32 | 1.25 |
| 1 | D | 1006 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | J | 1006 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | L | 1006 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | C | 1006 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | J | 338 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | N | 1006 | GLU | CD-OE2 | 5.93 | 1.32 | 1.25 |
| 1 | A | 1006 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | I | 1006 | GLU | CD-OE2 | 5.92 | 1.32 | 1.25 |
| 1 | E | 338 | GLU | CD-OE2 | 5.91 | 1.32 | 1.25 |
| 1 | K | 1006 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | M | 1006 | GLU | CD-OE2 | 5.89 | 1.32 | 1.25 |
| 1 | H | 1006 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | G | 1006 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | K | 871 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | N | 871 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | O | 871 | GLU | CD-OE2 | 5.86 | 1.32 | 1.25 |
| 1 | I | 871 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | L | 871 | GLU | CD-OE2 | 5.84 | 1.32 | 1.25 |
| 1 | J | 871 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | E | 871 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | G | 871 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | B | 871 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | A | 871 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | O | 525 | SER | CB-OG | 5.82 | 1.49 | 1.42 |
| 1 | P | 871 | GLU | CD-OE2 | 5.82 | 1.32 | 1.25 |
| 1 | E | 525 | SER | CB-OG | 5.81 | 1.49 | 1.42 |
| 1 | D | 871 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | F | 871 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | H | 525 | SER | CB-OG | 5.80 | 1.49 | 1.42 |
| 1 | C | 871 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | N | 525 | SER | CB-OG | 5.80 | 1.49 | 1.42 |
| 1 | B | 525 | SER | CB-OG | 5.79 | 1.49 | 1.42 |
| 1 | C | 525 | SER | CB-OG | 5.79 | 1.49 | 1.42 |
| 1 | I | 334 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | K | 525 | SER | CB-OG | 5.78 | 1.49 | 1.42 |
| 1 | H | 871 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | M | 871 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | P | 334 | GLU | CD-OE2 | 5.78 | 1.32 | 1.25 |
| 1 | L | 525 | SER | CB-OG | 5.78 | 1.49 | 1.42 |
| 1 | N | 334 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | G | 334 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | B | 304 | GLU | CD-OE1 | -5.76 | 1.19 | 1.25 |
| 1 | G | 525 | SER | CB-OG | 5.76 | 1.49 | 1.42 |
| 1 | B | 334 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | I | 525 | SER | CB-OG | 5.76 | 1.49 | 1.42 |
| 1 | L | 334 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | F | 525 | SER | CB-OG | 5.75 | 1.49 | 1.42 |
| 1 | J | 334 | GLU | CD-OE2 | 5.75 | 1.31 | 1.25 |
| 1 | A | 525 | SER | CB-OG | 5.74 | 1.49 | 1.42 |
| 1 | D | 334 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | C | 334 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | D | 525 | SER | CB-OG | 5.74 | 1.49 | 1.42 |
| 1 | P | 525 | SER | CB-OG | 5.73 | 1.49 | 1.42 |
| 1 | J | 525 | SER | CB-OG | 5.73 | 1.49 | 1.42 |
| 1 | M | 304 | GLU | CD-OE1 | -5.72 | 1.19 | 1.25 |
| 1 | A | 334 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | F | 334 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | E | 304 | GLU | CD-OE1 | -5.72 | 1.19 | 1.25 |
| 1 | K | 334 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | M | 525 | SER | CB-OG | 5.71 | 1.49 | 1.42 |
| 1 | M | 334 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | P | 304 | GLU | CD-OE1 | -5.70 | 1.19 | 1.25 |
| 1 | E | 334 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | H | 334 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | A | 304 | GLU | CD-OE1 | -5.69 | 1.19 | 1.25 |
| 1 | C | 304 | GLU | CD-OE1 | -5.68 | 1.19 | 1.25 |
| 1 | O | 334 | GLU | CD-OE2 | 5.68 | 1.31 | 1.25 |
| 1 | K | 304 | GLU | CD-OE1 | -5.68 | 1.19 | 1.25 |
| 1 | O | 304 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 1 | G | 304 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 1 | J | 304 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 1 | D | 304 | GLU | CD-OE1 | -5.66 | 1.19 | 1.25 |
| 1 | I | 304 | GLU | CD-OE1 | -5.66 | 1.19 | 1.25 |
| 1 | N | 304 | GLU | CD-OE1 | -5.65 | 1.19 | 1.25 |
| 1 | E | 619 | GLU | CD-OE2 | 5.64 | 1.31 | 1.25 |
| 1 | F | 304 | GLU | CD-OE1 | -5.63 | 1.19 | 1.25 |
| 1 | F | 461 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | L | 304 | GLU | CD-OE1 | -5.61 | 1.19 | 1.25 |
| 1 | F | 619 | GLU | CD-OE2 | 5.61 | 1.31 | 1.25 |
| 1 | H | 304 | GLU | CD-OE1 | -5.60 | 1.19 | 1.25 |
| 1 | C | 461 | GLU | CD-OE2 | 5.59 | 1.31 | 1.25 |
| 1 | A | 461 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | G | 619 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | P | 461 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | C | 619 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | E | 461 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | G | 461 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | H | 461 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | J | 619 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | N | 461 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | I | 619 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | N | 619 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | O | 619 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | B | 461 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | I | 461 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | A | 619 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | M | 461 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | K | 461 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | L | 461 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | L | 619 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | K | 619 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | D | 461 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | D | 619 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | J | 461 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | M | 619 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | O | 461 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | B | 619 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | H | 619 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | P | 619 | GLU | CD-OE2 | 5.50 | 1.31 | 1.25 |
| 1 | C | 324 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | G | 324 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | J | 934 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | P | 324 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | O | 324 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | K | 934 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 1 | H | 324 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 1 | A | 934 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | I | 324 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | N | 324 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | D | 934 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | A | 324 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 1 | J | 324 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | F | 324 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | G | 934 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | D | 324 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | C | 979 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | N | 979 | GLU | CD-OE2 | 5.41 | 1.31 | 1.25 |
| 1 | E | 324 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | E | 934 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | L | 934 | GLU | CD-OE2 | 5.40 | 1.31 | 1.25 |
| 1 | B | 934 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | O | 934 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | K | 324 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | I | 934 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | I | 979 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 1 | K | 979 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | B | 324 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | M | 934 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | L | 324 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | N | 934 | GLU | CD-OE2 | 5.37 | 1.31 | 1.25 |
| 1 | M | 324 | GLU | CD-OE2 | 5.37 | 1.31 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | H | 934 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | P | 934 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 979 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | O | 979 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | B | 979 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | M | 979 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | C | 934 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | F | 934 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | D | 979 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | P | 979 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | E | 71 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | H | 979 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | L | 979 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | G | 979 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | J | 979 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | B | 71 | GLU | CD-OE2 | 5.32 | 1.31 | 1.25 |
| 1 | E | 979 | GLU | CD-OE2 | 5.32 | 1.31 | 1.25 |
| 1 | A | 71 | GLU | CD-OE2 | 5.30 | 1.31 | 1.25 |
| 1 | D | 71 | GLU | CD-OE2 | 5.29 | 1.31 | 1.25 |
| 1 | C | 71 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | K | 71 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | F | 979 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | M | 71 | GLU | CD-OE2 | 5.25 | 1.31 | 1.25 |
| 1 | I | 71 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | G | 750 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | G | 71 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | P | 71 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | H | 71 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | I | 750 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | F | 71 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 1 | H | 750 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | L | 71 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | E | 750 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | L | 750 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | O | 71 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 |
| 1 | J | 71 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | N | 71 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | F | 750 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | J | 750 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | P | 750 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | A | 750 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 1 | K | 750 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | N | 750 | GLU | CD-OE2 | 5.15 | 1.31 | 1.25 |
| 1 | M | 750 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | C | 750 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | B | 750 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | D | 750 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | B | 17 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | O | 750 | GLU | CD-OE2 | 5.12 | 1.31 | 1.25 |
| 1 | C | 800 | ARG | NE-CZ | 5.11 | 1.39 | 1.33 |
| 1 | C | 17 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | B | 800 | ARG | NE-CZ | 5.11 | 1.39 | 1.33 |
| 1 | P | 17 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | A | 800 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.33 |
| 1 | K | 800 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.33 |
| 1 | O | 800 | ARG | NE-CZ | 5.10 | 1.39 | 1.33 |
| 1 | I | 41 | GLU | CD-OE2 | 5.10 | 1.31 | 1.25 |
| 1 | J | 17 | GLU | CD-OE2 | 5.10 | 1.31 | 1.25 |
| 1 | F | 800 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.33 |
| 1 | G | 800 | ARG | CZ-NH1 | 5.09 | 1.39 | 1.33 |
| 1 | N | 800 | ARG | CZ-NH1 | 5.09 | 1.39 | 1.33 |
| 1 | I | 800 | ARG | NE-CZ | 5.09 | 1.39 | 1.33 |
| 1 | N | 17 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | G | 17 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | I | 17 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | K | 17 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 1 | F | 17 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | E | 800 | ARG | CZ-NH1 | 5.08 | 1.39 | 1.33 |
| 1 | L | 800 | ARG | NE-CZ | 5.08 | 1.39 | 1.33 |
| 1 | H | 17 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | P | 41 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | P | 800 | ARG | CZ-NH1 | 5.08 | 1.39 | 1.33 |
| 1 | D | 17 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | A | 800 | ARG | NE-CZ | 5.08 | 1.39 | 1.33 |
| 1 | E | 17 | GLU | CD-OE2 | 5.08 | 1.31 | 1.25 |
| 1 | G | 800 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 1 | A | 17 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | H | 800 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 1 | N | 800 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 1 | B | 800 | ARG | CZ-NH1 | 5.07 | 1.39 | 1.33 |
| 1 | J | 800 | ARG | NE-CZ | 5.07 | 1.39 | 1.33 |
| 1 | L | 17 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | O | 17 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | C | 800 | ARG | CZ-NH1 | 5.06 | 1.39 | 1.33 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | M | 41 | GLU | CD-OE2 | 5.06 | 1.31 | 1.25 |
| 1 | D | 800 | ARG | NE-CZ | 5.06 | 1.39 | 1.33 |
| 1 | M | 17 | GLU | CD-OE2 | 5.06 | 1.31 | 1.25 |
| 1 | I | 800 | ARG | CZ-NH1 | 5.06 | 1.39 | 1.33 |
| 1 | C | 41 | GLU | CD-OE2 | 5.06 | 1.31 | 1.25 |
| 1 | B | 41 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | M | 800 | ARG | NE-CZ | 5.05 | 1.39 | 1.33 |
| 1 | E | 41 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | K | 41 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | M | 800 | ARG | CZ-NH1 | 5.05 | 1.39 | 1.33 |
| 1 | P | 800 | ARG | NE-CZ | 5.05 | 1.39 | 1.33 |
| 1 | D | 800 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.33 |
| 1 | O | 41 | GLU | CD-OE2 | 5.04 | 1.31 | 1.25 |
| 1 | O | 800 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.33 |
| 1 | J | 800 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.33 |
| 1 | L | 41 | GLU | CD-OE2 | 5.04 | 1.31 | 1.25 |
| 1 | A | 41 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | F | 800 | ARG | NE-CZ | 5.03 | 1.39 | 1.33 |
| 1 | H | 41 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | N | 41 | GLU | CD-OE2 | 5.03 | 1.31 | 1.25 |
| 1 | D | 170 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | H | 170 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | K | 800 | ARG | NE-CZ | 5.02 | 1.39 | 1.33 |
| 1 | L | 800 | ARG | CZ-NH1 | 5.01 | 1.39 | 1.33 |
| 1 | G | 41 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | E | 800 | ARG | NE-CZ | 5.01 | 1.39 | 1.33 |
| 1 | O | 416 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |
| 1 | J | 41 | GLU | CD-OE2 | 5.00 | 1.31 | 1.25 |

All (3010) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | I | 210 | ARG | NE-CZ-NH1 | 18.08 | 129.34 | 120.30 |
| 1 | L | 210 | ARG | NE-CZ-NH1 | 18.07 | 129.34 | 120.30 |
| 1 | J | 210 | ARG | NE-CZ-NH1 | 18.07 | 129.33 | 120.30 |
| 1 | M | 210 | ARG | NE-CZ-NH1 | 18.03 | 129.31 | 120.30 |
| 1 | G | 210 | ARG | NE-CZ-NH1 | 18.01 | 129.30 | 120.30 |
| 1 | P | 210 | ARG | NE-CZ-NH1 | 18.01 | 129.30 | 120.30 |
| 1 | D | 210 | ARG | NE-CZ-NH1 | 18.00 | 129.30 | 120.30 |
| 1 | A | 210 | ARG | NE-CZ-NH1 | 17.99 | 129.30 | 120.30 |
| 1 | H | 210 | ARG | NE-CZ-NH1 | 17.98 | 129.29 | 120.30 |
| 1 | C | 210 | ARG | NE-CZ-NH1 | 17.98 | 129.29 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | E | 210 | ARG | NE-CZ-NH1 | 17.98 | 129.29 | 120.30 |
| 1 | F | 210 | ARG | NE-CZ-NH1 | 17.94 | 129.27 | 120.30 |
| 1 | N | 210 | ARG | NE-CZ-NH1 | 17.92 | 129.26 | 120.30 |
| 1 | K | 210 | ARG | NE-CZ-NH1 | 17.91 | 129.26 | 120.30 |
| 1 | O | 210 | ARG | NE-CZ-NH1 | 17.91 | 129.25 | 120.30 |
| 1 | B | 210 | ARG | NE-CZ-NH1 | 17.89 | 129.25 | 120.30 |
| 1 | C | 448 | ARG | NE-CZ-NH2 | -16.64 | 111.98 | 120.30 |
| 1 | G | 448 | ARG | NE-CZ-NH2 | -16.60 | 112.00 | 120.30 |
| 1 | D | 448 | ARG | NE-CZ-NH2 | -16.58 | 112.01 | 120.30 |
| 1 | L | 448 | ARG | NE-CZ-NH2 | -16.57 | 112.01 | 120.30 |
| 1 | H | 448 | ARG | NE-CZ-NH2 | -16.57 | 112.02 | 120.30 |
| 1 | N | 448 | ARG | NE-CZ-NH2 | -16.55 | 112.02 | 120.30 |
| 1 | I | 448 | ARG | NE-CZ-NH2 | -16.55 | 112.03 | 120.30 |
| 1 | A | 448 | ARG | NE-CZ-NH2 | -16.54 | 112.03 | 120.30 |
| 1 | F | 448 | ARG | NE-CZ-NH2 | -16.54 | 112.03 | 120.30 |
| 1 | B | 448 | ARG | NE-CZ-NH2 | -16.53 | 112.03 | 120.30 |
| 1 | K | 448 | ARG | NE-CZ-NH2 | -16.53 | 112.03 | 120.30 |
| 1 | M | 448 | ARG | NE-CZ-NH2 | -16.52 | 112.04 | 120.30 |
| 1 | E | 448 | ARG | NE-CZ-NH2 | -16.52 | 112.04 | 120.30 |
| 1 | O | 448 | ARG | NE-CZ-NH2 | -16.50 | 112.05 | 120.30 |
| 1 | J | 448 | ARG | NE-CZ-NH2 | -16.49 | 112.05 | 120.30 |
| 1 | P | 448 | ARG | NE-CZ-NH2 | -16.49 | 112.06 | 120.30 |
| 1 | H | 881 | ARG | NE-CZ-NH2 | -16.26 | 112.17 | 120.30 |
| 1 | J | 881 | ARG | NE-CZ-NH2 | -16.25 | 112.17 | 120.30 |
| 1 | K | 881 | ARG | NE-CZ-NH2 | -16.25 | 112.17 | 120.30 |
| 1 | L | 881 | ARG | NE-CZ-NH2 | -16.22 | 112.19 | 120.30 |
| 1 | C | 881 | ARG | NE-CZ-NH2 | -16.21 | 112.19 | 120.30 |
| 1 | N | 881 | ARG | NE-CZ-NH2 | -16.20 | 112.20 | 120.30 |
| 1 | P | 881 | ARG | NE-CZ-NH2 | -16.20 | 112.20 | 120.30 |
| 1 | F | 881 | ARG | NE-CZ-NH2 | -16.20 | 112.20 | 120.30 |
| 1 | G | 881 | ARG | NE-CZ-NH2 | -16.20 | 112.20 | 120.30 |
| 1 | B | 881 | ARG | NE-CZ-NH2 | -16.19 | 112.20 | 120.30 |
| 1 | E | 881 | ARG | NE-CZ-NH2 | -16.17 | 112.21 | 120.30 |
| 1 | A | 881 | ARG | NE-CZ-NH2 | -16.16 | 112.22 | 120.30 |
| 1 | M | 881 | ARG | NE-CZ-NH2 | -16.15 | 112.22 | 120.30 |
| 1 | I | 881 | ARG | NE-CZ-NH2 | -16.12 | 112.24 | 120.30 |
| 1 | D | 881 | ARG | NE-CZ-NH2 | -16.12 | 112.24 | 120.30 |
| 1 | O | 881 | ARG | NE-CZ-NH2 | -16.11 | 112.24 | 120.30 |
| 1 | E | 938 | ARG | NE-CZ-NH2 | -15.54 | 112.53 | 120.30 |
| 1 | A | 938 | ARG | NE-CZ-NH2 | -15.53 | 112.53 | 120.30 |
| 1 | M | 938 | ARG | NE-CZ-NH2 | -15.53 | 112.53 | 120.30 |
| 1 | F | 938 | ARG | NE-CZ-NH2 | -15.50 | 112.55 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | D | 938 | ARG | NE-CZ-NH2 | -15.50 | 112.55 | 120.30 |
| 1 | I | 938 | ARG | NE-CZ-NH2 | -15.49 | 112.55 | 120.30 |
| 1 | O | 938 | ARG | NE-CZ-NH2 | -15.49 | 112.56 | 120.30 |
| 1 | C | 881 | ARG | NE-CZ-NH1 | 15.48 | 128.04 | 120.30 |
| 1 | J | 938 | ARG | NE-CZ-NH2 | -15.46 | 112.57 | 120.30 |
| 1 | G | 881 | ARG | NE-CZ-NH1 | 15.45 | 128.03 | 120.30 |
| 1 | H | 938 | ARG | NE-CZ-NH2 | -15.45 | 112.58 | 120.30 |
| 1 | G | 938 | ARG | NE-CZ-NH2 | -15.44 | 112.58 | 120.30 |
| 1 | C | 938 | ARG | NE-CZ-NH2 | -15.44 | 112.58 | 120.30 |
| 1 | F | 881 | ARG | NE-CZ-NH1 | 15.44 | 128.02 | 120.30 |
| 1 | N | 881 | ARG | NE-CZ-NH1 | 15.44 | 128.02 | 120.30 |
| 1 | P | 938 | ARG | NE-CZ-NH2 | -15.44 | 112.58 | 120.30 |
| 1 | K | 938 | ARG | NE-CZ-NH2 | -15.42 | 112.59 | 120.30 |
| 1 | N | 938 | ARG | NE-CZ-NH2 | -15.42 | 112.59 | 120.30 |
| 1 | L | 881 | ARG | NE-CZ-NH1 | 15.40 | 128.00 | 120.30 |
| 1 | B | 881 | ARG | NE-CZ-NH1 | 15.40 | 128.00 | 120.30 |
| 1 | H | 881 | ARG | NE-CZ-NH1 | 15.39 | 128.00 | 120.30 |
| 1 | M | 881 | ARG | NE-CZ-NH1 | 15.39 | 127.99 | 120.30 |
| 1 | B | 938 | ARG | NE-CZ-NH2 | -15.38 | 112.61 | 120.30 |
| 1 | O | 881 | ARG | NE-CZ-NH1 | 15.38 | 127.99 | 120.30 |
| 1 | J | 881 | ARG | NE-CZ-NH1 | 15.38 | 127.99 | 120.30 |
| 1 | K | 881 | ARG | NE-CZ-NH1 | 15.35 | 127.98 | 120.30 |
| 1 | A | 881 | ARG | NE-CZ-NH1 | 15.34 | 127.97 | 120.30 |
| 1 | L | 938 | ARG | NE-CZ-NH2 | -15.34 | 112.63 | 120.30 |
| 1 | E | 881 | ARG | NE-CZ-NH1 | 15.33 | 127.96 | 120.30 |
| 1 | P | 881 | ARG | NE-CZ-NH1 | 15.28 | 127.94 | 120.30 |
| 1 | I | 881 | ARG | NE-CZ-NH1 | 15.24 | 127.92 | 120.30 |
| 1 | D | 881 | ARG | NE-CZ-NH1 | 15.20 | 127.90 | 120.30 |
| 1 | C | 210 | ARG | NE-CZ-NH2 | -14.78 | 112.91 | 120.30 |
| 1 | D | 210 | ARG | NE-CZ-NH2 | -14.77 | 112.91 | 120.30 |
| 1 | J | 210 | ARG | NE-CZ-NH2 | -14.77 | 112.92 | 120.30 |
| 1 | A | 210 | ARG | NE-CZ-NH2 | -14.76 | 112.92 | 120.30 |
| 1 | P | 210 | ARG | NE-CZ-NH2 | -14.74 | 112.93 | 120.30 |
| 1 | H | 210 | ARG | NE-CZ-NH2 | -14.74 | 112.93 | 120.30 |
| 1 | G | 210 | ARG | NE-CZ-NH2 | -14.73 | 112.94 | 120.30 |
| 1 | E | 210 | ARG | NE-CZ-NH2 | -14.72 | 112.94 | 120.30 |
| 1 | B | 210 | ARG | NE-CZ-NH2 | -14.69 | 112.95 | 120.30 |
| 1 | O | 210 | ARG | NE-CZ-NH2 | -14.68 | 112.96 | 120.30 |
| 1 | M | 210 | ARG | NE-CZ-NH2 | -14.68 | 112.96 | 120.30 |
| 1 | L | 166 | ARG | NE-CZ-NH1 | 14.68 | 127.64 | 120.30 |
| 1 | L | 210 | ARG | NE-CZ-NH2 | -14.68 | 112.96 | 120.30 |
| 1 | O | 166 | ARG | NE-CZ-NH1 | 14.67 | 127.63 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | I | 166 | ARG | NE-CZ-NH1 | 14.66 | 127.63 | 120.30 |
| 1 | N | 210 | ARG | NE-CZ-NH2 | -14.66 | 112.97 | 120.30 |
| 1 | I | 210 | ARG | NE-CZ-NH2 | -14.65 | 112.98 | 120.30 |
| 1 | K | 210 | ARG | NE-CZ-NH2 | -14.62 | 112.99 | 120.30 |
| 1 | D | 166 | ARG | NE-CZ-NH1 | 14.62 | 127.61 | 120.30 |
| 1 | F | 210 | ARG | NE-CZ-NH2 | -14.61 | 113.00 | 120.30 |
| 1 | C | 166 | ARG | NE-CZ-NH1 | 14.60 | 127.60 | 120.30 |
| 1 | E | 166 | ARG | NE-CZ-NH1 | 14.60 | 127.60 | 120.30 |
| 1 | K | 166 | ARG | NE-CZ-NH1 | 14.60 | 127.60 | 120.30 |
| 1 | J | 166 | ARG | NE-CZ-NH1 | 14.59 | 127.59 | 120.30 |
| 1 | M | 166 | ARG | NE-CZ-NH1 | 14.59 | 127.59 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH1 | 14.58 | 127.59 | 120.30 |
| 1 | N | 166 | ARG | NE-CZ-NH1 | 14.58 | 127.59 | 120.30 |
| 1 | G | 166 | ARG | NE-CZ-NH1 | 14.56 | 127.58 | 120.30 |
| 1 | H | 166 | ARG | NE-CZ-NH1 | 14.56 | 127.58 | 120.30 |
| 1 | F | 166 | ARG | NE-CZ-NH1 | 14.54 | 127.57 | 120.30 |
| 1 | B | 166 | ARG | NE-CZ-NH1 | 14.53 | 127.56 | 120.30 |
| 1 | P | 166 | ARG | NE-CZ-NH1 | 14.53 | 127.56 | 120.30 |
| 1 | D | 938 | ARG | NE-CZ-NH1 | 13.60 | 127.10 | 120.30 |
| 1 | E | 938 | ARG | NE-CZ-NH1 | 13.57 | 127.08 | 120.30 |
| 1 | F | 938 | ARG | NE-CZ-NH1 | 13.55 | 127.08 | 120.30 |
| 1 | B | 938 | ARG | NE-CZ-NH1 | 13.54 | 127.07 | 120.30 |
| 1 | M | 938 | ARG | NE-CZ-NH1 | 13.53 | 127.07 | 120.30 |
| 1 | I | 938 | ARG | NE-CZ-NH1 | 13.52 | 127.06 | 120.30 |
| 1 | O | 938 | ARG | NE-CZ-NH1 | 13.51 | 127.06 | 120.30 |
| 1 | H | 938 | ARG | NE-CZ-NH1 | 13.51 | 127.05 | 120.30 |
| 1 | C | 938 | ARG | NE-CZ-NH1 | 13.51 | 127.05 | 120.30 |
| 1 | P | 938 | ARG | NE-CZ-NH1 | 13.49 | 127.05 | 120.30 |
| 1 | A | 938 | ARG | NE-CZ-NH1 | 13.49 | 127.04 | 120.30 |
| 1 | K | 938 | ARG | NE-CZ-NH1 | 13.48 | 127.04 | 120.30 |
| 1 | G | 938 | ARG | NE-CZ-NH1 | 13.46 | 127.03 | 120.30 |
| 1 | N | 938 | ARG | NE-CZ-NH1 | 13.45 | 127.02 | 120.30 |
| 1 | L | 938 | ARG | NE-CZ-NH1 | 13.44 | 127.02 | 120.30 |
| 1 | J | 938 | ARG | NE-CZ-NH1 | 13.43 | 127.02 | 120.30 |
| 1 | D | 746 | ASP | CB-CG-OD2 | -12.36 | 107.17 | 118.30 |
| 1 | E | 746 | ASP | CB-CG-OD2 | -12.35 | 107.19 | 118.30 |
| 1 | J | 746 | ASP | CB-CG-OD2 | -12.34 | 107.19 | 118.30 |
| 1 | L | 746 | ASP | CB-CG-OD2 | -12.34 | 107.19 | 118.30 |
| 1 | G | 746 | ASP | CB-CG-OD2 | -12.33 | 107.20 | 118.30 |
| 1 | I | 746 | ASP | CB-CG-OD2 | -12.33 | 107.21 | 118.30 |
| 1 | H | 746 | ASP | CB-CG-OD2 | -12.32 | 107.21 | 118.30 |
| 1 | M | 746 | ASP | CB-CG-OD2 | -12.31 | 107.22 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | C | 746 | ASP | CB-CG-OD2 | -12.31 | 107.22 | 118.30 |
| 1 | N | 746 | ASP | CB-CG-OD2 | -12.31 | 107.22 | 118.30 |
| 1 | P | 746 | ASP | CB-CG-OD2 | -12.31 | 107.22 | 118.30 |
| 1 | A | 746 | ASP | CB-CG-OD2 | -12.30 | 107.23 | 118.30 |
| 1 | B | 746 | ASP | CB-CG-OD2 | -12.29 | 107.24 | 118.30 |
| 1 | K | 746 | ASP | CB-CG-OD2 | -12.29 | 107.24 | 118.30 |
| 1 | O | 746 | ASP | CB-CG-OD2 | -12.28 | 107.25 | 118.30 |
| 1 | F | 746 | ASP | CB-CG-OD2 | -12.27 | 107.26 | 118.30 |
| 1 | H | 809 | ARG | NE-CZ-NH1 | 11.03 | 125.81 | 120.30 |
| 1 | N | 809 | ARG | NE-CZ-NH1 | 10.98 | 125.79 | 120.30 |
| 1 | A | 809 | ARG | NE-CZ-NH1 | 10.97 | 125.78 | 120.30 |
| 1 | I | 809 | ARG | NE-CZ-NH1 | 10.96 | 125.78 | 120.30 |
| 1 | J | 809 | ARG | NE-CZ-NH1 | 10.95 | 125.78 | 120.30 |
| 1 | P | 809 | ARG | NE-CZ-NH1 | 10.95 | 125.78 | 120.30 |
| 1 | C | 809 | ARG | NE-CZ-NH1 | 10.94 | 125.77 | 120.30 |
| 1 | K | 809 | ARG | NE-CZ-NH1 | 10.94 | 125.77 | 120.30 |
| 1 | O | 809 | ARG | NE-CZ-NH1 | 10.94 | 125.77 | 120.30 |
| 1 | L | 809 | ARG | NE-CZ-NH1 | 10.93 | 125.77 | 120.30 |
| 1 | D | 809 | ARG | NE-CZ-NH1 | 10.92 | 125.76 | 120.30 |
| 1 | F | 809 | ARG | NE-CZ-NH1 | 10.92 | 125.76 | 120.30 |
| 1 | M | 809 | ARG | NE-CZ-NH1 | 10.89 | 125.75 | 120.30 |
| 1 | E | 809 | ARG | NE-CZ-NH1 | 10.88 | 125.74 | 120.30 |
| 1 | G | 809 | ARG | NE-CZ-NH1 | 10.87 | 125.73 | 120.30 |
| 1 | B | 809 | ARG | NE-CZ-NH1 | 10.84 | 125.72 | 120.30 |
| 1 | I | 473 | ARG | NE-CZ-NH1 | 10.06 | 125.33 | 120.30 |
| 1 | N | 473 | ARG | NE-CZ-NH1 | 10.05 | 125.33 | 120.30 |
| 1 | D | 473 | ARG | NE-CZ-NH1 | 10.05 | 125.33 | 120.30 |
| 1 | J | 473 | ARG | NE-CZ-NH1 | 10.04 | 125.32 | 120.30 |
| 1 | G | 473 | ARG | NE-CZ-NH1 | 10.04 | 125.32 | 120.30 |
| 1 | P | 473 | ARG | NE-CZ-NH1 | 10.03 | 125.31 | 120.30 |
| 1 | A | 473 | ARG | NE-CZ-NH1 | 10.02 | 125.31 | 120.30 |
| 1 | B | 473 | ARG | NE-CZ-NH1 | 10.01 | 125.31 | 120.30 |
| 1 | M | 473 | ARG | NE-CZ-NH1 | 10.00 | 125.30 | 120.30 |
| 1 | E | 473 | ARG | NE-CZ-NH1 | 10.00 | 125.30 | 120.30 |
| 1 | L | 473 | ARG | NE-CZ-NH1 | 9.99 | 125.30 | 120.30 |
| 1 | H | 473 | ARG | NE-CZ-NH1 | 9.99 | 125.30 | 120.30 |
| 1 | D | 645 | ARG | NE-CZ-NH1 | 9.98 | 125.29 | 120.30 |
| 1 | H | 645 | ARG | NE-CZ-NH1 | 9.98 | 125.29 | 120.30 |
| 1 | M | 645 | ARG | NE-CZ-NH1 | 9.96 | 125.28 | 120.30 |
| 1 | C | 473 | ARG | NE-CZ-NH1 | 9.95 | 125.28 | 120.30 |
| 1 | D | 1018 | LEU | CB-CA-C | -9.94 | 91.31 | 110.20 |
| 1 | K | 1018 | LEU | CB-CA-C | -9.94 | 91.31 | 110.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | E | 1018 | LEU | CB-CA-C | -9.93 | 91.33 | 110.20 |
| 1 | C | 1018 | LEU | CB-CA-C | -9.93 | 91.34 | 110.20 |
| 1 | L | 1018 | LEU | CB-CA-C | -9.93 | 91.34 | 110.20 |
| 1 | A | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | F | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | O | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | P | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | B | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | H | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | M | 1018 | LEU | CB-CA-C | -9.92 | 91.35 | 110.20 |
| 1 | F | 473 | ARG | NE-CZ-NH1 | 9.92 | 125.26 | 120.30 |
| 1 | G | 1018 | LEU | CB-CA-C | -9.92 | 91.36 | 110.20 |
| 1 | O | 473 | ARG | NE-CZ-NH1 | 9.92 | 125.26 | 120.30 |
| 1 | I | 1018 | LEU | CB-CA-C | -9.91 | 91.37 | 110.20 |
| 1 | K | 473 | ARG | NE-CZ-NH1 | 9.91 | 125.26 | 120.30 |
| 1 | J | 1018 | LEU | CB-CA-C | -9.91 | 91.37 | 110.20 |
| 1 | E | 645 | ARG | NE-CZ-NH1 | 9.89 | 125.25 | 120.30 |
| 1 | N | 1018 | LEU | CB-CA-C | -9.89 | 91.41 | 110.20 |
| 1 | G | 645 | ARG | NE-CZ-NH1 | 9.89 | 125.24 | 120.30 |
| 1 | I | 645 | ARG | NE-CZ-NH1 | 9.88 | 125.24 | 120.30 |
| 1 | N | 645 | ARG | NE-CZ-NH1 | 9.88 | 125.24 | 120.30 |
| 1 | A | 645 | ARG | NE-CZ-NH1 | 9.88 | 125.24 | 120.30 |
| 1 | O | 645 | ARG | NE-CZ-NH1 | 9.87 | 125.23 | 120.30 |
| 1 | K | 645 | ARG | NE-CZ-NH1 | 9.87 | 125.23 | 120.30 |
| 1 | C | 645 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 |
| 1 | J | 645 | ARG | NE-CZ-NH1 | 9.84 | 125.22 | 120.30 |
| 1 | P | 645 | ARG | NE-CZ-NH1 | 9.82 | 125.21 | 120.30 |
| 1 | E | 447 | ASP | CB-CG-OD2 | -9.80 | 109.48 | 118.30 |
| 1 | L | 645 | ARG | NE-CZ-NH1 | 9.79 | 125.20 | 120.30 |
| 1 | F | 645 | ARG | NE-CZ-NH1 | 9.79 | 125.19 | 120.30 |
| 1 | P | 447 | ASP | CB-CG-OD2 | -9.78 | 109.50 | 118.30 |
| 1 | G | 447 | ASP | CB-CG-OD2 | -9.77 | 109.51 | 118.30 |
| 1 | N | 233 | ASP | CB-CG-OD1 | 9.77 | 127.09 | 118.30 |
| 1 | G | 233 | ASP | CB-CG-OD1 | 9.77 | 127.09 | 118.30 |
| 1 | E | 233 | ASP | CB-CG-OD1 | 9.76 | 127.09 | 118.30 |
| 1 | O | 233 | ASP | CB-CG-OD1 | 9.76 | 127.09 | 118.30 |
| 1 | D | 447 | ASP | CB-CG-OD2 | -9.76 | 109.52 | 118.30 |
| 1 | J | 447 | ASP | CB-CG-OD2 | -9.76 | 109.52 | 118.30 |
| 1 | B | 233 | ASP | CB-CG-OD1 | 9.76 | 127.08 | 118.30 |
| 1 | M | 233 | ASP | CB-CG-OD1 | 9.75 | 127.08 | 118.30 |
| 1 | A | 447 | ASP | CB-CG-OD2 | -9.75 | 109.53 | 118.30 |
| 1 | F | 233 | ASP | CB-CG-OD1 | 9.75 | 127.07 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | L | 233 | ASP | CB-CG-OD1 | 9.75 | 127.07 | 118.30 |
| 1 | B | 645 | ARG | NE-CZ-NH1 | 9.74 | 125.17 | 120.30 |
| 1 | M | 447 | ASP | CB-CG-OD2 | -9.74 | 109.53 | 118.30 |
| 1 | O | 447 | ASP | CB-CG-OD2 | -9.74 | 109.53 | 118.30 |
| 1 | C | 233 | ASP | CB-CG-OD1 | 9.73 | 127.06 | 118.30 |
| 1 | L | 447 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | H | 447 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | N | 447 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | B | 447 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | F | 447 | ASP | CB-CG-OD2 | -9.73 | 109.54 | 118.30 |
| 1 | K | 233 | ASP | CB-CG-OD1 | 9.73 | 127.06 | 118.30 |
| 1 | C | 447 | ASP | CB-CG-OD2 | -9.73 | 109.55 | 118.30 |
| 1 | J | 233 | ASP | CB-CG-OD1 | 9.73 | 127.06 | 118.30 |
| 1 | D | 781 | ARG | NE-CZ-NH2 | -9.72 | 115.44 | 120.30 |
| 1 | H | 233 | ASP | CB-CG-OD1 | 9.72 | 127.05 | 118.30 |
| 1 | I | 447 | ASP | CB-CG-OD2 | -9.72 | 109.55 | 118.30 |
| 1 | L | 781 | ARG | NE-CZ-NH2 | -9.72 | 115.44 | 120.30 |
| 1 | K | 447 | ASP | CB-CG-OD2 | -9.72 | 109.55 | 118.30 |
| 1 | P | 781 | ARG | NE-CZ-NH2 | -9.72 | 115.44 | 120.30 |
| 1 | G | 781 | ARG | NE-CZ-NH2 | -9.71 | 115.44 | 120.30 |
| 1 | P | 233 | ASP | CB-CG-OD1 | 9.71 | 127.04 | 118.30 |
| 1 | B | 781 | ARG | NE-CZ-NH2 | -9.71 | 115.45 | 120.30 |
| 1 | D | 233 | ASP | CB-CG-OD1 | 9.71 | 127.03 | 118.30 |
| 1 | I | 233 | ASP | CB-CG-OD1 | 9.71 | 127.03 | 118.30 |
| 1 | A | 233 | ASP | CB-CG-OD1 | 9.68 | 127.01 | 118.30 |
| 1 | E | 431 | ARG | NE-CZ-NH1 | 9.68 | 125.14 | 120.30 |
| 1 | K | 199 | ASP | CB-CG-OD2 | -9.68 | 109.59 | 118.30 |
| 1 | K | 431 | ARG | NE-CZ-NH1 | 9.68 | 125.14 | 120.30 |
| 1 | L | 199 | ASP | CB-CG-OD2 | -9.67 | 109.59 | 118.30 |
| 1 | P | 199 | ASP | CB-CG-OD2 | -9.66 | 109.60 | 118.30 |
| 1 | I | 199 | ASP | CB-CG-OD2 | -9.65 | 109.61 | 118.30 |
| 1 | J | 199 | ASP | CB-CG-OD2 | -9.65 | 109.61 | 118.30 |
| 1 | A | 781 | ARG | NE-CZ-NH2 | -9.64 | 115.48 | 120.30 |
| 1 | D | 199 | ASP | CB-CG-OD2 | -9.64 | 109.62 | 118.30 |
| 1 | D | 431 | ARG | NE-CZ-NH1 | 9.64 | 125.12 | 120.30 |
| 1 | A | 199 | ASP | CB-CG-OD2 | -9.64 | 109.63 | 118.30 |
| 1 | O | 199 | ASP | CB-CG-OD2 | -9.64 | 109.63 | 118.30 |
| 1 | C | 781 | ARG | NE-CZ-NH2 | -9.63 | 115.48 | 120.30 |
| 1 | K | 781 | ARG | NE-CZ-NH2 | -9.63 | 115.48 | 120.30 |
| 1 | H | 199 | ASP | CB-CG-OD2 | -9.63 | 109.63 | 118.30 |
| 1 | M | 781 | ARG | NE-CZ-NH2 | -9.63 | 115.48 | 120.30 |
| 1 | B | 199 | ASP | CB-CG-OD2 | -9.62 | 109.64 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 199 | ASP | CB-CG-OD2 | -9.62 | 109.64 | 118.30 |
| 1 | G | 199 | ASP | CB-CG-OD2 | -9.62 | 109.64 | 118.30 |
| 1 | N | 199 | ASP | CB-CG-OD2 | -9.62 | 109.64 | 118.30 |
| 1 | H | 781 | ARG | NE-CZ-NH2 | -9.62 | 115.49 | 120.30 |
| 1 | P | 431 | ARG | NE-CZ-NH1 | 9.62 | 125.11 | 120.30 |
| 1 | F | 199 | ASP | CB-CG-OD2 | -9.61 | 109.65 | 118.30 |
| 1 | M | 199 | ASP | CB-CG-OD2 | -9.61 | 109.65 | 118.30 |
| 1 | E | 199 | ASP | CB-CG-OD2 | -9.61 | 109.65 | 118.30 |
| 1 | J | 431 | ARG | NE-CZ-NH1 | 9.60 | 125.10 | 120.30 |
| 1 | I | 431 | ARG | NE-CZ-NH1 | 9.60 | 125.10 | 120.30 |
| 1 | F | 781 | ARG | NE-CZ-NH2 | -9.59 | 115.51 | 120.30 |
| 1 | I | 781 | ARG | NE-CZ-NH2 | -9.58 | 115.51 | 120.30 |
| 1 | F | 431 | ARG | NE-CZ-NH1 | 9.58 | 125.09 | 120.30 |
| 1 | M | 431 | ARG | NE-CZ-NH1 | 9.58 | 125.09 | 120.30 |
| 1 | N | 781 | ARG | NE-CZ-NH2 | -9.58 | 115.51 | 120.30 |
| 1 | A | 431 | ARG | NE-CZ-NH1 | 9.57 | 125.09 | 120.30 |
| 1 | J | 781 | ARG | NE-CZ-NH2 | -9.57 | 115.52 | 120.30 |
| 1 | O | 431 | ARG | NE-CZ-NH1 | 9.57 | 125.08 | 120.30 |
| 1 | B | 431 | ARG | NE-CZ-NH1 | 9.56 | 125.08 | 120.30 |
| 1 | H | 431 | ARG | NE-CZ-NH1 | 9.56 | 125.08 | 120.30 |
| 1 | O | 781 | ARG | NE-CZ-NH2 | -9.56 | 115.52 | 120.30 |
| 1 | E | 781 | ARG | NE-CZ-NH2 | -9.55 | 115.53 | 120.30 |
| 1 | L | 431 | ARG | NE-CZ-NH1 | 9.53 | 125.07 | 120.30 |
| 1 | N | 431 | ARG | NE-CZ-NH1 | 9.53 | 125.06 | 120.30 |
| 1 | C | 431 | ARG | NE-CZ-NH1 | 9.51 | 125.06 | 120.30 |
| 1 | G | 431 | ARG | NE-CZ-NH1 | 9.50 | 125.05 | 120.30 |
| 1 | M | 809 | ARG | NE-CZ-NH2 | -9.49 | 115.55 | 120.30 |
| 1 | K | 13 | ARG | NE-CZ-NH1 | 9.49 | 125.04 | 120.30 |
| 1 | C | 809 | ARG | NE-CZ-NH2 | -9.46 | 115.57 | 120.30 |
| 1 | N | 809 | ARG | NE-CZ-NH2 | -9.46 | 115.57 | 120.30 |
| 1 | P | 809 | ARG | NE-CZ-NH2 | -9.45 | 115.57 | 120.30 |
| 1 | F | 809 | ARG | NE-CZ-NH2 | -9.45 | 115.58 | 120.30 |
| 1 | H | 809 | ARG | NE-CZ-NH2 | -9.44 | 115.58 | 120.30 |
| 1 | A | 809 | ARG | NE-CZ-NH2 | -9.43 | 115.58 | 120.30 |
| 1 | M | 13 | ARG | NE-CZ-NH1 | 9.43 | 125.02 | 120.30 |
| 1 | L | 809 | ARG | NE-CZ-NH2 | -9.43 | 115.59 | 120.30 |
| 1 | F | 13 | ARG | NE-CZ-NH1 | 9.42 | 125.01 | 120.30 |
| 1 | G | 809 | ARG | NE-CZ-NH2 | -9.42 | 115.59 | 120.30 |
| 1 | O | 13 | ARG | NE-CZ-NH1 | 9.41 | 125.01 | 120.30 |
| 1 | O | 809 | ARG | NE-CZ-NH2 | -9.41 | 115.59 | 120.30 |
| 1 | I | 13 | ARG | NE-CZ-NH1 | 9.41 | 125.00 | 120.30 |
| 1 | I | 809 | ARG | NE-CZ-NH2 | -9.41 | 115.60 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 13 | ARG | NE-CZ-NH1 | 9.40 | 125.00 | 120.30 |
| 1 | J | 809 | ARG | NE-CZ-NH2 | -9.39 | 115.61 | 120.30 |
| 1 | H | 13 | ARG | NE-CZ-NH1 | 9.39 | 124.99 | 120.30 |
| 1 | K | 809 | ARG | NE-CZ-NH2 | -9.38 | 115.61 | 120.30 |
| 1 | A | 13 | ARG | NE-CZ-NH1 | 9.37 | 124.98 | 120.30 |
| 1 | L | 13 | ARG | NE-CZ-NH1 | 9.36 | 124.98 | 120.30 |
| 1 | E | 809 | ARG | NE-CZ-NH2 | -9.36 | 115.62 | 120.30 |
| 1 | D | 809 | ARG | NE-CZ-NH2 | -9.36 | 115.62 | 120.30 |
| 1 | B | 809 | ARG | NE-CZ-NH2 | -9.35 | 115.62 | 120.30 |
| 1 | J | 13 | ARG | NE-CZ-NH1 | 9.35 | 124.98 | 120.30 |
| 1 | G | 13 | ARG | NE-CZ-NH1 | 9.35 | 124.97 | 120.30 |
| 1 | B | 13 | ARG | NE-CZ-NH1 | 9.33 | 124.97 | 120.30 |
| 1 | N | 13 | ARG | NE-CZ-NH1 | 9.33 | 124.97 | 120.30 |
| 1 | C | 13 | ARG | NE-CZ-NH1 | 9.31 | 124.95 | 120.30 |
| 1 | D | 13 | ARG | NE-CZ-NH1 | 9.30 | 124.95 | 120.30 |
| 1 | E | 13 | ARG | NE-CZ-NH1 | 9.29 | 124.94 | 120.30 |
| 1 | O | 509 | ASP | CB-CG-OD2 | -9.19 | 110.03 | 118.30 |
| 1 | H | 509 | ASP | CB-CG-OD2 | -9.18 | 110.04 | 118.30 |
| 1 | G | 509 | ASP | CB-CG-OD2 | -9.17 | 110.05 | 118.30 |
| 1 | P | 509 | ASP | CB-CG-OD2 | -9.16 | 110.06 | 118.30 |
| 1 | N | 509 | ASP | CB-CG-OD2 | -9.15 | 110.07 | 118.30 |
| 1 | B | 509 | ASP | CB-CG-OD2 | -9.14 | 110.08 | 118.30 |
| 1 | A | 509 | ASP | CB-CG-OD2 | -9.13 | 110.08 | 118.30 |
| 1 | K | 509 | ASP | CB-CG-OD2 | -9.13 | 110.08 | 118.30 |
| 1 | F | 509 | ASP | CB-CG-OD2 | -9.13 | 110.08 | 118.30 |
| 1 | L | 509 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | J | 509 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | M | 509 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | B | 429 | ASP | CB-CG-OD2 | -9.12 | 110.09 | 118.30 |
| 1 | J | 429 | ASP | CB-CG-OD2 | -9.11 | 110.10 | 118.30 |
| 1 | E | 509 | ASP | CB-CG-OD2 | -9.11 | 110.10 | 118.30 |
| 1 | O | 429 | ASP | CB-CG-OD2 | -9.11 | 110.11 | 118.30 |
| 1 | D | 509 | ASP | CB-CG-OD2 | -9.10 | 110.11 | 118.30 |
| 1 | N | 429 | ASP | CB-CG-OD2 | -9.10 | 110.11 | 118.30 |
| 1 | C | 429 | ASP | CB-CG-OD2 | -9.10 | 110.11 | 118.30 |
| 1 | C | 509 | ASP | CB-CG-OD2 | -9.09 | 110.12 | 118.30 |
| 1 | I | 509 | ASP | CB-CG-OD2 | -9.09 | 110.12 | 118.30 |
| 1 | A | 429 | ASP | CB-CG-OD2 | -9.09 | 110.12 | 118.30 |
| 1 | F | 429 | ASP | CB-CG-OD2 | -9.08 | 110.12 | 118.30 |
| 1 | K | 429 | ASP | CB-CG-OD2 | -9.08 | 110.12 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD2 | -9.08 | 110.13 | 118.30 |
| 1 | L | 429 | ASP | CB-CG-OD2 | -9.07 | 110.13 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | M | 429 | ASP | CB-CG-OD2 | -9.07 | 110.14 | 118.30 |
| 1 | E | 429 | ASP | CB-CG-OD2 | -9.07 | 110.14 | 118.30 |
| 1 | I | 429 | ASP | CB-CG-OD2 | -9.07 | 110.14 | 118.30 |
| 1 | G | 429 | ASP | CB-CG-OD2 | -9.05 | 110.16 | 118.30 |
| 1 | H | 429 | ASP | CB-CG-OD2 | -9.04 | 110.17 | 118.30 |
| 1 | P | 429 | ASP | CB-CG-OD2 | -9.01 | 110.19 | 118.30 |
| 1 | B | 473 | ARG | NE-CZ-NH2 | -8.94 | 115.83 | 120.30 |
| 1 | K | 473 | ARG | NE-CZ-NH2 | -8.91 | 115.84 | 120.30 |
| 1 | K | 287 | ASP | CB-CG-OD2 | -8.89 | 110.30 | 118.30 |
| 1 | N | 287 | ASP | CB-CG-OD2 | -8.89 | 110.30 | 118.30 |
| 1 | M | 473 | ARG | NE-CZ-NH2 | -8.89 | 115.86 | 120.30 |
| 1 | I | 287 | ASP | CB-CG-OD2 | -8.89 | 110.30 | 118.30 |
| 1 | D | 473 | ARG | NE-CZ-NH2 | -8.88 | 115.86 | 120.30 |
| 1 | H | 287 | ASP | CB-CG-OD2 | -8.89 | 110.30 | 118.30 |
| 1 | D | 287 | ASP | CB-CG-OD2 | -8.87 | 110.32 | 118.30 |
| 1 | C | 287 | ASP | CB-CG-OD2 | -8.87 | 110.32 | 118.30 |
| 1 | A | 287 | ASP | CB-CG-OD2 | -8.86 | 110.33 | 118.30 |
| 1 | A | 473 | ARG | NE-CZ-NH2 | -8.86 | 115.87 | 120.30 |
| 1 | J | 287 | ASP | CB-CG-OD2 | -8.86 | 110.33 | 118.30 |
| 1 | E | 287 | ASP | CB-CG-OD2 | -8.85 | 110.33 | 118.30 |
| 1 | C | 473 | ARG | NE-CZ-NH2 | -8.85 | 115.87 | 120.30 |
| 1 | I | 473 | ARG | NE-CZ-NH2 | -8.85 | 115.87 | 120.30 |
| 1 | B | 287 | ASP | CB-CG-OD2 | -8.85 | 110.34 | 118.30 |
| 1 | J | 473 | ARG | NE-CZ-NH2 | -8.85 | 115.88 | 120.30 |
| 1 | L | 473 | ARG | NE-CZ-NH2 | -8.85 | 115.88 | 120.30 |
| 1 | H | 473 | ARG | NE-CZ-NH2 | -8.84 | 115.88 | 120.30 |
| 1 | P | 287 | ASP | CB-CG-OD2 | -8.84 | 110.34 | 118.30 |
| 1 | L | 287 | ASP | CB-CG-OD2 | -8.84 | 110.34 | 118.30 |
| 1 | G | 287 | ASP | CB-CG-OD2 | -8.84 | 110.35 | 118.30 |
| 1 | O | 473 | ARG | NE-CZ-NH2 | -8.84 | 115.88 | 120.30 |
| 1 | F | 287 | ASP | CB-CG-OD2 | -8.82 | 110.36 | 118.30 |
| 1 | O | 287 | ASP | CB-CG-OD2 | -8.82 | 110.36 | 118.30 |
| 1 | P | 473 | ARG | NE-CZ-NH2 | -8.82 | 115.89 | 120.30 |
| 1 | M | 287 | ASP | CB-CG-OD2 | -8.82 | 110.36 | 118.30 |
| 1 | G | 473 | ARG | NE-CZ-NH2 | -8.81 | 115.90 | 120.30 |
| 1 | E | 473 | ARG | NE-CZ-NH2 | -8.76 | 115.92 | 120.30 |
| 1 | N | 473 | ARG | NE-CZ-NH2 | -8.74 | 115.93 | 120.30 |
| 1 | F | 52 | ARG | NE-CZ-NH2 | -8.73 | 115.93 | 120.30 |
| 1 | K | 210 | ARG | CD-NE-CZ | 8.72 | 135.81 | 123.60 |
| 1 | L | 210 | ARG | CD-NE-CZ | 8.72 | 135.81 | 123.60 |
| 1 | I | 210 | ARG | CD-NE-CZ | 8.72 | 135.80 | 123.60 |
| 1 | H | 210 | ARG | CD-NE-CZ | 8.71 | 135.80 | 123.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | O | 210 | ARG | CD-NE-CZ | 8.71 | 135.79 | 123.60 |
| 1 | N | 210 | ARG | CD-NE-CZ | 8.71 | 135.79 | 123.60 |
| 1 | C | 210 | ARG | CD-NE-CZ | 8.70 | 135.78 | 123.60 |
| 1 | F | 210 | ARG | CD-NE-CZ | 8.70 | 135.78 | 123.60 |
| 1 | F | 473 | ARG | NE-CZ-NH2 | -8.70 | 115.95 | 120.30 |
| 1 | A | 210 | ARG | CD-NE-CZ | 8.70 | 135.78 | 123.60 |
| 1 | B | 210 | ARG | CD-NE-CZ | 8.70 | 135.77 | 123.60 |
| 1 | O | 52 | ARG | NE-CZ-NH2 | -8.70 | 115.95 | 120.30 |
| 1 | P | 210 | ARG | CD-NE-CZ | 8.70 | 135.77 | 123.60 |
| 1 | D | 210 | ARG | CD-NE-CZ | 8.69 | 135.77 | 123.60 |
| 1 | G | 210 | ARG | CD-NE-CZ | 8.69 | 135.76 | 123.60 |
| 1 | E | 210 | ARG | CD-NE-CZ | 8.68 | 135.76 | 123.60 |
| 1 | J | 210 | ARG | CD-NE-CZ | 8.68 | 135.75 | 123.60 |
| 1 | M | 210 | ARG | CD-NE-CZ | 8.68 | 135.76 | 123.60 |
| 1 | I | 52 | ARG | NE-CZ-NH2 | -8.67 | 115.97 | 120.30 |
| 1 | B | 52 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 |
| 1 | N | 52 | ARG | NE-CZ-NH2 | -8.63 | 115.98 | 120.30 |
| 1 | P | 52 | ARG | NE-CZ-NH2 | -8.63 | 115.99 | 120.30 |
| 1 | E | 52 | ARG | NE-CZ-NH2 | -8.60 | 116.00 | 120.30 |
| 1 | H | 52 | ARG | NE-CZ-NH2 | -8.60 | 116.00 | 120.30 |
| 1 | D | 52 | ARG | NE-CZ-NH2 | -8.59 | 116.00 | 120.30 |
| 1 | J | 52 | ARG | NE-CZ-NH2 | -8.59 | 116.00 | 120.30 |
| 1 | A | 52 | ARG | NE-CZ-NH2 | -8.59 | 116.01 | 120.30 |
| 1 | B | 448 | ARG | NE-CZ-NH1 | 8.59 | 124.59 | 120.30 |
| 1 | K | 368 | ASP | CB-CG-OD2 | -8.58 | 110.58 | 118.30 |
| 1 | O | 368 | ASP | CB-CG-OD2 | -8.58 | 110.58 | 118.30 |
| 1 | G | 52 | ARG | NE-CZ-NH2 | -8.57 | 116.01 | 120.30 |
| 1 | E | 368 | ASP | CB-CG-OD2 | -8.57 | 110.59 | 118.30 |
| 1 | O | 429 | ASP | CB-CG-OD1 | 8.57 | 126.01 | 118.30 |
| 1 | J | 368 | ASP | CB-CG-OD2 | -8.56 | 110.59 | 118.30 |
| 1 | L | 52 | ARG | NE-CZ-NH2 | -8.56 | 116.02 | 120.30 |
| 1 | M | 368 | ASP | CB-CG-OD2 | -8.56 | 110.59 | 118.30 |
| 1 | D | 429 | ASP | CB-CG-OD1 | 8.56 | 126.00 | 118.30 |
| 1 | F | 429 | ASP | CB-CG-OD1 | 8.55 | 126.00 | 118.30 |
| 1 | K | 429 | ASP | CB-CG-OD1 | 8.55 | 126.00 | 118.30 |
| 1 | K | 52 | ARG | NE-CZ-NH2 | -8.55 | 116.03 | 120.30 |
| 1 | P | 368 | ASP | CB-CG-OD2 | -8.55 | 110.61 | 118.30 |
| 1 | C | 368 | ASP | CB-CG-OD2 | -8.55 | 110.61 | 118.30 |
| 1 | H | 368 | ASP | CB-CG-OD2 | -8.54 | 110.61 | 118.30 |
| 1 | M | 429 | ASP | CB-CG-OD1 | 8.55 | 125.99 | 118.30 |
| 1 | N | 429 | ASP | CB-CG-OD1 | 8.55 | 125.99 | 118.30 |
| 1 | J | 429 | ASP | CB-CG-OD1 | 8.54 | 125.99 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | N | 448 | ARG | NE-CZ-NH1 | 8.54 | 124.57 | 120.30 |
| 1 | C | 52 | ARG | NE-CZ-NH2 | -8.54 | 116.03 | 120.30 |
| 1 | L | 368 | ASP | CB-CG-OD2 | -8.54 | 110.62 | 118.30 |
| 1 | C | 429 | ASP | CB-CG-OD1 | 8.53 | 125.98 | 118.30 |
| 1 | E | 429 | ASP | CB-CG-OD1 | 8.54 | 125.98 | 118.30 |
| 1 | H | 448 | ARG | NE-CZ-NH1 | 8.53 | 124.57 | 120.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | -8.53 | 110.62 | 118.30 |
| 1 | I | 368 | ASP | CB-CG-OD2 | -8.53 | 110.62 | 118.30 |
| 1 | A | 429 | ASP | CB-CG-OD1 | 8.53 | 125.97 | 118.30 |
| 1 | I | 429 | ASP | CB-CG-OD1 | 8.53 | 125.97 | 118.30 |
| 1 | G | 448 | ARG | NE-CZ-NH1 | 8.52 | 124.56 | 120.30 |
| 1 | B | 368 | ASP | CB-CG-OD2 | -8.52 | 110.63 | 118.30 |
| 1 | I | 448 | ARG | NE-CZ-NH1 | 8.52 | 124.56 | 120.30 |
| 1 | D | 368 | ASP | CB-CG-OD2 | -8.52 | 110.64 | 118.30 |
| 1 | F | 368 | ASP | CB-CG-OD2 | -8.51 | 110.64 | 118.30 |
| 1 | K | 448 | ARG | NE-CZ-NH1 | 8.51 | 124.56 | 120.30 |
| 1 | P | 448 | ARG | NE-CZ-NH1 | 8.51 | 124.56 | 120.30 |
| 1 | D | 448 | ARG | NE-CZ-NH1 | 8.51 | 124.56 | 120.30 |
| 1 | G | 429 | ASP | CB-CG-OD1 | 8.51 | 125.96 | 118.30 |
| 1 | H | 429 | ASP | CB-CG-OD1 | 8.51 | 125.96 | 118.30 |
| 1 | M | 52 | ARG | NE-CZ-NH2 | -8.51 | 116.05 | 120.30 |
| 1 | B | 429 | ASP | CB-CG-OD1 | 8.51 | 125.95 | 118.30 |
| 1 | G | 368 | ASP | CB-CG-OD2 | -8.51 | 110.65 | 118.30 |
| 1 | A | 448 | ARG | NE-CZ-NH1 | 8.50 | 124.55 | 120.30 |
| 1 | N | 368 | ASP | CB-CG-OD2 | -8.50 | 110.65 | 118.30 |
| 1 | P | 571 | VAL | CB-CA-C | -8.49 | 95.27 | 111.40 |
| 1 | F | 448 | ARG | NE-CZ-NH1 | 8.49 | 124.55 | 120.30 |
| 1 | L | 571 | VAL | CB-CA-C | -8.49 | 95.27 | 111.40 |
| 1 | O | 448 | ARG | NE-CZ-NH1 | 8.49 | 124.54 | 120.30 |
| 1 | P | 429 | ASP | CB-CG-OD1 | 8.49 | 125.94 | 118.30 |
| 1 | F | 571 | VAL | CB-CA-C | -8.48 | 95.28 | 111.40 |
| 1 | E | 448 | ARG | NE-CZ-NH1 | 8.48 | 124.54 | 120.30 |
| 1 | E | 571 | VAL | CB-CA-C | -8.48 | 95.28 | 111.40 |
| 1 | L | 429 | ASP | CB-CG-OD1 | 8.48 | 125.93 | 118.30 |
| 1 | M | 571 | VAL | CB-CA-C | -8.48 | 95.29 | 111.40 |
| 1 | C | 571 | VAL | CB-CA-C | -8.48 | 95.30 | 111.40 |
| 1 | A | 571 | VAL | CB-CA-C | -8.47 | 95.30 | 111.40 |
| 1 | C | 448 | ARG | NE-CZ-NH1 | 8.47 | 124.54 | 120.30 |
| 1 | O | 571 | VAL | CB-CA-C | -8.47 | 95.30 | 111.40 |
| 1 | H | 571 | VAL | CB-CA-C | -8.47 | 95.31 | 111.40 |
| 1 | J | 448 | ARG | NE-CZ-NH1 | 8.47 | 124.53 | 120.30 |
| 1 | K | 571 | VAL | CB-CA-C | -8.47 | 95.31 | 111.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | G | 571 | VAL | CB-CA-C | -8.47 | 95.31 | 111.40 |
| 1 | L | 448 | ARG | NE-CZ-NH1 | 8.47 | 124.53 | 120.30 |
| 1 | I | 571 | VAL | CB-CA-C | -8.46 | 95.32 | 111.40 |
| 1 | N | 5 | ASP | CB-CG-OD2 | -8.46 | 110.68 | 118.30 |
| 1 | B | 571 | VAL | CB-CA-C | -8.46 | 95.32 | 111.40 |
| 1 | D | 571 | VAL | CB-CA-C | -8.46 | 95.32 | 111.40 |
| 1 | N | 571 | VAL | CB-CA-C | -8.45 | 95.35 | 111.40 |
| 1 | J | 571 | VAL | CB-CA-C | -8.45 | 95.35 | 111.40 |
| 1 | M | 448 | ARG | NE-CZ-NH1 | 8.43 | 124.51 | 120.30 |
| 1 | F | 5 | ASP | CB-CG-OD2 | -8.41 | 110.73 | 118.30 |
| 1 | F | 13 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 1 | K | 5 | ASP | CB-CG-OD2 | -8.40 | 110.74 | 118.30 |
| 1 | D | 5 | ASP | CB-CG-OD2 | -8.39 | 110.75 | 118.30 |
| 1 | O | 5 | ASP | CB-CG-OD2 | -8.39 | 110.75 | 118.30 |
| 1 | A | 5 | ASP | CB-CG-OD2 | -8.38 | 110.76 | 118.30 |
| 1 | I | 13 | ARG | NE-CZ-NH2 | -8.38 | 116.11 | 120.30 |
| 1 | P | 5 | ASP | CB-CG-OD2 | -8.38 | 110.76 | 118.30 |
| 1 | J | 5 | ASP | CB-CG-OD2 | -8.37 | 110.77 | 118.30 |
| 1 | B | 5 | ASP | CB-CG-OD2 | -8.37 | 110.77 | 118.30 |
| 1 | H | 5 | ASP | CB-CG-OD2 | -8.36 | 110.77 | 118.30 |
| 1 | M | 13 | ARG | NE-CZ-NH2 | -8.35 | 116.12 | 120.30 |
| 1 | G | 5 | ASP | CB-CG-OD2 | -8.35 | 110.78 | 118.30 |
| 1 | M | 5 | ASP | CB-CG-OD2 | -8.35 | 110.78 | 118.30 |
| 1 | G | 13 | ARG | NE-CZ-NH2 | -8.35 | 116.12 | 120.30 |
| 1 | L | 5 | ASP | CB-CG-OD2 | -8.35 | 110.79 | 118.30 |
| 1 | C | 5 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | E | 13 | ARG | NE-CZ-NH2 | -8.33 | 116.14 | 120.30 |
| 1 | G | 428 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | J | 428 | ASP | CB-CG-OD2 | -8.33 | 110.80 | 118.30 |
| 1 | J | 13 | ARG | NE-CZ-NH2 | -8.32 | 116.14 | 120.30 |
| 1 | I | 5 | ASP | CB-CG-OD2 | -8.31 | 110.82 | 118.30 |
| 1 | E | 5 | ASP | CB-CG-OD2 | -8.31 | 110.82 | 118.30 |
| 1 | N | 428 | ASP | CB-CG-OD2 | -8.30 | 110.83 | 118.30 |
| 1 | A | 13 | ARG | NE-CZ-NH2 | -8.29 | 116.15 | 120.30 |
| 1 | H | 13 | ARG | NE-CZ-NH2 | -8.29 | 116.15 | 120.30 |
| 1 | B | 13 | ARG | NE-CZ-NH2 | -8.29 | 116.16 | 120.30 |
| 1 | K | 428 | ASP | CB-CG-OD2 | -8.29 | 110.84 | 118.30 |
| 1 | H | 428 | ASP | CB-CG-OD2 | -8.28 | 110.84 | 118.30 |
| 1 | L | 428 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | E | 428 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | C | 428 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | K | 13 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | O | 13 | ARG | NE-CZ-NH2 | -8.28 | 116.16 | 120.30 |
| 1 | A | 428 | ASP | CB-CG-OD2 | -8.28 | 110.85 | 118.30 |
| 1 | B | 428 | ASP | CB-CG-OD2 | -8.27 | 110.85 | 118.30 |
| 1 | C | 13 | ARG | NE-CZ-NH2 | -8.27 | 116.16 | 120.30 |
| 1 | O | 428 | ASP | CB-CG-OD2 | -8.27 | 110.85 | 118.30 |
| 1 | M | 428 | ASP | CB-CG-OD2 | -8.27 | 110.86 | 118.30 |
| 1 | P | 428 | ASP | CB-CG-OD2 | -8.27 | 110.86 | 118.30 |
| 1 | D | 13 | ARG | NE-CZ-NH2 | -8.26 | 116.17 | 120.30 |
| 1 | F | 428 | ASP | CB-CG-OD2 | -8.26 | 110.87 | 118.30 |
| 1 | I | 428 | ASP | CB-CG-OD2 | -8.25 | 110.88 | 118.30 |
| 1 | L | 13 | ARG | NE-CZ-NH2 | -8.25 | 116.18 | 120.30 |
| 1 | P | 13 | ARG | NE-CZ-NH2 | -8.25 | 116.18 | 120.30 |
| 1 | D | 428 | ASP | CB-CG-OD2 | -8.24 | 110.88 | 118.30 |
| 1 | N | 13 | ARG | NE-CZ-NH2 | -8.20 | 116.20 | 120.30 |
| 1 | D | 329 | ASP | CB-CG-OD2 | -8.18 | 110.94 | 118.30 |
| 1 | E | 329 | ASP | CB-CG-OD2 | -8.18 | 110.94 | 118.30 |
| 1 | H | 329 | ASP | CB-CG-OD2 | -8.15 | 110.97 | 118.30 |
| 1 | L | 329 | ASP | CB-CG-OD2 | -8.14 | 110.97 | 118.30 |
| 1 | F | 329 | ASP | CB-CG-OD2 | -8.13 | 110.98 | 118.30 |
| 1 | J | 329 | ASP | CB-CG-OD2 | -8.12 | 110.99 | 118.30 |
| 1 | A | 329 | ASP | CB-CG-OD2 | -8.11 | 111.00 | 118.30 |
| 1 | N | 329 | ASP | CB-CG-OD2 | -8.11 | 111.00 | 118.30 |
| 1 | B | 329 | ASP | CB-CG-OD2 | -8.10 | 111.01 | 118.30 |
| 1 | P | 329 | ASP | CB-CG-OD2 | -8.10 | 111.01 | 118.30 |
| 1 | K | 329 | ASP | CB-CG-OD2 | -8.10 | 111.01 | 118.30 |
| 1 | G | 329 | ASP | CB-CG-OD2 | -8.08 | 111.03 | 118.30 |
| 1 | M | 329 | ASP | CB-CG-OD2 | -8.08 | 111.03 | 118.30 |
| 1 | I | 329 | ASP | CB-CG-OD2 | -8.08 | 111.03 | 118.30 |
| 1 | C | 329 | ASP | CB-CG-OD2 | -8.07 | 111.03 | 118.30 |
| 1 | O | 329 | ASP | CB-CG-OD2 | -8.07 | 111.04 | 118.30 |
| 1 | E | 130 | ASP | CB-CG-OD1 | 7.96 | 125.46 | 118.30 |
| 1 | G | 130 | ASP | CB-CG-OD1 | 7.94 | 125.44 | 118.30 |
| 1 | A | 130 | ASP | CB-CG-OD1 | 7.93 | 125.44 | 118.30 |
| 1 | M | 130 | ASP | CB-CG-OD1 | 7.93 | 125.44 | 118.30 |
| 1 | H | 130 | ASP | CB-CG-OD1 | 7.91 | 125.42 | 118.30 |
| 1 | B | 130 | ASP | CB-CG-OD1 | 7.91 | 125.42 | 118.30 |
| 1 | D | 130 | ASP | CB-CG-OD1 | 7.90 | 125.41 | 118.30 |
| 1 | N | 130 | ASP | CB-CG-OD1 | 7.90 | 125.41 | 118.30 |
| 1 | I | 130 | ASP | CB-CG-OD1 | 7.89 | 125.40 | 118.30 |
| 1 | H | 916 | ASP | CB-CG-OD1 | 7.89 | 125.40 | 118.30 |
| 1 | L | 916 | ASP | CB-CG-OD1 | 7.88 | 125.39 | 118.30 |
| 1 | O | 130 | ASP | CB-CG-OD1 | 7.88 | 125.39 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | F | 130 | ASP | CB-CG-OD1 | 7.88 | 125.39 | 118.30 |
| 1 | P | 130 | ASP | CB-CG-OD1 | 7.88 | 125.39 | 118.30 |
| 1 | C | 130 | ASP | CB-CG-OD1 | 7.87 | 125.39 | 118.30 |
| 1 | F | 916 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 1 | M | 916 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 1 | N | 916 | ASP | CB-CG-OD1 | 7.87 | 125.38 | 118.30 |
| 1 | K | 916 | ASP | CB-CG-OD1 | 7.86 | 125.38 | 118.30 |
| 1 | C | 916 | ASP | CB-CG-OD1 | 7.86 | 125.37 | 118.30 |
| 1 | D | 916 | ASP | CB-CG-OD1 | 7.86 | 125.37 | 118.30 |
| 1 | L | 130 | ASP | CB-CG-OD1 | 7.85 | 125.37 | 118.30 |
| 1 | P | 916 | ASP | CB-CG-OD1 | 7.84 | 125.36 | 118.30 |
| 1 | A | 916 | ASP | CB-CG-OD1 | 7.84 | 125.36 | 118.30 |
| 1 | O | 916 | ASP | CB-CG-OD1 | 7.84 | 125.36 | 118.30 |
| 1 | B | 916 | ASP | CB-CG-OD1 | 7.84 | 125.35 | 118.30 |
| 1 | G | 916 | ASP | CB-CG-OD1 | 7.84 | 125.35 | 118.30 |
| 1 | K | 130 | ASP | CB-CG-OD1 | 7.83 | 125.35 | 118.30 |
| 1 | J | 130 | ASP | CB-CG-OD1 | 7.83 | 125.34 | 118.30 |
| 1 | O | 659 | ASP | CB-CG-OD2 | -7.82 | 111.26 | 118.30 |
| 1 | E | 659 | ASP | CB-CG-OD2 | -7.81 | 111.27 | 118.30 |
| 1 | F | 659 | ASP | CB-CG-OD2 | -7.81 | 111.27 | 118.30 |
| 1 | D | 659 | ASP | CB-CG-OD2 | -7.81 | 111.27 | 118.30 |
| 1 | P | 659 | ASP | CB-CG-OD2 | -7.81 | 111.27 | 118.30 |
| 1 | J | 659 | ASP | CB-CG-OD2 | -7.80 | 111.28 | 118.30 |
| 1 | N | 659 | ASP | CB-CG-OD2 | -7.80 | 111.28 | 118.30 |
| 1 | I | 916 | ASP | CB-CG-OD1 | 7.79 | 125.32 | 118.30 |
| 1 | E | 916 | ASP | CB-CG-OD1 | 7.79 | 125.31 | 118.30 |
| 1 | I | 659 | ASP | CB-CG-OD2 | -7.79 | 111.29 | 118.30 |
| 1 | L | 659 | ASP | CB-CG-OD2 | -7.79 | 111.29 | 118.30 |
| 1 | J | 916 | ASP | CB-CG-OD1 | 7.79 | 125.31 | 118.30 |
| 1 | B | 659 | ASP | CB-CG-OD2 | -7.78 | 111.30 | 118.30 |
| 1 | K | 659 | ASP | CB-CG-OD2 | -7.78 | 111.30 | 118.30 |
| 1 | M | 659 | ASP | CB-CG-OD2 | -7.78 | 111.30 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD2 | -7.77 | 111.31 | 118.30 |
| 1 | A | 659 | ASP | CB-CG-OD2 | -7.76 | 111.31 | 118.30 |
| 1 | H | 659 | ASP | CB-CG-OD2 | -7.76 | 111.31 | 118.30 |
| 1 | G | 659 | ASP | CB-CG-OD2 | -7.72 | 111.35 | 118.30 |
| 1 | C | 442 | ARG | NE-CZ-NH2 | -7.64 | 116.48 | 120.30 |
| 1 | F | 442 | ARG | NE-CZ-NH2 | -7.63 | 116.48 | 120.30 |
| 1 | G | 442 | ARG | NE-CZ-NH2 | -7.62 | 116.49 | 120.30 |
| 1 | I | 442 | ARG | NE-CZ-NH2 | -7.62 | 116.49 | 120.30 |
| 1 | K | 442 | ARG | NE-CZ-NH2 | -7.62 | 116.49 | 120.30 |
| 1 | H | 442 | ARG | NE-CZ-NH2 | -7.61 | 116.49 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 442 | ARG | NE-CZ-NH2 | -7.60 | 116.50 | 120.30 |
| 1 | I | 356 | ARG | NE-CZ-NH1 | 7.60 | 124.10 | 120.30 |
| 1 | J | 442 | ARG | NE-CZ-NH2 | -7.60 | 116.50 | 120.30 |
| 1 | P | 442 | ARG | NE-CZ-NH2 | -7.60 | 116.50 | 120.30 |
| 1 | E | 442 | ARG | NE-CZ-NH2 | -7.58 | 116.51 | 120.30 |
| 1 | O | 442 | ARG | NE-CZ-NH2 | -7.58 | 116.51 | 120.30 |
| 1 | B | 442 | ARG | NE-CZ-NH2 | -7.57 | 116.51 | 120.30 |
| 1 | E | 447 | ASP | CB-CG-OD1 | 7.57 | 125.11 | 118.30 |
| 1 | J | 447 | ASP | CB-CG-OD1 | 7.56 | 125.11 | 118.30 |
| 1 | B | 447 | ASP | CB-CG-OD1 | 7.56 | 125.10 | 118.30 |
| 1 | A | 442 | ARG | NE-CZ-NH2 | -7.55 | 116.52 | 120.30 |
| 1 | B | 356 | ARG | NE-CZ-NH1 | 7.55 | 124.08 | 120.30 |
| 1 | C | 447 | ASP | CB-CG-OD1 | 7.55 | 125.10 | 118.30 |
| 1 | H | 447 | ASP | CB-CG-OD1 | 7.55 | 125.09 | 118.30 |
| 1 | D | 447 | ASP | CB-CG-OD1 | 7.54 | 125.09 | 118.30 |
| 1 | J | 356 | ARG | NE-CZ-NH1 | 7.54 | 124.07 | 120.30 |
| 1 | L | 442 | ARG | NE-CZ-NH2 | -7.54 | 116.53 | 120.30 |
| 1 | A | 447 | ASP | CB-CG-OD1 | 7.54 | 125.08 | 118.30 |
| 1 | N | 442 | ARG | NE-CZ-NH2 | -7.53 | 116.53 | 120.30 |
| 1 | G | 447 | ASP | CB-CG-OD1 | 7.53 | 125.08 | 118.30 |
| 1 | N | 447 | ASP | CB-CG-OD1 | 7.53 | 125.08 | 118.30 |
| 1 | G | 356 | ARG | NE-CZ-NH1 | 7.52 | 124.06 | 120.30 |
| 1 | O | 447 | ASP | CB-CG-OD1 | 7.52 | 125.06 | 118.30 |
| 1 | D | 249 | GLU | N-CA-CB | 7.52 | 124.13 | 110.60 |
| 1 | K | 249 | GLU | N-CA-CB | 7.52 | 124.13 | 110.60 |
| 1 | A | 249 | GLU | N-CA-CB | 7.51 | 124.12 | 110.60 |
| 1 | E | 249 | GLU | N-CA-CB | 7.51 | 124.13 | 110.60 |
| 1 | F | 447 | ASP | CB-CG-OD1 | 7.51 | 125.06 | 118.30 |
| 1 | M | 447 | ASP | CB-CG-OD1 | 7.51 | 125.06 | 118.30 |
| 1 | B | 249 | GLU | N-CA-CB | 7.51 | 124.11 | 110.60 |
| 1 | F | 249 | GLU | N-CA-CB | 7.51 | 124.11 | 110.60 |
| 1 | I | 447 | ASP | CB-CG-OD1 | 7.51 | 125.06 | 118.30 |
| 1 | O | 249 | GLU | N-CA-CB | 7.51 | 124.11 | 110.60 |
| 1 | O | 356 | ARG | NE-CZ-NH1 | 7.51 | 124.05 | 120.30 |
| 1 | G | 249 | GLU | N-CA-CB | 7.50 | 124.10 | 110.60 |
| 1 | P | 447 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | L | 447 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | K | 447 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | N | 249 | GLU | N-CA-CB | 7.50 | 124.09 | 110.60 |
| 1 | F | 356 | ARG | NE-CZ-NH1 | 7.49 | 124.05 | 120.30 |
| 1 | L | 249 | GLU | N-CA-CB | 7.49 | 124.08 | 110.60 |
| 1 | C | 249 | GLU | N-CA-CB | 7.49 | 124.08 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 249 | GLU | N-CA-CB | 7.49 | 124.08 | 110.60 |
| 1 | M | 249 | GLU | N-CA-CB | 7.49 | 124.08 | 110.60 |
| 1 | N | 356 | ARG | NE-CZ-NH1 | 7.49 | 124.04 | 120.30 |
| 1 | M | 442 | ARG | NE-CZ-NH2 | -7.48 | 116.56 | 120.30 |
| 1 | E | 356 | ARG | NE-CZ-NH1 | 7.48 | 124.04 | 120.30 |
| 1 | L | 356 | ARG | NE-CZ-NH1 | 7.48 | 124.04 | 120.30 |
| 1 | H | 249 | GLU | N-CA-CB | 7.48 | 124.06 | 110.60 |
| 1 | A | 356 | ARG | NE-CZ-NH1 | 7.48 | 124.04 | 120.30 |
| 1 | I | 249 | GLU | N-CA-CB | 7.48 | 124.06 | 110.60 |
| 1 | M | 356 | ARG | NE-CZ-NH1 | 7.47 | 124.04 | 120.30 |
| 1 | J | 249 | GLU | N-CA-CB | 7.47 | 124.04 | 110.60 |
| 1 | K | 431 | ARG | NE-CZ-NH2 | -7.45 | 116.57 | 120.30 |
| 1 | K | 356 | ARG | NE-CZ-NH1 | 7.45 | 124.03 | 120.30 |
| 1 | P | 356 | ARG | NE-CZ-NH1 | 7.45 | 124.02 | 120.30 |
| 1 | H | 356 | ARG | NE-CZ-NH1 | 7.45 | 124.02 | 120.30 |
| 1 | C | 356 | ARG | NE-CZ-NH1 | 7.44 | 124.02 | 120.30 |
| 1 | D | 356 | ARG | NE-CZ-NH1 | 7.43 | 124.02 | 120.30 |
| 1 | J | 431 | ARG | NE-CZ-NH2 | -7.41 | 116.59 | 120.30 |
| 1 | D | 431 | ARG | NE-CZ-NH2 | -7.41 | 116.60 | 120.30 |
| 1 | B | 431 | ARG | NE-CZ-NH2 | -7.39 | 116.60 | 120.30 |
| 1 | F | 431 | ARG | NE-CZ-NH2 | -7.38 | 116.61 | 120.30 |
| 1 | O | 531 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 1 | G | 431 | ARG | NE-CZ-NH2 | -7.37 | 116.62 | 120.30 |
| 1 | A | 431 | ARG | NE-CZ-NH2 | -7.36 | 116.62 | 120.30 |
| 1 | I | 431 | ARG | NE-CZ-NH2 | -7.36 | 116.62 | 120.30 |
| 1 | O | 431 | ARG | NE-CZ-NH2 | -7.36 | 116.62 | 120.30 |
| 1 | H | 431 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | P | 431 | ARG | NE-CZ-NH2 | -7.33 | 116.64 | 120.30 |
| 1 | E | 431 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | C | 431 | ARG | NE-CZ-NH2 | -7.31 | 116.64 | 120.30 |
| 1 | I | 292 | ARG | NE-CZ-NH1 | 7.31 | 123.96 | 120.30 |
| 1 | D | 292 | ARG | NE-CZ-NH1 | 7.31 | 123.95 | 120.30 |
| 1 | H | 292 | ARG | NE-CZ-NH1 | 7.30 | 123.95 | 120.30 |
| 1 | I | 531 | ARG | NE-CZ-NH1 | 7.29 | 123.95 | 120.30 |
| 1 | N | 431 | ARG | NE-CZ-NH2 | -7.29 | 116.65 | 120.30 |
| 1 | J | 531 | ARG | NE-CZ-NH1 | 7.29 | 123.94 | 120.30 |
| 1 | L | 938 | ARG | CD-NE-CZ | 7.29 | 133.80 | 123.60 |
| 1 | F | 292 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 1 | M | 431 | ARG | NE-CZ-NH2 | -7.28 | 116.66 | 120.30 |
| 1 | B | 938 | ARG | CD-NE-CZ | 7.28 | 133.79 | 123.60 |
| 1 | L | 431 | ARG | NE-CZ-NH2 | -7.28 | 116.66 | 120.30 |
| 1 | A | 832 | ASP | CB-CG-OD2 | -7.28 | 111.75 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | K | 938 | ARG | CD-NE-CZ | 7.28 | 133.79 | 123.60 |
| 1 | P | 531 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 1 | C | 292 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 |
| 1 | N | 938 | ARG | CD-NE-CZ | 7.27 | 133.78 | 123.60 |
| 1 | A | 938 | ARG | CD-NE-CZ | 7.26 | 133.77 | 123.60 |
| 1 | C | 938 | ARG | CD-NE-CZ | 7.26 | 133.77 | 123.60 |
| 1 | L | 531 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | D | 531 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | G | 938 | ARG | CD-NE-CZ | 7.26 | 133.76 | 123.60 |
| 1 | M | 531 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | N | 292 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | B | 292 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | B | 531 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | M | 832 | ASP | CB-CG-OD2 | -7.26 | 111.77 | 118.30 |
| 1 | C | 531 | ARG | NE-CZ-NH1 | 7.25 | 123.93 | 120.30 |
| 1 | A | 292 | ARG | NE-CZ-NH1 | 7.25 | 123.93 | 120.30 |
| 1 | K | 292 | ARG | NE-CZ-NH1 | 7.25 | 123.93 | 120.30 |
| 1 | E | 292 | ARG | NE-CZ-NH1 | 7.25 | 123.92 | 120.30 |
| 1 | J | 938 | ARG | CD-NE-CZ | 7.25 | 133.75 | 123.60 |
| 1 | P | 938 | ARG | CD-NE-CZ | 7.25 | 133.75 | 123.60 |
| 1 | E | 531 | ARG | NE-CZ-NH1 | 7.25 | 123.92 | 120.30 |
| 1 | O | 938 | ARG | CD-NE-CZ | 7.25 | 133.75 | 123.60 |
| 1 | G | 832 | ASP | CB-CG-OD2 | -7.24 | 111.78 | 118.30 |
| 1 | A | 531 | ARG | NE-CZ-NH1 | 7.24 | 123.92 | 120.30 |
| 1 | E | 938 | ARG | CD-NE-CZ | 7.24 | 133.74 | 123.60 |
| 1 | M | 292 | ARG | NE-CZ-NH1 | 7.24 | 123.92 | 120.30 |
| 1 | F | 832 | ASP | CB-CG-OD2 | -7.24 | 111.79 | 118.30 |
| 1 | M | 938 | ARG | CD-NE-CZ | 7.24 | 133.74 | 123.60 |
| 1 | N | 832 | ASP | CB-CG-OD2 | -7.24 | 111.79 | 118.30 |
| 1 | D | 938 | ARG | CD-NE-CZ | 7.23 | 133.72 | 123.60 |
| 1 | F | 531 | ARG | NE-CZ-NH1 | 7.23 | 123.92 | 120.30 |
| 1 | H | 938 | ARG | CD-NE-CZ | 7.23 | 133.72 | 123.60 |
| 1 | I | 938 | ARG | CD-NE-CZ | 7.23 | 133.73 | 123.60 |
| 1 | K | 832 | ASP | CB-CG-OD2 | -7.23 | 111.79 | 118.30 |
| 1 | P | 52 | ARG | NE-CZ-NH1 | 7.23 | 123.92 | 120.30 |
| 1 | F | 938 | ARG | CD-NE-CZ | 7.23 | 133.72 | 123.60 |
| 1 | M | 233 | ASP | CB-CG-OD2 | -7.23 | 111.79 | 118.30 |
| 1 | P | 832 | ASP | CB-CG-OD2 | -7.23 | 111.79 | 118.30 |
| 1 | C | 832 | ASP | CB-CG-OD2 | -7.23 | 111.80 | 118.30 |
| 1 | H | 832 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |
| 1 | J | 832 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |
| 1 | L | 832 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 832 | ASP | CB-CG-OD2 | -7.22 | 111.81 | 118.30 |
| 1 | G | 233 | ASP | CB-CG-OD2 | -7.22 | 111.81 | 118.30 |
| 1 | I | 832 | ASP | CB-CG-OD2 | -7.22 | 111.81 | 118.30 |
| 1 | O | 292 | ARG | NE-CZ-NH1 | 7.21 | 123.91 | 120.30 |
| 1 | O | 832 | ASP | CB-CG-OD2 | -7.21 | 111.81 | 118.30 |
| 1 | J | 292 | ARG | NE-CZ-NH1 | 7.21 | 123.90 | 120.30 |
| 1 | L | 292 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 1 | H | 199 | ASP | CB-CG-OD1 | 7.20 | 124.78 | 118.30 |
| 1 | G | 531 | ARG | NE-CZ-NH1 | 7.19 | 123.90 | 120.30 |
| 1 | L | 233 | ASP | CB-CG-OD2 | -7.19 | 111.83 | 118.30 |
| 1 | I | 233 | ASP | CB-CG-OD2 | -7.19 | 111.83 | 118.30 |
| 1 | D | 52 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 1 | D | 832 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | E | 233 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | P | 292 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 1 | E | 832 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | J | 233 | ASP | CB-CG-OD2 | -7.18 | 111.84 | 118.30 |
| 1 | K | 199 | ASP | CB-CG-OD1 | 7.18 | 124.76 | 118.30 |
| 1 | F | 52 | ARG | NE-CZ-NH1 | 7.17 | 123.89 | 120.30 |
| 1 | O | 233 | ASP | CB-CG-OD2 | -7.17 | 111.84 | 118.30 |
| 1 | N | 233 | ASP | CB-CG-OD2 | -7.17 | 111.84 | 118.30 |
| 1 | H | 52 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 1 | I | 199 | ASP | CB-CG-OD1 | 7.17 | 124.75 | 118.30 |
| 1 | N | 531 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 1 | H | 531 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 1 | P | 233 | ASP | CB-CG-OD2 | -7.16 | 111.85 | 118.30 |
| 1 | P | 909 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 1 | E | 199 | ASP | CB-CG-OD1 | 7.16 | 124.75 | 118.30 |
| 1 | J | 909 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 1 | L | 909 | ARG | NE-CZ-NH2 | -7.15 | 116.72 | 120.30 |
| 1 | C | 233 | ASP | CB-CG-OD2 | -7.15 | 111.86 | 118.30 |
| 1 | G | 292 | ARG | NE-CZ-NH1 | 7.15 | 123.88 | 120.30 |
| 1 | D | 233 | ASP | CB-CG-OD2 | -7.15 | 111.87 | 118.30 |
| 1 | M | 199 | ASP | CB-CG-OD1 | 7.15 | 124.73 | 118.30 |
| 1 | F | 233 | ASP | CB-CG-OD2 | -7.15 | 111.87 | 118.30 |
| 1 | I | 52 | ARG | NE-CZ-NH1 | 7.15 | 123.87 | 120.30 |
| 1 | D | 199 | ASP | CB-CG-OD1 | 7.14 | 124.73 | 118.30 |
| 1 | K | 193 | ASP | CB-CG-OD1 | 7.14 | 124.73 | 118.30 |
| 1 | B | 199 | ASP | CB-CG-OD1 | 7.14 | 124.73 | 118.30 |
| 1 | B | 233 | ASP | CB-CG-OD2 | -7.14 | 111.87 | 118.30 |
| 1 | M | 52 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | O | 52 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | F | 909 | ARG | NE-CZ-NH2 | -7.14 | 116.73 | 120.30 |
| 1 | C | 193 | ASP | CB-CG-OD1 | 7.14 | 124.73 | 118.30 |
| 1 | D | 193 | ASP | CB-CG-OD1 | 7.14 | 124.72 | 118.30 |
| 1 | D | 909 | ARG | NE-CZ-NH2 | -7.14 | 116.73 | 120.30 |
| 1 | G | 909 | ARG | NE-CZ-NH2 | -7.13 | 116.73 | 120.30 |
| 1 | K | 909 | ARG | NE-CZ-NH2 | -7.13 | 116.73 | 120.30 |
| 1 | O | 199 | ASP | CB-CG-OD1 | 7.13 | 124.72 | 118.30 |
| 1 | A | 52 | ARG | NE-CZ-NH1 | 7.13 | 123.87 | 120.30 |
| 1 | K | 233 | ASP | CB-CG-OD2 | -7.13 | 111.88 | 118.30 |
| 1 | A | 199 | ASP | CB-CG-OD1 | 7.13 | 124.72 | 118.30 |
| 1 | P | 199 | ASP | CB-CG-OD1 | 7.13 | 124.72 | 118.30 |
| 1 | K | 287 | ASP | CB-CG-OD1 | 7.12 | 124.71 | 118.30 |
| 1 | C | 199 | ASP | CB-CG-OD1 | 7.12 | 124.71 | 118.30 |
| 1 | C | 52 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | G | 52 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | H | 233 | ASP | CB-CG-OD2 | -7.12 | 111.89 | 118.30 |
| 1 | J | 52 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | A | 233 | ASP | CB-CG-OD2 | -7.12 | 111.89 | 118.30 |
| 1 | C | 909 | ARG | NE-CZ-NH2 | -7.12 | 116.74 | 120.30 |
| 1 | E | 52 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | J | 199 | ASP | CB-CG-OD1 | 7.12 | 124.71 | 118.30 |
| 1 | L | 52 | ARG | NE-CZ-NH1 | 7.11 | 123.86 | 120.30 |
| 1 | L | 199 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | A | 909 | ARG | NE-CZ-NH2 | -7.11 | 116.75 | 120.30 |
| 1 | G | 193 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | G | 199 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | J | 193 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | I | 193 | ASP | CB-CG-OD1 | 7.10 | 124.69 | 118.30 |
| 1 | N | 199 | ASP | CB-CG-OD1 | 7.10 | 124.69 | 118.30 |
| 1 | O | 572 | ASP | CB-CG-OD2 | -7.09 | 111.92 | 118.30 |
| 1 | O | 909 | ARG | NE-CZ-NH2 | -7.09 | 116.75 | 120.30 |
| 1 | B | 287 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | K | 52 | ARG | NE-CZ-NH1 | 7.09 | 123.84 | 120.30 |
| 1 | L | 193 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | P | 193 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | P | 287 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | A | 193 | ASP | CB-CG-OD1 | 7.09 | 124.68 | 118.30 |
| 1 | G | 572 | ASP | CB-CG-OD2 | -7.09 | 111.92 | 118.30 |
| 1 | K | 531 | ARG | NE-CZ-NH1 | 7.08 | 123.84 | 120.30 |
| 1 | C | 572 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | F | 199 | ASP | CB-CG-OD1 | 7.08 | 124.68 | 118.30 |
| 1 | D | 572 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | H | 287 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | I | 287 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | O | 193 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | M | 572 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | N | 193 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | N | 52 | ARG | NE-CZ-NH1 | 7.08 | 123.84 | 120.30 |
| 1 | C | 287 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | H | 572 | ASP | CB-CG-OD2 | -7.07 | 111.93 | 118.30 |
| 1 | F | 442 | ARG | NE-CZ-NH1 | 7.07 | 123.84 | 120.30 |
| 1 | A | 287 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | H | 193 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | F | 287 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | B | 572 | ASP | CB-CG-OD2 | -7.07 | 111.94 | 118.30 |
| 1 | N | 287 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | O | 287 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | E | 572 | ASP | CB-CG-OD2 | -7.06 | 111.94 | 118.30 |
| 1 | M | 909 | ARG | NE-CZ-NH2 | -7.06 | 116.77 | 120.30 |
| 1 | D | 287 | ASP | CB-CG-OD1 | 7.06 | 124.65 | 118.30 |
| 1 | B | 193 | ASP | CB-CG-OD1 | 7.06 | 124.65 | 118.30 |
| 1 | B | 909 | ARG | NE-CZ-NH2 | -7.06 | 116.77 | 120.30 |
| 1 | F | 193 | ASP | CB-CG-OD1 | 7.06 | 124.65 | 118.30 |
| 1 | A | 572 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | F | 572 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | N | 572 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | B | 52 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 1 | J | 287 | ASP | CB-CG-OD1 | 7.05 | 124.65 | 118.30 |
| 1 | J | 442 | ARG | NE-CZ-NH1 | 7.05 | 123.83 | 120.30 |
| 1 | N | 909 | ARG | NE-CZ-NH2 | -7.05 | 116.78 | 120.30 |
| 1 | P | 572 | ASP | CB-CG-OD2 | -7.05 | 111.95 | 118.30 |
| 1 | E | 909 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 1 | M | 287 | ASP | CB-CG-OD1 | 7.04 | 124.64 | 118.30 |
| 1 | G | 287 | ASP | CB-CG-OD1 | 7.04 | 124.64 | 118.30 |
| 1 | E | 193 | ASP | CB-CG-OD1 | 7.04 | 124.63 | 118.30 |
| 1 | I | 442 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 1 | H | 909 | ARG | NE-CZ-NH2 | -7.03 | 116.78 | 120.30 |
| 1 | M | 193 | ASP | CB-CG-OD1 | 7.03 | 124.63 | 118.30 |
| 1 | I | 572 | ASP | CB-CG-OD2 | -7.03 | 111.97 | 118.30 |
| 1 | L | 572 | ASP | CB-CG-OD2 | -7.03 | 111.97 | 118.30 |
| 1 | D | 442 | ARG | NE-CZ-NH1 | 7.03 | 123.81 | 120.30 |
| 1 | L | 287 | ASP | CB-CG-OD1 | 7.03 | 124.62 | 118.30 |
| 1 | J | 572 | ASP | CB-CG-OD2 | -7.02 | 111.98 | 118.30 |
| 1 | P | 769 | TRP | CB-CA-C | -7.02 | 96.36 | 110.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 769 | TRP | CB-CA-C | -7.02 | 96.36 | 110.40 |
| 1 | B | 786 | ARG | NE-CZ-NH1 | 7.02 | 123.81 | 120.30 |
| 1 | I | 909 | ARG | NE-CZ-NH2 | -7.01 | 116.79 | 120.30 |
| 1 | I | 769 | TRP | CB-CA-C | -7.01 | 96.37 | 110.40 |
| 1 | A | 769 | TRP | CB-CA-C | -7.01 | 96.38 | 110.40 |
| 1 | J | 769 | TRP | CB-CA-C | -7.01 | 96.38 | 110.40 |
| 1 | K | 572 | ASP | CB-CG-OD2 | -7.01 | 111.99 | 118.30 |
| 1 | B | 442 | ARG | NE-CZ-NH1 | 7.01 | 123.81 | 120.30 |
| 1 | H | 442 | ARG | NE-CZ-NH1 | 7.01 | 123.80 | 120.30 |
| 1 | O | 769 | TRP | CB-CA-C | -7.00 | 96.39 | 110.40 |
| 1 | E | 769 | TRP | CB-CA-C | -7.00 | 96.40 | 110.40 |
| 1 | G | 769 | TRP | CB-CA-C | -7.00 | 96.40 | 110.40 |
| 1 | G | 442 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 1 | K | 769 | TRP | CB-CA-C | -7.00 | 96.40 | 110.40 |
| 1 | P | 786 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 1 | D | 769 | TRP | CB-CA-C | -6.99 | 96.42 | 110.40 |
| 1 | E | 287 | ASP | CB-CG-OD1 | 6.99 | 124.59 | 118.30 |
| 1 | L | 769 | TRP | CB-CA-C | -6.99 | 96.41 | 110.40 |
| 1 | N | 769 | TRP | CB-CA-C | -6.99 | 96.41 | 110.40 |
| 1 | N | 786 | ARG | NE-CZ-NH1 | 6.99 | 123.80 | 120.30 |
| 1 | C | 769 | TRP | CB-CA-C | -6.99 | 96.42 | 110.40 |
| 1 | F | 769 | TRP | CB-CA-C | -6.99 | 96.42 | 110.40 |
| 1 | H | 769 | TRP | CB-CA-C | -6.99 | 96.42 | 110.40 |
| 1 | M | 769 | TRP | CB-CA-C | -6.99 | 96.42 | 110.40 |
| 1 | K | 442 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 1 | C | 442 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 1 | M | 442 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 1 | L | 442 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 1 | A | 442 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 1 | N | 442 | ARG | NE-CZ-NH1 | 6.96 | 123.78 | 120.30 |
| 1 | O | 442 | ARG | NE-CZ-NH1 | 6.95 | 123.77 | 120.30 |
| 1 | G | 746 | ASP | CB-CG-OD1 | 6.94 | 124.55 | 118.30 |
| 1 | P | 442 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 1 | J | 648 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |
| 1 | D | 645 | ARG | NE-CZ-NH2 | -6.93 | 116.83 | 120.30 |
| 1 | F | 648 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |
| 1 | A | 786 | ARG | NE-CZ-NH1 | 6.93 | 123.76 | 120.30 |
| 1 | L | 746 | ASP | CB-CG-OD1 | 6.93 | 124.53 | 118.30 |
| 1 | C | 786 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 1 | K | 166 | ARG | N-CA-CB | 6.92 | 123.06 | 110.60 |
| 1 | D | 746 | ASP | CB-CG-OD1 | 6.92 | 124.53 | 118.30 |
| 1 | I | 746 | ASP | CB-CG-OD1 | 6.92 | 124.53 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | E | 166 | ARG | N-CA-CB | 6.92 | 123.05 | 110.60 |
| 1 | E | 648 | ASP | CB-CG-OD2 | -6.92 | 112.08 | 118.30 |
| 1 | B | 648 | ASP | CB-CG-OD2 | -6.92 | 112.08 | 118.30 |
| 1 | I | 786 | ARG | NE-CZ-NH1 | 6.92 | 123.76 | 120.30 |
| 1 | J | 166 | ARG | N-CA-CB | 6.91 | 123.05 | 110.60 |
| 1 | K | 746 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 1 | N | 746 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 1 | C | 166 | ARG | N-CA-CB | 6.91 | 123.04 | 110.60 |
| 1 | G | 166 | ARG | N-CA-CB | 6.91 | 123.04 | 110.60 |
| 1 | L | 648 | ASP | CB-CG-OD2 | -6.91 | 112.08 | 118.30 |
| 1 | L | 166 | ARG | N-CA-CB | 6.91 | 123.04 | 110.60 |
| 1 | N | 166 | ARG | N-CA-CB | 6.91 | 123.03 | 110.60 |
| 1 | E | 442 | ARG | NE-CZ-NH1 | 6.91 | 123.75 | 120.30 |
| 1 | E | 746 | ASP | CB-CG-OD1 | 6.91 | 124.52 | 118.30 |
| 1 | N | 1004 | SER | N-CA-CB | 6.91 | 120.86 | 110.50 |
| 1 | A | 648 | ASP | CB-CG-OD2 | -6.90 | 112.09 | 118.30 |
| 1 | L | 1004 | SER | N-CA-CB | 6.90 | 120.86 | 110.50 |
| 1 | I | 166 | ARG | N-CA-CB | 6.90 | 123.03 | 110.60 |
| 1 | O | 166 | ARG | N-CA-CB | 6.90 | 123.03 | 110.60 |
| 1 | A | 166 | ARG | N-CA-CB | 6.90 | 123.02 | 110.60 |
| 1 | H | 746 | ASP | CB-CG-OD1 | 6.90 | 124.51 | 118.30 |
| 1 | P | 166 | ARG | N-CA-CB | 6.90 | 123.02 | 110.60 |
| 1 | C | 561 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | E | 687 | GLN | C-N-CD | -6.90 | 105.42 | 120.60 |
| 1 | E | 786 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | I | 648 | ASP | CB-CG-OD2 | -6.90 | 112.09 | 118.30 |
| 1 | J | 786 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | O | 648 | ASP | CB-CG-OD2 | -6.90 | 112.09 | 118.30 |
| 1 | C | 687 | GLN | C-N-CD | -6.90 | 105.43 | 120.60 |
| 1 | K | 561 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | A | 746 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | D | 687 | GLN | C-N-CD | -6.89 | 105.43 | 120.60 |
| 1 | C | 1004 | SER | N-CA-CB | 6.89 | 120.84 | 110.50 |
| 1 | F | 561 | ARG | NE-CZ-NH1 | 6.89 | 123.75 | 120.30 |
| 1 | M | 687 | GLN | C-N-CD | -6.89 | 105.44 | 120.60 |
| 1 | M | 786 | ARG | NE-CZ-NH1 | 6.89 | 123.75 | 120.30 |
| 1 | B | 166 | ARG | N-CA-CB | 6.89 | 123.00 | 110.60 |
| 1 | F | 1004 | SER | N-CA-CB | 6.89 | 120.84 | 110.50 |
| 1 | M | 645 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | M | 746 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | F | 746 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | P | 687 | GLN | C-N-CD | -6.89 | 105.45 | 120.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 645 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | C | 648 | ASP | CB-CG-OD2 | -6.89 | 112.10 | 118.30 |
| 1 | C | 746 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | F | 687 | GLN | C-N-CD | -6.89 | 105.45 | 120.60 |
| 1 | G | 687 | GLN | C-N-CD | -6.89 | 105.45 | 120.60 |
| 1 | H | 166 | ARG | N-CA-CB | 6.89 | 123.00 | 110.60 |
| 1 | H | 1004 | SER | N-CA-CB | 6.89 | 120.83 | 110.50 |
| 1 | P | 648 | ASP | CB-CG-OD2 | -6.89 | 112.10 | 118.30 |
| 1 | P | 746 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | H | 648 | ASP | CB-CG-OD2 | -6.88 | 112.11 | 118.30 |
| 1 | M | 648 | ASP | CB-CG-OD2 | -6.88 | 112.10 | 118.30 |
| 1 | A | 1004 | SER | N-CA-CB | 6.88 | 120.82 | 110.50 |
| 1 | F | 166 | ARG | N-CA-CB | 6.88 | 122.99 | 110.60 |
| 1 | A | 687 | GLN | C-N-CD | -6.88 | 105.46 | 120.60 |
| 1 | D | 561 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | J | 1004 | SER | N-CA-CB | 6.88 | 120.82 | 110.50 |
| 1 | L | 561 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | M | 1004 | SER | N-CA-CB | 6.88 | 120.82 | 110.50 |
| 1 | O | 1004 | SER | N-CA-CB | 6.88 | 120.82 | 110.50 |
| 1 | N | 5 | ASP | CB-CG-OD1 | 6.88 | 124.49 | 118.30 |
| 1 | C | 828 | ASP | CB-CG-OD2 | -6.88 | 112.11 | 118.30 |
| 1 | F | 786 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | H | 368 | ASP | CB-CG-OD1 | 6.88 | 124.49 | 118.30 |
| 1 | J | 746 | ASP | CB-CG-OD1 | 6.88 | 124.49 | 118.30 |
| 1 | G | 786 | ARG | NE-CZ-NH1 | 6.88 | 123.74 | 120.30 |
| 1 | M | 166 | ARG | N-CA-CB | 6.88 | 122.97 | 110.60 |
| 1 | N | 687 | GLN | C-N-CD | -6.88 | 105.47 | 120.60 |
| 1 | P | 1004 | SER | N-CA-CB | 6.88 | 120.81 | 110.50 |
| 1 | B | 746 | ASP | CB-CG-OD1 | 6.87 | 124.49 | 118.30 |
| 1 | F | 645 | ARG | NE-CZ-NH2 | -6.87 | 116.86 | 120.30 |
| 1 | J | 687 | GLN | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | K | 786 | ARG | NE-CZ-NH1 | 6.87 | 123.74 | 120.30 |
| 1 | L | 687 | GLN | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | O | 687 | GLN | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | B | 1004 | SER | N-CA-CB | 6.87 | 120.81 | 110.50 |
| 1 | D | 648 | ASP | CB-CG-OD2 | -6.87 | 112.12 | 118.30 |
| 1 | E | 1004 | SER | N-CA-CB | 6.87 | 120.81 | 110.50 |
| 1 | H | 687 | GLN | C-N-CD | -6.87 | 105.48 | 120.60 |
| 1 | I | 687 | GLN | C-N-CD | -6.87 | 105.49 | 120.60 |
| 1 | N | 648 | ASP | CB-CG-OD2 | -6.87 | 112.12 | 118.30 |
| 1 | D | 166 | ARG | N-CA-CB | 6.87 | 122.96 | 110.60 |
| 1 | G | 648 | ASP | CB-CG-OD2 | -6.87 | 112.12 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | O | 746 | ASP | CB-CG-OD1 | 6.87 | 124.48 | 118.30 |
| 1 | O | 786 | ARG | NE-CZ-NH1 | 6.87 | 123.73 | 120.30 |
| 1 | D | 786 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 1 | K | 1004 | SER | N-CA-CB | 6.86 | 120.80 | 110.50 |
| 1 | B | 687 | GLN | C-N-CD | -6.86 | 105.50 | 120.60 |
| 1 | I | 1004 | SER | N-CA-CB | 6.86 | 120.79 | 110.50 |
| 1 | O | 5 | ASP | CB-CG-OD1 | 6.86 | 124.48 | 118.30 |
| 1 | D | 1004 | SER | N-CA-CB | 6.86 | 120.79 | 110.50 |
| 1 | G | 1004 | SER | N-CA-CB | 6.86 | 120.79 | 110.50 |
| 1 | K | 687 | GLN | C-N-CD | -6.86 | 105.51 | 120.60 |
| 1 | B | 5 | ASP | CB-CG-OD1 | 6.86 | 124.47 | 118.30 |
| 1 | K | 648 | ASP | CB-CG-OD2 | -6.86 | 112.13 | 118.30 |
| 1 | A | 561 | ARG | NE-CZ-NH1 | 6.85 | 123.73 | 120.30 |
| 1 | F | 5 | ASP | CB-CG-OD1 | 6.85 | 124.47 | 118.30 |
| 1 | I | 828 | ASP | CB-CG-OD2 | -6.85 | 112.13 | 118.30 |
| 1 | H | 786 | ARG | NE-CZ-NH1 | 6.85 | 123.72 | 120.30 |
| 1 | M | 368 | ASP | CB-CG-OD1 | 6.85 | 124.46 | 118.30 |
| 1 | A | 5 | ASP | CB-CG-OD1 | 6.85 | 124.46 | 118.30 |
| 1 | C | 368 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | E | 561 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 1 | K | 5 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | L | 786 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 1 | N | 828 | ASP | CB-CG-OD2 | -6.84 | 112.14 | 118.30 |
| 1 | G | 5 | ASP | CB-CG-OD1 | 6.84 | 124.45 | 118.30 |
| 1 | H | 329 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | L | 5 | ASP | CB-CG-OD1 | 6.84 | 124.46 | 118.30 |
| 1 | H | 5 | ASP | CB-CG-OD1 | 6.84 | 124.45 | 118.30 |
| 1 | G | 561 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 1 | H | 645 | ARG | NE-CZ-NH2 | -6.84 | 116.88 | 120.30 |
| 1 | H | 828 | ASP | CB-CG-OD2 | -6.84 | 112.15 | 118.30 |
| 1 | M | 5 | ASP | CB-CG-OD1 | 6.84 | 124.45 | 118.30 |
| 1 | O | 828 | ASP | CB-CG-OD2 | -6.83 | 112.15 | 118.30 |
| 1 | G | 828 | ASP | CB-CG-OD2 | -6.83 | 112.15 | 118.30 |
| 1 | B | 211 | ASP | CB-CG-OD1 | 6.83 | 124.45 | 118.30 |
| 1 | C | 645 | ARG | NE-CZ-NH2 | -6.83 | 116.89 | 120.30 |
| 1 | O | 561 | ARG | NE-CZ-NH1 | 6.83 | 123.71 | 120.30 |
| 1 | P | 5 | ASP | CB-CG-OD1 | 6.83 | 124.44 | 118.30 |
| 1 | A | 368 | ASP | CB-CG-OD1 | 6.83 | 124.44 | 118.30 |
| 1 | I | 5 | ASP | CB-CG-OD1 | 6.83 | 124.44 | 118.30 |
| 1 | P | 828 | ASP | CB-CG-OD2 | -6.83 | 112.16 | 118.30 |
| 1 | E | 828 | ASP | CB-CG-OD2 | -6.82 | 112.16 | 118.30 |
| 1 | M | 828 | ASP | CB-CG-OD2 | -6.82 | 112.16 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 5 | ASP | CB-CG-OD1 | 6.82 | 124.44 | 118.30 |
| 1 | L | 368 | ASP | CB-CG-OD1 | 6.82 | 124.44 | 118.30 |
| 1 | N | 561 | ARG | NE-CZ-NH1 | 6.82 | 123.71 | 120.30 |
| 1 | O | 645 | ARG | NE-CZ-NH2 | -6.82 | 116.89 | 120.30 |
| 1 | J | 329 | ASP | CB-CG-OD1 | 6.82 | 124.44 | 118.30 |
| 1 | D | 5 | ASP | CB-CG-OD1 | 6.82 | 124.44 | 118.30 |
| 1 | F | 828 | ASP | CB-CG-OD2 | -6.82 | 112.17 | 118.30 |
| 1 | K | 610 | ASP | CB-CG-OD2 | -6.82 | 112.16 | 118.30 |
| 1 | L | 828 | ASP | CB-CG-OD2 | -6.82 | 112.17 | 118.30 |
| 1 | O | 492 | ASP | CB-CG-OD2 | -6.81 | 112.17 | 118.30 |
| 1 | D | 368 | ASP | CB-CG-OD1 | 6.81 | 124.43 | 118.30 |
| 1 | O | 610 | ASP | CB-CG-OD2 | -6.81 | 112.17 | 118.30 |
| 1 | I | 561 | ARG | NE-CZ-NH1 | 6.81 | 123.71 | 120.30 |
| 1 | A | 828 | ASP | CB-CG-OD2 | -6.81 | 112.17 | 118.30 |
| 1 | F | 368 | ASP | CB-CG-OD1 | 6.81 | 124.43 | 118.30 |
| 1 | E | 5 | ASP | CB-CG-OD1 | 6.81 | 124.42 | 118.30 |
| 1 | L | 329 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | L | 610 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | P | 211 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | P | 645 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | J | 561 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 1 | E | 645 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | H | 610 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | K | 329 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | M | 610 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | N | 329 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | D | 45 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | G | 610 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | J | 828 | ASP | CB-CG-OD2 | -6.80 | 112.18 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | F | 329 | ASP | CB-CG-OD1 | 6.80 | 124.42 | 118.30 |
| 1 | H | 561 | ARG | NE-CZ-NH1 | 6.80 | 123.70 | 120.30 |
| 1 | L | 645 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | B | 645 | ARG | NE-CZ-NH2 | -6.79 | 116.90 | 120.30 |
| 1 | E | 329 | ASP | CB-CG-OD1 | 6.79 | 124.42 | 118.30 |
| 1 | P | 329 | ASP | CB-CG-OD1 | 6.79 | 124.42 | 118.30 |
| 1 | C | 610 | ASP | CB-CG-OD2 | -6.79 | 112.19 | 118.30 |
| 1 | G | 368 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | P | 368 | ASP | CB-CG-OD1 | 6.79 | 124.42 | 118.30 |
| 1 | P | 561 | ARG | NE-CZ-NH1 | 6.79 | 123.70 | 120.30 |
| 1 | D | 211 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | I | 610 | ASP | CB-CG-OD2 | -6.79 | 112.19 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | I | 645 | ARG | NE-CZ-NH2 | -6.79 | 116.90 | 120.30 |
| 1 | A | 329 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | O | 329 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | K | 368 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 1 | N | 645 | ARG | NE-CZ-NH2 | -6.79 | 116.91 | 120.30 |
| 1 | B | 561 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 1 | B | 828 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | D | 329 | ASP | CB-CG-OD1 | 6.78 | 124.41 | 118.30 |
| 1 | D | 610 | ASP | CB-CG-OD2 | -6.78 | 112.19 | 118.30 |
| 1 | I | 368 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | J | 211 | ASP | CB-CG-OD1 | 6.78 | 124.41 | 118.30 |
| 1 | O | 368 | ASP | CB-CG-OD1 | 6.78 | 124.41 | 118.30 |
| 1 | P | 610 | ASP | CB-CG-OD2 | -6.78 | 112.19 | 118.30 |
| 1 | K | 211 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | K | 828 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | A | 211 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | F | 211 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | N | 610 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | M | 329 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | E | 368 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | F | 610 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | G | 645 | ARG | NE-CZ-NH2 | -6.78 | 116.91 | 120.30 |
| 1 | J | 5 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | J | 368 | ASP | CB-CG-OD1 | 6.78 | 124.40 | 118.30 |
| 1 | N | 425 | ARG | NE-CZ-NH1 | 6.78 | 123.69 | 120.30 |
| 1 | M | 561 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 1 | O | 211 | ASP | CB-CG-OD1 | 6.77 | 124.40 | 118.30 |
| 1 | C | 211 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 1 | D | 828 | ASP | CB-CG-OD2 | -6.77 | 112.21 | 118.30 |
| 1 | A | 610 | ASP | CB-CG-OD2 | -6.77 | 112.21 | 118.30 |
| 1 | N | 368 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 1 | B | 610 | ASP | CB-CG-OD2 | -6.77 | 112.21 | 118.30 |
| 1 | I | 211 | ASP | CB-CG-OD1 | 6.77 | 124.39 | 118.30 |
| 1 | D | 492 | ASP | CB-CG-OD2 | -6.76 | 112.21 | 118.30 |
| 1 | E | 492 | ASP | CB-CG-OD2 | -6.76 | 112.21 | 118.30 |
| 1 | L | 45 | ASP | CB-CG-OD1 | 6.76 | 124.39 | 118.30 |
| 1 | C | 45 | ASP | CB-CG-OD1 | 6.76 | 124.39 | 118.30 |
| 1 | K | 645 | ARG | NE-CZ-NH2 | -6.76 | 116.92 | 120.30 |
| 1 | B | 329 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | C | 329 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | F | 45 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | K | 492 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | N | 211 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | G | 329 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | L | 492 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |
| 1 | N | 492 | ASP | CB-CG-OD2 | -6.76 | 112.22 | 118.30 |
| 1 | G | 211 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | J | 610 | ASP | CB-CG-OD2 | -6.75 | 112.22 | 118.30 |
| 1 | C | 492 | ASP | CB-CG-OD2 | -6.75 | 112.22 | 118.30 |
| 1 | E | 211 | ASP | CB-CG-OD1 | 6.75 | 124.37 | 118.30 |
| 1 | P | 492 | ASP | CB-CG-OD2 | -6.75 | 112.23 | 118.30 |
| 1 | A | 492 | ASP | CB-CG-OD2 | -6.75 | 112.23 | 118.30 |
| 1 | E | 59 | ARG | NE-CZ-NH1 | 6.74 | 123.67 | 120.30 |
| 1 | E | 610 | ASP | CB-CG-OD2 | -6.74 | 112.23 | 118.30 |
| 1 | O | 45 | ASP | CB-CG-OD1 | 6.74 | 124.36 | 118.30 |
| 1 | H | 211 | ASP | CB-CG-OD1 | 6.74 | 124.36 | 118.30 |
| 1 | I | 45 | ASP | CB-CG-OD1 | 6.74 | 124.36 | 118.30 |
| 1 | I | 329 | ASP | CB-CG-OD1 | 6.74 | 124.36 | 118.30 |
| 1 | N | 45 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | M | 211 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | A | 45 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | B | 45 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | G | 45 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 1 | G | 492 | ASP | CB-CG-OD2 | -6.73 | 112.25 | 118.30 |
| 1 | J | 645 | ARG | NE-CZ-NH2 | -6.73 | 116.94 | 120.30 |
| 1 | J | 492 | ASP | CB-CG-OD2 | -6.72 | 112.25 | 118.30 |
| 1 | B | 492 | ASP | CB-CG-OD2 | -6.72 | 112.25 | 118.30 |
| 1 | E | 45 | ASP | CB-CG-OD1 | 6.72 | 124.35 | 118.30 |
| 1 | F | 492 | ASP | CB-CG-OD2 | -6.72 | 112.25 | 118.30 |
| 1 | M | 492 | ASP | CB-CG-OD2 | -6.71 | 112.26 | 118.30 |
| 1 | I | 492 | ASP | CB-CG-OD2 | -6.71 | 112.26 | 118.30 |
| 1 | K | 45 | ASP | CB-CG-OD1 | 6.71 | 124.34 | 118.30 |
| 1 | A | 425 | ARG | NE-CZ-NH1 | 6.71 | 123.65 | 120.30 |
| 1 | P | 45 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | E | 425 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 1 | H | 45 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | M | 425 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 1 | M | 45 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | J | 45 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | L | 211 | ASP | CB-CG-OD1 | 6.70 | 124.33 | 118.30 |
| 1 | L | 425 | ARG | NE-CZ-NH1 | 6.70 | 123.65 | 120.30 |
| 1 | H | 425 | ARG | NE-CZ-NH1 | 6.69 | 123.64 | 120.30 |
| 1 | H | 492 | ASP | CB-CG-OD2 | -6.69 | 112.28 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | N | 59 | ARG | NE-CZ-NH1 | 6.68 | 123.64 | 120.30 |
| 1 | M | 59 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | G | 59 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | I | 425 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | K | 425 | ARG | NE-CZ-NH1 | 6.67 | 123.64 | 120.30 |
| 1 | C | 411 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | M | 411 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | B | 411 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | H | 411 | ASP | CB-CG-OD1 | 6.66 | 124.30 | 118.30 |
| 1 | I | 411 | ASP | CB-CG-OD1 | 6.66 | 124.30 | 118.30 |
| 1 | D | 425 | ARG | NE-CZ-NH1 | 6.66 | 123.63 | 120.30 |
| 1 | L | 411 | ASP | CB-CG-OD1 | 6.65 | 124.29 | 118.30 |
| 1 | A | 411 | ASP | CB-CG-OD1 | 6.65 | 124.29 | 118.30 |
| 1 | O | 411 | ASP | CB-CG-OD1 | 6.65 | 124.29 | 118.30 |
| 1 | E | 411 | ASP | CB-CG-OD1 | 6.65 | 124.29 | 118.30 |
| 1 | L | 59 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | K | 411 | ASP | CB-CG-OD1 | 6.64 | 124.28 | 118.30 |
| 1 | N | 411 | ASP | CB-CG-OD1 | 6.64 | 124.28 | 118.30 |
| 1 | O | 59 | ARG | NE-CZ-NH1 | 6.64 | 123.62 | 120.30 |
| 1 | B | 59 | ARG | NE-CZ-NH1 | 6.63 | 123.62 | 120.30 |
| 1 | D | 59 | ARG | NE-CZ-NH1 | 6.63 | 123.62 | 120.30 |
| 1 | O | 425 | ARG | NE-CZ-NH1 | 6.63 | 123.62 | 120.30 |
| 1 | F | 411 | ASP | CB-CG-OD1 | 6.63 | 124.27 | 118.30 |
| 1 | A | 59 | ARG | NE-CZ-NH1 | 6.63 | 123.61 | 120.30 |
| 1 | B | 425 | ARG | NE-CZ-NH1 | 6.63 | 123.61 | 120.30 |
| 1 | J | 59 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | G | 425 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | H | 59 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | P | 411 | ASP | CB-CG-OD1 | 6.61 | 124.25 | 118.30 |
| 1 | F | 59 | ARG | NE-CZ-NH1 | 6.61 | 123.60 | 120.30 |
| 1 | C | 59 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | J | 425 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | C | 425 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | E | 954 | ASP | CB-CG-OD1 | 6.60 | 124.24 | 118.30 |
| 1 | K | 59 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | J | 411 | ASP | CB-CG-OD1 | 6.59 | 124.23 | 118.30 |
| 1 | H | 954 | ASP | CB-CG-OD1 | 6.58 | 124.23 | 118.30 |
| 1 | I | 59 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | G | 411 | ASP | CB-CG-OD1 | 6.58 | 124.22 | 118.30 |
| 1 | F | 425 | ARG | NE-CZ-NH1 | 6.57 | 123.58 | 120.30 |
| 1 | M | 954 | ASP | CB-CG-OD1 | 6.57 | 124.21 | 118.30 |
| 1 | P | 954 | ASP | CB-CG-OD1 | 6.56 | 124.21 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | G | 954 | ASP | CB-CG-OD1 | 6.56 | 124.20 | 118.30 |
| 1 | P | 425 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | B | 252 | ASP | CB-CG-OD2 | -6.55 | 112.41 | 118.30 |
| 1 | A | 252 | ASP | CB-CG-OD2 | -6.54 | 112.42 | 118.30 |
| 1 | J | 252 | ASP | CB-CG-OD2 | -6.54 | 112.42 | 118.30 |
| 1 | D | 954 | ASP | CB-CG-OD1 | 6.54 | 124.18 | 118.30 |
| 1 | A | 954 | ASP | CB-CG-OD1 | 6.53 | 124.18 | 118.30 |
| 1 | I | 252 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |
| 1 | P | 59 | ARG | NE-CZ-NH1 | 6.53 | 123.57 | 120.30 |
| 1 | F | 252 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |
| 1 | E | 130 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |
| 1 | H | 509 | ASP | CB-CG-OD1 | 6.53 | 124.17 | 118.30 |
| 1 | B | 130 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 1 | O | 509 | ASP | CB-CG-OD1 | 6.52 | 124.17 | 118.30 |
| 1 | K | 509 | ASP | CB-CG-OD1 | 6.52 | 124.17 | 118.30 |
| 1 | O | 252 | ASP | CB-CG-OD2 | -6.52 | 112.43 | 118.30 |
| 1 | K | 954 | ASP | CB-CG-OD1 | 6.52 | 124.16 | 118.30 |
| 1 | C | 130 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | I | 954 | ASP | CB-CG-OD1 | 6.51 | 124.16 | 118.30 |
| 1 | N | 252 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | L | 252 | ASP | CB-CG-OD2 | -6.51 | 112.44 | 118.30 |
| 1 | E | 252 | ASP | CB-CG-OD2 | -6.50 | 112.44 | 118.30 |
| 1 | B | 954 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | L | 509 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | M | 130 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | O | 130 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | F | 954 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | J | 509 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | D | 130 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | G | 130 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | D | 252 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | N | 509 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | P | 252 | ASP | CB-CG-OD2 | -6.50 | 112.45 | 118.30 |
| 1 | K | 252 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 1 | E | 367 | MET | CG-SD-CE | -6.49 | 89.81 | 100.20 |
| 1 | N | 954 | ASP | CB-CG-OD1 | 6.49 | 124.14 | 118.30 |
| 1 | B | 367 | MET | CG-SD-CE | -6.49 | 89.81 | 100.20 |
| 1 | F | 367 | MET | CG-SD-CE | -6.49 | 89.82 | 100.20 |
| 1 | D | 509 | ASP | CB-CG-OD1 | 6.49 | 124.14 | 118.30 |
| 1 | H | 367 | MET | CG-SD-CE | -6.49 | 89.82 | 100.20 |
| 1 | I | 509 | ASP | CB-CG-OD1 | 6.49 | 124.14 | 118.30 |
| 1 | J | 130 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | K | 367 | MET | CG-SD-CE | -6.49 | 89.82 | 100.20 |
| 1 | F | 130 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | J | 954 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | C | 509 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | D | 367 | MET | CG-SD-CE | -6.48 | 89.83 | 100.20 |
| 1 | H | 130 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | A | 509 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | C | 252 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | L | 954 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | P | 367 | MET | CG-SD-CE | -6.48 | 89.84 | 100.20 |
| 1 | G | 252 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | M | 252 | ASP | CB-CG-OD2 | -6.48 | 112.47 | 118.30 |
| 1 | A | 367 | MET | CG-SD-CE | -6.47 | 89.84 | 100.20 |
| 1 | J | 367 | MET | CG-SD-CE | -6.47 | 89.84 | 100.20 |
| 1 | O | 367 | MET | CG-SD-CE | -6.47 | 89.84 | 100.20 |
| 1 | B | 509 | ASP | CB-CG-OD1 | 6.47 | 124.13 | 118.30 |
| 1 | C | 367 | MET | CG-SD-CE | -6.47 | 89.84 | 100.20 |
| 1 | H | 252 | ASP | CB-CG-OD2 | -6.47 | 112.47 | 118.30 |
| 1 | L | 367 | MET | CG-SD-CE | -6.47 | 89.84 | 100.20 |
| 1 | C | 954 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | F | 509 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | L | 130 | ASP | CB-CG-OD2 | -6.47 | 112.48 | 118.30 |
| 1 | M | 509 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | N | 367 | MET | CG-SD-CE | -6.47 | 89.85 | 100.20 |
| 1 | I | 367 | MET | CG-SD-CE | -6.47 | 89.85 | 100.20 |
| 1 | G | 509 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | N | 130 | ASP | CB-CG-OD2 | -6.47 | 112.48 | 118.30 |
| 1 | P | 130 | ASP | CB-CG-OD2 | -6.47 | 112.48 | 118.30 |
| 1 | A | 130 | ASP | CB-CG-OD2 | -6.46 | 112.48 | 118.30 |
| 1 | I | 130 | ASP | CB-CG-OD2 | -6.46 | 112.48 | 118.30 |
| 1 | G | 367 | MET | CG-SD-CE | -6.46 | 89.86 | 100.20 |
| 1 | M | 367 | MET | CG-SD-CE | -6.46 | 89.86 | 100.20 |
| 1 | K | 130 | ASP | CB-CG-OD2 | -6.45 | 112.49 | 118.30 |
| 1 | P | 509 | ASP | CB-CG-OD1 | 6.45 | 124.10 | 118.30 |
| 1 | O | 954 | ASP | CB-CG-OD1 | 6.44 | 124.10 | 118.30 |
| 1 | E | 509 | ASP | CB-CG-OD1 | 6.43 | 124.09 | 118.30 |
| 1 | D | 15 | ASP | CB-CG-OD2 | -6.40 | 112.54 | 118.30 |
| 1 | K | 15 | ASP | CB-CG-OD2 | -6.40 | 112.54 | 118.30 |
| 1 | J | 15 | ASP | CB-CG-OD2 | -6.39 | 112.55 | 118.30 |
| 1 | D | 938 | ARG | N-CA-CB | 6.38 | 122.09 | 110.60 |
| 1 | N | 938 | ARG | N-CA-CB | 6.38 | 122.08 | 110.60 |
| 1 | L | 15 | ASP | CB-CG-OD2 | -6.38 | 112.56 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | L | 46 | ARG | CA-CB-CG | -6.38 | 99.37 | 113.40 |
| 1 | I | 46 | ARG | CA-CB-CG | -6.37 | 99.38 | 113.40 |
| 1 | M | 938 | ARG | N-CA-CB | 6.37 | 122.07 | 110.60 |
| 1 | O | 46 | ARG | CA-CB-CG | -6.37 | 99.39 | 113.40 |
| 1 | M | 46 | ARG | CA-CB-CG | -6.37 | 99.39 | 113.40 |
| 1 | E | 938 | ARG | N-CA-CB | 6.37 | 122.06 | 110.60 |
| 1 | I | 938 | ARG | N-CA-CB | 6.37 | 122.06 | 110.60 |
| 1 | H | 46 | ARG | CA-CB-CG | -6.36 | 99.40 | 113.40 |
| 1 | H | 15 | ASP | CB-CG-OD2 | -6.36 | 112.57 | 118.30 |
| 1 | E | 219 | THR | CA-CB-CG2 | -6.36 | 103.50 | 112.40 |
| 1 | G | 46 | ARG | CA-CB-CG | -6.36 | 99.41 | 113.40 |
| 1 | G | 938 | ARG | N-CA-CB | 6.36 | 122.05 | 110.60 |
| 1 | B | 46 | ARG | CA-CB-CG | -6.36 | 99.41 | 113.40 |
| 1 | H | 938 | ARG | N-CA-CB | 6.36 | 122.04 | 110.60 |
| 1 | K | 938 | ARG | N-CA-CB | 6.36 | 122.05 | 110.60 |
| 1 | O | 938 | ARG | N-CA-CB | 6.36 | 122.05 | 110.60 |
| 1 | C | 938 | ARG | N-CA-CB | 6.36 | 122.04 | 110.60 |
| 1 | J | 938 | ARG | N-CA-CB | 6.36 | 122.04 | 110.60 |
| 1 | A | 46 | ARG | CA-CB-CG | -6.35 | 99.42 | 113.40 |
| 1 | P | 46 | ARG | CA-CB-CG | -6.35 | 99.43 | 113.40 |
| 1 | E | 46 | ARG | CA-CB-CG | -6.35 | 99.43 | 113.40 |
| 1 | J | 46 | ARG | CA-CB-CG | -6.35 | 99.43 | 113.40 |
| 1 | C | 46 | ARG | CA-CB-CG | -6.35 | 99.43 | 113.40 |
| 1 | F | 46 | ARG | CA-CB-CG | -6.35 | 99.44 | 113.40 |
| 1 | F | 938 | ARG | N-CA-CB | 6.35 | 122.02 | 110.60 |
| 1 | N | 46 | ARG | CA-CB-CG | -6.35 | 99.44 | 113.40 |
| 1 | A | 938 | ARG | N-CA-CB | 6.35 | 122.02 | 110.60 |
| 1 | B | 938 | ARG | N-CA-CB | 6.35 | 122.02 | 110.60 |
| 1 | C | 15 | ASP | CB-CG-OD2 | -6.34 | 112.59 | 118.30 |
| 1 | G | 802 | ASP | CB-CG-OD2 | -6.34 | 112.59 | 118.30 |
| 1 | L | 938 | ARG | N-CA-CB | 6.34 | 122.01 | 110.60 |
| 1 | O | 15 | ASP | CB-CG-OD2 | -6.34 | 112.59 | 118.30 |
| 1 | D | 46 | ARG | CA-CB-CG | -6.34 | 99.45 | 113.40 |
| 1 | E | 15 | ASP | CB-CG-OD2 | -6.34 | 112.60 | 118.30 |
| 1 | P | 938 | ARG | N-CA-CB | 6.34 | 122.00 | 110.60 |
| 1 | F | 15 | ASP | CB-CG-OD2 | -6.33 | 112.60 | 118.30 |
| 1 | J | 219 | THR | CA-CB-CG2 | -6.33 | 103.54 | 112.40 |
| 1 | K | 219 | THR | CA-CB-CG2 | -6.33 | 103.54 | 112.40 |
| 1 | A | 15 | ASP | CB-CG-OD2 | -6.33 | 112.60 | 118.30 |
| 1 | I | 591 | ASP | CB-CG-OD2 | -6.33 | 112.61 | 118.30 |
| 1 | K | 46 | ARG | CA-CB-CG | -6.33 | 99.48 | 113.40 |
| 1 | P | 15 | ASP | CB-CG-OD2 | -6.33 | 112.61 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | M | 15 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | M | 659 | ASP | CB-CG-OD1 | 6.32 | 123.99 | 118.30 |
| 1 | B | 15 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | G | 219 | THR | CA-CB-CG2 | -6.32 | 103.55 | 112.40 |
| 1 | H | 219 | THR | CA-CB-CG2 | -6.32 | 103.55 | 112.40 |
| 1 | F | 219 | THR | CA-CB-CG2 | -6.32 | 103.56 | 112.40 |
| 1 | L | 219 | THR | CA-CB-CG2 | -6.32 | 103.55 | 112.40 |
| 1 | N | 802 | ASP | CB-CG-OD2 | -6.32 | 112.61 | 118.30 |
| 1 | A | 219 | THR | CA-CB-CG2 | -6.32 | 103.56 | 112.40 |
| 1 | P | 428 | ASP | CB-CG-OD1 | 6.31 | 123.98 | 118.30 |
| 1 | J | 802 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 1 | E | 428 | ASP | CB-CG-OD1 | 6.31 | 123.98 | 118.30 |
| 1 | G | 15 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 1 | O | 591 | ASP | CB-CG-OD2 | -6.31 | 112.62 | 118.30 |
| 1 | D | 219 | THR | CA-CB-CG2 | -6.31 | 103.57 | 112.40 |
| 1 | B | 591 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | I | 15 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | J | 659 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | O | 428 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | F | 802 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | G | 591 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | M | 219 | THR | CA-CB-CG2 | -6.30 | 103.58 | 112.40 |
| 1 | O | 917 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 1 | I | 219 | THR | CA-CB-CG2 | -6.30 | 103.58 | 112.40 |
| 1 | P | 219 | THR | CA-CB-CG2 | -6.30 | 103.58 | 112.40 |
| 1 | B | 219 | THR | CA-CB-CG2 | -6.30 | 103.58 | 112.40 |
| 1 | M | 802 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | N | 15 | ASP | CB-CG-OD2 | -6.30 | 112.63 | 118.30 |
| 1 | O | 659 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | C | 219 | THR | CA-CB-CG2 | -6.29 | 103.59 | 112.40 |
| 1 | N | 219 | THR | CA-CB-CG2 | -6.29 | 103.59 | 112.40 |
| 1 | E | 802 | ASP | CB-CG-OD2 | -6.29 | 112.64 | 118.30 |
| 1 | O | 219 | THR | CA-CB-CG2 | -6.29 | 103.60 | 112.40 |
| 1 | D | 659 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | E | 659 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | H | 802 | ASP | CB-CG-OD2 | -6.28 | 112.64 | 118.30 |
| 1 | A | 802 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | G | 917 | ARG | NE-CZ-NH2 | -6.28 | 117.16 | 120.30 |
| 1 | M | 591 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | P | 659 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | P | 802 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | F | 659 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | I | 802 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | J | 428 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | K | 428 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | K | 591 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | H | 591 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | K | 802 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | N | 428 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | O | 802 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | A | 591 | ASP | CB-CG-OD2 | -6.27 | 112.66 | 118.30 |
| 1 | D | 428 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | G | 428 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | K | 659 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | I | 659 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | C | 802 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 1 | F | 591 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 1 | A | 428 | ASP | CB-CG-OD1 | 6.26 | 123.94 | 118.30 |
| 1 | L | 428 | ASP | CB-CG-OD1 | 6.26 | 123.94 | 118.30 |
| 1 | L | 802 | ASP | CB-CG-OD2 | -6.26 | 112.66 | 118.30 |
| 1 | N | 591 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | D | 917 | ARG | NE-CZ-NH2 | -6.26 | 117.17 | 120.30 |
| 1 | J | 591 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | P | 591 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | C | 591 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | F | 428 | ASP | CB-CG-OD1 | 6.26 | 123.93 | 118.30 |
| 1 | C | 428 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | C | 659 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | N | 917 | ARG | NE-CZ-NH2 | -6.25 | 117.17 | 120.30 |
| 1 | B | 428 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | B | 659 | ASP | CB-CG-OD1 | 6.25 | 123.93 | 118.30 |
| 1 | H | 428 | ASP | CB-CG-OD1 | 6.25 | 123.92 | 118.30 |
| 1 | B | 802 | ASP | CB-CG-OD2 | -6.25 | 112.68 | 118.30 |
| 1 | L | 591 | ASP | CB-CG-OD2 | -6.25 | 112.68 | 118.30 |
| 1 | D | 802 | ASP | CB-CG-OD2 | -6.25 | 112.68 | 118.30 |
| 1 | B | 917 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 1 | N | 659 | ASP | CB-CG-OD1 | 6.24 | 123.92 | 118.30 |
| 1 | G | 17 | GLU | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 1 | F | 917 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 1 | G | 659 | ASP | CB-CG-OD1 | 6.24 | 123.91 | 118.30 |
| 1 | H | 659 | ASP | CB-CG-OD1 | 6.24 | 123.91 | 118.30 |
| 1 | I | 428 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | M | 428 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | I | 917 | ARG | NE-CZ-NH2 | -6.23 | 117.18 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 591 | ASP | CB-CG-OD2 | -6.23 | 112.69 | 118.30 |
| 1 | O | 96 | ASP | CB-CG-OD2 | -6.23 | 112.69 | 118.30 |
| 1 | L | 659 | ASP | CB-CG-OD1 | 6.23 | 123.90 | 118.30 |
| 1 | A | 917 | ARG | NE-CZ-NH2 | -6.22 | 117.19 | 120.30 |
| 1 | H | 17 | GLU | N-CA-CB | 6.22 | 121.79 | 110.60 |
| 1 | K | 96 | ASP | CB-CG-OD2 | -6.22 | 112.71 | 118.30 |
| 1 | A | 659 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | D | 17 | GLU | N-CA-CB | 6.21 | 121.78 | 110.60 |
| 1 | K | 17 | GLU | N-CA-CB | 6.21 | 121.78 | 110.60 |
| 1 | E | 917 | ARG | NE-CZ-NH2 | -6.21 | 117.19 | 120.30 |
| 1 | F | 17 | GLU | N-CA-CB | 6.21 | 121.78 | 110.60 |
| 1 | B | 17 | GLU | N-CA-CB | 6.21 | 121.78 | 110.60 |
| 1 | E | 591 | ASP | CB-CG-OD2 | -6.21 | 112.71 | 118.30 |
| 1 | O | 17 | GLU | N-CA-CB | 6.21 | 121.77 | 110.60 |
| 1 | P | 17 | GLU | N-CA-CB | 6.21 | 121.77 | 110.60 |
| 1 | M | 17 | GLU | N-CA-CB | 6.21 | 121.77 | 110.60 |
| 1 | A | 17 | GLU | N-CA-CB | 6.20 | 121.77 | 110.60 |
| 1 | J | 17 | GLU | N-CA-CB | 6.20 | 121.77 | 110.60 |
| 1 | L | 96 | ASP | CB-CG-OD2 | -6.20 | 112.72 | 118.30 |
| 1 | P | 96 | ASP | CB-CG-OD2 | -6.20 | 112.72 | 118.30 |
| 1 | L | 17 | GLU | N-CA-CB | 6.20 | 121.76 | 110.60 |
| 1 | N | 17 | GLU | N-CA-CB | 6.20 | 121.76 | 110.60 |
| 1 | J | 917 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 1 | C | 17 | GLU | N-CA-CB | 6.20 | 121.75 | 110.60 |
| 1 | H | 96 | ASP | CB-CG-OD2 | -6.20 | 112.72 | 118.30 |
| 1 | H | 917 | ARG | NE-CZ-NH2 | -6.20 | 117.20 | 120.30 |
| 1 | I | 17 | GLU | N-CA-CB | 6.19 | 121.75 | 110.60 |
| 1 | B | 96 | ASP | CB-CG-OD2 | -6.19 | 112.73 | 118.30 |
| 1 | G | 96 | ASP | CB-CG-OD2 | -6.18 | 112.74 | 118.30 |
| 1 | D | 96 | ASP | CB-CG-OD2 | -6.18 | 112.74 | 118.30 |
| 1 | E | 17 | GLU | N-CA-CB | 6.18 | 121.72 | 110.60 |
| 1 | A | 96 | ASP | CB-CG-OD2 | -6.17 | 112.74 | 118.30 |
| 1 | E | 96 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | L | 411 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | D | 411 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | J | 96 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | I | 96 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | K | 917 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 1 | M | 917 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 1 | H | 411 | ASP | CB-CG-OD2 | -6.16 | 112.76 | 118.30 |
| 1 | I | 772 | ASP | CB-CG-OD1 | 6.16 | 123.84 | 118.30 |
| 1 | C | 917 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | L | 917 | ARG | NE-CZ-NH2 | -6.15 | 117.22 | 120.30 |
| 1 | N | 411 | ASP | CB-CG-OD2 | -6.15 | 112.76 | 118.30 |
| 1 | M | 411 | ASP | CB-CG-OD2 | -6.15 | 112.76 | 118.30 |
| 1 | P | 772 | ASP | CB-CG-OD1 | 6.15 | 123.84 | 118.30 |
| 1 | C | 96 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | N | 96 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | F | 411 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | M | 96 | ASP | CB-CG-OD2 | -6.15 | 112.77 | 118.30 |
| 1 | O | 772 | ASP | CB-CG-OD1 | 6.14 | 123.83 | 118.30 |
| 1 | B | 411 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | E | 411 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | J | 411 | ASP | CB-CG-OD2 | -6.14 | 112.77 | 118.30 |
| 1 | P | 211 | ASP | CB-CG-OD2 | -6.13 | 112.78 | 118.30 |
| 1 | O | 411 | ASP | CB-CG-OD2 | -6.13 | 112.78 | 118.30 |
| 1 | A | 411 | ASP | CB-CG-OD2 | -6.13 | 112.78 | 118.30 |
| 1 | P | 917 | ARG | NE-CZ-NH2 | -6.13 | 117.24 | 120.30 |
| 1 | C | 411 | ASP | CB-CG-OD2 | -6.13 | 112.78 | 118.30 |
| 1 | F | 211 | ASP | CB-CG-OD2 | -6.13 | 112.79 | 118.30 |
| 1 | N | 772 | ASP | CB-CG-OD1 | 6.13 | 123.81 | 118.30 |
| 1 | M | 772 | ASP | CB-CG-OD1 | 6.12 | 123.81 | 118.30 |
| 1 | A | 772 | ASP | CB-CG-OD1 | 6.12 | 123.80 | 118.30 |
| 1 | F | 772 | ASP | CB-CG-OD1 | 6.12 | 123.80 | 118.30 |
| 1 | I | 411 | ASP | CB-CG-OD2 | -6.12 | 112.80 | 118.30 |
| 1 | F | 96 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 1 | J | 772 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | C | 211 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 1 | C | 772 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | O | 211 | ASP | CB-CG-OD2 | -6.11 | 112.81 | 118.30 |
| 1 | B | 211 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | D | 909 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 1 | F | 909 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 1 | G | 772 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | K | 411 | ASP | CB-CG-OD2 | -6.10 | 112.81 | 118.30 |
| 1 | N | 987 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | P | 411 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |
| 1 | A | 909 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | C | 909 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | J | 211 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |
| 1 | K | 211 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |
| 1 | N | 909 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | J | 909 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | E | 211 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | L | 909 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 1 | A | 211 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 1 | K | 909 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 1 | G | 211 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 1 | E | 772 | ASP | CB-CG-OD1 | 6.08 | 123.77 | 118.30 |
| 1 | H | 211 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 1 | H | 772 | ASP | CB-CG-OD1 | 6.07 | 123.77 | 118.30 |
| 1 | E | 987 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 1 | D | 211 | ASP | CB-CG-OD2 | -6.07 | 112.84 | 118.30 |
| 1 | F | 179 | ALA | N-CA-CB | 6.07 | 118.60 | 110.10 |
| 1 | G | 411 | ASP | CB-CG-OD2 | -6.07 | 112.84 | 118.30 |
| 1 | A | 987 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 1 | M | 987 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 1 | I | 909 | ARG | NE-CZ-NH1 | 6.07 | 123.33 | 120.30 |
| 1 | K | 772 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 1 | J | 987 | ASP | CB-CG-OD1 | 6.06 | 123.76 | 118.30 |
| 1 | C | 292 | ARG | NE-CZ-NH2 | -6.06 | 117.27 | 120.30 |
| 1 | D | 772 | ASP | CB-CG-OD1 | 6.06 | 123.76 | 118.30 |
| 1 | O | 987 | ASP | CB-CG-OD1 | 6.06 | 123.75 | 118.30 |
| 1 | H | 292 | ARG | NE-CZ-NH2 | -6.06 | 117.27 | 120.30 |
| 1 | G | 909 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 1 | I | 292 | ARG | NE-CZ-NH2 | -6.05 | 117.27 | 120.30 |
| 1 | K | 987 | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | M | 179 | ALA | N-CA-CB | 6.05 | 118.58 | 110.10 |
| 1 | O | 1006 | GLU | CG-CD-OE2 | -6.05 | 106.19 | 118.30 |
| 1 | B | 772 | ASP | CB-CG-OD1 | 6.05 | 123.75 | 118.30 |
| 1 | J | 179 | ALA | N-CA-CB | 6.05 | 118.57 | 110.10 |
| 1 | O | 179 | ALA | N-CA-CB | 6.05 | 118.57 | 110.10 |
| 1 | D | 987 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | N | 211 | ASP | CB-CG-OD2 | -6.05 | 112.86 | 118.30 |
| 1 | G | 292 | ARG | NE-CZ-NH2 | -6.05 | 117.28 | 120.30 |
| 1 | L | 987 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | C | 987 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | E | 1006 | GLU | CG-CD-OE2 | -6.05 | 106.21 | 118.30 |
| 1 | G | 179 | ALA | N-CA-CB | 6.05 | 118.56 | 110.10 |
| 1 | J | 1006 | GLU | CG-CD-OE2 | -6.05 | 106.20 | 118.30 |
| 1 | K | 179 | ALA | N-CA-CB | 6.05 | 118.56 | 110.10 |
| 1 | P | 987 | ASP | CB-CG-OD1 | 6.05 | 123.74 | 118.30 |
| 1 | B | 1006 | GLU | CG-CD-OE2 | -6.04 | 106.21 | 118.30 |
| 1 | B | 987 | ASP | CB-CG-OD1 | 6.04 | 123.74 | 118.30 |
| 1 | K | 1018 | LEU | CB-CG-CD2 | -6.04 | 100.73 | 111.00 |
| 1 | L | 211 | ASP | CB-CG-OD2 | -6.04 | 112.86 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | L | 292 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 1 | P | 909 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 |
| 1 | P | 1006 | GLU | CG-CD-OE2 | -6.04 | 106.21 | 118.30 |
| 1 | H | 987 | ASP | CB-CG-OD1 | 6.04 | 123.74 | 118.30 |
| 1 | L | 179 | ALA | N-CA-CB | 6.04 | 118.56 | 110.10 |
| 1 | I | 211 | ASP | CB-CG-OD2 | -6.04 | 112.86 | 118.30 |
| 1 | A | 179 | ALA | N-CA-CB | 6.04 | 118.55 | 110.10 |
| 1 | E | 179 | ALA | N-CA-CB | 6.04 | 118.55 | 110.10 |
| 1 | E | 292 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 1 | A | 292 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 1 | F | 1006 | GLU | CG-CD-OE2 | -6.04 | 106.23 | 118.30 |
| 1 | A | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.23 | 118.30 |
| 1 | G | 1018 | LEU | CB-CG-CD2 | -6.03 | 100.74 | 111.00 |
| 1 | L | 772 | ASP | CB-CG-OD1 | 6.03 | 123.73 | 118.30 |
| 1 | P | 1018 | LEU | CB-CG-CD2 | -6.03 | 100.75 | 111.00 |
| 1 | M | 211 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 |
| 1 | D | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.24 | 118.30 |
| 1 | G | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.24 | 118.30 |
| 1 | H | 179 | ALA | N-CA-CB | 6.03 | 118.54 | 110.10 |
| 1 | I | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.25 | 118.30 |
| 1 | M | 909 | ARG | NE-CZ-NH1 | 6.03 | 123.31 | 120.30 |
| 1 | N | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.25 | 118.30 |
| 1 | N | 1018 | LEU | CB-CG-CD2 | -6.03 | 100.75 | 111.00 |
| 1 | C | 1006 | GLU | CG-CD-OE2 | -6.03 | 106.25 | 118.30 |
| 1 | C | 1018 | LEU | CB-CG-CD2 | -6.03 | 100.76 | 111.00 |
| 1 | I | 987 | ASP | CB-CG-OD1 | 6.03 | 123.72 | 118.30 |
| 1 | B | 909 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | C | 179 | ALA | N-CA-CB | 6.02 | 118.53 | 110.10 |
| 1 | E | 1018 | LEU | CB-CG-CD2 | -6.02 | 100.76 | 111.00 |
| 1 | G | 987 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |
| 1 | K | 1006 | GLU | CG-CD-OE2 | -6.02 | 106.25 | 118.30 |
| 1 | L | 1018 | LEU | CB-CG-CD2 | -6.02 | 100.77 | 111.00 |
| 1 | A | 1018 | LEU | CB-CG-CD2 | -6.02 | 100.77 | 111.00 |
| 1 | D | 1018 | LEU | CB-CG-CD2 | -6.02 | 100.77 | 111.00 |
| 1 | F | 987 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |
| 1 | N | 179 | ALA | N-CA-CB | 6.02 | 118.53 | 110.10 |
| 1 | F | 292 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 1 | L | 1006 | GLU | CG-CD-OE2 | -6.02 | 106.27 | 118.30 |
| 1 | B | 179 | ALA | N-CA-CB | 6.02 | 118.52 | 110.10 |
| 1 | J | 1018 | LEU | CB-CG-CD2 | -6.01 | 100.77 | 111.00 |
| 1 | M | 1018 | LEU | CB-CG-CD2 | -6.01 | 100.78 | 111.00 |
| 1 | D | 179 | ALA | N-CA-CB | 6.01 | 118.51 | 110.10 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | F | 1018 | LEU | CB-CG-CD2 | -6.01 | 100.78 | 111.00 |
| 1 | H | 1006 | GLU | CG-CD-OE2 | -6.01 | 106.28 | 118.30 |
| 1 | O | 1018 | LEU | CB-CG-CD2 | -6.01 | 100.78 | 111.00 |
| 1 | I | 1018 | LEU | CB-CG-CD2 | -6.01 | 100.79 | 111.00 |
| 1 | K | 292 | ARG | NE-CZ-NH2 | -6.01 | 117.30 | 120.30 |
| 1 | M | 1006 | GLU | CG-CD-OE2 | -6.01 | 106.29 | 118.30 |
| 1 | M | 292 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 1 | I | 179 | ALA | N-CA-CB | 6.00 | 118.50 | 110.10 |
| 1 | B | 1018 | LEU | CB-CG-CD2 | -6.00 | 100.80 | 111.00 |
| 1 | H | 1018 | LEU | CB-CG-CD2 | -6.00 | 100.80 | 111.00 |
| 1 | P | 179 | ALA | N-CA-CB | 5.99 | 118.49 | 110.10 |
| 1 | L | 800 | ARG | NE-CZ-NH2 | -5.99 | 117.31 | 120.30 |
| 1 | O | 333 | ARG | NE-CZ-NH1 | 5.99 | 123.30 | 120.30 |
| 1 | J | 292 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 1 | D | 919 | ASP | CB-CG-OD1 | 5.98 | 123.68 | 118.30 |
| 1 | E | 909 | ARG | NE-CZ-NH1 | 5.97 | 123.29 | 120.30 |
| 1 | J | 919 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 1 | E | 648 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 1 | D | 292 | ARG | NE-CZ-NH2 | -5.97 | 117.32 | 120.30 |
| 1 | N | 333 | ARG | NE-CZ-NH1 | 5.97 | 123.28 | 120.30 |
| 1 | M | 1013 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | H | 909 | ARG | NE-CZ-NH1 | 5.96 | 123.28 | 120.30 |
| 1 | C | 234 | ASP | CB-CG-OD2 | -5.96 | 112.94 | 118.30 |
| 1 | C | 958 | ASN | N-CA-CB | 5.96 | 121.33 | 110.60 |
| 1 | N | 292 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | A | 919 | ASP | CB-CG-OD1 | 5.96 | 123.66 | 118.30 |
| 1 | C | 919 | ASP | CB-CG-OD1 | 5.96 | 123.66 | 118.30 |
| 1 | E | 919 | ASP | CB-CG-OD1 | 5.96 | 123.66 | 118.30 |
| 1 | O | 909 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 1 | G | 255 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 1 | P | 919 | ASP | CB-CG-OD1 | 5.95 | 123.66 | 118.30 |
| 1 | F | 648 | ASP | CB-CG-OD1 | 5.95 | 123.66 | 118.30 |
| 1 | B | 234 | ASP | CB-CG-OD2 | -5.95 | 112.95 | 118.30 |
| 1 | N | 1013 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | O | 255 | ARG | NE-CZ-NH1 | 5.95 | 123.28 | 120.30 |
| 1 | E | 958 | ASN | N-CA-CB | 5.95 | 121.30 | 110.60 |
| 1 | I | 919 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | F | 919 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | I | 255 | ARG | NE-CZ-NH1 | 5.95 | 123.27 | 120.30 |
| 1 | I | 800 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | K | 919 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | G | 1013 | ARG | NE-CZ-NH2 | -5.94 | 117.33 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | M | 648 | ASP | CB-CG-OD1 | 5.94 | 123.65 | 118.30 |
| 1 | D | 45 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | C | 333 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 1 | L | 648 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 |
| 1 | N | 919 | ASP | CB-CG-OD1 | 5.94 | 123.64 | 118.30 |
| 1 | A | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | I | 648 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | P | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | B | 919 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | B | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | N | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | O | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | F | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | G | 958 | ASN | N-CA-CB | 5.93 | 121.28 | 110.60 |
| 1 | D | 1013 | ARG | NE-CZ-NH2 | -5.93 | 117.34 | 120.30 |
| 1 | L | 919 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | M | 333 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 1 | J | 648 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 1 | M | 919 | ASP | CB-CG-OD1 | 5.93 | 123.63 | 118.30 |
| 1 | G | 45 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | H | 958 | ASN | N-CA-CB | 5.92 | 121.26 | 110.60 |
| 1 | F | 234 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | O | 234 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | F | 45 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | L | 958 | ASN | N-CA-CB | 5.92 | 121.26 | 110.60 |
| 1 | H | 919 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | A | 648 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | E | 1013 | ARG | NE-CZ-NH2 | -5.92 | 117.34 | 120.30 |
| 1 | F | 333 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | G | 919 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | I | 958 | ASN | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 1 | K | 958 | ASN | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 1 | P | 255 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | D | 958 | ASN | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 1 | H | 648 | ASP | CB-CG-OD1 | 5.92 | 123.62 | 118.30 |
| 1 | A | 234 | ASP | CB-CG-OD2 | -5.92 | 112.98 | 118.30 |
| 1 | J | 45 | ASP | CB-CG-OD2 | -5.92 | 112.98 | 118.30 |
| 1 | J | 958 | ASN | N-CA-CB | 5.91 | 121.25 | 110.60 |
| 1 | O | 648 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | P | 292 | ARG | NE-CZ-NH2 | -5.91 | 117.34 | 120.30 |
| 1 | O | 800 | ARG | NE-CZ-NH2 | -5.91 | 117.34 | 120.30 |
| 1 | B | 45 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 648 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | K | 234 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | L | 255 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 1 | K | 648 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | B | 292 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | B | 648 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 1 | M | 958 | ASN | N-CA-CB | 5.90 | 121.22 | 110.60 |
| 1 | F | 255 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | J | 255 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | K | 800 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | L | 45 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | O | 45 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | C | 800 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | G | 234 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | N | 648 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 1 | B | 255 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | E | 45 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | A | 45 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | P | 234 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | D | 648 | ASP | CB-CG-OD1 | 5.89 | 123.60 | 118.30 |
| 1 | C | 45 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | H | 800 | ARG | NE-CZ-NH2 | -5.89 | 117.36 | 120.30 |
| 1 | B | 1013 | ARG | NE-CZ-NH2 | -5.89 | 117.36 | 120.30 |
| 1 | H | 1013 | ARG | NE-CZ-NH2 | -5.89 | 117.36 | 120.30 |
| 1 | P | 45 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | P | 333 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | P | 648 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | H | 234 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | L | 234 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | P | 800 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | G | 648 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | K | 333 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | N | 234 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | B | 800 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | D | 800 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | L | 1013 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | M | 875 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | E | 234 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | M | 234 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | N | 45 | ASP | CB-CG-OD2 | -5.88 | 113.01 | 118.30 |
| 1 | O | 919 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | B | 333 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 559 | TYR | CB-CG-CD1 | 5.88 | 124.53 | 121.00 |
| 1 | K | 45 | ASP | CB-CG-OD2 | -5.87 | 113.01 | 118.30 |
| 1 | M | 255 | ARG | NE-CZ-NH1 | 5.87 | 123.23 | 120.30 |
| 1 | A | 1013 | ARG | NE-CZ-NH2 | -5.87 | 117.37 | 120.30 |
| 1 | D | 255 | ARG | NE-CZ-NH1 | 5.87 | 123.23 | 120.30 |
| 1 | I | 45 | ASP | CB-CG-OD2 | -5.87 | 113.02 | 118.30 |
| 1 | J | 234 | ASP | CB-CG-OD2 | -5.87 | 113.02 | 118.30 |
| 1 | A | 333 | ARG | NE-CZ-NH1 | 5.87 | 123.23 | 120.30 |
| 1 | J | 800 | ARG | NE-CZ-NH2 | -5.87 | 117.37 | 120.30 |
| 1 | D | 333 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | H | 333 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | D | 234 | ASP | CB-CG-OD2 | -5.86 | 113.03 | 118.30 |
| 1 | C | 1013 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | G | 46 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | H | 206 | SER | N-CA-CB | 5.86 | 119.29 | 110.50 |
| 1 | M | 45 | ASP | CB-CG-OD2 | -5.86 | 113.03 | 118.30 |
| 1 | O | 292 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | F | 1013 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | G | 875 | ASP | CB-CG-OD2 | -5.86 | 113.03 | 118.30 |
| 1 | M | 206 | SER | N-CA-CB | 5.85 | 119.27 | 110.50 |
| 1 | L | 333 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | E | 333 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | N | 206 | SER | N-CA-CB | 5.85 | 119.27 | 110.50 |
| 1 | E | 255 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | F | 206 | SER | N-CA-CB | 5.84 | 119.27 | 110.50 |
| 1 | B | 206 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | K | 206 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | N | 800 | ARG | NE-CZ-NH2 | -5.84 | 117.38 | 120.30 |
| 1 | C | 206 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | D | 875 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | O | 559 | TYR | CB-CG-CD1 | 5.84 | 124.50 | 121.00 |
| 1 | P | 206 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | E | 875 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | G | 800 | ARG | NE-CZ-NH2 | -5.84 | 117.38 | 120.30 |
| 1 | I | 234 | ASP | CB-CG-OD2 | -5.84 | 113.05 | 118.30 |
| 1 | I | 333 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | J | 206 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | A | 255 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | J | 333 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | K | 255 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | A | 206 | SER | N-CA-CB | 5.83 | 119.25 | 110.50 |
| 1 | L | 875 | ASP | CB-CG-OD2 | -5.83 | 113.05 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | G | 126 | THR | CA-CB-CG2 | -5.83 | 104.24 | 112.40 |
| 1 | H | 255 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | O | 206 | SER | N-CA-CB | 5.83 | 119.24 | 110.50 |
| 1 | F | 800 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 1 | H | 45 | ASP | CB-CG-OD2 | -5.83 | 113.06 | 118.30 |
| 1 | A | 875 | ASP | CB-CG-OD2 | -5.83 | 113.06 | 118.30 |
| 1 | C | 255 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | K | 1013 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 1 | P | 1013 | ARG | NE-CZ-NH2 | -5.83 | 117.39 | 120.30 |
| 1 | E | 800 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |
| 1 | L | 559 | TYR | CB-CG-CD1 | 5.82 | 124.50 | 121.00 |
| 1 | B | 387 | VAL | CG1-CB-CG2 | -5.82 | 101.58 | 110.90 |
| 1 | F | 875 | ASP | CB-CG-OD2 | -5.82 | 113.06 | 118.30 |
| 1 | P | 875 | ASP | CB-CG-OD2 | -5.82 | 113.06 | 118.30 |
| 1 | D | 46 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | D | 206 | SER | N-CA-CB | 5.82 | 119.23 | 110.50 |
| 1 | I | 206 | SER | N-CA-CB | 5.82 | 119.22 | 110.50 |
| 1 | M | 800 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |
| 1 | H | 126 | THR | CA-CB-CG2 | -5.81 | 104.26 | 112.40 |
| 1 | L | 206 | SER | N-CA-CB | 5.81 | 119.22 | 110.50 |
| 1 | E | 46 | ARG | NE-CZ-NH1 | 5.81 | 123.21 | 120.30 |
| 1 | C | 387 | VAL | CG1-CB-CG2 | -5.81 | 101.61 | 110.90 |
| 1 | D | 387 | VAL | CG1-CB-CG2 | -5.81 | 101.60 | 110.90 |
| 1 | E | 206 | SER | N-CA-CB | 5.81 | 119.22 | 110.50 |
| 1 | G | 206 | SER | N-CA-CB | 5.81 | 119.22 | 110.50 |
| 1 | K | 387 | VAL | CG1-CB-CG2 | -5.81 | 101.61 | 110.90 |
| 1 | M | 387 | VAL | CG1-CB-CG2 | -5.81 | 101.61 | 110.90 |
| 1 | N | 255 | ARG | NE-CZ-NH1 | 5.81 | 123.20 | 120.30 |
| 1 | B | 126 | THR | CA-CB-CG2 | -5.81 | 104.27 | 112.40 |
| 1 | H | 875 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 |
| 1 | F | 387 | VAL | CG1-CB-CG2 | -5.80 | 101.62 | 110.90 |
| 1 | J | 46 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | L | 126 | THR | CA-CB-CG2 | -5.80 | 104.28 | 112.40 |
| 1 | J | 1013 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | O | 1013 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | B | 46 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | C | 46 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | N | 875 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 |
| 1 | O | 679 | LEU | CA-CB-CG | -5.80 | 101.97 | 115.30 |
| 1 | G | 679 | LEU | CA-CB-CG | -5.80 | 101.97 | 115.30 |
| 1 | I | 1013 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | M | 126 | THR | CA-CB-CG2 | -5.80 | 104.28 | 112.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | N | 679 | LEU | CA-CB-CG | -5.80 | 101.97 | 115.30 |
| 1 | B | 679 | LEU | CA-CB-CG | -5.79 | 101.97 | 115.30 |
| 1 | B | 875 | ASP | CB-CG-OD2 | -5.79 | 113.08 | 118.30 |
| 1 | D | 126 | THR | CA-CB-CG2 | -5.79 | 104.29 | 112.40 |
| 1 | I | 387 | VAL | CG1-CB-CG2 | -5.79 | 101.63 | 110.90 |
| 1 | K | 671 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | A | 800 | ARG | NE-CZ-NH2 | -5.79 | 117.40 | 120.30 |
| 1 | C | 166 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | H | 1006 | GLU | CB-CA-C | -5.79 | 98.82 | 110.40 |
| 1 | I | 559 | TYR | CB-CG-CD1 | 5.79 | 124.47 | 121.00 |
| 1 | I | 679 | LEU | CA-CB-CG | -5.79 | 101.98 | 115.30 |
| 1 | E | 559 | TYR | CB-CG-CD1 | 5.79 | 124.47 | 121.00 |
| 1 | E | 679 | LEU | CA-CB-CG | -5.79 | 101.98 | 115.30 |
| 1 | J | 166 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | B | 166 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | I | 126 | THR | CA-CB-CG2 | -5.79 | 104.30 | 112.40 |
| 1 | J | 126 | THR | CA-CB-CG2 | -5.79 | 104.30 | 112.40 |
| 1 | M | 679 | LEU | CA-CB-CG | -5.79 | 101.99 | 115.30 |
| 1 | O | 387 | VAL | CG1-CB-CG2 | -5.79 | 101.64 | 110.90 |
| 1 | P | 679 | LEU | CA-CB-CG | -5.79 | 101.98 | 115.30 |
| 1 | F | 679 | LEU | CA-CB-CG | -5.79 | 101.99 | 115.30 |
| 1 | J | 387 | VAL | CG1-CB-CG2 | -5.79 | 101.64 | 110.90 |
| 1 | K | 875 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | A | 559 | TYR | CB-CG-CD1 | 5.79 | 124.47 | 121.00 |
| 1 | A | 679 | LEU | CA-CB-CG | -5.79 | 101.99 | 115.30 |
| 1 | E | 492 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 1 | E | 1006 | GLU | CB-CA-C | -5.79 | 98.83 | 110.40 |
| 1 | A | 126 | THR | CA-CB-CG2 | -5.78 | 104.30 | 112.40 |
| 1 | C | 679 | LEU | CA-CB-CG | -5.78 | 102.00 | 115.30 |
| 1 | K | 126 | THR | CA-CB-CG2 | -5.78 | 104.30 | 112.40 |
| 1 | D | 166 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | J | 679 | LEU | CA-CB-CG | -5.78 | 102.00 | 115.30 |
| 1 | J | 875 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | A | 387 | VAL | CG1-CB-CG2 | -5.78 | 101.65 | 110.90 |
| 1 | D | 679 | LEU | CA-CB-CG | -5.78 | 102.00 | 115.30 |
| 1 | L | 497 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 1 | L | 671 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | M | 492 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 1 | O | 126 | THR | CA-CB-CG2 | -5.78 | 104.31 | 112.40 |
| 1 | C | 875 | ASP | CB-CG-OD2 | -5.78 | 113.10 | 118.30 |
| 1 | E | 126 | THR | CA-CB-CG2 | -5.78 | 104.31 | 112.40 |
| 1 | H | 679 | LEU | CA-CB-CG | -5.78 | 102.01 | 115.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | K | 679 | LEU | CA-CB-CG | -5.78 | 102.01 | 115.30 |
| 1 | N | 559 | TYR | CB-CG-CD1 | 5.78 | 124.47 | 121.00 |
| 1 | P | 387 | VAL | CG1-CB-CG2 | -5.78 | 101.66 | 110.90 |
| 1 | N | 569 | ASP | CB-CG-OD2 | -5.77 | 113.10 | 118.30 |
| 1 | O | 875 | ASP | CB-CG-OD2 | -5.77 | 113.10 | 118.30 |
| 1 | G | 387 | VAL | CG1-CB-CG2 | -5.77 | 101.67 | 110.90 |
| 1 | L | 387 | VAL | CG1-CB-CG2 | -5.77 | 101.67 | 110.90 |
| 1 | M | 166 | ARG | NE-CZ-NH2 | -5.77 | 117.41 | 120.30 |
| 1 | N | 126 | THR | CA-CB-CG2 | -5.77 | 104.32 | 112.40 |
| 1 | H | 375 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | M | 388 | ARG | NE-CZ-NH1 | 5.77 | 123.19 | 120.30 |
| 1 | B | 497 | ASP | CB-CG-OD1 | 5.77 | 123.49 | 118.30 |
| 1 | E | 387 | VAL | CG1-CB-CG2 | -5.77 | 101.67 | 110.90 |
| 1 | F | 559 | TYR | CB-CG-CD1 | 5.77 | 124.46 | 121.00 |
| 1 | F | 671 | ASP | CB-CG-OD2 | -5.77 | 113.11 | 118.30 |
| 1 | G | 1006 | GLU | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 1 | M | 1006 | GLU | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 1 | P | 126 | THR | CA-CB-CG2 | -5.77 | 104.32 | 112.40 |
| 1 | L | 1006 | GLU | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 1 | P | 1006 | GLU | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 1 | A | 1006 | GLU | CB-CA-C | -5.77 | 98.87 | 110.40 |
| 1 | C | 126 | THR | CA-CB-CG2 | -5.77 | 104.33 | 112.40 |
| 1 | F | 126 | THR | CA-CB-CG2 | -5.77 | 104.33 | 112.40 |
| 1 | B | 1006 | GLU | CB-CA-C | -5.76 | 98.87 | 110.40 |
| 1 | C | 559 | TYR | CB-CG-CD1 | 5.76 | 124.46 | 121.00 |
| 1 | D | 569 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | D | 671 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | H | 569 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | L | 679 | LEU | CA-CB-CG | -5.76 | 102.04 | 115.30 |
| 1 | N | 497 | ASP | CB-CG-OD1 | 5.76 | 123.49 | 118.30 |
| 1 | G | 333 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 1 | J | 559 | TYR | CB-CG-CD1 | 5.76 | 124.46 | 121.00 |
| 1 | G | 671 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | H | 559 | TYR | CB-CG-CD1 | 5.76 | 124.46 | 121.00 |
| 1 | I | 1006 | GLU | CB-CA-C | -5.76 | 98.88 | 110.40 |
| 1 | J | 671 | ASP | CB-CG-OD2 | -5.76 | 113.11 | 118.30 |
| 1 | M | 559 | TYR | CB-CG-CD1 | 5.76 | 124.46 | 121.00 |
| 1 | N | 1006 | GLU | CB-CA-C | -5.76 | 98.88 | 110.40 |
| 1 | A | 46 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 1 | C | 671 | ASP | CB-CG-OD2 | -5.76 | 113.12 | 118.30 |
| 1 | C | 1006 | GLU | CB-CA-C | -5.76 | 98.88 | 110.40 |
| 1 | G | 492 | ASP | CB-CG-OD1 | 5.76 | 123.48 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | H | 387 | VAL | CG1-CB-CG2 | -5.76 | 101.69 | 110.90 |
| 1 | N | 387 | VAL | CG1-CB-CG2 | -5.76 | 101.68 | 110.90 |
| 1 | P | 671 | ASP | CB-CG-OD2 | -5.76 | 113.12 | 118.30 |
| 1 | K | 492 | ASP | CB-CG-OD1 | 5.76 | 123.48 | 118.30 |
| 1 | N | 166 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 1 | K | 1006 | GLU | CB-CA-C | -5.76 | 98.89 | 110.40 |
| 1 | L | 166 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 1 | N | 671 | ASP | CB-CG-OD2 | -5.76 | 113.12 | 118.30 |
| 1 | A | 671 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | J | 388 | ARG | NE-CZ-NH1 | 5.75 | 123.18 | 120.30 |
| 1 | D | 1006 | GLU | CB-CA-C | -5.75 | 98.90 | 110.40 |
| 1 | I | 594 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | I | 875 | ASP | CB-CG-OD2 | -5.75 | 113.12 | 118.30 |
| 1 | J | 1006 | GLU | CB-CA-C | -5.75 | 98.90 | 110.40 |
| 1 | O | 166 | ARG | NE-CZ-NH2 | -5.75 | 117.42 | 120.30 |
| 1 | F | 1006 | GLU | CB-CA-C | -5.75 | 98.90 | 110.40 |
| 1 | K | 166 | ARG | NE-CZ-NH2 | -5.75 | 117.42 | 120.30 |
| 1 | B | 559 | TYR | CB-CG-CD1 | 5.75 | 124.45 | 121.00 |
| 1 | K | 594 | ASP | CB-CG-OD2 | -5.75 | 113.13 | 118.30 |
| 1 | L | 492 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | O | 497 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | O | 1006 | GLU | CB-CA-C | -5.75 | 98.91 | 110.40 |
| 1 | I | 166 | ARG | NE-CZ-NH2 | -5.75 | 117.43 | 120.30 |
| 1 | I | 497 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | J | 497 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | P | 497 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | H | 671 | ASP | CB-CG-OD2 | -5.75 | 113.13 | 118.30 |
| 1 | P | 559 | TYR | CB-CG-CD1 | 5.75 | 124.45 | 121.00 |
| 1 | A | 497 | ASP | CB-CG-OD1 | 5.74 | 123.47 | 118.30 |
| 1 | N | 492 | ASP | CB-CG-OD1 | 5.74 | 123.47 | 118.30 |
| 1 | H | 46 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 1 | P | 594 | ASP | CB-CG-OD2 | -5.74 | 113.14 | 118.30 |
| 1 | F | 594 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | I | 671 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | J | 569 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | N | 388 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 1 | A | 166 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 1 | A | 569 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | B | 671 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | O | 492 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 1 | O | 671 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | C | 388 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 492 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 1 | M | 671 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | K | 388 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 1 | O | 594 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | E | 497 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 1 | F | 46 | ARG | NE-CZ-NH1 | 5.73 | 123.16 | 120.30 |
| 1 | H | 166 | ARG | NE-CZ-NH2 | -5.73 | 117.44 | 120.30 |
| 1 | L | 569 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 |
| 1 | M | 497 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 1 | P | 46 | ARG | NE-CZ-NH1 | 5.73 | 123.16 | 120.30 |
| 1 | A | 492 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 1 | C | 497 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 1 | K | 559 | TYR | CB-CG-CD1 | 5.73 | 124.44 | 121.00 |
| 1 | A | 594 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | D | 497 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | H | 594 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | I | 46 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | I | 388 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | K | 569 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | H | 388 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | O | 388 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | O | 610 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | E | 594 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | F | 497 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | G | 559 | TYR | CB-CG-CD1 | 5.72 | 124.43 | 121.00 |
| 1 | H | 492 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | B | 375 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | G | 497 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 1 | H | 186 | VAL | CA-CB-CG1 | -5.72 | 102.32 | 110.90 |
| 1 | B | 492 | ASP | CB-CG-OD1 | 5.72 | 123.44 | 118.30 |
| 1 | C | 186 | VAL | CA-CB-CG1 | -5.72 | 102.32 | 110.90 |
| 1 | C | 569 | ASP | CB-CG-OD2 | -5.72 | 113.16 | 118.30 |
| 1 | K | 497 | ASP | CB-CG-OD1 | 5.72 | 123.44 | 118.30 |
| 1 | E | 186 | VAL | CA-CB-CG1 | -5.71 | 102.33 | 110.90 |
| 1 | I | 492 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | I | 772 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | M | 375 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | P | 569 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | N | 186 | VAL | CA-CB-CG1 | -5.71 | 102.33 | 110.90 |
| 1 | P | 375 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | A | 388 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | E | 671 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | G | 186 | VAL | CA-CB-CG1 | -5.71 | 102.34 | 110.90 |
| 1 | N | 594 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | G | 388 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | B | 569 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | C | 375 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | G | 594 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | I | 569 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | J | 594 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | M | 569 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | B | 186 | VAL | CA-CB-CG1 | -5.70 | 102.35 | 110.90 |
| 1 | F | 166 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 1 | J | 553 | TRP | CA-CB-CG | -5.70 | 102.87 | 113.70 |
| 1 | K | 186 | VAL | CA-CB-CG1 | -5.70 | 102.35 | 110.90 |
| 1 | K | 375 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | A | 375 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | D | 594 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | C | 553 | TRP | CA-CB-CG | -5.70 | 102.87 | 113.70 |
| 1 | C | 594 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | D | 186 | VAL | CA-CB-CG1 | -5.70 | 102.35 | 110.90 |
| 1 | E | 166 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 1 | F | 569 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | N | 46 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 1 | B | 553 | TRP | CA-CB-CG | -5.70 | 102.88 | 113.70 |
| 1 | C | 492 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | D | 388 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 1 | H | 497 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | I | 186 | VAL | CA-CB-CG1 | -5.70 | 102.36 | 110.90 |
| 1 | M | 594 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | O | 46 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 1 | P | 492 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | B | 594 | ASP | CB-CG-OD2 | -5.69 | 113.18 | 118.30 |
| 1 | E | 375 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | E | 553 | TRP | CA-CB-CG | -5.69 | 102.88 | 113.70 |
| 1 | I | 375 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | N | 772 | ASP | CB-CG-OD2 | -5.69 | 113.18 | 118.30 |
| 1 | J | 186 | VAL | CA-CB-CG1 | -5.69 | 102.36 | 110.90 |
| 1 | A | 186 | VAL | CA-CB-CG1 | -5.69 | 102.37 | 110.90 |
| 1 | D | 375 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | F | 186 | VAL | CA-CB-CG1 | -5.69 | 102.37 | 110.90 |
| 1 | F | 375 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | F | 772 | ASP | CB-CG-OD2 | -5.69 | 113.18 | 118.30 |
| 1 | N | 610 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 772 | ASP | CB-CG-OD2 | -5.69 | 113.18 | 118.30 |
| 1 | M | 46 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 1 | O | 375 | ASP | CB-CG-OD1 | 5.69 | 123.42 | 118.30 |
| 1 | G | 569 | ASP | CB-CG-OD2 | -5.68 | 113.18 | 118.30 |
| 1 | I | 553 | TRP | CA-CB-CG | -5.68 | 102.90 | 113.70 |
| 1 | K | 46 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | L | 46 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | L | 186 | VAL | CA-CB-CG1 | -5.68 | 102.37 | 110.90 |
| 1 | L | 375 | ASP | CB-CG-OD1 | 5.68 | 123.42 | 118.30 |
| 1 | L | 610 | ASP | CB-CG-OD1 | 5.68 | 123.42 | 118.30 |
| 1 | M | 186 | VAL | CA-CB-CG1 | -5.68 | 102.37 | 110.90 |
| 1 | C | 772 | ASP | CB-CG-OD2 | -5.68 | 113.19 | 118.30 |
| 1 | E | 388 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | D | 553 | TRP | CA-CB-CG | -5.68 | 102.91 | 113.70 |
| 1 | E | 569 | ASP | CB-CG-OD2 | -5.68 | 113.19 | 118.30 |
| 1 | G | 375 | ASP | CB-CG-OD1 | 5.68 | 123.41 | 118.30 |
| 1 | F | 492 | ASP | CB-CG-OD1 | 5.68 | 123.41 | 118.30 |
| 1 | K | 553 | TRP | CA-CB-CG | -5.68 | 102.91 | 113.70 |
| 1 | P | 553 | TRP | CA-CB-CG | -5.68 | 102.92 | 113.70 |
| 1 | A | 553 | TRP | CA-CB-CG | -5.67 | 102.92 | 113.70 |
| 1 | M | 553 | TRP | CA-CB-CG | -5.67 | 102.92 | 113.70 |
| 1 | N | 375 | ASP | CB-CG-OD1 | 5.67 | 123.41 | 118.30 |
| 1 | A | 772 | ASP | CB-CG-OD2 | -5.67 | 113.19 | 118.30 |
| 1 | M | 772 | ASP | CB-CG-OD2 | -5.67 | 113.19 | 118.30 |
| 1 | P | 961 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 1 | F | 553 | TRP | CA-CB-CG | -5.67 | 102.92 | 113.70 |
| 1 | L | 594 | ASP | CB-CG-OD2 | -5.67 | 113.20 | 118.30 |
| 1 | O | 553 | TRP | CA-CB-CG | -5.67 | 102.92 | 113.70 |
| 1 | N | 553 | TRP | CA-CB-CG | -5.67 | 102.93 | 113.70 |
| 1 | O | 569 | ASP | CB-CG-OD2 | -5.67 | 113.20 | 118.30 |
| 1 | H | 553 | TRP | CA-CB-CG | -5.67 | 102.93 | 113.70 |
| 1 | J | 375 | ASP | CB-CG-OD1 | 5.67 | 123.40 | 118.30 |
| 1 | L | 388 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 1 | P | 388 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 1 | O | 186 | VAL | CA-CB-CG1 | -5.67 | 102.40 | 110.90 |
| 1 | P | 186 | VAL | CA-CB-CG1 | -5.67 | 102.40 | 110.90 |
| 1 | K | 96 | ASP | N-CA-CB | 5.67 | 120.80 | 110.60 |
| 1 | L | 553 | TRP | CA-CB-CG | -5.66 | 102.94 | 113.70 |
| 1 | F | 96 | ASP | N-CA-CB | 5.66 | 120.79 | 110.60 |
| 1 | B | 388 | ARG | NE-CZ-NH1 | 5.66 | 123.13 | 120.30 |
| 1 | G | 166 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | G | 610 | ASP | CB-CG-OD1 | 5.66 | 123.39 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | J | 492 | ASP | CB-CG-OD1 | 5.66 | 123.39 | 118.30 |
| 1 | E | 610 | ASP | CB-CG-OD1 | 5.66 | 123.39 | 118.30 |
| 1 | J | 772 | ASP | CB-CG-OD2 | -5.66 | 113.21 | 118.30 |
| 1 | O | 772 | ASP | CB-CG-OD2 | -5.66 | 113.21 | 118.30 |
| 1 | F | 388 | ARG | NE-CZ-NH1 | 5.65 | 123.13 | 120.30 |
| 1 | G | 553 | TRP | CA-CB-CG | -5.65 | 102.96 | 113.70 |
| 1 | J | 96 | ASP | N-CA-CB | 5.65 | 120.77 | 110.60 |
| 1 | E | 772 | ASP | CB-CG-OD2 | -5.65 | 113.21 | 118.30 |
| 1 | L | 96 | ASP | N-CA-CB | 5.65 | 120.77 | 110.60 |
| 1 | C | 15 | ASP | CB-CG-OD1 | 5.65 | 123.38 | 118.30 |
| 1 | H | 96 | ASP | N-CA-CB | 5.65 | 120.76 | 110.60 |
| 1 | I | 610 | ASP | CB-CG-OD1 | 5.65 | 123.38 | 118.30 |
| 1 | C | 96 | ASP | N-CA-CB | 5.64 | 120.76 | 110.60 |
| 1 | H | 772 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | M | 610 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | P | 166 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | D | 201 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | D | 610 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | P | 610 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | C | 201 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | D | 772 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | G | 96 | ASP | N-CA-CB | 5.64 | 120.75 | 110.60 |
| 1 | K | 610 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 1 | K | 800 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | O | 800 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | P | 201 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | D | 96 | ASP | N-CA-CB | 5.64 | 120.75 | 110.60 |
| 1 | L | 15 | ASP | CB-CG-OD1 | 5.64 | 123.37 | 118.30 |
| 1 | A | 96 | ASP | N-CA-CB | 5.64 | 120.75 | 110.60 |
| 1 | B | 96 | ASP | N-CA-CB | 5.64 | 120.75 | 110.60 |
| 1 | E | 201 | ASP | CB-CG-OD2 | -5.64 | 113.23 | 118.30 |
| 1 | H | 961 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | P | 980 | GLU | C-N-CA | -5.64 | 110.46 | 122.30 |
| 1 | B | 772 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | I | 800 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | L | 772 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | P | 96 | ASP | N-CA-CB | 5.63 | 120.74 | 110.60 |
| 1 | A | 610 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | C | 610 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | F | 610 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | G | 961 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | J | 610 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | K | 772 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | M | 96 | ASP | N-CA-CB | 5.63 | 120.74 | 110.60 |
| 1 | N | 961 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | G | 15 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | E | 96 | ASP | N-CA-CB | 5.63 | 120.73 | 110.60 |
| 1 | G | 772 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | K | 201 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | B | 610 | ASP | CB-CG-OD1 | 5.63 | 123.36 | 118.30 |
| 1 | E | 800 | ARG | NE-CZ-NH1 | 5.63 | 123.11 | 120.30 |
| 1 | H | 610 | ASP | CB-CG-OD1 | 5.63 | 123.36 | 118.30 |
| 1 | N | 96 | ASP | N-CA-CB | 5.63 | 120.73 | 110.60 |
| 1 | O | 980 | GLU | C-N-CA | -5.63 | 110.48 | 122.30 |
| 1 | E | 15 | ASP | CB-CG-OD1 | 5.62 | 123.36 | 118.30 |
| 1 | I | 96 | ASP | N-CA-CB | 5.62 | 120.73 | 110.60 |
| 1 | I | 980 | GLU | C-N-CA | -5.62 | 110.49 | 122.30 |
| 1 | H | 980 | GLU | C-N-CA | -5.62 | 110.50 | 122.30 |
| 1 | J | 980 | GLU | C-N-CA | -5.62 | 110.49 | 122.30 |
| 1 | O | 96 | ASP | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 1 | F | 201 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | K | 980 | GLU | C-N-CA | -5.62 | 110.50 | 122.30 |
| 1 | N | 980 | GLU | C-N-CA | -5.62 | 110.50 | 122.30 |
| 1 | E | 980 | GLU | C-N-CA | -5.62 | 110.51 | 122.30 |
| 1 | M | 980 | GLU | C-N-CA | -5.62 | 110.51 | 122.30 |
| 1 | A | 980 | GLU | C-N-CA | -5.61 | 110.51 | 122.30 |
| 1 | D | 800 | ARG | NE-CZ-NH1 | 5.61 | 123.11 | 120.30 |
| 1 | I | 201 | ASP | CB-CG-OD2 | -5.61 | 113.25 | 118.30 |
| 1 | P | 800 | ARG | NE-CZ-NH1 | 5.61 | 123.11 | 120.30 |
| 1 | L | 980 | GLU | C-N-CA | -5.61 | 110.52 | 122.30 |
| 1 | N | 425 | ARG | NE-CZ-NH2 | -5.61 | 117.50 | 120.30 |
| 1 | B | 980 | GLU | C-N-CA | -5.61 | 110.53 | 122.30 |
| 1 | C | 980 | GLU | C-N-CA | -5.61 | 110.53 | 122.30 |
| 1 | F | 980 | GLU | C-N-CA | -5.61 | 110.53 | 122.30 |
| 1 | G | 980 | GLU | C-N-CA | -5.61 | 110.53 | 122.30 |
| 1 | H | 15 | ASP | CB-CG-OD1 | 5.61 | 123.34 | 118.30 |
| 1 | A | 201 | ASP | CB-CG-OD2 | -5.60 | 113.26 | 118.30 |
| 1 | D | 980 | GLU | C-N-CA | -5.60 | 110.53 | 122.30 |
| 1 | J | 599 | ARG | NE-CZ-NH2 | 5.60 | 123.10 | 120.30 |
| 1 | L | 201 | ASP | CB-CG-OD2 | -5.60 | 113.26 | 118.30 |
| 1 | L | 800 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | O | 961 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | H | 201 | ASP | CB-CG-OD2 | -5.59 | 113.27 | 118.30 |
| 1 | N | 201 | ASP | CB-CG-OD2 | -5.59 | 113.27 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | I | 961 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | B | 800 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | C | 800 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | F | 961 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | J | 961 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | M | 15 | ASP | CB-CG-OD1 | 5.58 | 123.33 | 118.30 |
| 1 | A | 15 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | B | 201 | ASP | CB-CG-OD2 | -5.58 | 113.28 | 118.30 |
| 1 | H | 800 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | I | 938 | ARG | CG-CD-NE | -5.58 | 100.08 | 111.80 |
| 1 | O | 15 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | D | 15 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | F | 15 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | K | 15 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | A | 961 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | G | 201 | ASP | CB-CG-OD2 | -5.58 | 113.28 | 118.30 |
| 1 | J | 201 | ASP | CB-CG-OD2 | -5.57 | 113.28 | 118.30 |
| 1 | O | 938 | ARG | CG-CD-NE | -5.57 | 100.10 | 111.80 |
| 1 | H | 938 | ARG | CG-CD-NE | -5.57 | 100.10 | 111.80 |
| 1 | M | 201 | ASP | CB-CG-OD2 | -5.57 | 113.29 | 118.30 |
| 1 | B | 479 | ASP | CB-CG-OD2 | -5.57 | 113.29 | 118.30 |
| 1 | E | 954 | ASP | CB-CG-OD2 | -5.57 | 113.29 | 118.30 |
| 1 | I | 15 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | J | 938 | ARG | CG-CD-NE | -5.57 | 100.11 | 111.80 |
| 1 | D | 938 | ARG | CG-CD-NE | -5.57 | 100.11 | 111.80 |
| 1 | E | 938 | ARG | CG-CD-NE | -5.57 | 100.11 | 111.80 |
| 1 | N | 15 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 1 | G | 938 | ARG | CG-CD-NE | -5.56 | 100.12 | 111.80 |
| 1 | H | 594 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | K | 961 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |
| 1 | M | 938 | ARG | CG-CD-NE | -5.56 | 100.13 | 111.80 |
| 1 | A | 938 | ARG | CG-CD-NE | -5.56 | 100.13 | 111.80 |
| 1 | J | 15 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | E | 961 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | F | 938 | ARG | CG-CD-NE | -5.55 | 100.13 | 111.80 |
| 1 | L | 938 | ARG | CG-CD-NE | -5.55 | 100.13 | 111.80 |
| 1 | N | 938 | ARG | CG-CD-NE | -5.55 | 100.14 | 111.80 |
| 1 | B | 15 | ASP | CB-CG-OD1 | 5.55 | 123.30 | 118.30 |
| 1 | H | 699[A] | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | H | 699[B] | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | I | 479 | ASP | CB-CG-OD2 | -5.55 | 113.30 | 118.30 |
| 1 | F | 800 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | K | 938 | ARG | CG-CD-NE | -5.55 | 100.15 | 111.80 |
| 1 | K | 699[A] | ARG | NE-CZ-NH1 | 5.55 | 123.07 | 120.30 |
| 1 | K | 699[B] | ARG | NE-CZ-NH1 | 5.55 | 123.07 | 120.30 |
| 1 | P | 599 | ARG | NE-CZ-NH2 | 5.55 | 123.07 | 120.30 |
| 1 | P | 938 | ARG | CG-CD-NE | -5.55 | 100.15 | 111.80 |
| 1 | D | 425 | ARG | NE-CZ-NH2 | -5.54 | 117.53 | 120.30 |
| 1 | B | 599 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | C | 699[A] | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | C | 699[B] | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | C | 938 | ARG | CG-CD-NE | -5.54 | 100.16 | 111.80 |
| 1 | I | 599 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | J | 425 | ARG | NE-CZ-NH2 | -5.54 | 117.53 | 120.30 |
| 1 | M | 800 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | N | 800 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | O | 201 | ASP | CB-CG-OD2 | -5.54 | 113.31 | 118.30 |
| 1 | B | 938 | ARG | CG-CD-NE | -5.54 | 100.17 | 111.80 |
| 1 | K | 594 | ASP | CB-CG-OD1 | 5.54 | 123.28 | 118.30 |
| 1 | G | 599 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | H | 599 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | J | 800 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 1 | M | 961 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 1 | D | 271 | THR | CA-CB-CG2 | -5.53 | 104.66 | 112.40 |
| 1 | H | 954 | ASP | CB-CG-OD2 | -5.53 | 113.33 | 118.30 |
| 1 | I | 271 | THR | CA-CB-CG2 | -5.53 | 104.67 | 112.40 |
| 1 | P | 594 | ASP | CB-CG-OD1 | 5.53 | 123.27 | 118.30 |
| 1 | D | 954 | ASP | CB-CG-OD2 | -5.52 | 113.33 | 118.30 |
| 1 | J | 594 | ASP | CB-CG-OD1 | 5.52 | 123.27 | 118.30 |
| 1 | N | 594 | ASP | CB-CG-OD1 | 5.52 | 123.27 | 118.30 |
| 1 | O | 271 | THR | CA-CB-CG2 | -5.52 | 104.67 | 112.40 |
| 1 | P | 15 | ASP | CB-CG-OD1 | 5.52 | 123.27 | 118.30 |
| 1 | L | 425 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 1 | E | 479 | ASP | CB-CG-OD2 | -5.52 | 113.33 | 118.30 |
| 1 | B | 100 | TYR | N-CA-CB | 5.52 | 120.53 | 110.60 |
| 1 | C | 954 | ASP | CB-CG-OD2 | -5.52 | 113.33 | 118.30 |
| 1 | O | 100 | TYR | N-CA-CB | 5.52 | 120.53 | 110.60 |
| 1 | F | 71 | GLU | CB-CA-C | 5.52 | 121.43 | 110.40 |
| 1 | D | 71 | GLU | CB-CA-C | 5.51 | 121.43 | 110.40 |
| 1 | F | 271 | THR | CA-CB-CG2 | -5.51 | 104.68 | 112.40 |
| 1 | G | 100 | TYR | N-CA-CB | 5.51 | 120.52 | 110.60 |
| 1 | L | 961 | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 1 | A | 599 | ARG | NE-CZ-NH2 | 5.51 | 123.06 | 120.30 |
| 1 | B | 954 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | D | 699[A] | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 1 | D | 699[B] | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 1 | F | 594 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | H | 425 | ARG | NE-CZ-NH2 | -5.51 | 117.54 | 120.30 |
| 1 | H | 100 | TYR | N-CA-CB | 5.51 | 120.52 | 110.60 |
| 1 | J | 100 | TYR | N-CA-CB | 5.51 | 120.52 | 110.60 |
| 1 | A | 425 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 1 | C | 479 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | D | 100 | TYR | N-CA-CB | 5.51 | 120.52 | 110.60 |
| 1 | F | 479 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | I | 594 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | K | 954 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | C | 828 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | G | 71 | GLU | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 1 | G | 425 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 1 | A | 479 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | A | 699[A] | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 1 | A | 699[B] | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 1 | D | 828 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | K | 425 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 1 | O | 71 | GLU | CB-CA-C | 5.51 | 121.41 | 110.40 |
| 1 | I | 100 | TYR | N-CA-CB | 5.50 | 120.51 | 110.60 |
| 1 | L | 599 | ARG | NE-CZ-NH2 | 5.50 | 123.05 | 120.30 |
| 1 | A | 100 | TYR | N-CA-CB | 5.50 | 120.51 | 110.60 |
| 1 | E | 100 | TYR | N-CA-CB | 5.50 | 120.51 | 110.60 |
| 1 | G | 800 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | H | 271 | THR | CA-CB-CG2 | -5.50 | 104.70 | 112.40 |
| 1 | J | 71 | GLU | CB-CA-C | 5.50 | 121.40 | 110.40 |
| 1 | L | 71 | GLU | CB-CA-C | 5.50 | 121.40 | 110.40 |
| 1 | L | 100 | TYR | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | N | 100 | TYR | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | E | 699[A] | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | E | 699[B] | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | H | 479 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |
| 1 | A | 271 | THR | CA-CB-CG2 | -5.50 | 104.70 | 112.40 |
| 1 | B | 271 | THR | CA-CB-CG2 | -5.50 | 104.70 | 112.40 |
| 1 | C | 100 | TYR | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | E | 271 | THR | CA-CB-CG2 | -5.50 | 104.70 | 112.40 |
| 1 | H | 92 | MET | CG-SD-CE | -5.50 | 91.40 | 100.20 |
| 1 | M | 100 | TYR | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | M | 954 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |
| 1 | O | 954 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | A | 71 | GLU | CB-CA-C | 5.50 | 121.39 | 110.40 |
| 1 | F | 100 | TYR | N-CA-CB | 5.50 | 120.49 | 110.60 |
| 1 | P | 479 | ASP | CB-CG-OD2 | -5.50 | 113.35 | 118.30 |
| 1 | C | 71 | GLU | CB-CA-C | 5.50 | 121.39 | 110.40 |
| 1 | E | 71 | GLU | CB-CA-C | 5.50 | 121.39 | 110.40 |
| 1 | G | 594 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | L | 594 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | A | 954 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | D | 599 | ARG | NE-CZ-NH2 | 5.49 | 123.05 | 120.30 |
| 1 | G | 954 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | N | 954 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | B | 594 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | D | 479 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | G | 479 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | I | 699[A] | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 1 | I | 699[B] | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 1 | M | 271 | THR | CA-CB-CG2 | -5.49 | 104.71 | 112.40 |
| 1 | K | 71 | GLU | CB-CA-C | 5.49 | 121.38 | 110.40 |
| 1 | K | 479 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | P | 699[A] | ARG | NE-CZ-NH1 | 5.49 | 123.04 | 120.30 |
| 1 | P | 699[B] | ARG | NE-CZ-NH1 | 5.49 | 123.04 | 120.30 |
| 1 | K | 100 | TYR | N-CA-CB | 5.49 | 120.48 | 110.60 |
| 1 | L | 271 | THR | CA-CB-CG2 | -5.49 | 104.72 | 112.40 |
| 1 | C | 961 | ARG | NE-CZ-NH1 | 5.49 | 123.04 | 120.30 |
| 1 | D | 961 | ARG | NE-CZ-NH1 | 5.49 | 123.04 | 120.30 |
| 1 | H | 71 | GLU | CB-CA-C | 5.49 | 121.37 | 110.40 |
| 1 | J | 271 | THR | CA-CB-CG2 | -5.49 | 104.72 | 112.40 |
| 1 | L | 828 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | M | 71 | GLU | CB-CA-C | 5.49 | 121.37 | 110.40 |
| 1 | N | 271 | THR | CA-CB-CG2 | -5.49 | 104.72 | 112.40 |
| 1 | N | 479 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | P | 71 | GLU | CB-CA-C | 5.49 | 121.37 | 110.40 |
| 1 | A | 594 | ASP | CB-CG-OD1 | 5.48 | 123.24 | 118.30 |
| 1 | J | 954 | ASP | CB-CG-OD2 | -5.48 | 113.37 | 118.30 |
| 1 | K | 271 | THR | CA-CB-CG2 | -5.48 | 104.72 | 112.40 |
| 1 | N | 92 | MET | CG-SD-CE | -5.48 | 91.43 | 100.20 |
| 1 | O | 92 | MET | CG-SD-CE | -5.48 | 91.43 | 100.20 |
| 1 | G | 271 | THR | CA-CB-CG2 | -5.48 | 104.73 | 112.40 |
| 1 | G | 832 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | I | 71 | GLU | CB-CA-C | 5.48 | 121.36 | 110.40 |
| 1 | I | 92 | MET | CG-SD-CE | -5.48 | 91.43 | 100.20 |
| 1 | J | 479 | ASP | CB-CG-OD2 | -5.48 | 113.37 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | O | 594 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | P | 100 | TYR | N-CA-CB | 5.48 | 120.47 | 110.60 |
| 1 | F | 92 | MET | CG-SD-CE | -5.48 | 91.43 | 100.20 |
| 1 | K | 403 | ASP | CB-CG-OD2 | -5.48 | 113.37 | 118.30 |
| 1 | A | 92 | MET | CG-SD-CE | -5.48 | 91.44 | 100.20 |
| 1 | D | 92 | MET | CG-SD-CE | -5.48 | 91.44 | 100.20 |
| 1 | L | 954 | ASP | CB-CG-OD2 | -5.48 | 113.37 | 118.30 |
| 1 | N | 828 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 1 | F | 699[A] | ARG | NE-CZ-NH1 | 5.47 | 123.04 | 120.30 |
| 1 | F | 699[B] | ARG | NE-CZ-NH1 | 5.47 | 123.04 | 120.30 |
| 1 | F | 954 | ASP | CB-CG-OD2 | -5.47 | 113.37 | 118.30 |
| 1 | N | 71 | GLU | CB-CA-C | 5.47 | 121.34 | 110.40 |
| 1 | N | 599 | ARG | NE-CZ-NH2 | 5.47 | 123.04 | 120.30 |
| 1 | M | 92 | MET | CG-SD-CE | -5.47 | 91.45 | 100.20 |
| 1 | O | 403 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | B | 961 | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | L | 92 | MET | CG-SD-CE | -5.47 | 91.45 | 100.20 |
| 1 | M | 599 | ARG | NE-CZ-NH2 | 5.47 | 123.03 | 120.30 |
| 1 | M | 828 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | P | 92 | MET | CG-SD-CE | -5.47 | 91.45 | 100.20 |
| 1 | B | 71 | GLU | CB-CA-C | 5.47 | 121.33 | 110.40 |
| 1 | B | 92 | MET | CG-SD-CE | -5.47 | 91.45 | 100.20 |
| 1 | C | 403 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | J | 699[A] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | J | 699[B] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | O | 479 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | O | 828 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | C | 271 | THR | CA-CB-CG2 | -5.47 | 104.75 | 112.40 |
| 1 | F | 599 | ARG | NE-CZ-NH2 | 5.47 | 123.03 | 120.30 |
| 1 | G | 699[A] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | G | 699[B] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | G | 828 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | J | 92 | MET | CG-SD-CE | -5.47 | 91.45 | 100.20 |
| 1 | L | 479 | ASP | CB-CG-OD2 | -5.47 | 113.38 | 118.30 |
| 1 | L | 699[A] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | L | 699[B] | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | A | 828 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | F | 828 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | G | 92 | MET | CG-SD-CE | -5.46 | 91.46 | 100.20 |
| 1 | P | 271 | THR | CA-CB-CG2 | -5.46 | 104.75 | 112.40 |
| 1 | E | 92 | MET | CG-SD-CE | -5.46 | 91.46 | 100.20 |
| 1 | M | 479 | ASP | CB-CG-OD2 | -5.46 | 113.38 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | C | 92 | MET | CG-SD-CE | -5.46 | 91.46 | 100.20 |
| 1 | K | 92 | MET | CG-SD-CE | -5.46 | 91.46 | 100.20 |
| 1 | D | 594 | ASP | CB-CG-OD1 | 5.46 | 123.21 | 118.30 |
| 1 | H | 828 | ASP | CB-CG-OD1 | 5.46 | 123.21 | 118.30 |
| 1 | I | 954 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | B | 403 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | E | 599 | ARG | NE-CZ-NH2 | 5.46 | 123.03 | 120.30 |
| 1 | C | 425 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | M | 425 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | N | 699[A] | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | N | 699[B] | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | P | 954 | ASP | CB-CG-OD2 | -5.46 | 113.39 | 118.30 |
| 1 | A | 832 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 1 | D | 178 | ARG | NE-CZ-NH1 | -5.45 | 117.57 | 120.30 |
| 1 | I | 828 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 1 | P | 828 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 1 | M | 699[A] | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 1 | M | 699[B] | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 1 | N | 832 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 |
| 1 | K | 832 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 |
| 1 | E | 425 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | E | 594 | ASP | CB-CG-OD1 | 5.44 | 123.20 | 118.30 |
| 1 | O | 425 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | P | 178 | ARG | NE-CZ-NH1 | -5.44 | 117.58 | 120.30 |
| 1 | M | 594 | ASP | CB-CG-OD1 | 5.44 | 123.19 | 118.30 |
| 1 | N | 403 | ASP | CB-CG-OD2 | -5.44 | 113.41 | 118.30 |
| 1 | P | 425 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | A | 800 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 1 | M | 77 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | C | 599 | ARG | NE-CZ-NH2 | 5.43 | 123.02 | 120.30 |
| 1 | J | 828 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 1 | G | 403 | ASP | CB-CG-OD2 | -5.43 | 113.41 | 118.30 |
| 1 | P | 403 | ASP | CB-CG-OD2 | -5.43 | 113.42 | 118.30 |
| 1 | B | 425 | ARG | NE-CZ-NH2 | -5.43 | 117.59 | 120.30 |
| 1 | O | 599 | ARG | NE-CZ-NH2 | 5.42 | 123.01 | 120.30 |
| 1 | C | 594 | ASP | CB-CG-OD1 | 5.42 | 123.18 | 118.30 |
| 1 | H | 403 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | I | 425 | ARG | NE-CZ-NH2 | -5.42 | 117.59 | 120.30 |
| 1 | L | 403 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | A | 403 | ASP | CB-CG-OD2 | -5.42 | 113.42 | 118.30 |
| 1 | F | 832 | ASP | CB-CG-OD1 | 5.42 | 123.17 | 118.30 |
| 1 | E | 996 | ASP | CB-CG-OD2 | -5.42 | 113.43 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | P | 832 | ASP | CB-CG-OD1 | 5.42 | 123.17 | 118.30 |
| 1 | D | 403 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | E | 828 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | B | 996 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | J | 77 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | I | 832 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | P | 77 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | B | 77 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | B | 828 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | F | 77 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | I | 403 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | I | 77 | ASP | N-CA-CB | 5.40 | 120.33 | 110.60 |
| 1 | J | 832 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | M | 832 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | O | 832 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | D | 996 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | E | 210 | ARG | N-CA-CB | 5.40 | 120.32 | 110.60 |
| 1 | J | 403 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | L | 832 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | B | 403 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | J | 77 | ASP | N-CA-CB | 5.40 | 120.32 | 110.60 |
| 1 | O | 996 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | C | 77 | ASP | N-CA-CB | 5.40 | 120.31 | 110.60 |
| 1 | C | 832 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | D | 77 | ASP | N-CA-CB | 5.40 | 120.31 | 110.60 |
| 1 | D | 210 | ARG | N-CA-CB | 5.40 | 120.31 | 110.60 |
| 1 | O | 699[A] | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 1 | O | 699[B] | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 1 | J | 210 | ARG | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 1 | K | 828 | ASP | CB-CG-OD1 | 5.39 | 123.16 | 118.30 |
| 1 | P | 210 | ARG | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 1 | C | 77 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | F | 77 | ASP | N-CA-CB | 5.39 | 120.31 | 110.60 |
| 1 | M | 77 | ASP | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | A | 77 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | F | 425 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 1 | H | 77 | ASP | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | K | 599 | ARG | NE-CZ-NH2 | 5.39 | 122.99 | 120.30 |
| 1 | L | 77 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | N | 210 | ARG | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | O | 77 | ASP | N-CA-CB | 5.39 | 120.30 | 110.60 |
| 1 | A | 210 | ARG | N-CA-CB | 5.38 | 120.29 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | B | 210 | ARG | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | C | 210 | ARG | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | E | 77 | ASP | CB-CG-OD1 | 5.38 | 123.15 | 118.30 |
| 1 | G | 210 | ARG | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | L | 210 | ARG | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | M | 996 | ASP | CB-CG-OD2 | -5.38 | 113.45 | 118.30 |
| 1 | A | 77 | ASP | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | D | 77 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | G | 77 | ASP | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | M | 403 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | E | 77 | ASP | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | J | 178 | ARG | NE-CZ-NH1 | -5.38 | 117.61 | 120.30 |
| 1 | E | 403 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | F | 210 | ARG | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | G | 77 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | H | 210 | ARG | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | I | 210 | ARG | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | I | 996 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | K | 210 | ARG | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | N | 77 | ASP | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | O | 210 | ARG | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | E | 832 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | P | 77 | ASP | N-CA-CB | 5.38 | 120.28 | 110.60 |
| 1 | E | 178 | ARG | NE-CZ-NH1 | -5.37 | 117.61 | 120.30 |
| 1 | I | 77 | ASP | CB-CG-OD1 | 5.37 | 123.14 | 118.30 |
| 1 | K | 77 | ASP | N-CA-CB | 5.37 | 120.27 | 110.60 |
| 1 | M | 210 | ARG | N-CA-CB | 5.37 | 120.27 | 110.60 |
| 1 | O | 403 | ASP | CB-CG-OD1 | 5.37 | 123.14 | 118.30 |
| 1 | A | 996 | ASP | CB-CG-OD2 | -5.37 | 113.47 | 118.30 |
| 1 | N | 996 | ASP | CB-CG-OD2 | -5.37 | 113.47 | 118.30 |
| 1 | K | 996 | ASP | CB-CG-OD2 | -5.37 | 113.47 | 118.30 |
| 1 | B | 178 | ARG | NE-CZ-NH1 | -5.37 | 117.62 | 120.30 |
| 1 | B | 832 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | B | 699[A] | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | B | 699[B] | ARG | NE-CZ-NH1 | 5.37 | 122.98 | 120.30 |
| 1 | L | 178 | ARG | NE-CZ-NH1 | -5.37 | 117.62 | 120.30 |
| 1 | O | 908 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | E | 908 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | C | 996 | ASP | CB-CG-OD2 | -5.36 | 113.47 | 118.30 |
| 1 | F | 403 | ASP | CB-CG-OD2 | -5.36 | 113.47 | 118.30 |
| 1 | M | 1013 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 1 | B | 77 | ASP | N-CA-CB | 5.36 | 120.25 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 832 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | G | 178 | ARG | NE-CZ-NH1 | -5.36 | 117.62 | 120.30 |
| 1 | H | 996 | ASP | CB-CG-OD2 | -5.36 | 113.48 | 118.30 |
| 1 | O | 77 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | P | 996 | ASP | CB-CG-OD2 | -5.36 | 113.48 | 118.30 |
| 1 | K | 864 | MET | CG-SD-CE | -5.36 | 91.62 | 100.20 |
| 1 | G | 996 | ASP | CB-CG-OD2 | -5.36 | 113.48 | 118.30 |
| 1 | J | 826 | THR | CA-CB-CG2 | -5.36 | 104.90 | 112.40 |
| 1 | N | 77 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | P | 908 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | D | 1018 | LEU | CB-CG-CD1 | -5.36 | 101.90 | 111.00 |
| 1 | E | 1018 | LEU | CB-CG-CD1 | -5.36 | 101.89 | 111.00 |
| 1 | J | 908 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | H | 77 | ASP | CB-CG-OD1 | 5.35 | 123.12 | 118.30 |
| 1 | N | 864 | MET | CG-SD-CE | -5.35 | 91.63 | 100.20 |
| 1 | L | 77 | ASP | N-CA-CB | 5.35 | 120.23 | 110.60 |
| 1 | M | 864 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | F | 996 | ASP | CB-CG-OD2 | -5.35 | 113.48 | 118.30 |
| 1 | F | 1018 | LEU | CB-CG-CD1 | -5.35 | 101.90 | 111.00 |
| 1 | J | 864 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | C | 864 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | G | 826 | THR | CA-CB-CG2 | -5.35 | 104.91 | 112.40 |
| 1 | L | 864 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | H | 864 | MET | CG-SD-CE | -5.35 | 91.65 | 100.20 |
| 1 | K | 77 | ASP | CB-CG-OD1 | 5.35 | 123.11 | 118.30 |
| 1 | L | 996 | ASP | CB-CG-OD2 | -5.35 | 113.49 | 118.30 |
| 1 | A | 864 | MET | CG-SD-CE | -5.34 | 91.65 | 100.20 |
| 1 | D | 864 | MET | CG-SD-CE | -5.34 | 91.65 | 100.20 |
| 1 | G | 864 | MET | CG-SD-CE | -5.34 | 91.65 | 100.20 |
| 1 | I | 178 | ARG | NE-CZ-NH1 | -5.34 | 117.63 | 120.30 |
| 1 | N | 403 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | D | 826 | THR | CA-CB-CG2 | -5.34 | 104.92 | 112.40 |
| 1 | H | 1018 | LEU | CB-CG-CD1 | -5.34 | 101.92 | 111.00 |
| 1 | A | 729 | THR | CA-C-N | -5.34 | 105.45 | 117.20 |
| 1 | D | 908 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | G | 1018 | LEU | CB-CG-CD1 | -5.34 | 101.92 | 111.00 |
| 1 | N | 178 | ARG | NE-CZ-NH1 | -5.34 | 117.63 | 120.30 |
| 1 | O | 864 | MET | CG-SD-CE | -5.34 | 91.66 | 100.20 |
| 1 | P | 826 | THR | CA-CB-CG2 | -5.34 | 104.92 | 112.40 |
| 1 | P | 864 | MET | CG-SD-CE | -5.34 | 91.65 | 100.20 |
| 1 | D | 1013 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 1 | J | 996 | ASP | CB-CG-OD2 | -5.34 | 113.49 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | M | 826 | THR | CA-CB-CG2 | -5.34 | 104.93 | 112.40 |
| 1 | P | 1018 | LEU | CB-CG-CD1 | -5.34 | 101.92 | 111.00 |
| 1 | A | 908 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |
| 1 | A | 1018 | LEU | CB-CG-CD1 | -5.34 | 101.93 | 111.00 |
| 1 | G | 183 | ARG | CD-NE-CZ | -5.34 | 116.13 | 123.60 |
| 1 | H | 427 | THR | CA-CB-CG2 | -5.34 | 104.93 | 112.40 |
| 1 | C | 826 | THR | CA-CB-CG2 | -5.33 | 104.93 | 112.40 |
| 1 | D | 403 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | F | 183 | ARG | CD-NE-CZ | -5.33 | 116.13 | 123.60 |
| 1 | N | 826 | THR | CA-CB-CG2 | -5.33 | 104.93 | 112.40 |
| 1 | P | 729 | THR | CA-C-N | -5.33 | 105.47 | 117.20 |
| 1 | C | 403 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | E | 864 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 1 | B | 695 | TRP | CB-CA-C | -5.33 | 99.74 | 110.40 |
| 1 | F | 427 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | F | 864 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 1 | H | 826 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | H | 832 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | I | 427 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | I | 864 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 1 | K | 1018 | LEU | CB-CG-CD1 | -5.33 | 101.94 | 111.00 |
| 1 | O | 826 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 1 | O | 1018 | LEU | CB-CG-CD1 | -5.33 | 101.94 | 111.00 |
| 1 | B | 729 | THR | CA-C-N | -5.33 | 105.48 | 117.20 |
| 1 | D | 729 | THR | CA-C-N | -5.33 | 105.48 | 117.20 |
| 1 | F | 908 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | G | 403 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | H | 178 | ARG | NE-CZ-NH1 | -5.33 | 117.64 | 120.30 |
| 1 | K | 729 | THR | CA-C-N | -5.33 | 105.49 | 117.20 |
| 1 | N | 1013 | ARG | NE-CZ-NH1 | 5.33 | 122.96 | 120.30 |
| 1 | P | 183 | ARG | CD-NE-CZ | -5.33 | 116.14 | 123.60 |
| 1 | C | 729 | THR | CA-C-N | -5.32 | 105.49 | 117.20 |
| 1 | D | 183 | ARG | CD-NE-CZ | -5.32 | 116.15 | 123.60 |
| 1 | I | 1018 | LEU | CB-CG-CD1 | -5.32 | 101.95 | 111.00 |
| 1 | J | 1018 | LEU | CB-CG-CD1 | -5.32 | 101.95 | 111.00 |
| 1 | P | 403 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | B | 1018 | LEU | CB-CG-CD1 | -5.32 | 101.95 | 111.00 |
| 1 | B | 864 | MET | CG-SD-CE | -5.32 | 91.69 | 100.20 |
| 1 | C | 183 | ARG | CD-NE-CZ | -5.32 | 116.15 | 123.60 |
| 1 | H | 729 | THR | CA-C-N | -5.32 | 105.50 | 117.20 |
| 1 | N | 729 | THR | CA-C-N | -5.32 | 105.49 | 117.20 |
| 1 | B | 183 | ARG | CD-NE-CZ | -5.32 | 116.15 | 123.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | I | 908 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | K | 183 | ARG | CD-NE-CZ | -5.32 | 116.15 | 123.60 |
| 1 | M | 183 | ARG | CD-NE-CZ | -5.32 | 116.15 | 123.60 |
| 1 | M | 729 | THR | CA-C-N | -5.32 | 105.50 | 117.20 |
| 1 | A | 178 | ARG | NE-CZ-NH1 | -5.32 | 117.64 | 120.30 |
| 1 | J | 427 | THR | CA-CB-CG2 | -5.32 | 104.95 | 112.40 |
| 1 | K | 908 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | L | 403 | ASP | CB-CG-OD1 | 5.32 | 123.08 | 118.30 |
| 1 | L | 729 | THR | CA-C-N | -5.32 | 105.50 | 117.20 |
| 1 | L | 1018 | LEU | CB-CG-CD1 | -5.32 | 101.96 | 111.00 |
| 1 | N | 1018 | LEU | CB-CG-CD1 | -5.32 | 101.96 | 111.00 |
| 1 | O | 729 | THR | CA-C-N | -5.32 | 105.50 | 117.20 |
| 1 | C | 427 | THR | CA-CB-CG2 | -5.32 | 104.96 | 112.40 |
| 1 | O | 695 | TRP | CB-CA-C | -5.32 | 99.77 | 110.40 |
| 1 | A | 427 | THR | CA-CB-CG2 | -5.31 | 104.96 | 112.40 |
| 1 | C | 1018 | LEU | CB-CG-CD1 | -5.31 | 101.97 | 111.00 |
| 1 | G | 427 | THR | CA-CB-CG2 | -5.31 | 104.96 | 112.40 |
| 1 | I | 183 | ARG | CD-NE-CZ | -5.31 | 116.16 | 123.60 |
| 1 | J | 729 | THR | CA-C-N | -5.31 | 105.51 | 117.20 |
| 1 | K | 403 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | M | 1018 | LEU | CB-CG-CD1 | -5.31 | 101.97 | 111.00 |
| 1 | P | 427 | THR | CA-CB-CG2 | -5.31 | 104.96 | 112.40 |
| 1 | A | 826 | THR | CA-CB-CG2 | -5.31 | 104.96 | 112.40 |
| 1 | N | 427 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | A | 183 | ARG | CD-NE-CZ | -5.31 | 116.17 | 123.60 |
| 1 | B | 826 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | C | 104 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | G | 729 | THR | CA-C-N | -5.31 | 105.52 | 117.20 |
| 1 | H | 183 | ARG | CD-NE-CZ | -5.31 | 116.17 | 123.60 |
| 1 | I | 729 | THR | CA-C-N | -5.31 | 105.52 | 117.20 |
| 1 | I | 826 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | L | 826 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | A | 403 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | C | 908 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | E | 729 | THR | CA-C-N | -5.31 | 105.53 | 117.20 |
| 1 | P | 104 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | D | 695 | TRP | CB-CA-C | -5.31 | 99.79 | 110.40 |
| 1 | H | 104 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 |
| 1 | O | 178 | ARG | NE-CZ-NH1 | -5.31 | 117.65 | 120.30 |
| 1 | F | 729 | THR | CA-C-N | -5.30 | 105.53 | 117.20 |
| 1 | N | 908 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | E | 183 | ARG | CD-NE-CZ | -5.30 | 116.18 | 123.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | E | 826 | THR | CA-CB-CG2 | -5.30 | 104.98 | 112.40 |
| 1 | C | 695 | TRP | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 1 | M | 427 | THR | CA-CB-CG2 | -5.30 | 104.98 | 112.40 |
| 1 | A | 695 | TRP | CB-CA-C | -5.30 | 99.80 | 110.40 |
| 1 | G | 802 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | H | 908 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | L | 908 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | B | 427 | THR | CA-CB-CG2 | -5.30 | 104.98 | 112.40 |
| 1 | C | 729 | THR | N-CA-CB | 5.30 | 120.37 | 110.30 |
| 1 | J | 695 | TRP | CB-CA-C | -5.30 | 99.81 | 110.40 |
| 1 | F | 729 | THR | N-CA-CB | 5.30 | 120.36 | 110.30 |
| 1 | H | 695 | TRP | CB-CA-C | -5.30 | 99.81 | 110.40 |
| 1 | I | 729 | THR | N-CA-CB | 5.30 | 120.36 | 110.30 |
| 1 | N | 729 | THR | N-CA-CB | 5.30 | 120.36 | 110.30 |
| 1 | O | 183 | ARG | CD-NE-CZ | -5.30 | 116.18 | 123.60 |
| 1 | G | 695 | TRP | CB-CA-C | -5.29 | 99.81 | 110.40 |
| 1 | M | 403 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | I | 403 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | I | 695 | TRP | CB-CA-C | -5.29 | 99.81 | 110.40 |
| 1 | L | 427 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | M | 695 | TRP | CB-CA-C | -5.29 | 99.81 | 110.40 |
| 1 | N | 695 | TRP | CB-CA-C | -5.29 | 99.81 | 110.40 |
| 1 | O | 427 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | B | 104 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | F | 826 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | K | 802 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | K | 178 | ARG | NE-CZ-NH1 | -5.29 | 117.66 | 120.30 |
| 1 | K | 695 | TRP | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | K | 826 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | L | 695 | TRP | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | M | 908 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | O | 104 | THR | CA-CB-CG2 | -5.29 | 104.99 | 112.40 |
| 1 | B | 729 | THR | N-CA-CB | 5.29 | 120.35 | 110.30 |
| 1 | E | 427 | THR | CA-CB-CG2 | -5.29 | 105.00 | 112.40 |
| 1 | F | 104 | THR | CA-CB-CG2 | -5.29 | 105.00 | 112.40 |
| 1 | F | 695 | TRP | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | H | 403 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | M | 729 | THR | N-CA-CB | 5.29 | 120.34 | 110.30 |
| 1 | P | 695 | TRP | CB-CA-C | -5.29 | 99.83 | 110.40 |
| 1 | A | 104 | THR | CA-CB-CG2 | -5.29 | 105.00 | 112.40 |
| 1 | B | 84 | VAL | N-CA-CB | -5.29 | 99.87 | 111.50 |
| 1 | G | 84 | VAL | N-CA-CB | -5.29 | 99.87 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | K | 427 | THR | CA-CB-CG2 | -5.28 | 105.00 | 112.40 |
| 1 | L | 802 | ASP | CB-CG-OD1 | 5.28 | 123.06 | 118.30 |
| 1 | J | 183 | ARG | CD-NE-CZ | -5.28 | 116.20 | 123.60 |
| 1 | A | 1013 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | D | 427 | THR | CA-CB-CG2 | -5.28 | 105.01 | 112.40 |
| 1 | J | 729 | THR | N-CA-CB | 5.28 | 120.33 | 110.30 |
| 1 | O | 84 | VAL | N-CA-CB | -5.28 | 99.89 | 111.50 |
| 1 | B | 114 | VAL | N-CA-CB | -5.28 | 99.89 | 111.50 |
| 1 | E | 695 | TRP | CB-CA-C | -5.28 | 99.85 | 110.40 |
| 1 | F | 84 | VAL | N-CA-CB | -5.28 | 99.89 | 111.50 |
| 1 | F | 403 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | F | 802 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | G | 1013 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | J | 104 | THR | CA-CB-CG2 | -5.28 | 105.01 | 112.40 |
| 1 | L | 729 | THR | N-CA-CB | 5.28 | 120.33 | 110.30 |
| 1 | O | 729 | THR | N-CA-CB | 5.28 | 120.33 | 110.30 |
| 1 | P | 729 | THR | N-CA-CB | 5.28 | 120.33 | 110.30 |
| 1 | C | 84 | VAL | N-CA-CB | -5.28 | 99.89 | 111.50 |
| 1 | G | 729 | THR | N-CA-CB | 5.28 | 120.32 | 110.30 |
| 1 | I | 1013 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | H | 114 | VAL | N-CA-CB | -5.27 | 99.90 | 111.50 |
| 1 | H | 802 | ASP | CB-CG-OD1 | 5.27 | 123.05 | 118.30 |
| 1 | N | 183 | ARG | CD-NE-CZ | -5.27 | 116.22 | 123.60 |
| 1 | P | 114 | VAL | N-CA-CB | -5.27 | 99.90 | 111.50 |
| 1 | E | 114 | VAL | N-CA-CB | -5.27 | 99.90 | 111.50 |
| 1 | K | 84 | VAL | N-CA-CB | -5.27 | 99.90 | 111.50 |
| 1 | M | 104 | THR | CA-CB-CG2 | -5.27 | 105.02 | 112.40 |
| 1 | P | 84 | VAL | N-CA-CB | -5.27 | 99.90 | 111.50 |
| 1 | D | 729 | THR | N-CA-CB | 5.27 | 120.31 | 110.30 |
| 1 | H | 729 | THR | N-CA-CB | 5.27 | 120.31 | 110.30 |
| 1 | B | 908 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | K | 729 | THR | N-CA-CB | 5.27 | 120.31 | 110.30 |
| 1 | L | 183 | ARG | CD-NE-CZ | -5.27 | 116.22 | 123.60 |
| 1 | M | 178 | ARG | NE-CZ-NH1 | -5.27 | 117.67 | 120.30 |
| 1 | N | 104 | THR | CA-CB-CG2 | -5.27 | 105.02 | 112.40 |
| 1 | A | 84 | VAL | N-CA-CB | -5.27 | 99.91 | 111.50 |
| 1 | E | 84 | VAL | N-CA-CB | -5.27 | 99.91 | 111.50 |
| 1 | E | 104 | THR | CA-CB-CG2 | -5.27 | 105.03 | 112.40 |
| 1 | E | 729 | THR | N-CA-CB | 5.27 | 120.31 | 110.30 |
| 1 | I | 104 | THR | CA-CB-CG2 | -5.27 | 105.03 | 112.40 |
| 1 | K | 104 | THR | CA-CB-CG2 | -5.27 | 105.02 | 112.40 |
| 1 | L | 84 | VAL | N-CA-CB | -5.27 | 99.91 | 111.50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | N | 114 | VAL | N-CA-CB | -5.27 | 99.91 | 111.50 |
| 1 | O | 114 | VAL | N-CA-CB | -5.27 | 99.91 | 111.50 |
| 1 | E | 403 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 |
| 1 | J | 403 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 |
| 1 | D | 84 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | D | 114 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | J | 114 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | K | 114 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | B | 1013 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 1 | G | 104 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 1 | I | 84 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | L | 104 | THR | CA-CB-CG2 | -5.26 | 105.03 | 112.40 |
| 1 | M | 84 | VAL | N-CA-CB | -5.26 | 99.92 | 111.50 |
| 1 | P | 802 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 |
| 1 | A | 114 | VAL | N-CA-CB | -5.26 | 99.93 | 111.50 |
| 1 | B | 782 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | C | 802 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | D | 104 | THR | CA-CB-CG2 | -5.26 | 105.04 | 112.40 |
| 1 | H | 84 | VAL | N-CA-CB | -5.26 | 99.93 | 111.50 |
| 1 | I | 114 | VAL | N-CA-CB | -5.26 | 99.93 | 111.50 |
| 1 | N | 84 | VAL | N-CA-CB | -5.26 | 99.93 | 111.50 |
| 1 | E | 802 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | F | 114 | VAL | N-CA-CB | -5.26 | 99.94 | 111.50 |
| 1 | E | 1013 | ARG | NE-CZ-NH1 | 5.25 | 122.93 | 120.30 |
| 1 | J | 84 | VAL | N-CA-CB | -5.25 | 99.94 | 111.50 |
| 1 | O | 1013 | ARG | NE-CZ-NH1 | 5.25 | 122.93 | 120.30 |
| 1 | A | 729 | THR | N-CA-CB | 5.25 | 120.28 | 110.30 |
| 1 | A | 802 | ASP | CB-CG-OD1 | 5.25 | 123.03 | 118.30 |
| 1 | G | 114 | VAL | N-CA-CB | -5.25 | 99.95 | 111.50 |
| 1 | K | 1013 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | D | 802 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | C | 114 | VAL | N-CA-CB | -5.25 | 99.96 | 111.50 |
| 1 | G | 908 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | J | 802 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |
| 1 | F | 178 | ARG | NE-CZ-NH1 | -5.25 | 117.68 | 120.30 |
| 1 | J | 1013 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | L | 114 | VAL | N-CA-CB | -5.24 | 99.96 | 111.50 |
| 1 | M | 114 | VAL | N-CA-CB | -5.24 | 99.97 | 111.50 |
| 1 | L | 761 | GLN | CA-CB-CG | -5.24 | 101.87 | 113.40 |
| 1 | H | 761 | GLN | CA-CB-CG | -5.24 | 101.88 | 113.40 |
| 1 | N | 802 | ASP | CB-CG-OD1 | 5.24 | 123.02 | 118.30 |
| 1 | O | 802 | ASP | CB-CG-OD1 | 5.24 | 123.01 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 178 | ARG | NE-CZ-NH1 | -5.24 | 117.68 | 120.30 |
| 1 | P | 761 | GLN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | C | 761 | GLN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | O | 761 | GLN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | P | 1013 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | E | 761 | GLN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | J | 761 | GLN | CA-CB-CG | -5.23 | 101.89 | 113.40 |
| 1 | C | 1013 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | I | 761 | GLN | CA-CB-CG | -5.23 | 101.90 | 113.40 |
| 1 | P | 782 | ASP | CB-CG-OD1 | 5.23 | 123.00 | 118.30 |
| 1 | G | 761 | GLN | CA-CB-CG | -5.23 | 101.90 | 113.40 |
| 1 | A | 761 | GLN | CA-CB-CG | -5.22 | 101.91 | 113.40 |
| 1 | E | 782 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | K | 761 | GLN | CA-CB-CG | -5.22 | 101.91 | 113.40 |
| 1 | B | 761 | GLN | CA-CB-CG | -5.22 | 101.92 | 113.40 |
| 1 | D | 761 | GLN | CA-CB-CG | -5.22 | 101.92 | 113.40 |
| 1 | M | 802 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | E | 651 | LEU | CB-CA-C | -5.22 | 100.29 | 110.20 |
| 1 | F | 761 | GLN | CA-CB-CG | -5.21 | 101.93 | 113.40 |
| 1 | M | 761 | GLN | CA-CB-CG | -5.21 | 101.93 | 113.40 |
| 1 | O | 651 | LEU | CB-CA-C | -5.21 | 100.30 | 110.20 |
| 1 | I | 802 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | N | 761 | GLN | CA-CB-CG | -5.21 | 101.93 | 113.40 |
| 1 | C | 651 | LEU | CB-CA-C | -5.21 | 100.31 | 110.20 |
| 1 | L | 1013 | ARG | NE-CZ-NH1 | 5.21 | 122.90 | 120.30 |
| 1 | L | 745 | MET | CB-CA-C | -5.21 | 99.99 | 110.40 |
| 1 | F | 651 | LEU | CB-CA-C | -5.20 | 100.31 | 110.20 |
| 1 | P | 651 | LEU | CB-CA-C | -5.20 | 100.31 | 110.20 |
| 1 | D | 651 | LEU | CB-CA-C | -5.20 | 100.32 | 110.20 |
| 1 | H | 1013 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 1 | O | 782 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | B | 802 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | F | 745 | MET | CB-CA-C | -5.20 | 100.00 | 110.40 |
| 1 | K | 745 | MET | CB-CA-C | -5.20 | 100.00 | 110.40 |
| 1 | K | 651 | LEU | CB-CA-C | -5.20 | 100.33 | 110.20 |
| 1 | C | 782 | ASP | CB-CG-OD1 | 5.20 | 122.97 | 118.30 |
| 1 | N | 651 | LEU | CB-CA-C | -5.20 | 100.33 | 110.20 |
| 1 | I | 782 | ASP | CB-CG-OD1 | 5.19 | 122.97 | 118.30 |
| 1 | J | 651 | LEU | CB-CA-C | -5.19 | 100.33 | 110.20 |
| 1 | A | 651 | LEU | CB-CA-C | -5.19 | 100.33 | 110.20 |
| 1 | H | 651 | LEU | CB-CA-C | -5.19 | 100.33 | 110.20 |
| 1 | B | 651 | LEU | CB-CA-C | -5.19 | 100.34 | 110.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | G | 651 | LEU | CB-CA-C | -5.19 | 100.34 | 110.20 |
| 1 | I | 651 | LEU | CB-CA-C | -5.19 | 100.34 | 110.20 |
| 1 | J | 745 | MET | CB-CA-C | -5.19 | 100.02 | 110.40 |
| 1 | H | 745 | MET | CB-CA-C | -5.19 | 100.03 | 110.40 |
| 1 | M | 745 | MET | CB-CA-C | -5.19 | 100.03 | 110.40 |
| 1 | A | 782 | ASP | CB-CG-OD1 | 5.19 | 122.97 | 118.30 |
| 1 | P | 745 | MET | CB-CA-C | -5.18 | 100.03 | 110.40 |
| 1 | J | 782 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | L | 651 | LEU | CB-CA-C | -5.18 | 100.35 | 110.20 |
| 1 | B | 745 | MET | CB-CA-C | -5.18 | 100.04 | 110.40 |
| 1 | G | 745 | MET | CB-CA-C | -5.18 | 100.04 | 110.40 |
| 1 | K | 782 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | M | 782 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | C | 745 | MET | CB-CA-C | -5.18 | 100.04 | 110.40 |
| 1 | E | 745 | MET | CB-CA-C | -5.18 | 100.04 | 110.40 |
| 1 | F | 782 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | F | 1013 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | A | 745 | MET | CB-CA-C | -5.18 | 100.05 | 110.40 |
| 1 | D | 745 | MET | CB-CA-C | -5.18 | 100.05 | 110.40 |
| 1 | M | 651 | LEU | CB-CA-C | -5.18 | 100.36 | 110.20 |
| 1 | N | 745 | MET | CB-CA-C | -5.18 | 100.05 | 110.40 |
| 1 | O | 745 | MET | CB-CA-C | -5.17 | 100.05 | 110.40 |
| 1 | D | 782 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 1 | K | 310 | ARG | N-CA-CB | 5.17 | 119.90 | 110.60 |
| 1 | L | 782 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 |
| 1 | I | 745 | MET | CB-CA-C | -5.16 | 100.08 | 110.40 |
| 1 | J | 147 | ASN | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | M | 147 | ASN | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | L | 147 | ASN | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | O | 310 | ARG | N-CA-CB | 5.16 | 119.88 | 110.60 |
| 1 | D | 310 | ARG | N-CA-CB | 5.15 | 119.88 | 110.60 |
| 1 | G | 147 | ASN | N-CA-CB | -5.15 | 101.32 | 110.60 |
| 1 | H | 782 | ASP | CB-CG-OD1 | 5.15 | 122.94 | 118.30 |
| 1 | A | 147 | ASN | N-CA-CB | -5.15 | 101.33 | 110.60 |
| 1 | B | 310 | ARG | N-CA-CB | 5.15 | 119.87 | 110.60 |
| 1 | I | 147 | ASN | N-CA-CB | -5.15 | 101.33 | 110.60 |
| 1 | G | 782 | ASP | CB-CG-OD1 | 5.14 | 122.93 | 118.30 |
| 1 | E | 508 | GLU | CA-CB-CG | 5.14 | 124.71 | 113.40 |
| 1 | H | 508 | GLU | CA-CB-CG | 5.14 | 124.71 | 113.40 |
| 1 | B | 147 | ASN | N-CA-CB | -5.14 | 101.35 | 110.60 |
| 1 | K | 508 | GLU | CA-CB-CG | 5.14 | 124.71 | 113.40 |
| 1 | C | 310 | ARG | N-CA-CB | 5.14 | 119.85 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 147 | ASN | N-CA-CB | -5.14 | 101.35 | 110.60 |
| 1 | C | 508 | GLU | CA-CB-CG | 5.13 | 124.69 | 113.40 |
| 1 | F | 147 | ASN | N-CA-CB | -5.13 | 101.36 | 110.60 |
| 1 | N | 310 | ARG | N-CA-CB | 5.13 | 119.84 | 110.60 |
| 1 | N | 508 | GLU | CA-CB-CG | 5.13 | 124.70 | 113.40 |
| 1 | A | 310 | ARG | N-CA-CB | 5.13 | 119.84 | 110.60 |
| 1 | O | 147 | ASN | N-CA-CB | -5.13 | 101.36 | 110.60 |
| 1 | I | 524 | LEU | CB-CA-C | -5.13 | 100.45 | 110.20 |
| 1 | I | 508 | GLU | CA-CB-CG | 5.13 | 124.69 | 113.40 |
| 1 | A | 508 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 |
| 1 | B | 598 | ASP | CB-CG-OD2 | -5.13 | 113.69 | 118.30 |
| 1 | D | 147 | ASN | N-CA-CB | -5.13 | 101.37 | 110.60 |
| 1 | K | 147 | ASN | N-CA-CB | -5.13 | 101.37 | 110.60 |
| 1 | L | 508 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 |
| 1 | L | 848 | THR | CA-CB-CG2 | -5.13 | 105.22 | 112.40 |
| 1 | B | 508 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 |
| 1 | F | 508 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 |
| 1 | H | 147 | ASN | N-CA-CB | -5.13 | 101.37 | 110.60 |
| 1 | N | 782 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | E | 147 | ASN | N-CA-CB | -5.12 | 101.38 | 110.60 |
| 1 | E | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | G | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | H | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | O | 848 | THR | CA-CB-CG2 | -5.12 | 105.23 | 112.40 |
| 1 | P | 147 | ASN | N-CA-CB | -5.12 | 101.38 | 110.60 |
| 1 | F | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | F | 598 | ASP | CB-CG-OD2 | -5.12 | 113.69 | 118.30 |
| 1 | I | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | E | 848 | THR | CA-CB-CG2 | -5.12 | 105.23 | 112.40 |
| 1 | M | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | M | 508 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | P | 310 | ARG | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | H | 524 | LEU | CB-CA-C | -5.12 | 100.47 | 110.20 |
| 1 | L | 310 | ARG | N-CA-CB | 5.12 | 119.81 | 110.60 |
| 1 | P | 508 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | B | 524 | LEU | CB-CA-C | -5.12 | 100.48 | 110.20 |
| 1 | H | 598 | ASP | CB-CG-OD2 | -5.12 | 113.70 | 118.30 |
| 1 | J | 508 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | J | 710 | GLU | CB-CA-C | -5.12 | 100.17 | 110.40 |
| 1 | O | 508 | GLU | CB-CA-C | -5.12 | 100.17 | 110.40 |
| 1 | O | 508 | GLU | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | O | 524 | LEU | CB-CA-C | -5.12 | 100.48 | 110.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 508 | GLU | CB-CA-C | -5.11 | 100.17 | 110.40 |
| 1 | F | 524 | LEU | CB-CA-C | -5.11 | 100.49 | 110.20 |
| 1 | J | 524 | LEU | CB-CA-C | -5.11 | 100.48 | 110.20 |
| 1 | K | 598 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | N | 147 | ASN | N-CA-CB | -5.11 | 101.40 | 110.60 |
| 1 | O | 710 | GLU | CB-CA-C | -5.11 | 100.17 | 110.40 |
| 1 | P | 524 | LEU | CB-CA-C | -5.11 | 100.48 | 110.20 |
| 1 | I | 710 | GLU | CB-CA-C | -5.11 | 100.17 | 110.40 |
| 1 | M | 524 | LEU | CB-CA-C | -5.11 | 100.49 | 110.20 |
| 1 | A | 524 | LEU | CB-CA-C | -5.11 | 100.49 | 110.20 |
| 1 | D | 710 | GLU | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 1 | E | 710 | GLU | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 1 | J | 310 | ARG | N-CA-CB | 5.11 | 119.80 | 110.60 |
| 1 | K | 226 | HIS | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 1 | L | 524 | LEU | CB-CA-C | -5.11 | 100.49 | 110.20 |
| 1 | O | 226 | HIS | CB-CA-C | -5.11 | 100.18 | 110.40 |
| 1 | L | 598 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | C | 710 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | D | 508 | GLU | CA-CB-CG | 5.11 | 124.64 | 113.40 |
| 1 | D | 524 | LEU | CB-CA-C | -5.11 | 100.50 | 110.20 |
| 1 | I | 508 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | A | 710 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | B | 710 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | D | 598 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | N | 710 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | P | 710 | GLU | CB-CA-C | -5.11 | 100.19 | 110.40 |
| 1 | C | 524 | LEU | CB-CA-C | -5.10 | 100.50 | 110.20 |
| 1 | D | 226 | HIS | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | G | 710 | GLU | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | N | 226 | HIS | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | B | 848 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |
| 1 | G | 508 | GLU | CA-CB-CG | 5.10 | 124.63 | 113.40 |
| 1 | K | 848 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |
| 1 | M | 710 | GLU | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | M | 848 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |
| 1 | N | 598 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 1 | P | 508 | GLU | CB-CA-C | -5.10 | 100.19 | 110.40 |
| 1 | A | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | F | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | F | 710 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | G | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | K | 524 | LEU | CB-CA-C | -5.10 | 100.51 | 110.20 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 226 | HIS | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | G | 524 | LEU | CB-CA-C | -5.10 | 100.51 | 110.20 |
| 1 | H | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | H | 1014 | TYR | CB-CG-CD2 | -5.10 | 117.94 | 121.00 |
| 1 | I | 598 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 1 | H | 226 | HIS | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | J | 336 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | J | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | L | 710 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | M | 508 | GLU | CB-CA-C | -5.10 | 100.20 | 110.40 |
| 1 | P | 848 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |
| 1 | A | 598 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |
| 1 | E | 524 | LEU | CB-CA-C | -5.09 | 100.52 | 110.20 |
| 1 | I | 226 | HIS | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | L | 508 | GLU | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | N | 508 | GLU | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | L | 226 | HIS | CB-CA-C | -5.09 | 100.21 | 110.40 |
| 1 | A | 226 | HIS | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | C | 848 | THR | CA-CB-CG2 | -5.09 | 105.27 | 112.40 |
| 1 | D | 848 | THR | CA-CB-CG2 | -5.09 | 105.27 | 112.40 |
| 1 | J | 598 | ASP | CB-CG-OD2 | -5.09 | 113.72 | 118.30 |
| 1 | J | 848 | THR | CA-CB-CG2 | -5.09 | 105.27 | 112.40 |
| 1 | N | 524 | LEU | CB-CA-C | -5.09 | 100.53 | 110.20 |
| 1 | B | 226 | HIS | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | I | 750 | GLU | N-CA-CB | -5.09 | 101.44 | 110.60 |
| 1 | M | 226 | HIS | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | A | 848 | THR | CA-CB-CG2 | -5.09 | 105.28 | 112.40 |
| 1 | G | 226 | HIS | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | E | 508 | GLU | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | F | 848 | THR | CA-CB-CG2 | -5.09 | 105.28 | 112.40 |
| 1 | I | 848 | THR | CA-CB-CG2 | -5.09 | 105.28 | 112.40 |
| 1 | H | 710 | GLU | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | K | 508 | GLU | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | H | 848 | THR | CA-CB-CG2 | -5.08 | 105.28 | 112.40 |
| 1 | K | 710 | GLU | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | B | 508 | GLU | CB-CA-C | -5.08 | 100.23 | 110.40 |
| 1 | C | 508 | GLU | CB-CA-C | -5.08 | 100.24 | 110.40 |
| 1 | E | 612 | THR | N-CA-CB | 5.08 | 119.95 | 110.30 |
| 1 | G | 598 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | J | 750 | GLU | N-CA-CB | -5.08 | 101.45 | 110.60 |
| 1 | N | 612 | THR | N-CA-CB | 5.08 | 119.95 | 110.30 |
| 1 | N | 750 | GLU | N-CA-CB | -5.08 | 101.45 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 612 | THR | N-CA-CB | 5.08 | 119.95 | 110.30 |
| 1 | N | 848 | THR | CA-CB-CG2 | -5.08 | 105.29 | 112.40 |
| 1 | B | 750 | GLU | N-CA-CB | -5.08 | 101.46 | 110.60 |
| 1 | C | 598 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | F | 226 | HIS | CB-CA-C | -5.08 | 100.24 | 110.40 |
| 1 | H | 750 | GLU | N-CA-CB | -5.08 | 101.46 | 110.60 |
| 1 | M | 750 | GLU | N-CA-CB | -5.08 | 101.46 | 110.60 |
| 1 | B | 612 | THR | N-CA-CB | 5.08 | 119.95 | 110.30 |
| 1 | E | 226 | HIS | CB-CA-C | -5.08 | 100.25 | 110.40 |
| 1 | P | 750 | GLU | N-CA-CB | -5.08 | 101.46 | 110.60 |
| 1 | M | 598 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | E | 598 | ASP | CB-CG-OD2 | -5.07 | 113.73 | 118.30 |
| 1 | G | 750 | GLU | N-CA-CB | -5.07 | 101.47 | 110.60 |
| 1 | I | 363 | HIS | CA-CB-CG | -5.07 | 104.97 | 113.60 |
| 1 | M | 336 | ARG | NE-CZ-NH1 | 5.07 | 122.84 | 120.30 |
| 1 | P | 226 | HIS | CB-CA-C | -5.07 | 100.26 | 110.40 |
| 1 | E | 750 | GLU | N-CA-CB | -5.07 | 101.47 | 110.60 |
| 1 | O | 612 | THR | N-CA-CB | 5.07 | 119.93 | 110.30 |
| 1 | I | 612 | THR | N-CA-CB | 5.07 | 119.93 | 110.30 |
| 1 | J | 226 | HIS | CB-CA-C | -5.07 | 100.27 | 110.40 |
| 1 | K | 750 | GLU | N-CA-CB | -5.07 | 101.48 | 110.60 |
| 1 | P | 598 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 1 | F | 750 | GLU | N-CA-CB | -5.07 | 101.48 | 110.60 |
| 1 | G | 363 | HIS | CA-CB-CG | -5.07 | 104.99 | 113.60 |
| 1 | L | 750 | GLU | N-CA-CB | -5.07 | 101.48 | 110.60 |
| 1 | K | 59 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | A | 612 | THR | N-CA-CB | 5.06 | 119.92 | 110.30 |
| 1 | A | 750 | GLU | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 1 | C | 750 | GLU | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 1 | F | 363 | HIS | CA-CB-CG | -5.06 | 104.99 | 113.60 |
| 1 | H | 612 | THR | N-CA-CB | 5.06 | 119.92 | 110.30 |
| 1 | L | 336 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | L | 612 | THR | N-CA-CB | 5.06 | 119.92 | 110.30 |
| 1 | N | 336 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | O | 750 | GLU | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 1 | C | 363 | HIS | CA-CB-CG | -5.06 | 105.00 | 113.60 |
| 1 | D | 612 | THR | N-CA-CB | 5.06 | 119.91 | 110.30 |
| 1 | G | 848 | THR | CA-CB-CG2 | -5.06 | 105.32 | 112.40 |
| 1 | M | 612 | THR | N-CA-CB | 5.06 | 119.91 | 110.30 |
| 1 | G | 336 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 1 | F | 612 | THR | N-CA-CB | 5.05 | 119.90 | 110.30 |
| 1 | A | 363 | HIS | CA-CB-CG | -5.05 | 105.01 | 113.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 363 | HIS | CA-CB-CG | -5.05 | 105.01 | 113.60 |
| 1 | G | 612 | THR | N-CA-CB | 5.05 | 119.90 | 110.30 |
| 1 | K | 612 | THR | N-CA-CB | 5.05 | 119.90 | 110.30 |
| 1 | C | 612 | THR | N-CA-CB | 5.05 | 119.89 | 110.30 |
| 1 | N | 1014 | TYR | CB-CG-CD2 | -5.05 | 117.97 | 121.00 |
| 1 | E | 336 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | G | 172 | ASP | CB-CG-OD2 | -5.05 | 113.76 | 118.30 |
| 1 | H | 363 | HIS | CA-CB-CG | -5.05 | 105.02 | 113.60 |
| 1 | P | 363 | HIS | CA-CB-CG | -5.05 | 105.02 | 113.60 |
| 1 | M | 59 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | N | 363 | HIS | CA-CB-CG | -5.04 | 105.02 | 113.60 |
| 1 | O | 172 | ASP | CB-CG-OD2 | -5.04 | 113.76 | 118.30 |
| 1 | D | 750 | GLU | N-CA-CB | -5.04 | 101.52 | 110.60 |
| 1 | I | 1014 | TYR | CB-CG-CD2 | -5.04 | 117.97 | 121.00 |
| 1 | J | 363 | HIS | CA-CB-CG | -5.04 | 105.03 | 113.60 |
| 1 | J | 612 | THR | N-CA-CB | 5.04 | 119.88 | 110.30 |
| 1 | K | 336 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | K | 363 | HIS | CA-CB-CG | -5.04 | 105.03 | 113.60 |
| 1 | P | 1014 | TYR | CB-CG-CD2 | -5.04 | 117.97 | 121.00 |
| 1 | H | 336 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | L | 363 | HIS | CA-CB-CG | -5.04 | 105.03 | 113.60 |
| 1 | O | 598 | ASP | CB-CG-OD2 | -5.04 | 113.76 | 118.30 |
| 1 | E | 172 | ASP | CB-CG-OD2 | -5.04 | 113.77 | 118.30 |
| 1 | O | 363 | HIS | CA-CB-CG | -5.04 | 105.03 | 113.60 |
| 1 | M | 363 | HIS | CA-CB-CG | -5.04 | 105.04 | 113.60 |
| 1 | C | 336 | ARG | NE-CZ-NH1 | 5.03 | 122.82 | 120.30 |
| 1 | K | 172 | ASP | CB-CG-OD2 | -5.03 | 113.77 | 118.30 |
| 1 | B | 120 | THR | CA-CB-CG2 | -5.03 | 105.36 | 112.40 |
| 1 | B | 172 | ASP | CB-CG-OD2 | -5.03 | 113.78 | 118.30 |
| 1 | O | 336 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 1 | H | 859 | ASP | CB-CG-OD2 | -5.03 | 113.78 | 118.30 |
| 1 | E | 363 | HIS | CA-CB-CG | -5.02 | 105.06 | 113.60 |
| 1 | D | 172 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | G | 1014 | TYR | CB-CG-CD2 | -5.02 | 117.99 | 121.00 |
| 1 | A | 1014 | TYR | CB-CG-CD2 | -5.02 | 117.99 | 121.00 |
| 1 | M | 343 | LEU | CB-CA-C | -5.02 | 100.66 | 110.20 |
| 1 | A | 336 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | D | 363 | HIS | CA-CB-CG | -5.02 | 105.07 | 113.60 |
| 1 | J | 1014 | TYR | CB-CG-CD2 | -5.02 | 117.99 | 121.00 |
| 1 | A | 172 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | O | 343 | LEU | CB-CA-C | -5.02 | 100.67 | 110.20 |
| 1 | B | 336 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | D | 336 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 1 | I | 172 | ASP | CB-CG-OD2 | -5.01 | 113.79 | 118.30 |
| 1 | E | 59 | ARG | NE-CZ-NH2 | -5.01 | 117.79 | 120.30 |
| 1 | G | 343 | LEU | CB-CA-C | -5.01 | 100.68 | 110.20 |
| 1 | D | 859 | ASP | CB-CG-OD2 | -5.01 | 113.79 | 118.30 |
| 1 | J | 120 | THR | CA-CB-CG2 | -5.01 | 105.39 | 112.40 |
| 1 | B | 59 | ARG | NE-CZ-NH2 | -5.01 | 117.80 | 120.30 |
| 1 | C | 859 | ASP | CB-CG-OD2 | -5.01 | 113.80 | 118.30 |
| 1 | E | 1014 | TYR | CB-CG-CD2 | -5.00 | 118.00 | 121.00 |
| 1 | I | 343 | LEU | CB-CA-C | -5.00 | 100.69 | 110.20 |
| 1 | K | 120 | THR | CA-CB-CG2 | -5.00 | 105.39 | 112.40 |
| 1 | H | 343 | LEU | CB-CA-C | -5.00 | 100.69 | 110.20 |
| 1 | L | 1014 | TYR | CB-CG-CD2 | -5.00 | 118.00 | 121.00 |
| 1 | C | 343 | LEU | CB-CA-C | -5.00 | 100.70 | 110.20 |
| 1 | F | 120 | THR | CA-CB-CG2 | -5.00 | 105.40 | 112.40 |
| 1 | L | 172 | ASP | CB-CG-OD2 | -5.00 | 113.80 | 118.30 |
| 1 | M | 172 | ASP | CB-CG-OD2 | -5.00 | 113.80 | 118.30 |
| 1 | P | 343 | LEU | CB-CA-C | -5.00 | 100.70 | 110.20 |

All (32) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 166 | ARG | CA |
| 1 | A | 249 | GLU | CA |
| 1 | B | 166 | ARG | CA |
| 1 | B | 249 | GLU | CA |
| 1 | C | 166 | ARG | CA |
| 1 | C | 249 | GLU | CA |
| 1 | D | 166 | ARG | CA |
| 1 | D | 249 | GLU | CA |
| 1 | E | 166 | ARG | CA |
| 1 | E | 249 | GLU | CA |
| 1 | F | 166 | ARG | CA |
| 1 | F | 249 | GLU | CA |
| 1 | G | 166 | ARG | CA |
| 1 | G | 249 | GLU | CA |
| 1 | H | 166 | ARG | CA |
| 1 | H | 249 | GLU | CA |
| 1 | I | 166 | ARG | CA |
| 1 | I | 249 | GLU | CA |
| 1 | J | 166 | ARG | CA |
| 1 | J | 249 | GLU | CA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | K | 166 | ARG | CA |
| 1 | K | 249 | GLU | CA |
| 1 | L | 166 | ARG | CA |
| 1 | L | 249 | GLU | CA |
| 1 | M | 166 | ARG | CA |
| 1 | M | 249 | GLU | CA |
| 1 | N | 166 | ARG | CA |
| 1 | N | 249 | GLU | CA |
| 1 | O | 166 | ARG | CA |
| 1 | O | 249 | GLU | CA |
| 1 | P | 166 | ARG | CA |
| 1 | P | 249 | GLU | CA |

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 8232 | 0 | 7817 | 270 | 3 |
| 1 | B | 8232 | 0 | 7817 | 267 | 4 |
| 1 | C | 8232 | 0 | 7817 | 262 | 1 |
| 1 | D | 8232 | 0 | 7817 | 275 | 0 |
| 1 | E | 8232 | 0 | 7817 | 266 | 0 |
| 1 | F | 8232 | 0 | 7817 | 269 | 0 |
| 1 | G | 8232 | 0 | 7817 | 267 | 0 |
| 1 | H | 8232 | 0 | 7817 | 261 | 0 |
| 1 | I | 8232 | 0 | 7817 | 269 | 1 |
| 1 | J | 8232 | 0 | 7817 | 274 | 0 |
| 1 | K | 8232 | 0 | 7817 | 277 | 0 |
| 1 | L | 8232 | 0 | 7817 | 264 | 0 |
| 1 | M | 8232 | 0 | 7817 | 271 | 0 |
| 1 | N | 8232 | 0 | 7817 | 269 | 0 |
| 1 | O | 8232 | 0 | 7817 | 271 | 0 |
| 1 | P | 8232 | 0 | 7817 | 269 | 1 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 2 | E | 2 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | G | 2 | 0 | 0 | 0 | 0 |
| 2 | H | 2 | 0 | 0 | 0 | 0 |
| 2 | I | 2 | 0 | 0 | 0 | 0 |
| 2 | J | 2 | 0 | 0 | 0 | 0 |
| 2 | K | 2 | 0 | 0 | 0 | 0 |
| 2 | L | 2 | 0 | 0 | 0 | 0 |
| 2 | M | 2 | 0 | 0 | 0 | 0 |
| 2 | N | 2 | 0 | 0 | 0 | 0 |
| 2 | O | 2 | 0 | 0 | 0 | 0 |
| 2 | P | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 434 | 0 | 0 | 13 | 0 |
| 3 | B | 436 | 0 | 0 | 13 | 0 |
| 3 | C | 433 | 0 | 0 | 13 | 0 |
| 3 | D | 437 | 0 | 0 | 13 | 0 |
| 3 | E | 435 | 0 | 0 | 13 | 0 |
| 3 | F | 436 | 0 | 0 | 13 | 0 |
| 3 | G | 434 | 0 | 0 | 13 | 0 |
| 3 | H | 435 | 0 | 0 | 13 | 0 |
| 3 | I | 434 | 0 | 0 | 13 | 0 |
| 3 | J | 436 | 0 | 0 | 13 | 0 |
| 3 | K | 435 | 0 | 0 | 13 | 0 |
| 3 | L | 435 | 0 | 0 | 13 | 0 |
| 3 | M | 434 | 0 | 0 | 13 | 0 |
| 3 | N | 436 | 0 | 0 | 13 | 0 |
| 3 | O | 433 | 0 | 0 | 13 | 0 |
| 3 | P | 437 | 0 | 0 | 13 | 0 |
| All | All | 138704 | 0 | 125072 | 4201 | 5 |

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 16.

All (4201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:L:427:THR:HA | 1:L:436:MET:HE1 | 1.43 | 1.01 |
| 1:E:427:THR:HA | 1:E:436:MET:HE1 | 1.41 | 1.00 |
| 1:M:427:THR:HA | 1:M:436:MET:HE1 | 1.43 | 1.00 |
| 1:J:427:THR:HA | 1:J:436:MET:HE1 | 1.44 | 0.99 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:427:THR:HA | 1:C:436:MET:HE1 | 1.45 | 0.98 |
| 1:K:427:THR:HA | 1:K:436:MET:HE1 | 1.47 | 0.97 |
| 1:I:427:THR:HA | 1:I:436:MET:HE1 | 1.47 | 0.96 |
| 1:G:427:THR:HA | 1:G:436:MET:HE1 | 1.47 | 0.96 |
| 1:P:427:THR:HA | 1:P:436:MET:HE1 | 1.47 | 0.95 |
| 1:B:525:SER:HB3 | 3:B:3101:HOH:O | 1.68 | 0.94 |
| 1:O:427:THR:HA | 1:O:436:MET:HE1 | 1.50 | 0.93 |
| 1:D:427:THR:HA | 1:D:436:MET:HE1 | 1.48 | 0.93 |
| 1:B:427:THR:HA | 1:B:436:MET:HE1 | 1.50 | 0.93 |
| 1:A:427:THR:HA | 1:A:436:MET:HE1 | 1.53 | 0.90 |
| 1:F:427:THR:HA | 1:F:436:MET:HE1 | 1.53 | 0.90 |
| 1:N:427:THR:HA | 1:N:436:MET:HE1 | 1.53 | 0.90 |
| 1:H:427:THR:HA | 1:H:436:MET:CE | 2.02 | 0.89 |
| 1:L:427:THR:HA | 1:L:436:MET:CE | 2.02 | 0.89 |
| 1:D:427:THR:HA | 1:D:436:MET:CE | 2.02 | 0.89 |
| 1:G:427:THR:HA | 1:G:436:MET:CE | 2.02 | 0.89 |
| 1:C:427:THR:HA | 1:C:436:MET:CE | 2.02 | 0.89 |
| 1:N:427:THR:HA | 1:N:436:MET:CE | 2.02 | 0.89 |
| 1:F:427:THR:HA | 1:F:436:MET:CE | 2.02 | 0.89 |
| 1:H:427:THR:HA | 1:H:436:MET:HE1 | 1.53 | 0.89 |
| 1:A:427:THR:HA | 1:A:436:MET:CE | 2.02 | 0.88 |
| 1:K:427:THR:HA | 1:K:436:MET:CE | 2.02 | 0.88 |
| 1:E:427:THR:HA | 1:E:436:MET:CE | 2.02 | 0.88 |
| 1:J:427:THR:HA | 1:J:436:MET:CE | 2.03 | 0.88 |
| 1:I:427:THR:HA | 1:I:436:MET:CE | 2.02 | 0.88 |
| 1:B:427:THR:HA | 1:B:436:MET:CE | 2.03 | 0.88 |
| 1:M:427:THR:HA | 1:M:436:MET:CE | 2.02 | 0.88 |
| 1:O:427:THR:HA | 1:O:436:MET:CE | 2.02 | 0.87 |
| 1:N:595:THR:HG23 | 1:N:596:PRO:HA | 1.57 | 0.87 |
| 1:F:595:THR:HG23 | 1:F:596:PRO:HA | 1.57 | 0.87 |
| 1:P:427:THR:HA | 1:P:436:MET:CE | 2.02 | 0.87 |
| 1:H:595:THR:HG23 | 1:H:596:PRO:HA | 1.57 | 0.87 |
| 1:P:595:THR:HG23 | 1:P:596:PRO:HA | 1.57 | 0.87 |
| 1:K:525:SER:HB3 | 3:K:4178:HOH:O | 1.74 | 0.87 |
| 1:E:595:THR:HG23 | 1:E:596:PRO:HA | 1.57 | 0.86 |
| 1:M:595:THR:HG23 | 1:M:596:PRO:HA | 1.57 | 0.86 |
| 1:A:595:THR:HG23 | 1:A:596:PRO:HA | 1.57 | 0.86 |
| 1:C:595:THR:HG23 | 1:C:596:PRO:HA | 1.57 | 0.86 |
| 1:K:595:THR:HG23 | 1:K:596:PRO:HA | 1.57 | 0.86 |
| 1:L:595:THR:HG23 | 1:L:596:PRO:HA | 1.57 | 0.85 |
| 1:B:595:THR:HG23 | 1:B:596:PRO:HA | 1.57 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:595:THR:HG23 | 1:D:596:PRO:HA | 1.57 | 0.85 |
| 1:O:525:SER:HB3 | 3:O:3528:HOH:O | 1.76 | 0.85 |
| 1:I:595:THR:HG23 | 1:I:596:PRO:HA | 1.57 | 0.84 |
| 1:G:595:THR:HG23 | 1:G:596:PRO:HA | 1.57 | 0.84 |
| 1:O:595:THR:HG23 | 1:O:596:PRO:HA | 1.57 | 0.84 |
| 1:J:595:THR:HG23 | 1:J:596:PRO:HA | 1.57 | 0.84 |
| 1:M:525:SER:HB3 | 3:M:4424:HOH:O | 1.76 | 0.84 |
| 1:B:434:PRO:HB3 | 1:C:434:PRO:HB3 | 1.58 | 0.83 |
| 1:H:525:SER:HB3 | 3:H:4178:HOH:O | 1.77 | 0.83 |
| 1:A:282:ARG:HD3 | 1:D:420:MET:O | 1.81 | 0.81 |
| 1:J:436:MET:CE | 1:J:467:ASN:HD22 | 1.95 | 0.80 |
| 1:G:436:MET:CE | 1:G:467:ASN:HD22 | 1.95 | 0.80 |
| 1:C:436:MET:CE | 1:C:467:ASN:HD22 | 1.95 | 0.80 |
| 1:F:436:MET:CE | 1:F:467:ASN:HD22 | 1.95 | 0.80 |
| 1:N:436:MET:CE | 1:N:467:ASN:HD22 | 1.95 | 0.80 |
| 1:M:436:MET:CE | 1:M:467:ASN:HD22 | 1.95 | 0.80 |
| 1:D:436:MET:CE | 1:D:467:ASN:HD22 | 1.95 | 0.80 |
| 1:E:436:MET:CE | 1:E:467:ASN:HD22 | 1.95 | 0.80 |
| 1:I:436:MET:CE | 1:I:467:ASN:HD22 | 1.95 | 0.79 |
| 1:L:436:MET:CE | 1:L:467:ASN:HD22 | 1.95 | 0.79 |
| 1:A:436:MET:CE | 1:A:467:ASN:HD22 | 1.95 | 0.79 |
| 1:I:525:SER:HB3 | 3:I:4424:HOH:O | 1.81 | 0.79 |
| 1:L:525:SER:HB3 | 3:L:3107:HOH:O | 1.81 | 0.79 |
| 1:K:436:MET:CE | 1:K:467:ASN:HD22 | 1.95 | 0.78 |
| 1:P:436:MET:CE | 1:P:467:ASN:HD22 | 1.95 | 0.78 |
| 1:I:316:HIS:HA | 1:I:323:ILE:HD12 | 1.66 | 0.78 |
| 1:H:436:MET:CE | 1:H:467:ASN:HD22 | 1.95 | 0.78 |
| 1:D:316:HIS:HA | 1:D:323:ILE:HD12 | 1.66 | 0.78 |
| 1:B:436:MET:CE | 1:B:467:ASN:HD22 | 1.95 | 0.78 |
| 1:P:316:HIS:HA | 1:P:323:ILE:HD12 | 1.66 | 0.78 |
| 1:O:436:MET:CE | 1:O:467:ASN:HD22 | 1.95 | 0.78 |
| 1:C:316:HIS:HA | 1:C:323:ILE:HD12 | 1.66 | 0.78 |
| 1:L:316:HIS:HA | 1:L:323:ILE:HD12 | 1.66 | 0.78 |
| 1:J:316:HIS:HA | 1:J:323:ILE:HD12 | 1.66 | 0.78 |
| 1:K:316:HIS:HA | 1:K:323:ILE:HD12 | 1.66 | 0.78 |
| 1:A:436:MET:HE1 | 1:A:467:ASN:HD22 | 1.49 | 0.77 |
| 1:N:436:MET:HE1 | 1:N:467:ASN:HD22 | 1.49 | 0.77 |
| 1:H:316:HIS:HA | 1:H:323:ILE:HD12 | 1.66 | 0.77 |
| 1:F:436:MET:HE1 | 1:F:467:ASN:HD22 | 1.49 | 0.77 |
| 1:H:436:MET:HE1 | 1:H:467:ASN:HD22 | 1.49 | 0.77 |
| 1:B:316:HIS:HA | 1:B:323:ILE:HD12 | 1.66 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:525:SER:HB3 | 3:G:3531:HOH:O | 1.85 | 0.77 |
| 1:E:316:HIS:HA | 1:E:323:ILE:HD12 | 1.66 | 0.77 |
| 1:G:316:HIS:HA | 1:G:323:ILE:HD12 | 1.66 | 0.77 |
| 1:O:316:HIS:HA | 1:O:323:ILE:HD12 | 1.66 | 0.77 |
| 1:J:285:TYR:HB3 | 1:J:288:ARG:HG3 | 1.67 | 0.76 |
| 1:E:525:SER:HB3 | 3:E:4426:HOH:O | 1.85 | 0.76 |
| 1:L:949:HIS:CD2 | 1:L:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:B:285:TYR:HB3 | 1:B:288:ARG:HG3 | 1.67 | 0.76 |
| 1:M:316:HIS:HA | 1:M:323:ILE:HD12 | 1.66 | 0.76 |
| 1:A:316:HIS:HA | 1:A:323:ILE:HD12 | 1.66 | 0.76 |
| 1:L:57:GLU:HG2 | 1:L:83:THR:CG2 | 2.16 | 0.76 |
| 1:I:949:HIS:CD2 | 1:I:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:O:57:GLU:HG2 | 1:O:83:THR:CG2 | 2.16 | 0.76 |
| 1:B:949:HIS:CD2 | 1:B:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:N:316:HIS:HA | 1:N:323:ILE:HD12 | 1.66 | 0.76 |
| 1:J:57:GLU:HG2 | 1:J:83:THR:CG2 | 2.16 | 0.76 |
| 1:N:949:HIS:CD2 | 1:N:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:K:285:TYR:HB3 | 1:K:288:ARG:HG3 | 1.68 | 0.76 |
| 1:E:57:GLU:HG2 | 1:E:83:THR:CG2 | 2.16 | 0.76 |
| 1:F:949:HIS:CD2 | 1:F:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:M:57:GLU:HG2 | 1:M:83:THR:CG2 | 2.16 | 0.76 |
| 1:J:949:HIS:CD2 | 1:J:1020:TRP:HE1 | 2.04 | 0.76 |
| 1:F:316:HIS:HA | 1:F:323:ILE:HD12 | 1.66 | 0.76 |
| 1:D:525:SER:HB3 | 3:D:3109:HOH:O | 1.86 | 0.75 |
| 1:D:57:GLU:HG2 | 1:D:83:THR:CG2 | 2.16 | 0.75 |
| 1:K:57:GLU:HG2 | 1:K:83:THR:CG2 | 2.16 | 0.75 |
| 1:L:285:TYR:HB3 | 1:L:288:ARG:HG3 | 1.68 | 0.75 |
| 1:G:949:HIS:CD2 | 1:G:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:A:949:HIS:CD2 | 1:A:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:H:57:GLU:HG2 | 1:H:83:THR:CG2 | 2.16 | 0.75 |
| 1:I:285:TYR:HB3 | 1:I:288:ARG:HG3 | 1.67 | 0.75 |
| 1:P:57:GLU:HG2 | 1:P:83:THR:CG2 | 2.16 | 0.75 |
| 1:C:949:HIS:CD2 | 1:C:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:G:57:GLU:HG2 | 1:G:83:THR:CG2 | 2.16 | 0.75 |
| 1:A:57:GLU:HG2 | 1:A:83:THR:CG2 | 2.16 | 0.75 |
| 1:M:949:HIS:CD2 | 1:M:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:I:57:GLU:HG2 | 1:I:83:THR:CG2 | 2.16 | 0.75 |
| 1:C:57:GLU:HG2 | 1:C:83:THR:CG2 | 2.16 | 0.75 |
| 1:O:949:HIS:CD2 | 1:O:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:F:285:TYR:HB3 | 1:F:288:ARG:HG3 | 1.67 | 0.75 |
| 1:N:285:TYR:HB3 | 1:N:288:ARG:HG3 | 1.68 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:701:VAL:O | 1:K:703:PRO:HD3 | 1.87 | 0.75 |
| 1:F:701:VAL:O | 1:F:703:PRO:HD3 | 1.86 | 0.75 |
| 1:N:525:SER:HB3 | 3:N:3102:HOH:O | 1.87 | 0.75 |
| 1:H:285:TYR:HB3 | 1:H:288:ARG:HG3 | 1.68 | 0.75 |
| 1:A:701:VAL:O | 1:A:703:PRO:HD3 | 1.86 | 0.75 |
| 1:B:701:VAL:O | 1:B:703:PRO:HD3 | 1.86 | 0.75 |
| 1:E:949:HIS:CD2 | 1:E:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:C:701:VAL:O | 1:C:703:PRO:HD3 | 1.86 | 0.75 |
| 1:D:701:VAL:O | 1:D:703:PRO:HD3 | 1.86 | 0.75 |
| 1:D:78:LEU:HB3 | 1:D:79:PRO:HD2 | 1.69 | 0.75 |
| 1:I:701:VAL:O | 1:I:703:PRO:HD3 | 1.86 | 0.75 |
| 1:P:285:TYR:HB3 | 1:P:288:ARG:HG3 | 1.67 | 0.75 |
| 1:H:701:VAL:O | 1:H:703:PRO:HD3 | 1.86 | 0.75 |
| 1:P:949:HIS:CD2 | 1:P:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:J:78:LEU:HB3 | 1:J:79:PRO:HD2 | 1.69 | 0.75 |
| 1:N:57:GLU:HG2 | 1:N:83:THR:CG2 | 2.16 | 0.75 |
| 1:B:57:GLU:HG2 | 1:B:83:THR:CG2 | 2.16 | 0.75 |
| 1:D:949:HIS:CD2 | 1:D:1020:TRP:HE1 | 2.04 | 0.75 |
| 1:K:78:LEU:HB3 | 1:K:79:PRO:HD2 | 1.69 | 0.74 |
| 1:G:285:TYR:HB3 | 1:G:288:ARG:HG3 | 1.68 | 0.74 |
| 1:A:285:TYR:HB3 | 1:A:288:ARG:HG3 | 1.68 | 0.74 |
| 1:P:701:VAL:O | 1:P:703:PRO:HD3 | 1.86 | 0.74 |
| 1:O:285:TYR:HB3 | 1:O:288:ARG:HG3 | 1.67 | 0.74 |
| 1:K:949:HIS:CD2 | 1:K:1020:TRP:HE1 | 2.04 | 0.74 |
| 1:E:78:LEU:HB3 | 1:E:79:PRO:HD2 | 1.69 | 0.74 |
| 1:C:78:LEU:HB3 | 1:C:79:PRO:HD2 | 1.69 | 0.74 |
| 1:E:285:TYR:HB3 | 1:E:288:ARG:HG3 | 1.68 | 0.74 |
| 1:C:285:TYR:HB3 | 1:C:288:ARG:HG3 | 1.67 | 0.74 |
| 1:P:525:SER:HB3 | 3:P:3107:HOH:O | 1.86 | 0.74 |
| 1:F:57:GLU:HG2 | 1:F:83:THR:CG2 | 2.16 | 0.74 |
| 1:G:701:VAL:O | 1:G:703:PRO:HD3 | 1.86 | 0.74 |
| 1:P:78:LEU:HB3 | 1:P:79:PRO:HD2 | 1.69 | 0.74 |
| 1:M:285:TYR:HB3 | 1:M:288:ARG:HG3 | 1.68 | 0.74 |
| 1:H:78:LEU:HB3 | 1:H:79:PRO:HD2 | 1.69 | 0.74 |
| 1:L:701:VAL:O | 1:L:703:PRO:HD3 | 1.86 | 0.74 |
| 1:M:189:LEU:N | 1:M:189:LEU:HD23 | 2.03 | 0.74 |
| 1:M:78:LEU:HB3 | 1:M:79:PRO:HD2 | 1.69 | 0.74 |
| 1:J:189:LEU:N | 1:J:189:LEU:HD23 | 2.03 | 0.74 |
| 1:E:189:LEU:HD23 | 1:E:189:LEU:N | 2.03 | 0.74 |
| 1:M:745:MET:HA | 1:M:745:MET:HE2 | 1.70 | 0.74 |
| 1:K:189:LEU:HD23 | 1:K:189:LEU:N | 2.03 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:436:MET:HE1 | 1:O:467:ASN:HD22 | 1.52 | 0.74 |
| 1:M:701:VAL:O | 1:M:703:PRO:HD3 | 1.86 | 0.74 |
| 1:N:701:VAL:O | 1:N:703:PRO:HD3 | 1.86 | 0.74 |
| 1:P:316:HIS:HA | 1:P:323:ILE:CD1 | 2.18 | 0.74 |
| 1:J:701:VAL:O | 1:J:703:PRO:HD3 | 1.87 | 0.74 |
| 1:B:78:LEU:HB3 | 1:B:79:PRO:HD2 | 1.69 | 0.74 |
| 1:I:78:LEU:HB3 | 1:I:79:PRO:HD2 | 1.69 | 0.74 |
| 1:L:568:TRP:HE1 | 1:L:604:ASN:HD22 | 1.37 | 0.73 |
| 1:D:285:TYR:HB3 | 1:D:288:ARG:HG3 | 1.68 | 0.73 |
| 1:H:316:HIS:HA | 1:H:323:ILE:CD1 | 2.19 | 0.73 |
| 1:A:189:LEU:HD23 | 1:A:189:LEU:N | 2.03 | 0.73 |
| 1:J:568:TRP:HE1 | 1:J:604:ASN:HD22 | 1.36 | 0.73 |
| 1:K:316:HIS:HA | 1:K:323:ILE:CD1 | 2.18 | 0.73 |
| 1:E:316:HIS:HA | 1:E:323:ILE:CD1 | 2.18 | 0.73 |
| 1:M:316:HIS:HA | 1:M:323:ILE:CD1 | 2.19 | 0.73 |
| 1:B:189:LEU:HD23 | 1:B:189:LEU:N | 2.03 | 0.73 |
| 1:L:78:LEU:HB3 | 1:L:79:PRO:HD2 | 1.69 | 0.73 |
| 1:F:78:LEU:HB3 | 1:F:79:PRO:HD2 | 1.69 | 0.73 |
| 1:H:949:HIS:CD2 | 1:H:1020:TRP:HE1 | 2.04 | 0.73 |
| 1:E:701:VAL:O | 1:E:703:PRO:HD3 | 1.86 | 0.73 |
| 1:O:316:HIS:HA | 1:O:323:ILE:CD1 | 2.18 | 0.73 |
| 1:M:278:ILE:HD12 | 1:M:278:ILE:H | 1.54 | 0.73 |
| 1:N:78:LEU:HB3 | 1:N:79:PRO:HD2 | 1.69 | 0.73 |
| 1:L:189:LEU:HD23 | 1:L:189:LEU:N | 2.03 | 0.73 |
| 1:I:316:HIS:HA | 1:I:323:ILE:CD1 | 2.18 | 0.73 |
| 1:C:316:HIS:HA | 1:C:323:ILE:CD1 | 2.18 | 0.73 |
| 1:B:316:HIS:HA | 1:B:323:ILE:CD1 | 2.18 | 0.73 |
| 1:G:316:HIS:HA | 1:G:323:ILE:CD1 | 2.19 | 0.73 |
| 1:A:316:HIS:HA | 1:A:323:ILE:CD1 | 2.18 | 0.73 |
| 1:P:189:LEU:HD23 | 1:P:189:LEU:N | 2.03 | 0.73 |
| 1:I:745:MET:HA | 1:I:745:MET:HE2 | 1.70 | 0.73 |
| 1:E:278:ILE:HD12 | 1:E:278:ILE:H | 1.54 | 0.73 |
| 1:L:316:HIS:HA | 1:L:323:ILE:CD1 | 2.18 | 0.73 |
| 1:H:189:LEU:N | 1:H:189:LEU:HD23 | 2.03 | 0.73 |
| 1:J:316:HIS:HA | 1:J:323:ILE:CD1 | 2.18 | 0.73 |
| 1:D:894:ARG:NH2 | 1:D:921:PRO:HD3 | 2.04 | 0.73 |
| 1:C:189:LEU:HD23 | 1:C:189:LEU:N | 2.03 | 0.73 |
| 1:N:189:LEU:HD23 | 1:N:189:LEU:N | 2.03 | 0.73 |
| 1:M:568:TRP:HE1 | 1:M:604:ASN:HD22 | 1.37 | 0.73 |
| 1:L:278:ILE:HD12 | 1:L:278:ILE:H | 1.54 | 0.73 |
| 1:O:78:LEU:HB3 | 1:O:79:PRO:HD2 | 1.69 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:894:ARG:NH2 | 1:K:921:PRO:HD3 | 2.04 | 0.73 |
| 1:E:568:TRP:HE1 | 1:E:604:ASN:HD22 | 1.36 | 0.73 |
| 1:M:282:ARG:HD3 | 1:P:420:MET:O | 1.88 | 0.73 |
| 1:A:78:LEU:HB3 | 1:A:79:PRO:HD2 | 1.69 | 0.73 |
| 1:G:78:LEU:HB3 | 1:G:79:PRO:HD2 | 1.69 | 0.73 |
| 1:F:189:LEU:N | 1:F:189:LEU:HD23 | 2.03 | 0.73 |
| 1:G:189:LEU:HD23 | 1:G:189:LEU:N | 2.03 | 0.73 |
| 1:I:568:TRP:HE1 | 1:I:604:ASN:HD22 | 1.37 | 0.73 |
| 1:J:894:ARG:NH2 | 1:J:921:PRO:HD3 | 2.04 | 0.73 |
| 1:E:894:ARG:NH2 | 1:E:921:PRO:HD3 | 2.04 | 0.73 |
| 1:G:894:ARG:NH2 | 1:G:921:PRO:HD3 | 2.04 | 0.72 |
| 1:K:568:TRP:HE1 | 1:K:604:ASN:HD22 | 1.36 | 0.72 |
| 1:O:894:ARG:NH2 | 1:O:921:PRO:HD3 | 2.04 | 0.72 |
| 1:H:278:ILE:HD12 | 1:H:278:ILE:H | 1.54 | 0.72 |
| 1:O:701:VAL:O | 1:O:703:PRO:HD3 | 1.86 | 0.72 |
| 1:C:278:ILE:H | 1:C:278:ILE:HD12 | 1.54 | 0.72 |
| 1:D:189:LEU:HD23 | 1:D:189:LEU:N | 2.03 | 0.72 |
| 1:B:436:MET:HE1 | 1:B:467:ASN:HD22 | 1.52 | 0.72 |
| 1:L:894:ARG:NH2 | 1:L:921:PRO:HD3 | 2.04 | 0.72 |
| 1:N:316:HIS:HA | 1:N:323:ILE:CD1 | 2.18 | 0.72 |
| 1:F:316:HIS:HA | 1:F:323:ILE:CD1 | 2.18 | 0.72 |
| 1:F:894:ARG:NH2 | 1:F:921:PRO:HD3 | 2.04 | 0.72 |
| 1:A:894:ARG:NH2 | 1:A:921:PRO:HD3 | 2.04 | 0.72 |
| 1:D:316:HIS:HA | 1:D:323:ILE:CD1 | 2.18 | 0.72 |
| 1:M:894:ARG:NH2 | 1:M:921:PRO:HD3 | 2.04 | 0.72 |
| 1:C:894:ARG:NH2 | 1:C:921:PRO:HD3 | 2.04 | 0.72 |
| 1:N:894:ARG:NH2 | 1:N:921:PRO:HD3 | 2.04 | 0.72 |
| 1:P:278:ILE:H | 1:P:278:ILE:HD12 | 1.54 | 0.72 |
| 1:B:278:ILE:H | 1:B:278:ILE:HD12 | 1.54 | 0.72 |
| 1:K:436:MET:HE1 | 1:K:467:ASN:HD22 | 1.55 | 0.72 |
| 1:H:894:ARG:NH2 | 1:H:921:PRO:HD3 | 2.04 | 0.72 |
| 1:B:894:ARG:NH2 | 1:B:921:PRO:HD3 | 2.04 | 0.72 |
| 1:A:568:TRP:HE1 | 1:A:604:ASN:HD22 | 1.36 | 0.72 |
| 1:N:745:MET:HA | 1:N:745:MET:HE2 | 1.72 | 0.72 |
| 1:O:189:LEU:N | 1:O:189:LEU:HD23 | 2.03 | 0.72 |
| 1:I:189:LEU:HD23 | 1:I:189:LEU:N | 2.03 | 0.72 |
| 1:C:568:TRP:HE1 | 1:C:604:ASN:HD22 | 1.37 | 0.72 |
| 1:P:894:ARG:NH2 | 1:P:921:PRO:HD3 | 2.04 | 0.72 |
| 1:F:745:MET:HA | 1:F:745:MET:HE2 | 1.72 | 0.72 |
| 1:I:278:ILE:H | 1:I:278:ILE:HD12 | 1.54 | 0.72 |
| 1:M:425:ARG:NH2 | 1:P:287:ASP:OD2 | 2.23 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:183:ARG:HD3 | 3:C:4254:HOH:O | 1.90 | 0.72 |
| 1:B:568:TRP:HE1 | 1:B:604:ASN:HD22 | 1.37 | 0.72 |
| 1:D:278:ILE:HD12 | 1:D:278:ILE:H | 1.54 | 0.72 |
| 1:O:278:ILE:H | 1:O:278:ILE:HD12 | 1.54 | 0.72 |
| 1:C:7:LEU:CD1 | 1:C:74:LEU:HD11 | 2.20 | 0.72 |
| 1:D:436:MET:HE1 | 1:D:467:ASN:HD22 | 1.53 | 0.71 |
| 1:F:7:LEU:CD1 | 1:F:74:LEU:HD11 | 2.20 | 0.71 |
| 1:M:7:LEU:CD1 | 1:M:74:LEU:HD11 | 2.20 | 0.71 |
| 1:F:278:ILE:H | 1:F:278:ILE:HD12 | 1.54 | 0.71 |
| 1:N:278:ILE:HD12 | 1:N:278:ILE:H | 1.54 | 0.71 |
| 1:K:7:LEU:CD1 | 1:K:74:LEU:HD11 | 2.20 | 0.71 |
| 1:N:7:LEU:CD1 | 1:N:74:LEU:HD11 | 2.20 | 0.71 |
| 1:I:894:ARG:NH2 | 1:I:921:PRO:HD3 | 2.04 | 0.71 |
| 1:K:278:ILE:HD12 | 1:K:278:ILE:H | 1.54 | 0.71 |
| 1:E:7:LEU:CD1 | 1:E:74:LEU:HD11 | 2.20 | 0.71 |
| 1:N:183:ARG:HD3 | 3:N:3360:HOH:O | 1.90 | 0.71 |
| 1:A:278:ILE:H | 1:A:278:ILE:HD12 | 1.54 | 0.71 |
| 1:P:568:TRP:HE1 | 1:P:604:ASN:HD22 | 1.36 | 0.71 |
| 1:J:7:LEU:CD1 | 1:J:74:LEU:HD11 | 2.20 | 0.71 |
| 1:B:7:LEU:CD1 | 1:B:74:LEU:HD11 | 2.20 | 0.71 |
| 1:E:183:ARG:HD3 | 3:E:4253:HOH:O | 1.90 | 0.71 |
| 1:D:1021:CME:HE2 | 1:D:1021:CME:C | 2.21 | 0.71 |
| 1:G:7:LEU:CD1 | 1:G:74:LEU:HD11 | 2.20 | 0.71 |
| 1:G:278:ILE:H | 1:G:278:ILE:HD12 | 1.54 | 0.71 |
| 1:O:7:LEU:CD1 | 1:O:74:LEU:HD11 | 2.20 | 0.71 |
| 1:A:7:LEU:CD1 | 1:A:74:LEU:HD11 | 2.20 | 0.71 |
| 1:F:1021:CME:HE2 | 1:F:1021:CME:C | 2.21 | 0.71 |
| 1:N:568:TRP:HE1 | 1:N:604:ASN:HD22 | 1.37 | 0.71 |
| 1:I:436:MET:HE1 | 1:I:467:ASN:HD22 | 1.55 | 0.71 |
| 1:G:436:MET:HE1 | 1:G:467:ASN:HD22 | 1.55 | 0.71 |
| 1:D:568:TRP:HE1 | 1:D:604:ASN:HD22 | 1.37 | 0.71 |
| 1:H:568:TRP:HE1 | 1:H:604:ASN:HD22 | 1.36 | 0.71 |
| 1:D:183:ARG:HD3 | 3:D:3366:HOH:O | 1.90 | 0.71 |
| 1:I:7:LEU:CD1 | 1:I:74:LEU:HD11 | 2.20 | 0.71 |
| 1:P:7:LEU:CD1 | 1:P:74:LEU:HD11 | 2.20 | 0.71 |
| 1:L:183:ARG:HD3 | 3:L:3363:HOH:O | 1.90 | 0.71 |
| 1:F:568:TRP:HE1 | 1:F:604:ASN:HD22 | 1.37 | 0.71 |
| 1:C:436:MET:HE1 | 1:C:467:ASN:HD22 | 1.56 | 0.70 |
| 1:M:183:ARG:HD3 | 3:M:4253:HOH:O | 1.90 | 0.70 |
| 1:L:7:LEU:CD1 | 1:L:74:LEU:HD11 | 2.20 | 0.70 |
| 1:L:1021:CME:HE2 | 1:L:1021:CME:C | 2.21 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:1021:CME:HE2 | 1:E:1021:CME:C | 2.21 | 0.70 |
| 1:K:1021:CME:C | 1:K:1021:CME:HE2 | 2.21 | 0.70 |
| 1:H:7:LEU:CD1 | 1:H:74:LEU:HD11 | 2.20 | 0.70 |
| 1:G:183:ARG:HD3 | 3:G:3357:HOH:O | 1.90 | 0.70 |
| 1:O:183:ARG:HD3 | 3:O:3357:HOH:O | 1.90 | 0.70 |
| 1:K:183:ARG:HD3 | 3:K:4254:HOH:O | 1.90 | 0.70 |
| 1:B:183:ARG:HD3 | 3:B:3357:HOH:O | 1.90 | 0.70 |
| 1:J:183:ARG:HD3 | 3:J:3360:HOH:O | 1.90 | 0.70 |
| 1:D:7:LEU:CD1 | 1:D:74:LEU:HD11 | 2.20 | 0.70 |
| 1:F:183:ARG:HD3 | 3:F:3359:HOH:O | 1.90 | 0.70 |
| 1:N:1021:CME:HE2 | 1:N:1021:CME:C | 2.21 | 0.70 |
| 1:A:1021:CME:HE2 | 1:A:1021:CME:C | 2.21 | 0.70 |
| 1:J:278:ILE:HD12 | 1:J:278:ILE:H | 1.54 | 0.70 |
| 1:G:568:TRP:HE1 | 1:G:604:ASN:HD22 | 1.36 | 0.70 |
| 1:C:1021:CME:HE2 | 1:C:1021:CME:C | 2.21 | 0.70 |
| 1:O:568:TRP:HE1 | 1:O:604:ASN:HD22 | 1.37 | 0.70 |
| 1:I:1021:CME:HE2 | 1:I:1021:CME:C | 2.21 | 0.70 |
| 1:P:1021:CME:HE2 | 1:P:1021:CME:C | 2.21 | 0.70 |
| 1:P:183:ARG:HD3 | 3:P:3365:HOH:O | 1.90 | 0.70 |
| 1:M:579:ASP:OD1 | 1:M:583:ASN:HB2 | 1.92 | 0.70 |
| 1:I:183:ARG:HD3 | 3:I:4252:HOH:O | 1.90 | 0.70 |
| 1:J:579:ASP:OD1 | 1:J:583:ASN:HB2 | 1.92 | 0.70 |
| 1:P:436:MET:HE1 | 1:P:467:ASN:HD22 | 1.55 | 0.69 |
| 1:B:1021:CME:C | 1:B:1021:CME:HE2 | 2.21 | 0.69 |
| 1:P:166:ARG:HG3 | 1:P:392:TYR:HB2 | 1.74 | 0.69 |
| 1:G:166:ARG:HG3 | 1:G:392:TYR:HB2 | 1.74 | 0.69 |
| 1:E:579:ASP:OD1 | 1:E:583:ASN:HB2 | 1.92 | 0.69 |
| 1:K:579:ASP:OD1 | 1:K:583:ASN:HB2 | 1.92 | 0.69 |
| 1:A:183:ARG:HD3 | 3:A:4254:HOH:O | 1.90 | 0.69 |
| 1:O:166:ARG:HG3 | 1:O:392:TYR:HB2 | 1.74 | 0.69 |
| 1:B:579:ASP:OD1 | 1:B:583:ASN:HB2 | 1.92 | 0.69 |
| 1:P:579:ASP:OD1 | 1:P:583:ASN:HB2 | 1.93 | 0.69 |
| 1:D:166:ARG:HG3 | 1:D:392:TYR:HB2 | 1.74 | 0.69 |
| 1:G:579:ASP:OD1 | 1:G:583:ASN:HB2 | 1.92 | 0.69 |
| 1:H:166:ARG:HG3 | 1:H:392:TYR:HB2 | 1.74 | 0.69 |
| 1:O:1021:CME:C | 1:O:1021:CME:HE2 | 2.21 | 0.69 |
| 1:C:579:ASP:OD1 | 1:C:583:ASN:HB2 | 1.92 | 0.69 |
| 1:K:63:PHE:HB3 | 1:K:64:PRO:HD2 | 1.75 | 0.69 |
| 1:G:1021:CME:C | 1:G:1021:CME:HE2 | 2.21 | 0.69 |
| 1:H:183:ARG:HD3 | 3:H:4254:HOH:O | 1.90 | 0.69 |
| 1:I:63:PHE:HB3 | 1:I:64:PRO:HD2 | 1.75 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:166:ARG:HG3 | 1:B:392:TYR:HB2 | 1.74 | 0.69 |
| 1:F:579:ASP:OD1 | 1:F:583:ASN:HB2 | 1.92 | 0.69 |
| 1:B:745:MET:HE2 | 1:B:745:MET:HA | 1.73 | 0.69 |
| 1:J:1021:CME:HE2 | 1:J:1021:CME:C | 2.21 | 0.69 |
| 1:H:1021:CME:HE2 | 1:H:1021:CME:C | 2.21 | 0.69 |
| 1:G:63:PHE:HB3 | 1:G:64:PRO:HD2 | 1.75 | 0.69 |
| 1:O:63:PHE:HB3 | 1:O:64:PRO:HD2 | 1.75 | 0.69 |
| 1:N:166:ARG:HG3 | 1:N:392:TYR:HB2 | 1.74 | 0.69 |
| 1:E:856:TYR:HD2 | 1:E:864:MET:HE2 | 1.58 | 0.69 |
| 1:A:579:ASP:OD1 | 1:A:583:ASN:HB2 | 1.92 | 0.69 |
| 1:F:434:PRO:HB3 | 1:G:434:PRO:HB3 | 1.74 | 0.69 |
| 1:O:579:ASP:OD1 | 1:O:583:ASN:HB2 | 1.92 | 0.69 |
| 1:B:919:ASP:O | 1:B:920:LEU:HD23 | 1.93 | 0.69 |
| 1:F:166:ARG:HG3 | 1:F:392:TYR:HB2 | 1.74 | 0.69 |
| 1:C:166:ARG:HG3 | 1:C:392:TYR:HB2 | 1.74 | 0.69 |
| 1:J:166:ARG:HG3 | 1:J:392:TYR:HB2 | 1.74 | 0.69 |
| 1:B:63:PHE:HB3 | 1:B:64:PRO:HD2 | 1.75 | 0.69 |
| 1:E:166:ARG:HG3 | 1:E:392:TYR:HB2 | 1.74 | 0.69 |
| 1:O:952:ARG:HG2 | 1:O:952:ARG:NH1 | 2.08 | 0.69 |
| 1:M:1021:CME:C | 1:M:1021:CME:HE2 | 2.21 | 0.68 |
| 1:L:579:ASP:OD1 | 1:L:583:ASN:HB2 | 1.92 | 0.68 |
| 1:A:63:PHE:HB3 | 1:A:64:PRO:HD2 | 1.75 | 0.68 |
| 1:N:579:ASP:OD1 | 1:N:583:ASN:HB2 | 1.92 | 0.68 |
| 1:P:952:ARG:HG2 | 1:P:952:ARG:NH1 | 2.08 | 0.68 |
| 1:J:952:ARG:NH1 | 1:J:952:ARG:HG2 | 2.08 | 0.68 |
| 1:G:919:ASP:O | 1:G:920:LEU:HD23 | 1.93 | 0.68 |
| 1:C:525:SER:HB3 | 3:C:4178:HOH:O | 1.91 | 0.68 |
| 1:L:952:ARG:NH1 | 1:L:952:ARG:HG2 | 2.08 | 0.68 |
| 1:H:952:ARG:HG2 | 1:H:952:ARG:NH1 | 2.08 | 0.68 |
| 1:D:919:ASP:O | 1:D:920:LEU:HD23 | 1.94 | 0.68 |
| 1:A:919:ASP:O | 1:A:920:LEU:HD23 | 1.93 | 0.68 |
| 1:I:166:ARG:HG3 | 1:I:392:TYR:HB2 | 1.74 | 0.68 |
| 1:L:166:ARG:HG3 | 1:L:392:TYR:HB2 | 1.74 | 0.68 |
| 1:O:919:ASP:O | 1:O:920:LEU:HD23 | 1.93 | 0.68 |
| 1:I:919:ASP:O | 1:I:920:LEU:HD23 | 1.93 | 0.68 |
| 1:A:952:ARG:NH1 | 1:A:952:ARG:HG2 | 2.08 | 0.68 |
| 1:J:436:MET:HE1 | 1:J:467:ASN:HD22 | 1.58 | 0.68 |
| 1:H:919:ASP:O | 1:H:920:LEU:HD23 | 1.94 | 0.68 |
| 1:D:745:MET:HE2 | 1:D:745:MET:HA | 1.74 | 0.68 |
| 1:N:919:ASP:O | 1:N:920:LEU:HD23 | 1.94 | 0.68 |
| 1:M:166:ARG:HG3 | 1:M:392:TYR:HB2 | 1.74 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:166:ARG:HG3 | 1:A:392:TYR:HB2 | 1.74 | 0.68 |
| 1:J:63:PHE:HB3 | 1:J:64:PRO:HD2 | 1.75 | 0.68 |
| 1:D:856:TYR:HD2 | 1:D:864:MET:HE2 | 1.59 | 0.68 |
| 1:E:919:ASP:O | 1:E:920:LEU:HD23 | 1.93 | 0.68 |
| 1:L:63:PHE:HB3 | 1:L:64:PRO:HD2 | 1.75 | 0.68 |
| 1:I:579:ASP:OD1 | 1:I:583:ASN:HB2 | 1.92 | 0.68 |
| 1:D:63:PHE:HB3 | 1:D:64:PRO:HD2 | 1.75 | 0.68 |
| 1:I:920:LEU:HB3 | 1:I:921:PRO:HD2 | 1.76 | 0.68 |
| 1:H:43:ARG:HG2 | 1:H:43:ARG:HH11 | 1.59 | 0.68 |
| 1:B:43:ARG:HG2 | 1:B:43:ARG:HH11 | 1.59 | 0.68 |
| 1:P:745:MET:HE2 | 1:P:745:MET:HA | 1.75 | 0.68 |
| 1:I:890:GLN:HG3 | 1:I:891:VAL:N | 2.09 | 0.68 |
| 1:J:43:ARG:HH11 | 1:J:43:ARG:HG2 | 1.59 | 0.68 |
| 1:G:890:GLN:HG3 | 1:G:891:VAL:N | 2.09 | 0.68 |
| 1:J:919:ASP:O | 1:J:920:LEU:HD23 | 1.93 | 0.68 |
| 1:O:43:ARG:HH11 | 1:O:43:ARG:HG2 | 1.59 | 0.68 |
| 1:A:890:GLN:HG3 | 1:A:891:VAL:N | 2.09 | 0.68 |
| 1:D:579:ASP:OD1 | 1:D:583:ASN:HB2 | 1.92 | 0.68 |
| 1:L:919:ASP:O | 1:L:920:LEU:HD23 | 1.93 | 0.67 |
| 1:F:919:ASP:O | 1:F:920:LEU:HD23 | 1.94 | 0.67 |
| 1:M:919:ASP:O | 1:M:920:LEU:HD23 | 1.94 | 0.67 |
| 1:L:745:MET:HE2 | 1:L:745:MET:HA | 1.75 | 0.67 |
| 1:C:43:ARG:HG2 | 1:C:43:ARG:HH11 | 1.59 | 0.67 |
| 1:H:579:ASP:OD1 | 1:H:583:ASN:HB2 | 1.92 | 0.67 |
| 1:P:43:ARG:HH11 | 1:P:43:ARG:HG2 | 1.59 | 0.67 |
| 1:G:952:ARG:NH1 | 1:G:952:ARG:HG2 | 2.08 | 0.67 |
| 1:I:952:ARG:NH1 | 1:I:952:ARG:HG2 | 2.08 | 0.67 |
| 1:P:919:ASP:O | 1:P:920:LEU:HD23 | 1.94 | 0.67 |
| 1:E:745:MET:HA | 1:E:745:MET:HE2 | 1.76 | 0.67 |
| 1:M:43:ARG:HH11 | 1:M:43:ARG:HG2 | 1.59 | 0.67 |
| 1:G:43:ARG:HH11 | 1:G:43:ARG:HG2 | 1.59 | 0.67 |
| 1:K:166:ARG:HG3 | 1:K:392:TYR:HB2 | 1.74 | 0.67 |
| 1:E:43:ARG:HH11 | 1:E:43:ARG:HG2 | 1.59 | 0.67 |
| 1:N:890:GLN:HG3 | 1:N:891:VAL:N | 2.09 | 0.67 |
| 1:K:919:ASP:O | 1:K:920:LEU:HD23 | 1.94 | 0.67 |
| 1:E:920:LEU:HB3 | 1:E:921:PRO:HD2 | 1.76 | 0.67 |
| 1:L:920:LEU:HB3 | 1:L:921:PRO:HD2 | 1.76 | 0.67 |
| 1:M:920:LEU:HB3 | 1:M:921:PRO:HD2 | 1.76 | 0.67 |
| 1:J:890:GLN:HG3 | 1:J:891:VAL:N | 2.09 | 0.67 |
| 1:M:63:PHE:HB3 | 1:M:64:PRO:HD2 | 1.75 | 0.67 |
| 1:C:952:ARG:HG2 | 1:C:952:ARG:NH1 | 2.08 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:920:LEU:HB3 | 1:B:921:PRO:HD2 | 1.76 | 0.67 |
| 1:E:63:PHE:HB3 | 1:E:64:PRO:HD2 | 1.75 | 0.67 |
| 1:N:952:ARG:NH1 | 1:N:952:ARG:HG2 | 2.08 | 0.67 |
| 1:C:63:PHE:HB3 | 1:C:64:PRO:HD2 | 1.75 | 0.67 |
| 1:G:920:LEU:HB3 | 1:G:921:PRO:HD2 | 1.76 | 0.67 |
| 1:O:920:LEU:HB3 | 1:O:921:PRO:HD2 | 1.76 | 0.67 |
| 1:H:63:PHE:HB3 | 1:H:64:PRO:HD2 | 1.75 | 0.67 |
| 1:E:952:ARG:NH1 | 1:E:952:ARG:HG2 | 2.08 | 0.67 |
| 1:N:43:ARG:HG2 | 1:N:43:ARG:HH11 | 1.59 | 0.67 |
| 1:F:43:ARG:HH11 | 1:F:43:ARG:HG2 | 1.59 | 0.67 |
| 1:K:920:LEU:HB3 | 1:K:921:PRO:HD2 | 1.76 | 0.67 |
| 1:M:425:ARG:HH22 | 1:P:287:ASP:CG | 1.98 | 0.67 |
| 1:L:436:MET:HE1 | 1:L:467:ASN:HD22 | 1.59 | 0.67 |
| 1:M:7:LEU:HD13 | 1:M:74:LEU:HD11 | 1.77 | 0.67 |
| 1:M:952:ARG:NH1 | 1:M:952:ARG:HG2 | 2.08 | 0.67 |
| 1:K:952:ARG:NH1 | 1:K:952:ARG:HG2 | 2.08 | 0.67 |
| 1:F:63:PHE:HB3 | 1:F:64:PRO:HD2 | 1.75 | 0.67 |
| 1:F:952:ARG:NH1 | 1:F:952:ARG:HG2 | 2.08 | 0.67 |
| 1:F:890:GLN:HG3 | 1:F:891:VAL:N | 2.09 | 0.67 |
| 1:N:63:PHE:HB3 | 1:N:64:PRO:HD2 | 1.75 | 0.67 |
| 1:F:920:LEU:HB3 | 1:F:921:PRO:HD2 | 1.76 | 0.67 |
| 1:C:919:ASP:O | 1:C:920:LEU:HD23 | 1.94 | 0.67 |
| 1:B:278:ILE:N | 1:B:278:ILE:HD12 | 2.10 | 0.67 |
| 1:E:7:LEU:HD13 | 1:E:74:LEU:HD11 | 1.77 | 0.67 |
| 1:A:43:ARG:HH11 | 1:A:43:ARG:HG2 | 1.59 | 0.67 |
| 1:J:745:MET:HA | 1:J:745:MET:HE2 | 1.76 | 0.67 |
| 1:H:890:GLN:HG3 | 1:H:891:VAL:N | 2.09 | 0.67 |
| 1:P:278:ILE:N | 1:P:278:ILE:HD12 | 2.10 | 0.67 |
| 1:J:278:ILE:HD12 | 1:J:278:ILE:N | 2.10 | 0.67 |
| 1:O:745:MET:HE2 | 1:O:745:MET:HA | 1.76 | 0.67 |
| 1:A:856:TYR:HD2 | 1:A:864:MET:HE2 | 1.60 | 0.67 |
| 1:A:745:MET:HE2 | 1:A:745:MET:HA | 1.76 | 0.67 |
| 1:G:856:TYR:HD2 | 1:G:864:MET:HE2 | 1.59 | 0.67 |
| 1:K:43:ARG:HH11 | 1:K:43:ARG:HG2 | 1.59 | 0.67 |
| 1:H:278:ILE:HD12 | 1:H:278:ILE:N | 2.10 | 0.66 |
| 1:N:920:LEU:HB3 | 1:N:921:PRO:HD2 | 1.76 | 0.66 |
| 1:O:278:ILE:N | 1:O:278:ILE:HD12 | 2.10 | 0.66 |
| 1:G:278:ILE:N | 1:G:278:ILE:HD12 | 2.10 | 0.66 |
| 1:L:952:ARG:HH11 | 1:L:952:ARG:HG2 | 1.61 | 0.66 |
| 1:L:43:ARG:HG2 | 1:L:43:ARG:HH11 | 1.59 | 0.66 |
| 1:D:952:ARG:HG2 | 1:D:952:ARG:NH1 | 2.08 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:278:ILE:HD12 | 1:M:278:ILE:N | 2.10 | 0.66 |
| 1:L:278:ILE:HD12 | 1:L:278:ILE:N | 2.10 | 0.66 |
| 1:J:920:LEU:HB3 | 1:J:921:PRO:HD2 | 1.76 | 0.66 |
| 1:I:278:ILE:N | 1:I:278:ILE:HD12 | 2.10 | 0.66 |
| 1:A:7:LEU:HD13 | 1:A:74:LEU:HD11 | 1.77 | 0.66 |
| 1:C:890:GLN:HG3 | 1:C:891:VAL:N | 2.09 | 0.66 |
| 1:G:745:MET:HE2 | 1:G:745:MET:HA | 1.76 | 0.66 |
| 1:H:745:MET:HE2 | 1:H:745:MET:HA | 1.76 | 0.66 |
| 1:F:278:ILE:HD12 | 1:F:278:ILE:N | 2.10 | 0.66 |
| 1:N:278:ILE:N | 1:N:278:ILE:HD12 | 2.10 | 0.66 |
| 1:K:278:ILE:HD12 | 1:K:278:ILE:N | 2.10 | 0.66 |
| 1:L:890:GLN:HG3 | 1:L:891:VAL:N | 2.09 | 0.66 |
| 1:B:952:ARG:HH11 | 1:B:952:ARG:HG2 | 1.61 | 0.66 |
| 1:E:278:ILE:HD12 | 1:E:278:ILE:N | 2.10 | 0.66 |
| 1:C:952:ARG:HG2 | 1:C:952:ARG:HH11 | 1.61 | 0.66 |
| 1:O:890:GLN:HG3 | 1:O:891:VAL:N | 2.09 | 0.66 |
| 1:A:418:HIS:O | 1:D:282:ARG:HD2 | 1.96 | 0.66 |
| 1:I:43:ARG:HH11 | 1:I:43:ARG:HG2 | 1.59 | 0.66 |
| 1:P:63:PHE:HB3 | 1:P:64:PRO:HD2 | 1.75 | 0.66 |
| 1:D:278:ILE:N | 1:D:278:ILE:HD12 | 2.10 | 0.66 |
| 1:H:7:LEU:HD13 | 1:H:74:LEU:HD11 | 1.77 | 0.66 |
| 1:E:436:MET:HE3 | 1:E:467:ASN:HD22 | 1.60 | 0.66 |
| 1:P:7:LEU:HD13 | 1:P:74:LEU:HD11 | 1.77 | 0.66 |
| 1:B:952:ARG:NH1 | 1:B:952:ARG:HG2 | 2.08 | 0.66 |
| 1:D:890:GLN:HG3 | 1:D:891:VAL:N | 2.09 | 0.66 |
| 1:D:43:ARG:HH11 | 1:D:43:ARG:HG2 | 1.59 | 0.66 |
| 1:B:890:GLN:HG3 | 1:B:891:VAL:N | 2.09 | 0.66 |
| 1:J:7:LEU:HD13 | 1:J:74:LEU:HD11 | 1.77 | 0.66 |
| 1:L:7:LEU:HD13 | 1:L:74:LEU:HD11 | 1.77 | 0.66 |
| 1:D:7:LEU:HD13 | 1:D:74:LEU:HD11 | 1.77 | 0.66 |
| 1:A:525:SER:HB3 | 3:A:4178:HOH:O | 1.94 | 0.66 |
| 1:C:920:LEU:HB3 | 1:C:921:PRO:HD2 | 1.76 | 0.66 |
| 1:N:952:ARG:HG2 | 1:N:952:ARG:HH11 | 1.61 | 0.66 |
| 1:E:952:ARG:HG2 | 1:E:952:ARG:HH11 | 1.61 | 0.66 |
| 1:P:890:GLN:HG3 | 1:P:891:VAL:N | 2.09 | 0.66 |
| 1:C:745:MET:HE2 | 1:C:745:MET:HA | 1.76 | 0.66 |
| 1:M:890:GLN:HG3 | 1:M:891:VAL:N | 2.09 | 0.66 |
| 1:J:434:PRO:HB3 | 1:K:434:PRO:HB3 | 1.76 | 0.66 |
| 1:C:278:ILE:N | 1:C:278:ILE:HD12 | 2.10 | 0.66 |
| 1:A:278:ILE:HD12 | 1:A:278:ILE:N | 2.10 | 0.66 |
| 1:N:43:ARG:NH1 | 1:N:43:ARG:HG2 | 2.11 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:952:ARG:HH11 | 1:M:952:ARG:HG2 | 1.61 | 0.66 |
| 1:A:920:LEU:HB3 | 1:A:921:PRO:HD2 | 1.76 | 0.66 |
| 1:P:952:ARG:HG2 | 1:P:952:ARG:HH11 | 1.60 | 0.66 |
| 1:O:43:ARG:HG2 | 1:O:43:ARG:NH1 | 2.11 | 0.66 |
| 1:D:952:ARG:HH11 | 1:D:952:ARG:HG2 | 1.61 | 0.66 |
| 1:D:43:ARG:HG2 | 1:D:43:ARG:NH1 | 2.11 | 0.66 |
| 1:D:920:LEU:HB3 | 1:D:921:PRO:HD2 | 1.76 | 0.65 |
| 1:P:920:LEU:HB3 | 1:P:921:PRO:HD2 | 1.76 | 0.65 |
| 1:P:43:ARG:NH1 | 1:P:43:ARG:HG2 | 2.11 | 0.65 |
| 1:H:43:ARG:NH1 | 1:H:43:ARG:HG2 | 2.11 | 0.65 |
| 1:E:43:ARG:NH1 | 1:E:43:ARG:HG2 | 2.11 | 0.65 |
| 1:F:952:ARG:HH11 | 1:F:952:ARG:HG2 | 1.61 | 0.65 |
| 1:F:525:SER:HB3 | 3:F:3102:HOH:O | 1.95 | 0.65 |
| 1:J:334:GLU:OE1 | 1:J:336:ARG:NH1 | 2.30 | 0.65 |
| 1:B:367:MET:HB3 | 1:B:372:MET:HE3 | 1.78 | 0.65 |
| 1:K:890:GLN:HG3 | 1:K:891:VAL:N | 2.09 | 0.65 |
| 1:M:436:MET:HE1 | 1:M:467:ASN:HD22 | 1.59 | 0.65 |
| 1:M:436:MET:HE3 | 1:M:467:ASN:HD22 | 1.62 | 0.65 |
| 1:D:7:LEU:N | 1:D:71:GLU:OE2 | 2.30 | 0.65 |
| 1:H:952:ARG:HH11 | 1:H:952:ARG:HG2 | 1.61 | 0.65 |
| 1:K:43:ARG:HG2 | 1:K:43:ARG:NH1 | 2.11 | 0.65 |
| 1:D:334:GLU:OE1 | 1:D:336:ARG:NH1 | 2.30 | 0.65 |
| 1:H:59:ARG:NH2 | 1:H:81:ALA:O | 2.30 | 0.65 |
| 1:A:117:GLU:OE1 | 1:A:117:GLU:N | 2.29 | 0.65 |
| 1:F:7:LEU:N | 1:F:71:GLU:OE2 | 2.30 | 0.65 |
| 1:J:7:LEU:N | 1:J:71:GLU:OE2 | 2.30 | 0.65 |
| 1:B:7:LEU:N | 1:B:71:GLU:OE2 | 2.30 | 0.65 |
| 1:I:7:LEU:N | 1:I:71:GLU:OE2 | 2.30 | 0.65 |
| 1:K:952:ARG:HH11 | 1:K:952:ARG:HG2 | 1.61 | 0.65 |
| 1:L:334:GLU:OE1 | 1:L:336:ARG:NH1 | 2.30 | 0.65 |
| 1:P:59:ARG:NH2 | 1:P:81:ALA:O | 2.30 | 0.65 |
| 1:A:334:GLU:OE1 | 1:A:336:ARG:NH1 | 2.30 | 0.65 |
| 1:B:7:LEU:HD13 | 1:B:74:LEU:HD11 | 1.77 | 0.65 |
| 1:O:7:LEU:HD13 | 1:O:74:LEU:HD11 | 1.77 | 0.65 |
| 1:M:43:ARG:HG2 | 1:M:43:ARG:NH1 | 2.11 | 0.65 |
| 1:A:43:ARG:NH1 | 1:A:43:ARG:HG2 | 2.11 | 0.65 |
| 1:E:890:GLN:HG3 | 1:E:891:VAL:N | 2.09 | 0.65 |
| 1:I:681:GLU:OE2 | 1:I:681:GLU:HA | 1.97 | 0.65 |
| 1:F:367:MET:HB3 | 1:F:372:MET:HE3 | 1.79 | 0.65 |
| 1:H:920:LEU:HB3 | 1:H:921:PRO:HD2 | 1.76 | 0.65 |
| 1:L:7:LEU:N | 1:L:71:GLU:OE2 | 2.30 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:O:254:LEU:C | 1:O:255:ARG:HG2 | 2.17 | 0.65 |
| 1:I:59:ARG:NH2 | 1:I:81:ALA:O | 2.30 | 0.65 |
| 1:K:745:MET:HE2 | 1:K:745:MET:HA | 1.76 | 0.65 |
| 1:K:7:LEU:N | 1:K:71:GLU:OE2 | 2.30 | 0.65 |
| 1:J:952:ARG:HH11 | 1:J:952:ARG:HG2 | 1.61 | 0.65 |
| 1:J:59:ARG:NH2 | 1:J:81:ALA:O | 2.30 | 0.65 |
| 1:E:254:LEU:C | 1:E:255:ARG:HG2 | 2.17 | 0.65 |
| 1:M:117:GLU:OE1 | 1:M:117:GLU:N | 2.29 | 0.65 |
| 1:F:334:GLU:OE1 | 1:F:336:ARG:NH1 | 2.30 | 0.65 |
| 1:N:334:GLU:OE1 | 1:N:336:ARG:NH1 | 2.30 | 0.65 |
| 1:C:7:LEU:N | 1:C:71:GLU:OE2 | 2.30 | 0.65 |
| 1:N:7:LEU:HD13 | 1:N:74:LEU:HD11 | 1.77 | 0.65 |
| 1:G:7:LEU:HD13 | 1:G:74:LEU:HD11 | 1.77 | 0.65 |
| 1:B:59:ARG:NH2 | 1:B:81:ALA:O | 2.30 | 0.65 |
| 1:E:334:GLU:OE1 | 1:E:336:ARG:NH1 | 2.30 | 0.65 |
| 1:C:681:GLU:OE2 | 1:C:681:GLU:HA | 1.97 | 0.65 |
| 1:E:117:GLU:OE1 | 1:E:117:GLU:N | 2.29 | 0.65 |
| 1:D:367:MET:HB3 | 1:D:372:MET:HE3 | 1.77 | 0.65 |
| 1:J:43:ARG:NH1 | 1:J:43:ARG:HG2 | 2.11 | 0.65 |
| 1:F:43:ARG:HG2 | 1:F:43:ARG:NH1 | 2.11 | 0.65 |
| 1:L:59:ARG:NH2 | 1:L:81:ALA:O | 2.30 | 0.65 |
| 1:F:59:ARG:NH2 | 1:F:81:ALA:O | 2.30 | 0.65 |
| 1:G:254:LEU:C | 1:G:255:ARG:HG2 | 2.17 | 0.65 |
| 1:P:7:LEU:N | 1:P:71:GLU:OE2 | 2.30 | 0.64 |
| 1:A:952:ARG:HH11 | 1:A:952:ARG:HG2 | 1.61 | 0.64 |
| 1:B:43:ARG:HG2 | 1:B:43:ARG:NH1 | 2.11 | 0.64 |
| 1:G:952:ARG:HH11 | 1:G:952:ARG:HG2 | 1.61 | 0.64 |
| 1:G:43:ARG:NH1 | 1:G:43:ARG:HG2 | 2.11 | 0.64 |
| 1:J:917:ARG:NH2 | 1:J:943:GLU:OE1 | 2.30 | 0.64 |
| 1:C:59:ARG:NH2 | 1:C:81:ALA:O | 2.30 | 0.64 |
| 1:N:59:ARG:NH2 | 1:N:81:ALA:O | 2.30 | 0.64 |
| 1:M:334:GLU:OE1 | 1:M:336:ARG:NH1 | 2.30 | 0.64 |
| 1:D:917:ARG:NH2 | 1:D:943:GLU:OE1 | 2.30 | 0.64 |
| 1:F:7:LEU:HD13 | 1:F:74:LEU:HD11 | 1.77 | 0.64 |
| 1:H:7:LEU:N | 1:H:71:GLU:OE2 | 2.30 | 0.64 |
| 1:L:43:ARG:HG2 | 1:L:43:ARG:NH1 | 2.11 | 0.64 |
| 1:C:334:GLU:OE1 | 1:C:336:ARG:NH1 | 2.30 | 0.64 |
| 1:I:254:LEU:C | 1:I:255:ARG:HG2 | 2.17 | 0.64 |
| 1:C:917:ARG:NH2 | 1:C:943:GLU:OE1 | 2.30 | 0.64 |
| 1:I:367:MET:HB3 | 1:I:372:MET:HE3 | 1.79 | 0.64 |
| 1:F:753:ASN:OD1 | 1:F:753:ASN:N | 2.30 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:59:ARG:NH2 | 1:A:81:ALA:O | 2.30 | 0.64 |
| 1:L:254:LEU:C | 1:L:255:ARG:HG2 | 2.17 | 0.64 |
| 1:O:917:ARG:NH2 | 1:O:943:GLU:OE1 | 2.30 | 0.64 |
| 1:A:425:ARG:HH22 | 1:D:287:ASP:CG | 2.01 | 0.64 |
| 1:E:436:MET:HE1 | 1:E:467:ASN:HD22 | 1.61 | 0.64 |
| 1:A:7:LEU:N | 1:A:71:GLU:OE2 | 2.30 | 0.64 |
| 1:H:254:LEU:C | 1:H:255:ARG:HG2 | 2.17 | 0.64 |
| 1:B:254:LEU:C | 1:B:255:ARG:HG2 | 2.17 | 0.64 |
| 1:G:917:ARG:NH2 | 1:G:943:GLU:OE1 | 2.30 | 0.64 |
| 1:M:279:ILE:HD11 | 1:P:422:PRO:HG2 | 1.79 | 0.64 |
| 1:P:254:LEU:C | 1:P:255:ARG:HG2 | 2.17 | 0.64 |
| 1:K:334:GLU:OE1 | 1:K:336:ARG:NH1 | 2.30 | 0.64 |
| 1:N:753:ASN:N | 1:N:753:ASN:OD1 | 2.30 | 0.64 |
| 1:F:254:LEU:C | 1:F:255:ARG:HG2 | 2.17 | 0.64 |
| 1:B:334:GLU:OE1 | 1:B:336:ARG:NH1 | 2.30 | 0.64 |
| 1:E:7:LEU:N | 1:E:71:GLU:OE2 | 2.30 | 0.64 |
| 1:O:334:GLU:OE1 | 1:O:336:ARG:NH1 | 2.30 | 0.64 |
| 1:N:917:ARG:NH2 | 1:N:943:GLU:OE1 | 2.30 | 0.64 |
| 1:N:287:ASP:OD2 | 1:O:425:ARG:NH2 | 2.30 | 0.64 |
| 1:D:254:LEU:C | 1:D:255:ARG:HG2 | 2.17 | 0.64 |
| 1:G:59:ARG:NH2 | 1:G:81:ALA:O | 2.30 | 0.64 |
| 1:G:334:GLU:OE1 | 1:G:336:ARG:NH1 | 2.30 | 0.64 |
| 1:O:856:TYR:HD2 | 1:O:864:MET:HE2 | 1.61 | 0.64 |
| 1:L:917:ARG:NH2 | 1:L:943:GLU:OE1 | 2.30 | 0.64 |
| 1:I:7:LEU:HD13 | 1:I:74:LEU:HD11 | 1.77 | 0.64 |
| 1:I:952:ARG:HH11 | 1:I:952:ARG:HG2 | 1.61 | 0.64 |
| 1:J:117:GLU:OE1 | 1:J:117:GLU:N | 2.29 | 0.64 |
| 1:F:917:ARG:NH2 | 1:F:943:GLU:OE1 | 2.30 | 0.64 |
| 1:J:436:MET:HE3 | 1:J:467:ASN:HD22 | 1.63 | 0.64 |
| 1:N:287:ASP:CG | 1:O:425:ARG:HH22 | 2.01 | 0.64 |
| 1:I:334:GLU:OE1 | 1:I:336:ARG:NH1 | 2.30 | 0.64 |
| 1:G:681:GLU:HA | 1:G:681:GLU:OE2 | 1.97 | 0.64 |
| 1:C:117:GLU:N | 1:C:117:GLU:OE1 | 2.29 | 0.64 |
| 1:H:917:ARG:NH2 | 1:H:943:GLU:OE1 | 2.30 | 0.64 |
| 1:P:917:ARG:NH2 | 1:P:943:GLU:OE1 | 2.30 | 0.64 |
| 1:M:7:LEU:N | 1:M:71:GLU:OE2 | 2.30 | 0.64 |
| 1:C:43:ARG:HG2 | 1:C:43:ARG:NH1 | 2.11 | 0.64 |
| 1:M:59:ARG:NH2 | 1:M:81:ALA:O | 2.30 | 0.64 |
| 1:I:917:ARG:NH2 | 1:I:943:GLU:OE1 | 2.30 | 0.64 |
| 1:M:254:LEU:C | 1:M:255:ARG:HG2 | 2.17 | 0.64 |
| 1:H:334:GLU:OE1 | 1:H:336:ARG:NH1 | 2.30 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:7:LEU:HD13 | 1:C:74:LEU:HD11 | 1.77 | 0.64 |
| 1:N:7:LEU:N | 1:N:71:GLU:OE2 | 2.30 | 0.64 |
| 1:O:7:LEU:N | 1:O:71:GLU:OE2 | 2.30 | 0.64 |
| 1:I:43:ARG:NH1 | 1:I:43:ARG:HG2 | 2.11 | 0.64 |
| 1:P:334:GLU:OE1 | 1:P:336:ARG:NH1 | 2.30 | 0.64 |
| 1:B:917:ARG:NH2 | 1:B:943:GLU:OE1 | 2.30 | 0.64 |
| 1:J:525:SER:HB3 | 3:J:3103:HOH:O | 1.97 | 0.64 |
| 1:E:59:ARG:NH2 | 1:E:81:ALA:O | 2.30 | 0.64 |
| 1:L:436:MET:HE3 | 1:L:467:ASN:HD22 | 1.62 | 0.64 |
| 1:G:7:LEU:N | 1:G:71:GLU:OE2 | 2.30 | 0.64 |
| 1:O:681:GLU:HA | 1:O:681:GLU:OE2 | 1.97 | 0.64 |
| 1:O:59:ARG:NH2 | 1:O:81:ALA:O | 2.30 | 0.64 |
| 1:M:917:ARG:NH2 | 1:M:943:GLU:OE1 | 2.30 | 0.64 |
| 1:K:59:ARG:NH2 | 1:K:81:ALA:O | 2.30 | 0.64 |
| 1:B:681:GLU:HA | 1:B:681:GLU:OE2 | 1.97 | 0.64 |
| 1:D:681:GLU:OE2 | 1:D:681:GLU:HA | 1.97 | 0.64 |
| 1:D:59:ARG:NH2 | 1:D:81:ALA:O | 2.30 | 0.64 |
| 1:E:129:VAL:HG23 | 1:E:182:ASN:HD22 | 1.63 | 0.63 |
| 1:K:117:GLU:OE1 | 1:K:117:GLU:N | 2.29 | 0.63 |
| 1:L:367:MET:HB3 | 1:L:372:MET:HE3 | 1.79 | 0.63 |
| 1:C:367:MET:HB3 | 1:C:372:MET:HE3 | 1.79 | 0.63 |
| 1:F:117:GLU:OE1 | 1:F:117:GLU:N | 2.29 | 0.63 |
| 1:K:7:LEU:HD13 | 1:K:74:LEU:HD11 | 1.77 | 0.63 |
| 1:K:917:ARG:NH2 | 1:K:943:GLU:OE1 | 2.30 | 0.63 |
| 1:L:129:VAL:HG23 | 1:L:182:ASN:HD22 | 1.63 | 0.63 |
| 1:A:917:ARG:NH2 | 1:A:943:GLU:OE1 | 2.30 | 0.63 |
| 1:J:129:VAL:HG23 | 1:J:182:ASN:HD22 | 1.63 | 0.63 |
| 1:P:681:GLU:OE2 | 1:P:681:GLU:HA | 1.97 | 0.63 |
| 1:K:254:LEU:C | 1:K:255:ARG:HG2 | 2.17 | 0.63 |
| 1:O:129:VAL:HG23 | 1:O:182:ASN:HD22 | 1.63 | 0.63 |
| 1:P:117:GLU:OE1 | 1:P:117:GLU:N | 2.29 | 0.63 |
| 1:J:681:GLU:OE2 | 1:J:681:GLU:HA | 1.97 | 0.63 |
| 1:K:681:GLU:OE2 | 1:K:681:GLU:HA | 1.97 | 0.63 |
| 1:D:129:VAL:HG23 | 1:D:182:ASN:HD22 | 1.63 | 0.63 |
| 1:O:917:ARG:HH22 | 1:O:943:GLU:CD | 2.02 | 0.63 |
| 1:M:129:VAL:HG23 | 1:M:182:ASN:HD22 | 1.64 | 0.63 |
| 1:J:367:MET:HB3 | 1:J:372:MET:HE3 | 1.81 | 0.63 |
| 1:A:681:GLU:HA | 1:A:681:GLU:OE2 | 1.97 | 0.63 |
| 1:N:681:GLU:HA | 1:N:681:GLU:OE2 | 1.97 | 0.63 |
| 1:H:129:VAL:HG23 | 1:H:182:ASN:HD22 | 1.63 | 0.63 |
| 1:E:917:ARG:NH2 | 1:E:943:GLU:OE1 | 2.30 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:254:LEU:C | 1:C:255:ARG:HG2 | 2.17 | 0.63 |
| 1:M:681:GLU:OE2 | 1:M:681:GLU:HA | 1.97 | 0.63 |
| 1:E:681:GLU:HA | 1:E:681:GLU:OE2 | 1.97 | 0.63 |
| 1:J:254:LEU:C | 1:J:255:ARG:HG2 | 2.17 | 0.63 |
| 1:L:681:GLU:HA | 1:L:681:GLU:OE2 | 1.97 | 0.63 |
| 1:A:254:LEU:C | 1:A:255:ARG:HG2 | 2.17 | 0.63 |
| 1:L:917:ARG:HH22 | 1:L:943:GLU:CD | 2.02 | 0.63 |
| 1:A:917:ARG:HH22 | 1:A:943:GLU:CD | 2.02 | 0.63 |
| 1:F:681:GLU:OE2 | 1:F:681:GLU:HA | 1.97 | 0.63 |
| 1:K:367:MET:HB3 | 1:K:372:MET:HE3 | 1.79 | 0.63 |
| 1:N:254:LEU:C | 1:N:255:ARG:HG2 | 2.17 | 0.63 |
| 1:I:917:ARG:HH22 | 1:I:943:GLU:CD | 2.02 | 0.63 |
| 1:G:129:VAL:HG23 | 1:G:182:ASN:HD22 | 1.63 | 0.63 |
| 1:F:66:PRO:HB3 | 1:F:187:MET:CE | 2.29 | 0.63 |
| 1:E:66:PRO:HB3 | 1:E:187:MET:CE | 2.29 | 0.63 |
| 1:N:66:PRO:HB3 | 1:N:187:MET:CE | 2.29 | 0.63 |
| 1:E:367:MET:HB3 | 1:E:372:MET:HE3 | 1.79 | 0.63 |
| 1:P:129:VAL:HG23 | 1:P:182:ASN:HD22 | 1.63 | 0.63 |
| 1:G:917:ARG:HH22 | 1:G:943:GLU:CD | 2.02 | 0.62 |
| 1:K:917:ARG:HH22 | 1:K:943:GLU:CD | 2.02 | 0.62 |
| 1:A:129:VAL:HG23 | 1:A:182:ASN:HD22 | 1.63 | 0.62 |
| 1:N:367:MET:HB3 | 1:N:372:MET:HE3 | 1.81 | 0.62 |
| 1:K:129:VAL:HG23 | 1:K:182:ASN:HD22 | 1.63 | 0.62 |
| 1:J:66:PRO:HB3 | 1:J:187:MET:CE | 2.29 | 0.62 |
| 1:O:952:ARG:HG2 | 1:O:952:ARG:HH11 | 1.60 | 0.62 |
| 1:A:367:MET:HB3 | 1:A:372:MET:HE3 | 1.81 | 0.62 |
| 1:C:66:PRO:HB3 | 1:C:187:MET:CE | 2.29 | 0.62 |
| 1:D:917:ARG:HH22 | 1:D:943:GLU:CD | 2.02 | 0.62 |
| 1:B:66:PRO:HB3 | 1:B:187:MET:CE | 2.29 | 0.62 |
| 1:J:753:ASN:N | 1:J:753:ASN:OD1 | 2.30 | 0.62 |
| 1:M:917:ARG:HH22 | 1:M:943:GLU:CD | 2.02 | 0.62 |
| 1:M:66:PRO:HB3 | 1:M:187:MET:CE | 2.30 | 0.62 |
| 1:F:129:VAL:HG23 | 1:F:182:ASN:HD22 | 1.63 | 0.62 |
| 1:C:129:VAL:HG23 | 1:C:182:ASN:HD22 | 1.63 | 0.62 |
| 1:O:66:PRO:HB3 | 1:O:187:MET:CE | 2.29 | 0.62 |
| 1:N:129:VAL:HG23 | 1:N:182:ASN:HD22 | 1.63 | 0.62 |
| 1:G:66:PRO:HB3 | 1:G:187:MET:CE | 2.29 | 0.62 |
| 1:H:681:GLU:OE2 | 1:H:681:GLU:HA | 1.97 | 0.62 |
| 1:D:66:PRO:HB3 | 1:D:187:MET:CE | 2.30 | 0.62 |
| 1:E:917:ARG:HH22 | 1:E:943:GLU:CD | 2.02 | 0.62 |
| 1:M:367:MET:HB3 | 1:M:372:MET:HE3 | 1.79 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:66:PRO:HB3 | 1:L:187:MET:CE | 2.29 | 0.62 |
| 1:B:129:VAL:HG23 | 1:B:182:ASN:HD22 | 1.63 | 0.62 |
| 1:H:917:ARG:HH22 | 1:H:943:GLU:CD | 2.02 | 0.62 |
| 1:A:66:PRO:HB3 | 1:A:187:MET:CE | 2.29 | 0.62 |
| 1:K:856:TYR:HD2 | 1:K:864:MET:HE2 | 1.63 | 0.62 |
| 1:B:917:ARG:HH22 | 1:B:943:GLU:CD | 2.02 | 0.62 |
| 1:N:30:HIS:ND1 | 1:N:31:PRO:O | 2.30 | 0.62 |
| 1:I:117:GLU:N | 1:I:117:GLU:OE1 | 2.29 | 0.62 |
| 1:J:856:TYR:HD2 | 1:J:864:MET:HE2 | 1.63 | 0.62 |
| 1:C:917:ARG:HH22 | 1:C:943:GLU:CD | 2.02 | 0.62 |
| 1:H:117:GLU:OE1 | 1:H:117:GLU:N | 2.29 | 0.62 |
| 1:K:66:PRO:HB3 | 1:K:187:MET:CE | 2.29 | 0.62 |
| 1:O:367:MET:HB3 | 1:O:372:MET:HE3 | 1.81 | 0.62 |
| 1:K:753:ASN:OD1 | 1:K:753:ASN:N | 2.30 | 0.62 |
| 1:J:917:ARG:HH22 | 1:J:943:GLU:CD | 2.02 | 0.61 |
| 1:N:917:ARG:HH22 | 1:N:943:GLU:CD | 2.02 | 0.61 |
| 1:F:917:ARG:HH22 | 1:F:943:GLU:CD | 2.02 | 0.61 |
| 1:P:917:ARG:HH22 | 1:P:943:GLU:CD | 2.02 | 0.61 |
| 1:H:66:PRO:HB3 | 1:H:187:MET:CE | 2.29 | 0.61 |
| 1:I:129:VAL:HG23 | 1:I:182:ASN:HD22 | 1.63 | 0.61 |
| 1:P:66:PRO:HB3 | 1:P:187:MET:CE | 2.29 | 0.61 |
| 1:I:66:PRO:HB3 | 1:I:187:MET:CE | 2.29 | 0.61 |
| 1:A:30:HIS:ND1 | 1:A:31:PRO:O | 2.30 | 0.61 |
| 1:L:634:GLN:O | 1:L:682:LEU:HB2 | 2.01 | 0.61 |
| 1:C:436:MET:HE3 | 1:C:467:ASN:HD22 | 1.64 | 0.61 |
| 1:A:425:ARG:NH2 | 1:D:287:ASP:OD2 | 2.34 | 0.61 |
| 1:F:749:ILE:CD1 | 1:F:834:VAL:HG11 | 2.31 | 0.61 |
| 1:M:749:ILE:CD1 | 1:M:834:VAL:HG11 | 2.31 | 0.61 |
| 1:A:749:ILE:CD1 | 1:A:834:VAL:HG11 | 2.31 | 0.61 |
| 1:N:749:ILE:CD1 | 1:N:834:VAL:HG11 | 2.31 | 0.61 |
| 1:I:749:ILE:CD1 | 1:I:834:VAL:HG11 | 2.31 | 0.61 |
| 1:I:30:HIS:ND1 | 1:I:31:PRO:O | 2.30 | 0.61 |
| 1:L:753:ASN:N | 1:L:753:ASN:OD1 | 2.30 | 0.61 |
| 1:E:749:ILE:CD1 | 1:E:834:VAL:HG11 | 2.31 | 0.61 |
| 1:L:1020:TRP:HD1 | 1:L:1021:CME:N | 1.99 | 0.61 |
| 1:C:749:ILE:CD1 | 1:C:834:VAL:HG11 | 2.31 | 0.61 |
| 1:I:436:MET:HE3 | 1:I:467:ASN:HD22 | 1.66 | 0.61 |
| 1:O:1020:TRP:HD1 | 1:O:1021:CME:N | 1.99 | 0.61 |
| 1:O:129:VAL:HG23 | 1:O:182:ASN:ND2 | 2.16 | 0.61 |
| 1:F:129:VAL:HG23 | 1:F:182:ASN:ND2 | 2.16 | 0.61 |
| 1:N:129:VAL:HG23 | 1:N:182:ASN:ND2 | 2.16 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:749:ILE:CD1 | 1:O:834:VAL:HG11 | 2.31 | 0.61 |
| 1:G:749:ILE:CD1 | 1:G:834:VAL:HG11 | 2.31 | 0.61 |
| 1:H:634:GLN:O | 1:H:682:LEU:HB2 | 2.01 | 0.61 |
| 1:G:634:GLN:O | 1:G:682:LEU:HB2 | 2.01 | 0.61 |
| 1:F:1020:TRP:HD1 | 1:F:1021:CME:N | 1.99 | 0.61 |
| 1:P:1020:TRP:HD1 | 1:P:1021:CME:N | 1.99 | 0.61 |
| 1:C:634:GLN:O | 1:C:682:LEU:HB2 | 2.01 | 0.61 |
| 1:C:1020:TRP:HD1 | 1:C:1021:CME:N | 1.99 | 0.61 |
| 1:D:117:GLU:OE1 | 1:D:117:GLU:N | 2.29 | 0.61 |
| 1:G:436:MET:HE3 | 1:G:467:ASN:HD22 | 1.66 | 0.60 |
| 1:N:1020:TRP:HD1 | 1:N:1021:CME:N | 1.99 | 0.60 |
| 1:D:1020:TRP:HD1 | 1:D:1021:CME:N | 1.99 | 0.60 |
| 1:L:129:VAL:HG23 | 1:L:182:ASN:ND2 | 2.16 | 0.60 |
| 1:L:749:ILE:CD1 | 1:L:834:VAL:HG11 | 2.31 | 0.60 |
| 1:O:634:GLN:O | 1:O:682:LEU:HB2 | 2.01 | 0.60 |
| 1:P:634:GLN:O | 1:P:682:LEU:HB2 | 2.01 | 0.60 |
| 1:K:1020:TRP:HD1 | 1:K:1021:CME:N | 1.99 | 0.60 |
| 1:E:129:VAL:HG23 | 1:E:182:ASN:ND2 | 2.16 | 0.60 |
| 1:A:129:VAL:HG23 | 1:A:182:ASN:ND2 | 2.16 | 0.60 |
| 1:B:129:VAL:HG23 | 1:B:182:ASN:ND2 | 2.16 | 0.60 |
| 1:J:634:GLN:O | 1:J:682:LEU:HB2 | 2.01 | 0.60 |
| 1:H:749:ILE:CD1 | 1:H:834:VAL:HG11 | 2.31 | 0.60 |
| 1:D:749:ILE:CD1 | 1:D:834:VAL:HG11 | 2.31 | 0.60 |
| 1:H:427:THR:HA | 1:H:436:MET:HE2 | 1.83 | 0.60 |
| 1:H:1020:TRP:HD1 | 1:H:1021:CME:N | 1.99 | 0.60 |
| 1:C:129:VAL:HG23 | 1:C:182:ASN:ND2 | 2.16 | 0.60 |
| 1:O:682:LEU:HD22 | 1:O:683:PRO:HD2 | 1.83 | 0.60 |
| 1:B:634:GLN:O | 1:B:682:LEU:HB2 | 2.01 | 0.60 |
| 1:H:30:HIS:ND1 | 1:H:31:PRO:O | 2.30 | 0.60 |
| 1:G:117:GLU:N | 1:G:117:GLU:OE1 | 2.29 | 0.60 |
| 1:N:682:LEU:HD22 | 1:N:683:PRO:HD2 | 1.84 | 0.60 |
| 1:K:749:ILE:CD1 | 1:K:834:VAL:HG11 | 2.31 | 0.60 |
| 1:M:129:VAL:HG23 | 1:M:182:ASN:ND2 | 2.16 | 0.60 |
| 1:L:682:LEU:HD22 | 1:L:683:PRO:HD2 | 1.83 | 0.60 |
| 1:P:682:LEU:HD22 | 1:P:683:PRO:HD2 | 1.84 | 0.60 |
| 1:P:367:MET:HB3 | 1:P:372:MET:HE3 | 1.81 | 0.60 |
| 1:K:634:GLN:O | 1:K:682:LEU:HB2 | 2.01 | 0.60 |
| 1:K:682:LEU:HD22 | 1:K:683:PRO:HD2 | 1.84 | 0.60 |
| 1:D:30:HIS:ND1 | 1:D:31:PRO:O | 2.30 | 0.60 |
| 1:F:682:LEU:HD22 | 1:F:683:PRO:HD2 | 1.84 | 0.60 |
| 1:I:1020:TRP:HD1 | 1:I:1021:CME:N | 1.99 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:129:VAL:HG23 | 1:H:182:ASN:ND2 | 2.16 | 0.60 |
| 1:G:129:VAL:HG23 | 1:G:182:ASN:ND2 | 2.16 | 0.60 |
| 1:H:682:LEU:HD22 | 1:H:683:PRO:HD2 | 1.83 | 0.60 |
| 1:G:682:LEU:HD22 | 1:G:683:PRO:HD2 | 1.83 | 0.60 |
| 1:C:682:LEU:HD22 | 1:C:683:PRO:HD2 | 1.84 | 0.60 |
| 1:C:333:ARG:NH2 | 3:C:4202:HOH:O | 2.31 | 0.60 |
| 1:O:117:GLU:OE1 | 1:O:117:GLU:N | 2.29 | 0.60 |
| 1:J:749:ILE:CD1 | 1:J:834:VAL:HG11 | 2.31 | 0.60 |
| 1:G:322:LEU:HD23 | 1:G:324:GLU:N | 2.17 | 0.60 |
| 1:G:1020:TRP:HD1 | 1:G:1021:CME:N | 1.99 | 0.60 |
| 1:F:634:GLN:O | 1:F:682:LEU:HB2 | 2.01 | 0.60 |
| 1:E:634:GLN:O | 1:E:682:LEU:HB2 | 2.01 | 0.60 |
| 1:I:682:LEU:HD22 | 1:I:683:PRO:HD2 | 1.83 | 0.60 |
| 1:B:749:ILE:CD1 | 1:B:834:VAL:HG11 | 2.31 | 0.60 |
| 1:H:856:TYR:HD2 | 1:H:864:MET:HE2 | 1.66 | 0.60 |
| 1:L:178:ARG:NH1 | 1:L:181:GLU:O | 2.35 | 0.60 |
| 1:O:322:LEU:HD23 | 1:O:324:GLU:N | 2.17 | 0.60 |
| 1:B:1020:TRP:HD1 | 1:B:1021:CME:N | 1.99 | 0.60 |
| 1:K:129:VAL:HG23 | 1:K:182:ASN:ND2 | 2.16 | 0.60 |
| 1:N:634:GLN:O | 1:N:682:LEU:HB2 | 2.01 | 0.60 |
| 1:D:634:GLN:O | 1:D:682:LEU:HB2 | 2.01 | 0.60 |
| 1:A:634:GLN:O | 1:A:682:LEU:HB2 | 2.01 | 0.60 |
| 1:J:88:SER:HA | 1:J:366:VAL:HG21 | 1.84 | 0.60 |
| 1:F:178:ARG:NH1 | 1:F:181:GLU:O | 2.35 | 0.60 |
| 1:M:178:ARG:NH1 | 1:M:181:GLU:O | 2.35 | 0.60 |
| 1:P:322:LEU:HD23 | 1:P:324:GLU:N | 2.17 | 0.60 |
| 1:E:322:LEU:HD23 | 1:E:324:GLU:N | 2.17 | 0.60 |
| 1:N:322:LEU:HD23 | 1:N:324:GLU:N | 2.17 | 0.60 |
| 1:A:88:SER:HA | 1:A:366:VAL:HG21 | 1.84 | 0.60 |
| 1:H:360:HIS:CE1 | 1:H:362:LEU:HB2 | 2.37 | 0.60 |
| 1:K:178:ARG:NH1 | 1:K:181:GLU:O | 2.35 | 0.60 |
| 1:K:436:MET:HE3 | 1:K:467:ASN:HD22 | 1.66 | 0.60 |
| 1:H:322:LEU:HD23 | 1:H:324:GLU:N | 2.17 | 0.60 |
| 1:B:322:LEU:HD23 | 1:B:324:GLU:N | 2.17 | 0.60 |
| 1:A:1020:TRP:HD1 | 1:A:1021:CME:N | 1.99 | 0.60 |
| 1:G:367:MET:HB3 | 1:G:372:MET:HE3 | 1.82 | 0.60 |
| 1:K:577:LYS:O | 1:K:584:PRO:HA | 2.02 | 0.60 |
| 1:L:577:LYS:O | 1:L:584:PRO:HA | 2.02 | 0.60 |
| 1:B:178:ARG:NH1 | 1:B:181:GLU:O | 2.35 | 0.60 |
| 1:H:367:MET:HB3 | 1:H:372:MET:HE3 | 1.81 | 0.60 |
| 1:I:178:ARG:NH1 | 1:I:181:GLU:O | 2.35 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:753:ASN:OD1 | 1:M:753:ASN:N | 2.30 | 0.60 |
| 1:D:178:ARG:NH1 | 1:D:181:GLU:O | 2.35 | 0.60 |
| 1:P:577:LYS:O | 1:P:584:PRO:HA | 2.02 | 0.60 |
| 1:C:88:SER:HA | 1:C:366:VAL:HG21 | 1.84 | 0.60 |
| 1:M:682:LEU:HD22 | 1:M:683:PRO:HD2 | 1.83 | 0.60 |
| 1:J:322:LEU:HD23 | 1:J:324:GLU:N | 2.17 | 0.60 |
| 1:D:129:VAL:HG23 | 1:D:182:ASN:ND2 | 2.16 | 0.60 |
| 1:N:360:HIS:CE1 | 1:N:362:LEU:HB2 | 2.37 | 0.60 |
| 1:K:88:SER:HA | 1:K:366:VAL:HG21 | 1.84 | 0.60 |
| 1:B:360:HIS:CE1 | 1:B:362:LEU:HB2 | 2.37 | 0.60 |
| 1:A:577:LYS:O | 1:A:584:PRO:HA | 2.02 | 0.60 |
| 1:K:333:ARG:NH2 | 3:K:4202:HOH:O | 2.31 | 0.60 |
| 1:L:117:GLU:OE1 | 1:L:117:GLU:N | 2.29 | 0.60 |
| 1:K:360:HIS:CE1 | 1:K:362:LEU:HB2 | 2.37 | 0.60 |
| 1:H:577:LYS:O | 1:H:584:PRO:HA | 2.02 | 0.60 |
| 1:P:436:MET:HE3 | 1:P:467:ASN:HD22 | 1.66 | 0.59 |
| 1:F:427:THR:HA | 1:F:436:MET:HE2 | 1.83 | 0.59 |
| 1:N:427:THR:HA | 1:N:436:MET:HE2 | 1.83 | 0.59 |
| 1:L:322:LEU:HD23 | 1:L:324:GLU:N | 2.17 | 0.59 |
| 1:J:744:GLU:HB3 | 1:J:745:MET:HE3 | 1.84 | 0.59 |
| 1:P:129:VAL:HG23 | 1:P:182:ASN:ND2 | 2.16 | 0.59 |
| 1:J:682:LEU:HD22 | 1:J:683:PRO:HD2 | 1.83 | 0.59 |
| 1:M:88:SER:HA | 1:M:366:VAL:HG21 | 1.84 | 0.59 |
| 1:G:178:ARG:NH1 | 1:G:181:GLU:O | 2.35 | 0.59 |
| 1:N:178:ARG:NH1 | 1:N:181:GLU:O | 2.35 | 0.59 |
| 1:G:577:LYS:O | 1:G:584:PRO:HA | 2.02 | 0.59 |
| 1:E:753:ASN:OD1 | 1:E:753:ASN:N | 2.30 | 0.59 |
| 1:N:577:LYS:O | 1:N:584:PRO:HA | 2.02 | 0.59 |
| 1:E:178:ARG:NH1 | 1:E:181:GLU:O | 2.35 | 0.59 |
| 1:B:856:TYR:HD2 | 1:B:864:MET:HE2 | 1.67 | 0.59 |
| 1:F:360:HIS:CE1 | 1:F:362:LEU:HB2 | 2.37 | 0.59 |
| 1:F:30:HIS:ND1 | 1:F:31:PRO:O | 2.30 | 0.59 |
| 1:I:322:LEU:HD23 | 1:I:324:GLU:N | 2.17 | 0.59 |
| 1:D:322:LEU:HD23 | 1:D:324:GLU:N | 2.17 | 0.59 |
| 1:M:322:LEU:HD23 | 1:M:324:GLU:N | 2.17 | 0.59 |
| 1:O:744:GLU:HB3 | 1:O:745:MET:HE3 | 1.84 | 0.59 |
| 1:I:129:VAL:HG23 | 1:I:182:ASN:ND2 | 2.16 | 0.59 |
| 1:O:178:ARG:NH1 | 1:O:181:GLU:O | 2.35 | 0.59 |
| 1:P:178:ARG:NH1 | 1:P:181:GLU:O | 2.35 | 0.59 |
| 1:O:577:LYS:O | 1:O:584:PRO:HA | 2.02 | 0.59 |
| 1:P:360:HIS:CE1 | 1:P:362:LEU:HB2 | 2.37 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:322:LEU:HD23 | 1:K:324:GLU:N | 2.17 | 0.59 |
| 1:A:322:LEU:HD23 | 1:A:324:GLU:N | 2.17 | 0.59 |
| 1:J:1020:TRP:HD1 | 1:J:1021:CME:N | 1.99 | 0.59 |
| 1:E:1020:TRP:HD1 | 1:E:1021:CME:N | 1.99 | 0.59 |
| 1:B:744:GLU:HB3 | 1:B:745:MET:HE3 | 1.84 | 0.59 |
| 1:J:129:VAL:HG23 | 1:J:182:ASN:ND2 | 2.16 | 0.59 |
| 1:I:634:GLN:O | 1:I:682:LEU:HB2 | 2.01 | 0.59 |
| 1:H:178:ARG:NH1 | 1:H:181:GLU:O | 2.35 | 0.59 |
| 1:F:577:LYS:O | 1:F:584:PRO:HA | 2.02 | 0.59 |
| 1:J:360:HIS:CE1 | 1:J:362:LEU:HB2 | 2.37 | 0.59 |
| 1:J:786:ARG:HH11 | 1:J:990:HIS:CE1 | 2.21 | 0.59 |
| 1:E:786:ARG:HH11 | 1:E:990:HIS:CE1 | 2.21 | 0.59 |
| 1:N:117:GLU:N | 1:N:117:GLU:OE1 | 2.29 | 0.59 |
| 1:J:178:ARG:NH1 | 1:J:181:GLU:O | 2.35 | 0.59 |
| 1:G:88:SER:HA | 1:G:366:VAL:HG21 | 1.84 | 0.59 |
| 1:D:360:HIS:CE1 | 1:D:362:LEU:HB2 | 2.37 | 0.59 |
| 1:B:786:ARG:HH11 | 1:B:990:HIS:CE1 | 2.21 | 0.59 |
| 1:O:88:SER:HA | 1:O:366:VAL:HG21 | 1.84 | 0.59 |
| 1:F:287:ASP:OD2 | 1:G:425:ARG:NH2 | 2.35 | 0.59 |
| 1:M:1020:TRP:HD1 | 1:M:1021:CME:N | 1.99 | 0.59 |
| 1:N:894:ARG:NH1 | 1:N:919:ASP:OD2 | 2.36 | 0.59 |
| 1:F:744:GLU:HB3 | 1:F:745:MET:HE3 | 1.84 | 0.59 |
| 1:G:744:GLU:HB3 | 1:G:745:MET:HE3 | 1.84 | 0.59 |
| 1:E:682:LEU:HD22 | 1:E:683:PRO:HD2 | 1.83 | 0.59 |
| 1:D:682:LEU:HD22 | 1:D:683:PRO:HD2 | 1.83 | 0.59 |
| 1:A:682:LEU:HD22 | 1:A:683:PRO:HD2 | 1.84 | 0.59 |
| 1:G:360:HIS:CE1 | 1:G:362:LEU:HB2 | 2.37 | 0.59 |
| 1:A:360:HIS:CE1 | 1:A:362:LEU:HB2 | 2.37 | 0.59 |
| 1:B:577:LYS:O | 1:B:584:PRO:HA | 2.02 | 0.59 |
| 1:E:88:SER:HA | 1:E:366:VAL:HG21 | 1.84 | 0.59 |
| 1:A:786:ARG:HH11 | 1:A:990:HIS:CE1 | 2.21 | 0.59 |
| 1:A:178:ARG:NH1 | 1:A:181:GLU:O | 2.35 | 0.59 |
| 1:F:894:ARG:NH1 | 1:F:919:ASP:OD2 | 2.36 | 0.59 |
| 1:C:894:ARG:NH1 | 1:C:919:ASP:OD2 | 2.36 | 0.59 |
| 1:B:894:ARG:NH1 | 1:B:919:ASP:OD2 | 2.36 | 0.59 |
| 1:N:744:GLU:HB3 | 1:N:745:MET:HE3 | 1.84 | 0.59 |
| 1:A:744:GLU:HB3 | 1:A:745:MET:HE3 | 1.84 | 0.59 |
| 1:O:786:ARG:HH11 | 1:O:990:HIS:CE1 | 2.21 | 0.59 |
| 1:I:333:ARG:NH2 | 3:I:4200:HOH:O | 2.31 | 0.59 |
| 1:C:178:ARG:NH1 | 1:C:181:GLU:O | 2.35 | 0.59 |
| 1:L:786:ARG:HH11 | 1:L:990:HIS:CE1 | 2.21 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:786:ARG:HH11 | 1:G:990:HIS:CE1 | 2.21 | 0.59 |
| 1:N:786:ARG:HH11 | 1:N:990:HIS:CE1 | 2.21 | 0.59 |
| 1:C:322:LEU:HD23 | 1:C:324:GLU:N | 2.17 | 0.59 |
| 1:B:682:LEU:HD22 | 1:B:683:PRO:HD2 | 1.84 | 0.59 |
| 1:H:786:ARG:HH11 | 1:H:990:HIS:CE1 | 2.21 | 0.59 |
| 1:F:786:ARG:HH11 | 1:F:990:HIS:CE1 | 2.21 | 0.59 |
| 1:I:577:LYS:O | 1:I:584:PRO:HA | 2.02 | 0.59 |
| 1:P:749:ILE:CD1 | 1:P:834:VAL:HG11 | 2.31 | 0.59 |
| 1:C:577:LYS:O | 1:C:584:PRO:HA | 2.02 | 0.59 |
| 1:L:88:SER:HA | 1:L:366:VAL:HG21 | 1.84 | 0.59 |
| 1:G:894:ARG:NH1 | 1:G:919:ASP:OD2 | 2.36 | 0.59 |
| 1:H:88:SER:HA | 1:H:366:VAL:HG21 | 1.84 | 0.59 |
| 1:B:117:GLU:OE1 | 1:B:117:GLU:N | 2.29 | 0.59 |
| 1:K:894:ARG:NH1 | 1:K:919:ASP:OD2 | 2.36 | 0.59 |
| 1:M:894:ARG:NH1 | 1:M:919:ASP:OD2 | 2.36 | 0.59 |
| 1:D:744:GLU:HB3 | 1:D:745:MET:HE3 | 1.84 | 0.59 |
| 1:L:744:GLU:HB3 | 1:L:745:MET:HE3 | 1.84 | 0.59 |
| 1:I:786:ARG:HH11 | 1:I:990:HIS:CE1 | 2.21 | 0.59 |
| 1:B:333:ARG:NH2 | 3:B:3305:HOH:O | 2.31 | 0.59 |
| 1:F:322:LEU:HD23 | 1:F:324:GLU:N | 2.17 | 0.59 |
| 1:J:894:ARG:NH1 | 1:J:919:ASP:OD2 | 2.36 | 0.59 |
| 1:L:894:ARG:NH1 | 1:L:919:ASP:OD2 | 2.36 | 0.59 |
| 1:K:744:GLU:HB3 | 1:K:745:MET:HE3 | 1.84 | 0.59 |
| 1:C:249:GLU:OE1 | 1:C:251:ARG:NH1 | 2.34 | 0.59 |
| 1:M:746:ASP:HA | 1:M:760:ARG:HG3 | 1.85 | 0.59 |
| 1:P:786:ARG:HH11 | 1:P:990:HIS:CE1 | 2.21 | 0.59 |
| 1:D:786:ARG:HH11 | 1:D:990:HIS:CE1 | 2.21 | 0.59 |
| 1:D:786:ARG:HH11 | 1:D:990:HIS:HE1 | 1.51 | 0.59 |
| 1:N:333:ARG:NH2 | 3:N:3308:HOH:O | 2.31 | 0.59 |
| 1:E:746:ASP:HA | 1:E:760:ARG:HG3 | 1.85 | 0.59 |
| 1:A:746:ASP:HA | 1:A:760:ARG:HG3 | 1.85 | 0.59 |
| 1:M:577:LYS:O | 1:M:584:PRO:HA | 2.02 | 0.59 |
| 1:I:360:HIS:CE1 | 1:I:362:LEU:HB2 | 2.37 | 0.59 |
| 1:I:88:SER:HA | 1:I:366:VAL:HG21 | 1.84 | 0.59 |
| 1:D:753:ASN:OD1 | 1:D:753:ASN:N | 2.30 | 0.59 |
| 1:E:894:ARG:NH1 | 1:E:919:ASP:OD2 | 2.36 | 0.58 |
| 1:A:786:ARG:HH11 | 1:A:990:HIS:HE1 | 1.50 | 0.58 |
| 1:F:746:ASP:HA | 1:F:760:ARG:HG3 | 1.85 | 0.58 |
| 1:O:360:HIS:CE1 | 1:O:362:LEU:HB2 | 2.37 | 0.58 |
| 1:N:746:ASP:HA | 1:N:760:ARG:HG3 | 1.85 | 0.58 |
| 1:C:360:HIS:CE1 | 1:C:362:LEU:HB2 | 2.37 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:377:LEU:N | 1:J:377:LEU:HD23 | 2.18 | 0.58 |
| 1:D:577:LYS:O | 1:D:584:PRO:HA | 2.02 | 0.58 |
| 1:F:88:SER:HA | 1:F:366:VAL:HG21 | 1.84 | 0.58 |
| 1:A:427:THR:HA | 1:A:436:MET:HE2 | 1.83 | 0.58 |
| 1:H:744:GLU:HB3 | 1:H:745:MET:HE3 | 1.84 | 0.58 |
| 1:M:634:GLN:O | 1:M:682:LEU:HB2 | 2.01 | 0.58 |
| 1:E:786:ARG:HH11 | 1:E:990:HIS:HE1 | 1.50 | 0.58 |
| 1:P:786:ARG:HH11 | 1:P:990:HIS:HE1 | 1.50 | 0.58 |
| 1:L:746:ASP:HA | 1:L:760:ARG:HG3 | 1.85 | 0.58 |
| 1:P:88:SER:HA | 1:P:366:VAL:HG21 | 1.84 | 0.58 |
| 1:E:360:HIS:CE1 | 1:E:362:LEU:HB2 | 2.37 | 0.58 |
| 1:O:894:ARG:NH1 | 1:O:919:ASP:OD2 | 2.36 | 0.58 |
| 1:H:894:ARG:NH1 | 1:H:919:ASP:OD2 | 2.36 | 0.58 |
| 1:H:786:ARG:HH11 | 1:H:990:HIS:HE1 | 1.50 | 0.58 |
| 1:B:287:ASP:OD2 | 1:C:425:ARG:NH2 | 2.36 | 0.58 |
| 1:N:88:SER:HA | 1:N:366:VAL:HG21 | 1.84 | 0.58 |
| 1:C:786:ARG:HH11 | 1:C:990:HIS:CE1 | 2.21 | 0.58 |
| 1:I:746:ASP:HA | 1:I:760:ARG:HG3 | 1.85 | 0.58 |
| 1:D:88:SER:HA | 1:D:366:VAL:HG21 | 1.84 | 0.58 |
| 1:E:577:LYS:O | 1:E:584:PRO:HA | 2.02 | 0.58 |
| 1:L:166:ARG:HD3 | 3:L:3144:HOH:O | 2.04 | 0.58 |
| 1:M:360:HIS:CE1 | 1:M:362:LEU:HB2 | 2.37 | 0.58 |
| 1:G:272:ALA:HB1 | 1:G:273:PRO:HD2 | 1.86 | 0.58 |
| 1:O:272:ALA:HB1 | 1:O:273:PRO:HD2 | 1.86 | 0.58 |
| 1:J:746:ASP:HA | 1:J:760:ARG:HG3 | 1.85 | 0.58 |
| 1:D:746:ASP:HA | 1:D:760:ARG:HG3 | 1.85 | 0.58 |
| 1:P:894:ARG:NH1 | 1:P:919:ASP:OD2 | 2.36 | 0.58 |
| 1:N:166:ARG:HD3 | 3:N:3141:HOH:O | 2.04 | 0.58 |
| 1:F:166:ARG:HD3 | 3:F:3140:HOH:O | 2.04 | 0.58 |
| 1:C:744:GLU:HB3 | 1:C:745:MET:HE3 | 1.84 | 0.58 |
| 1:E:333:ARG:NH2 | 3:E:4201:HOH:O | 2.31 | 0.58 |
| 1:G:166:ARG:HD3 | 3:G:3138:HOH:O | 2.04 | 0.58 |
| 1:J:249:GLU:OE1 | 1:J:251:ARG:NH1 | 2.34 | 0.58 |
| 1:I:377:LEU:HD23 | 1:I:377:LEU:N | 2.19 | 0.58 |
| 1:M:786:ARG:HH11 | 1:M:990:HIS:CE1 | 2.21 | 0.58 |
| 1:M:786:ARG:HH11 | 1:M:990:HIS:HE1 | 1.50 | 0.58 |
| 1:L:360:HIS:CE1 | 1:L:362:LEU:HB2 | 2.37 | 0.58 |
| 1:L:272:ALA:HB1 | 1:L:273:PRO:HD2 | 1.86 | 0.58 |
| 1:J:577:LYS:O | 1:J:584:PRO:HA | 2.02 | 0.58 |
| 1:M:724:GLU:O | 1:N:847:LYS:NZ | 2.27 | 0.58 |
| 1:D:436:MET:HE3 | 1:D:467:ASN:HD22 | 1.67 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:894:ARG:NH1 | 1:I:919:ASP:OD2 | 2.36 | 0.58 |
| 1:P:744:GLU:HB3 | 1:P:745:MET:HE3 | 1.84 | 0.58 |
| 1:J:786:ARG:HH11 | 1:J:990:HIS:HE1 | 1.51 | 0.58 |
| 1:O:249:GLU:OE1 | 1:O:251:ARG:NH1 | 2.34 | 0.58 |
| 1:E:434:PRO:HB3 | 1:H:434:PRO:HB3 | 1.84 | 0.58 |
| 1:B:88:SER:HA | 1:B:366:VAL:HG21 | 1.84 | 0.58 |
| 1:G:249:GLU:OE1 | 1:G:251:ARG:NH1 | 2.34 | 0.58 |
| 1:C:856:TYR:HD2 | 1:C:864:MET:HE2 | 1.67 | 0.58 |
| 1:O:427:THR:HA | 1:O:436:MET:HE2 | 1.86 | 0.58 |
| 1:L:597:ASN:HD22 | 1:L:599:ARG:H | 1.52 | 0.58 |
| 1:I:272:ALA:HB1 | 1:I:273:PRO:HD2 | 1.86 | 0.58 |
| 1:H:746:ASP:HA | 1:H:760:ARG:HG3 | 1.86 | 0.58 |
| 1:K:597:ASN:HD22 | 1:K:599:ARG:H | 1.52 | 0.58 |
| 1:J:272:ALA:HB1 | 1:J:273:PRO:HD2 | 1.86 | 0.58 |
| 1:K:786:ARG:HH11 | 1:K:990:HIS:CE1 | 2.21 | 0.58 |
| 1:A:377:LEU:HD23 | 1:A:377:LEU:N | 2.18 | 0.58 |
| 1:B:377:LEU:N | 1:B:377:LEU:HD23 | 2.18 | 0.58 |
| 1:M:333:ARG:NH2 | 3:M:4201:HOH:O | 2.31 | 0.58 |
| 1:A:249:GLU:OE1 | 1:A:251:ARG:NH1 | 2.34 | 0.58 |
| 1:A:894:ARG:NH1 | 1:A:919:ASP:OD2 | 2.36 | 0.58 |
| 1:C:166:ARG:HD3 | 3:C:4034:HOH:O | 2.04 | 0.58 |
| 1:E:744:GLU:HB3 | 1:E:745:MET:HE3 | 1.84 | 0.58 |
| 1:B:786:ARG:HH11 | 1:B:990:HIS:HE1 | 1.51 | 0.58 |
| 1:K:786:ARG:HH11 | 1:K:990:HIS:HE1 | 1.51 | 0.58 |
| 1:M:830:LEU:HD11 | 1:N:830:LEU:HD11 | 1.86 | 0.58 |
| 1:E:597:ASN:HD22 | 1:E:599:ARG:H | 1.52 | 0.58 |
| 1:B:272:ALA:HB1 | 1:B:273:PRO:HD2 | 1.86 | 0.58 |
| 1:M:377:LEU:N | 1:M:377:LEU:HD23 | 2.19 | 0.58 |
| 1:N:377:LEU:HD23 | 1:N:377:LEU:N | 2.19 | 0.58 |
| 1:C:746:ASP:HA | 1:C:760:ARG:HG3 | 1.85 | 0.58 |
| 1:N:420:MET:O | 1:O:282:ARG:HD3 | 2.03 | 0.58 |
| 1:P:166:ARG:HG3 | 1:P:392:TYR:CB | 2.34 | 0.58 |
| 1:D:597:ASN:HD22 | 1:D:599:ARG:H | 1.52 | 0.58 |
| 1:A:272:ALA:HB1 | 1:A:273:PRO:HD2 | 1.86 | 0.58 |
| 1:N:272:ALA:HB1 | 1:N:273:PRO:HD2 | 1.86 | 0.58 |
| 1:G:668:VAL:HG13 | 1:G:669:PRO:HD2 | 1.86 | 0.58 |
| 1:P:746:ASP:HA | 1:P:760:ARG:HG3 | 1.85 | 0.58 |
| 1:F:272:ALA:HB1 | 1:F:273:PRO:HD2 | 1.86 | 0.58 |
| 1:B:166:ARG:HD3 | 3:B:3139:HOH:O | 2.04 | 0.57 |
| 1:C:786:ARG:HH11 | 1:C:990:HIS:HE1 | 1.50 | 0.57 |
| 1:C:753:ASN:N | 1:C:753:ASN:OD1 | 2.30 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:377:LEU:HD23 | 1:L:377:LEU:N | 2.18 | 0.57 |
| 1:O:668:VAL:HG13 | 1:O:669:PRO:HD2 | 1.87 | 0.57 |
| 1:K:272:ALA:HB1 | 1:K:273:PRO:HD2 | 1.86 | 0.57 |
| 1:A:333:ARG:NH2 | 3:A:4202:HOH:O | 2.31 | 0.57 |
| 1:M:597:ASN:HD22 | 1:M:599:ARG:H | 1.52 | 0.57 |
| 1:B:436:MET:HE3 | 1:B:467:ASN:HD22 | 1.69 | 0.57 |
| 1:A:668:VAL:HG13 | 1:A:669:PRO:HD2 | 1.87 | 0.57 |
| 1:I:668:VAL:HG13 | 1:I:669:PRO:HD2 | 1.87 | 0.57 |
| 1:M:249:GLU:OE1 | 1:M:251:ARG:NH1 | 2.34 | 0.57 |
| 1:L:30:HIS:ND1 | 1:L:31:PRO:O | 2.30 | 0.57 |
| 1:I:744:GLU:HB3 | 1:I:745:MET:HE3 | 1.85 | 0.57 |
| 1:E:166:ARG:HD3 | 3:E:4034:HOH:O | 2.04 | 0.57 |
| 1:M:166:ARG:HG3 | 1:M:392:TYR:CB | 2.34 | 0.57 |
| 1:N:434:PRO:HB3 | 1:O:434:PRO:HB3 | 1.85 | 0.57 |
| 1:M:744:GLU:HB3 | 1:M:745:MET:HE3 | 1.85 | 0.57 |
| 1:E:166:ARG:HG3 | 1:E:392:TYR:CB | 2.34 | 0.57 |
| 1:C:272:ALA:HB1 | 1:C:273:PRO:HD2 | 1.86 | 0.57 |
| 1:B:668:VAL:HG13 | 1:B:669:PRO:HD2 | 1.86 | 0.57 |
| 1:G:377:LEU:HD23 | 1:G:377:LEU:N | 2.18 | 0.57 |
| 1:O:377:LEU:N | 1:O:377:LEU:HD23 | 2.18 | 0.57 |
| 1:B:597:ASN:HD22 | 1:B:599:ARG:H | 1.52 | 0.57 |
| 1:D:166:ARG:HD3 | 3:D:3147:HOH:O | 2.04 | 0.57 |
| 1:L:668:VAL:HG13 | 1:L:669:PRO:HD2 | 1.86 | 0.57 |
| 1:D:377:LEU:N | 1:D:377:LEU:HD23 | 2.18 | 0.57 |
| 1:C:668:VAL:HG13 | 1:C:669:PRO:HD2 | 1.87 | 0.57 |
| 1:P:597:ASN:HD22 | 1:P:599:ARG:H | 1.52 | 0.57 |
| 1:G:166:ARG:HG3 | 1:G:392:TYR:CB | 2.34 | 0.57 |
| 1:O:166:ARG:HG3 | 1:O:392:TYR:CB | 2.34 | 0.57 |
| 1:O:746:ASP:HA | 1:O:760:ARG:HG3 | 1.85 | 0.57 |
| 1:G:746:ASP:HA | 1:G:760:ARG:HG3 | 1.85 | 0.57 |
| 1:A:279:ILE:HD11 | 1:D:422:PRO:HG2 | 1.86 | 0.57 |
| 1:C:377:LEU:N | 1:C:377:LEU:HD23 | 2.18 | 0.57 |
| 1:I:279:ILE:HD11 | 1:L:422:PRO:HG2 | 1.85 | 0.57 |
| 1:H:166:ARG:HG3 | 1:H:392:TYR:CB | 2.34 | 0.57 |
| 1:N:166:ARG:HG3 | 1:N:392:TYR:CB | 2.34 | 0.57 |
| 1:I:166:ARG:HG3 | 1:I:392:TYR:CB | 2.34 | 0.57 |
| 1:I:786:ARG:HH11 | 1:I:990:HIS:HE1 | 1.50 | 0.57 |
| 1:O:333:ARG:NH2 | 3:O:3305:HOH:O | 2.31 | 0.57 |
| 1:J:30:HIS:ND1 | 1:J:31:PRO:O | 2.30 | 0.57 |
| 1:K:30:HIS:ND1 | 1:K:31:PRO:O | 2.30 | 0.57 |
| 1:D:747:PHE:HE1 | 1:D:825:CYS:HG | 1.51 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:668:VAL:HG13 | 1:N:669:PRO:HD2 | 1.87 | 0.57 |
| 1:P:166:ARG:HD3 | 3:P:3146:HOH:O | 2.04 | 0.57 |
| 1:B:166:ARG:HG3 | 1:B:392:TYR:CB | 2.34 | 0.57 |
| 1:I:166:ARG:HD3 | 3:I:4034:HOH:O | 2.04 | 0.57 |
| 1:K:166:ARG:HD3 | 3:K:4034:HOH:O | 2.04 | 0.57 |
| 1:F:786:ARG:HH11 | 1:F:990:HIS:HE1 | 1.50 | 0.57 |
| 1:F:668:VAL:HG13 | 1:F:669:PRO:HD2 | 1.86 | 0.57 |
| 1:G:333:ARG:NH2 | 3:G:3305:HOH:O | 2.31 | 0.57 |
| 1:A:597:ASN:HD22 | 1:A:599:ARG:H | 1.52 | 0.57 |
| 1:B:249:GLU:OE1 | 1:B:251:ARG:NH1 | 2.34 | 0.57 |
| 1:D:894:ARG:NH1 | 1:D:919:ASP:OD2 | 2.36 | 0.57 |
| 1:D:166:ARG:HG3 | 1:D:392:TYR:CB | 2.34 | 0.57 |
| 1:E:856:TYR:CD2 | 1:E:864:MET:HE2 | 2.40 | 0.57 |
| 1:F:166:ARG:HG3 | 1:F:392:TYR:CB | 2.34 | 0.57 |
| 1:E:63:PHE:CB | 1:E:64:PRO:HD2 | 2.34 | 0.57 |
| 1:J:597:ASN:HD22 | 1:J:599:ARG:H | 1.52 | 0.57 |
| 1:D:249:GLU:OE1 | 1:D:251:ARG:NH1 | 2.34 | 0.57 |
| 1:O:166:ARG:HD3 | 3:O:3138:HOH:O | 2.04 | 0.57 |
| 1:J:166:ARG:HD3 | 3:J:3141:HOH:O | 2.04 | 0.57 |
| 1:M:272:ALA:HB1 | 1:M:273:PRO:HD2 | 1.86 | 0.57 |
| 1:P:272:ALA:HB1 | 1:P:273:PRO:HD2 | 1.86 | 0.57 |
| 1:E:249:GLU:OE1 | 1:E:251:ARG:NH1 | 2.34 | 0.57 |
| 1:C:30:HIS:ND1 | 1:C:31:PRO:O | 2.30 | 0.57 |
| 1:J:422:PRO:HG2 | 1:K:279:ILE:HD11 | 1.85 | 0.57 |
| 1:B:949:HIS:HD2 | 1:B:1020:TRP:HE1 | 1.53 | 0.56 |
| 1:P:30:HIS:ND1 | 1:P:31:PRO:O | 2.30 | 0.56 |
| 1:H:668:VAL:HG13 | 1:H:669:PRO:HD2 | 1.86 | 0.56 |
| 1:H:597:ASN:HD22 | 1:H:599:ARG:H | 1.52 | 0.56 |
| 1:N:249:GLU:OE1 | 1:N:251:ARG:NH1 | 2.34 | 0.56 |
| 1:A:166:ARG:HD3 | 3:A:4034:HOH:O | 2.04 | 0.56 |
| 1:A:166:ARG:HG3 | 1:A:392:TYR:CB | 2.34 | 0.56 |
| 1:L:786:ARG:HH11 | 1:L:990:HIS:HE1 | 1.50 | 0.56 |
| 1:F:249:GLU:OE1 | 1:F:251:ARG:NH1 | 2.35 | 0.56 |
| 1:L:949:HIS:HD2 | 1:L:1020:TRP:HE1 | 1.53 | 0.56 |
| 1:H:166:ARG:HD3 | 3:H:4034:HOH:O | 2.04 | 0.56 |
| 1:C:166:ARG:HG3 | 1:C:392:TYR:CB | 2.34 | 0.56 |
| 1:L:166:ARG:HG3 | 1:L:392:TYR:CB | 2.34 | 0.56 |
| 1:M:166:ARG:HD3 | 3:M:4034:HOH:O | 2.04 | 0.56 |
| 1:K:166:ARG:HG3 | 1:K:392:TYR:CB | 2.34 | 0.56 |
| 1:N:786:ARG:HH11 | 1:N:990:HIS:HE1 | 1.51 | 0.56 |
| 1:B:30:HIS:ND1 | 1:B:31:PRO:O | 2.30 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:377:LEU:HD23 | 1:K:377:LEU:N | 2.18 | 0.56 |
| 1:F:377:LEU:HD23 | 1:F:377:LEU:N | 2.19 | 0.56 |
| 1:C:597:ASN:HD22 | 1:C:599:ARG:H | 1.52 | 0.56 |
| 1:D:272:ALA:HB1 | 1:D:273:PRO:HD2 | 1.86 | 0.56 |
| 1:D:316:HIS:HD2 | 1:D:317:THR:O | 1.89 | 0.56 |
| 1:B:316:HIS:HD2 | 1:B:317:THR:O | 1.89 | 0.56 |
| 1:G:316:HIS:HD2 | 1:G:317:THR:O | 1.89 | 0.56 |
| 1:H:272:ALA:HB1 | 1:H:273:PRO:HD2 | 1.86 | 0.56 |
| 1:O:30:HIS:ND1 | 1:O:31:PRO:O | 2.30 | 0.56 |
| 1:D:668:VAL:HG13 | 1:D:669:PRO:HD2 | 1.87 | 0.56 |
| 1:H:333:ARG:NH2 | 3:H:4202:HOH:O | 2.31 | 0.56 |
| 1:E:316:HIS:HD2 | 1:E:317:THR:O | 1.89 | 0.56 |
| 1:N:316:HIS:HD2 | 1:N:317:THR:O | 1.89 | 0.56 |
| 1:K:493:THR:HG23 | 3:K:4019:HOH:O | 2.06 | 0.56 |
| 1:I:645:ARG:NH2 | 1:I:650:GLU:OE1 | 2.39 | 0.56 |
| 1:H:493:THR:HG23 | 3:H:4019:HOH:O | 2.06 | 0.56 |
| 1:B:746:ASP:HA | 1:B:760:ARG:HG3 | 1.85 | 0.56 |
| 1:E:30:HIS:ND1 | 1:E:31:PRO:O | 2.30 | 0.56 |
| 1:M:434:PRO:HB3 | 1:P:434:PRO:HB3 | 1.87 | 0.56 |
| 1:P:493:THR:HG23 | 3:P:3131:HOH:O | 2.06 | 0.56 |
| 1:M:316:HIS:HD2 | 1:M:317:THR:O | 1.89 | 0.56 |
| 1:A:316:HIS:HD2 | 1:A:317:THR:O | 1.89 | 0.56 |
| 1:G:786:ARG:HH11 | 1:G:990:HIS:HE1 | 1.50 | 0.56 |
| 1:F:493:THR:HG23 | 3:F:3125:HOH:O | 2.06 | 0.56 |
| 1:E:377:LEU:HD23 | 1:E:377:LEU:N | 2.18 | 0.56 |
| 1:E:645:ARG:NH2 | 1:E:650:GLU:OE1 | 2.39 | 0.56 |
| 1:D:949:HIS:HD2 | 1:D:1020:TRP:HE1 | 1.53 | 0.56 |
| 1:I:63:PHE:CB | 1:I:64:PRO:HD2 | 2.34 | 0.56 |
| 1:O:786:ARG:HH11 | 1:O:990:HIS:HE1 | 1.51 | 0.56 |
| 1:P:645:ARG:NH2 | 1:P:650:GLU:OE1 | 2.39 | 0.56 |
| 1:P:668:VAL:HG13 | 1:P:669:PRO:HD2 | 1.87 | 0.56 |
| 1:E:272:ALA:HB1 | 1:E:273:PRO:HD2 | 1.86 | 0.56 |
| 1:O:597:ASN:HD22 | 1:O:599:ARG:H | 1.52 | 0.56 |
| 1:K:746:ASP:HA | 1:K:760:ARG:HG3 | 1.85 | 0.56 |
| 1:G:597:ASN:HD22 | 1:G:599:ARG:H | 1.52 | 0.56 |
| 1:I:753:ASN:OD1 | 1:I:753:ASN:N | 2.30 | 0.56 |
| 1:D:645:ARG:NH2 | 1:D:650:GLU:OE1 | 2.39 | 0.56 |
| 1:I:493:THR:HG23 | 3:I:4019:HOH:O | 2.06 | 0.56 |
| 1:C:595:THR:HG23 | 1:C:596:PRO:CA | 2.35 | 0.56 |
| 1:I:894:ARG:HD3 | 1:I:919:ASP:OD2 | 2.06 | 0.56 |
| 1:F:63:PHE:CB | 1:F:64:PRO:HD2 | 2.34 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:597:ASN:HD22 | 1:F:599:ARG:H | 1.52 | 0.56 |
| 1:M:493:THR:HG23 | 3:M:4019:HOH:O | 2.06 | 0.56 |
| 1:P:377:LEU:HD23 | 1:P:377:LEU:N | 2.18 | 0.56 |
| 1:H:377:LEU:HD23 | 1:H:377:LEU:N | 2.19 | 0.56 |
| 1:M:856:TYR:HD2 | 1:M:864:MET:HE2 | 1.69 | 0.56 |
| 1:P:316:HIS:HD2 | 1:P:317:THR:O | 1.89 | 0.56 |
| 1:A:894:ARG:HD3 | 1:A:919:ASP:OD2 | 2.06 | 0.56 |
| 1:N:63:PHE:CB | 1:N:64:PRO:HD2 | 2.34 | 0.56 |
| 1:P:333:ARG:NH2 | 3:P:3313:HOH:O | 2.31 | 0.56 |
| 1:L:770:ILE:HD11 | 1:L:1022:GLN:HG2 | 1.88 | 0.56 |
| 1:N:645:ARG:NH2 | 1:N:650:GLU:OE1 | 2.39 | 0.56 |
| 1:A:493:THR:HG23 | 3:A:4019:HOH:O | 2.06 | 0.56 |
| 1:J:645:ARG:NH2 | 1:J:650:GLU:OE1 | 2.39 | 0.56 |
| 1:N:597:ASN:HD22 | 1:N:599:ARG:H | 1.52 | 0.56 |
| 1:F:645:ARG:NH2 | 1:F:650:GLU:OE1 | 2.39 | 0.56 |
| 1:H:316:HIS:HD2 | 1:H:317:THR:O | 1.89 | 0.55 |
| 1:L:894:ARG:HD3 | 1:L:919:ASP:OD2 | 2.06 | 0.55 |
| 1:J:166:ARG:HG3 | 1:J:392:TYR:CB | 2.34 | 0.55 |
| 1:O:645:ARG:NH2 | 1:O:650:GLU:OE1 | 2.39 | 0.55 |
| 1:F:333:ARG:NH2 | 3:F:3307:HOH:O | 2.31 | 0.55 |
| 1:J:493:THR:HG23 | 3:J:3126:HOH:O | 2.06 | 0.55 |
| 1:C:316:HIS:HD2 | 1:C:317:THR:O | 1.89 | 0.55 |
| 1:J:316:HIS:HD2 | 1:J:317:THR:O | 1.89 | 0.55 |
| 1:O:316:HIS:HD2 | 1:O:317:THR:O | 1.89 | 0.55 |
| 1:L:645:ARG:NH2 | 1:L:650:GLU:OE1 | 2.39 | 0.55 |
| 1:M:645:ARG:NH2 | 1:M:650:GLU:OE1 | 2.39 | 0.55 |
| 1:D:333:ARG:NH2 | 3:D:3314:HOH:O | 2.31 | 0.55 |
| 1:N:493:THR:HG23 | 3:N:3126:HOH:O | 2.06 | 0.55 |
| 1:G:770:ILE:HD11 | 1:G:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:J:668:VAL:HG13 | 1:J:669:PRO:HD2 | 1.87 | 0.55 |
| 1:K:645:ARG:NH2 | 1:K:650:GLU:OE1 | 2.39 | 0.55 |
| 1:D:493:THR:HG23 | 3:D:3132:HOH:O | 2.06 | 0.55 |
| 1:H:894:ARG:HD3 | 1:H:919:ASP:OD2 | 2.06 | 0.55 |
| 1:H:249:GLU:OE1 | 1:H:251:ARG:NH1 | 2.35 | 0.55 |
| 1:A:645:ARG:NH2 | 1:A:650:GLU:OE1 | 2.39 | 0.55 |
| 1:M:668:VAL:HG13 | 1:M:669:PRO:HD2 | 1.87 | 0.55 |
| 1:B:645:ARG:NH2 | 1:B:650:GLU:OE1 | 2.39 | 0.55 |
| 1:H:645:ARG:NH2 | 1:H:650:GLU:OE1 | 2.39 | 0.55 |
| 1:O:493:THR:HG23 | 3:O:3123:HOH:O | 2.06 | 0.55 |
| 1:O:770:ILE:HD11 | 1:O:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:K:668:VAL:HG13 | 1:K:669:PRO:HD2 | 1.87 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:316:HIS:HD2 | 1:L:317:THR:O | 1.89 | 0.55 |
| 1:F:949:HIS:HD2 | 1:F:1020:TRP:HE1 | 1.53 | 0.55 |
| 1:D:894:ARG:HD3 | 1:D:919:ASP:OD2 | 2.06 | 0.55 |
| 1:O:894:ARG:HD3 | 1:O:919:ASP:OD2 | 2.06 | 0.55 |
| 1:C:894:ARG:HD3 | 1:C:919:ASP:OD2 | 2.06 | 0.55 |
| 1:H:360:HIS:ND1 | 1:H:361:PRO:HD2 | 2.22 | 0.55 |
| 1:D:360:HIS:ND1 | 1:D:361:PRO:HD2 | 2.22 | 0.55 |
| 1:G:645:ARG:NH2 | 1:G:650:GLU:OE1 | 2.39 | 0.55 |
| 1:L:493:THR:HG23 | 3:L:3129:HOH:O | 2.06 | 0.55 |
| 1:P:249:GLU:OE1 | 1:P:251:ARG:NH1 | 2.34 | 0.55 |
| 1:P:824:GLN:O | 1:P:838:THR:HA | 2.07 | 0.55 |
| 1:J:824:GLN:O | 1:J:838:THR:HA | 2.07 | 0.55 |
| 1:K:824:GLN:O | 1:K:838:THR:HA | 2.07 | 0.55 |
| 1:C:493:THR:HG23 | 3:C:4019:HOH:O | 2.06 | 0.55 |
| 1:C:433:LEU:HB3 | 1:C:434:PRO:HD3 | 1.89 | 0.55 |
| 1:N:949:HIS:HD2 | 1:N:1020:TRP:HE1 | 1.53 | 0.55 |
| 1:J:894:ARG:HD3 | 1:J:919:ASP:OD2 | 2.06 | 0.55 |
| 1:G:856:TYR:CD2 | 1:G:864:MET:HE2 | 2.41 | 0.55 |
| 1:P:360:HIS:ND1 | 1:P:361:PRO:HD2 | 2.22 | 0.55 |
| 1:J:360:HIS:ND1 | 1:J:361:PRO:HD2 | 2.22 | 0.55 |
| 1:E:360:HIS:ND1 | 1:E:361:PRO:HD2 | 2.22 | 0.55 |
| 1:H:824:GLN:O | 1:H:838:THR:HA | 2.07 | 0.55 |
| 1:I:824:GLN:O | 1:I:838:THR:HA | 2.07 | 0.55 |
| 1:O:824:GLN:O | 1:O:838:THR:HA | 2.07 | 0.55 |
| 1:A:422:PRO:HG2 | 1:D:279:ILE:CD1 | 2.37 | 0.55 |
| 1:G:949:HIS:HD2 | 1:G:1020:TRP:HE1 | 1.53 | 0.55 |
| 1:K:894:ARG:HD3 | 1:K:919:ASP:OD2 | 2.06 | 0.55 |
| 1:B:894:ARG:HD3 | 1:B:919:ASP:OD2 | 2.06 | 0.55 |
| 1:K:43:ARG:NH1 | 1:K:44:THR:HG23 | 2.22 | 0.55 |
| 1:A:360:HIS:ND1 | 1:A:361:PRO:HD2 | 2.22 | 0.55 |
| 1:O:651:LEU:HD12 | 1:O:668:VAL:O | 2.07 | 0.55 |
| 1:N:43:ARG:NH1 | 1:N:44:THR:HG23 | 2.22 | 0.55 |
| 1:O:360:HIS:ND1 | 1:O:361:PRO:HD2 | 2.22 | 0.55 |
| 1:G:651:LEU:HD12 | 1:G:668:VAL:O | 2.07 | 0.55 |
| 1:F:651:LEU:HD12 | 1:F:668:VAL:O | 2.07 | 0.55 |
| 1:D:651:LEU:HD12 | 1:D:668:VAL:O | 2.07 | 0.55 |
| 1:B:824:GLN:O | 1:B:838:THR:HA | 2.07 | 0.55 |
| 1:A:770:ILE:HD11 | 1:A:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:C:645:ARG:NH2 | 1:C:650:GLU:OE1 | 2.39 | 0.55 |
| 1:J:770:ILE:HD11 | 1:J:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:E:668:VAL:HG13 | 1:E:669:PRO:HD2 | 1.87 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:894:ARG:HD3 | 1:F:919:ASP:OD2 | 2.06 | 0.55 |
| 1:N:894:ARG:HD3 | 1:N:919:ASP:OD2 | 2.06 | 0.55 |
| 1:J:43:ARG:NH1 | 1:J:44:THR:HG23 | 2.22 | 0.55 |
| 1:C:43:ARG:NH1 | 1:C:44:THR:HG23 | 2.22 | 0.55 |
| 1:F:43:ARG:NH1 | 1:F:44:THR:HG23 | 2.22 | 0.55 |
| 1:M:651:LEU:HD12 | 1:M:668:VAL:O | 2.07 | 0.55 |
| 1:A:422:PRO:HG2 | 1:D:279:ILE:HD11 | 1.89 | 0.55 |
| 1:M:30:HIS:ND1 | 1:M:31:PRO:O | 2.30 | 0.55 |
| 1:G:824:GLN:O | 1:G:838:THR:HA | 2.07 | 0.55 |
| 1:L:856:TYR:HD2 | 1:L:864:MET:HE2 | 1.71 | 0.55 |
| 1:B:493:THR:HG23 | 3:B:3124:HOH:O | 2.06 | 0.55 |
| 1:I:597:ASN:HD22 | 1:I:599:ARG:H | 1.52 | 0.55 |
| 1:I:316:HIS:HD2 | 1:I:317:THR:O | 1.89 | 0.55 |
| 1:F:316:HIS:HD2 | 1:F:317:THR:O | 1.89 | 0.55 |
| 1:P:949:HIS:HD2 | 1:P:1020:TRP:HE1 | 1.53 | 0.55 |
| 1:F:433:LEU:HB3 | 1:F:434:PRO:HD3 | 1.89 | 0.55 |
| 1:G:433:LEU:HB3 | 1:G:434:PRO:HD3 | 1.89 | 0.55 |
| 1:P:43:ARG:NH1 | 1:P:44:THR:HG23 | 2.22 | 0.55 |
| 1:E:43:ARG:NH1 | 1:E:44:THR:HG23 | 2.22 | 0.55 |
| 1:I:360:HIS:ND1 | 1:I:361:PRO:HD2 | 2.22 | 0.55 |
| 1:N:433:LEU:HB3 | 1:N:434:PRO:HD3 | 1.89 | 0.55 |
| 1:E:651:LEU:HD12 | 1:E:668:VAL:O | 2.07 | 0.55 |
| 1:L:740:LEU:HD12 | 1:L:741:THR:H | 1.72 | 0.55 |
| 1:E:493:THR:HG23 | 3:E:4019:HOH:O | 2.06 | 0.55 |
| 1:I:433:LEU:HB3 | 1:I:434:PRO:HD3 | 1.89 | 0.55 |
| 1:C:824:GLN:O | 1:C:838:THR:HA | 2.07 | 0.55 |
| 1:D:433:LEU:HB3 | 1:D:434:PRO:HD3 | 1.89 | 0.55 |
| 1:D:770:ILE:HD11 | 1:D:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:G:894:ARG:HD3 | 1:G:919:ASP:OD2 | 2.06 | 0.55 |
| 1:M:894:ARG:HD3 | 1:M:919:ASP:OD2 | 2.06 | 0.55 |
| 1:N:360:HIS:ND1 | 1:N:361:PRO:HD2 | 2.22 | 0.55 |
| 1:O:433:LEU:HB3 | 1:O:434:PRO:HD3 | 1.89 | 0.55 |
| 1:L:651:LEU:HD12 | 1:L:668:VAL:O | 2.07 | 0.55 |
| 1:M:824:GLN:O | 1:M:838:THR:HA | 2.07 | 0.55 |
| 1:N:279:ILE:HD11 | 1:O:422:PRO:HG2 | 1.89 | 0.55 |
| 1:B:770:ILE:HD11 | 1:B:1022:GLN:HG2 | 1.88 | 0.55 |
| 1:C:949:HIS:HD2 | 1:C:1020:TRP:HE1 | 1.53 | 0.54 |
| 1:E:894:ARG:HD3 | 1:E:919:ASP:OD2 | 2.06 | 0.54 |
| 1:H:43:ARG:NH1 | 1:H:44:THR:HG23 | 2.22 | 0.54 |
| 1:M:43:ARG:NH1 | 1:M:44:THR:HG23 | 2.22 | 0.54 |
| 1:A:856:TYR:CD2 | 1:A:864:MET:HE2 | 2.42 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:433:LEU:HB3 | 1:K:434:PRO:HD3 | 1.89 | 0.54 |
| 1:K:360:HIS:ND1 | 1:K:361:PRO:HD2 | 2.22 | 0.54 |
| 1:H:651:LEU:HD12 | 1:H:668:VAL:O | 2.07 | 0.54 |
| 1:P:651:LEU:HD12 | 1:P:668:VAL:O | 2.07 | 0.54 |
| 1:J:740:LEU:HD12 | 1:J:741:THR:H | 1.72 | 0.54 |
| 1:B:43:ARG:NH1 | 1:B:44:THR:HG23 | 2.22 | 0.54 |
| 1:I:43:ARG:NH1 | 1:I:44:THR:HG23 | 2.22 | 0.54 |
| 1:D:43:ARG:NH1 | 1:D:44:THR:HG23 | 2.22 | 0.54 |
| 1:J:433:LEU:HB3 | 1:J:434:PRO:HD3 | 1.89 | 0.54 |
| 1:I:254:LEU:O | 1:I:255:ARG:HG2 | 2.08 | 0.54 |
| 1:L:254:LEU:O | 1:L:255:ARG:HG2 | 2.08 | 0.54 |
| 1:P:254:LEU:O | 1:P:255:ARG:HG2 | 2.08 | 0.54 |
| 1:A:651:LEU:HD12 | 1:A:668:VAL:O | 2.07 | 0.54 |
| 1:I:651:LEU:HD12 | 1:I:668:VAL:O | 2.07 | 0.54 |
| 1:N:651:LEU:HD12 | 1:N:668:VAL:O | 2.07 | 0.54 |
| 1:L:433:LEU:HB3 | 1:L:434:PRO:HD3 | 1.89 | 0.54 |
| 1:I:249:GLU:OE1 | 1:I:251:ARG:NH1 | 2.34 | 0.54 |
| 1:N:856:TYR:HD2 | 1:N:864:MET:HE2 | 1.72 | 0.54 |
| 1:O:125:LEU:HG | 1:O:126:THR:N | 2.23 | 0.54 |
| 1:K:740:LEU:HD12 | 1:K:741:THR:H | 1.73 | 0.54 |
| 1:P:125:LEU:HG | 1:P:126:THR:N | 2.23 | 0.54 |
| 1:P:427:THR:HA | 1:P:436:MET:HE2 | 1.89 | 0.54 |
| 1:G:254:LEU:O | 1:G:255:ARG:HG2 | 2.08 | 0.54 |
| 1:G:360:HIS:ND1 | 1:G:361:PRO:HD2 | 2.22 | 0.54 |
| 1:B:651:LEU:HD12 | 1:B:668:VAL:O | 2.07 | 0.54 |
| 1:N:167:LEU:HB3 | 1:N:168:PRO:HD2 | 1.90 | 0.54 |
| 1:I:420:MET:O | 1:L:282:ARG:HD3 | 2.08 | 0.54 |
| 1:G:740:LEU:HD12 | 1:G:741:THR:H | 1.73 | 0.54 |
| 1:J:333:ARG:NH2 | 3:J:3308:HOH:O | 2.31 | 0.54 |
| 1:F:125:LEU:HG | 1:F:126:THR:N | 2.23 | 0.54 |
| 1:B:740:LEU:HD12 | 1:B:741:THR:H | 1.72 | 0.54 |
| 1:L:167:LEU:HB3 | 1:L:168:PRO:HD2 | 1.90 | 0.54 |
| 1:F:167:LEU:HB3 | 1:F:168:PRO:HD2 | 1.90 | 0.54 |
| 1:F:824:GLN:O | 1:F:838:THR:HA | 2.07 | 0.54 |
| 1:D:254:LEU:O | 1:D:255:ARG:HG2 | 2.08 | 0.54 |
| 1:A:254:LEU:O | 1:A:255:ARG:HG2 | 2.08 | 0.54 |
| 1:G:30:HIS:ND1 | 1:G:31:PRO:O | 2.30 | 0.54 |
| 1:I:167:LEU:HB3 | 1:I:168:PRO:HD2 | 1.90 | 0.54 |
| 1:P:167:LEU:HB3 | 1:P:168:PRO:HD2 | 1.90 | 0.54 |
| 1:I:740:LEU:HD12 | 1:I:741:THR:H | 1.73 | 0.54 |
| 1:G:493:THR:HG23 | 3:G:3123:HOH:O | 2.06 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:770:ILE:HD11 | 1:H:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:L:824:GLN:O | 1:L:838:THR:HA | 2.07 | 0.54 |
| 1:I:427:THR:HA | 1:I:436:MET:HE2 | 1.89 | 0.54 |
| 1:A:595:THR:HG23 | 1:A:596:PRO:CA | 2.35 | 0.54 |
| 1:P:894:ARG:HD3 | 1:P:919:ASP:OD2 | 2.06 | 0.54 |
| 1:H:63:PHE:CB | 1:H:64:PRO:HD2 | 2.34 | 0.54 |
| 1:H:254:LEU:O | 1:H:255:ARG:HG2 | 2.08 | 0.54 |
| 1:F:360:HIS:ND1 | 1:F:361:PRO:HD2 | 2.22 | 0.54 |
| 1:C:651:LEU:HD12 | 1:C:668:VAL:O | 2.07 | 0.54 |
| 1:A:824:GLN:O | 1:A:838:THR:HA | 2.07 | 0.54 |
| 1:G:73:TRP:CE2 | 1:G:122:CYS:HB3 | 2.43 | 0.54 |
| 1:A:73:TRP:CE2 | 1:A:122:CYS:HB3 | 2.43 | 0.54 |
| 1:H:125:LEU:HG | 1:H:126:THR:N | 2.23 | 0.54 |
| 1:O:73:TRP:CE2 | 1:O:122:CYS:HB3 | 2.43 | 0.54 |
| 1:M:167:LEU:HB3 | 1:M:168:PRO:HD2 | 1.90 | 0.54 |
| 1:P:73:TRP:CE2 | 1:P:122:CYS:HB3 | 2.43 | 0.54 |
| 1:D:73:TRP:CE2 | 1:D:122:CYS:HB3 | 2.43 | 0.54 |
| 1:G:43:ARG:NH1 | 1:G:44:THR:HG23 | 2.22 | 0.54 |
| 1:P:63:PHE:CB | 1:P:64:PRO:HD2 | 2.34 | 0.54 |
| 1:F:254:LEU:O | 1:F:255:ARG:HG2 | 2.08 | 0.54 |
| 1:K:254:LEU:O | 1:K:255:ARG:HG2 | 2.08 | 0.54 |
| 1:J:254:LEU:O | 1:J:255:ARG:HG2 | 2.08 | 0.54 |
| 1:N:254:LEU:O | 1:N:255:ARG:HG2 | 2.08 | 0.54 |
| 1:L:360:HIS:ND1 | 1:L:361:PRO:HD2 | 2.22 | 0.54 |
| 1:K:651:LEU:HD12 | 1:K:668:VAL:O | 2.07 | 0.54 |
| 1:H:167:LEU:HB3 | 1:H:168:PRO:HD2 | 1.90 | 0.54 |
| 1:F:770:ILE:HD11 | 1:F:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:N:770:ILE:HD11 | 1:N:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:J:127:PHE:HE2 | 1:J:184:LEU:HG | 1.73 | 0.54 |
| 1:J:50:GLN:O | 1:J:215:LEU:HA | 2.08 | 0.54 |
| 1:A:433:LEU:HB3 | 1:A:434:PRO:HD3 | 1.89 | 0.54 |
| 1:P:433:LEU:HB3 | 1:P:434:PRO:HD3 | 1.89 | 0.54 |
| 1:B:167:LEU:HB3 | 1:B:168:PRO:HD2 | 1.90 | 0.54 |
| 1:F:50:GLN:O | 1:F:215:LEU:HA | 2.08 | 0.54 |
| 1:L:333:ARG:NH2 | 3:L:3311:HOH:O | 2.31 | 0.54 |
| 1:C:50:GLN:O | 1:C:215:LEU:HA | 2.08 | 0.54 |
| 1:H:73:TRP:CE2 | 1:H:122:CYS:HB3 | 2.43 | 0.54 |
| 1:D:824:GLN:O | 1:D:838:THR:HA | 2.07 | 0.54 |
| 1:L:50:GLN:O | 1:L:215:LEU:HA | 2.08 | 0.54 |
| 1:K:427:THR:HA | 1:K:436:MET:HE2 | 1.89 | 0.54 |
| 1:H:436:MET:HE3 | 1:H:467:ASN:HD22 | 1.72 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:595:THR:HG23 | 1:D:596:PRO:CA | 2.35 | 0.54 |
| 1:K:316:HIS:HD2 | 1:K:317:THR:O | 1.89 | 0.54 |
| 1:B:254:LEU:O | 1:B:255:ARG:HG2 | 2.08 | 0.54 |
| 1:M:254:LEU:O | 1:M:255:ARG:HG2 | 2.08 | 0.54 |
| 1:C:254:LEU:O | 1:C:255:ARG:HG2 | 2.08 | 0.54 |
| 1:M:433:LEU:HB3 | 1:M:434:PRO:HD3 | 1.89 | 0.54 |
| 1:J:651:LEU:HD12 | 1:J:668:VAL:O | 2.07 | 0.54 |
| 1:C:167:LEU:HB3 | 1:C:168:PRO:HD2 | 1.90 | 0.54 |
| 1:I:770:ILE:HD11 | 1:I:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:C:770:ILE:HD11 | 1:C:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:J:125:LEU:HG | 1:J:126:THR:N | 2.23 | 0.54 |
| 1:O:43:ARG:NH1 | 1:O:44:THR:HG23 | 2.22 | 0.54 |
| 1:M:360:HIS:ND1 | 1:M:361:PRO:HD2 | 2.22 | 0.54 |
| 1:A:127:PHE:HE2 | 1:A:184:LEU:HG | 1.73 | 0.54 |
| 1:H:127:PHE:HE2 | 1:H:184:LEU:HG | 1.73 | 0.54 |
| 1:E:167:LEU:HB3 | 1:E:168:PRO:HD2 | 1.90 | 0.54 |
| 1:L:249:GLU:OE1 | 1:L:251:ARG:NH1 | 2.34 | 0.54 |
| 1:C:73:TRP:CE2 | 1:C:122:CYS:HB3 | 2.43 | 0.54 |
| 1:C:37:ARG:NH2 | 1:C:218:PRO:HD3 | 2.23 | 0.54 |
| 1:O:740:LEU:HD12 | 1:O:741:THR:H | 1.73 | 0.54 |
| 1:L:322:LEU:HD23 | 1:L:323:ILE:N | 2.23 | 0.54 |
| 1:B:322:LEU:HD23 | 1:B:323:ILE:N | 2.23 | 0.54 |
| 1:L:43:ARG:NH1 | 1:L:44:THR:HG23 | 2.22 | 0.54 |
| 1:B:360:HIS:ND1 | 1:B:361:PRO:HD2 | 2.22 | 0.54 |
| 1:E:125:LEU:HG | 1:E:126:THR:N | 2.23 | 0.54 |
| 1:N:127:PHE:HE2 | 1:N:184:LEU:HG | 1.73 | 0.54 |
| 1:H:50:GLN:O | 1:H:215:LEU:HA | 2.08 | 0.54 |
| 1:N:824:GLN:O | 1:N:838:THR:HA | 2.07 | 0.54 |
| 1:J:287:ASP:OD2 | 1:K:425:ARG:NH2 | 2.41 | 0.54 |
| 1:C:127:PHE:HE2 | 1:C:184:LEU:HG | 1.73 | 0.54 |
| 1:B:73:TRP:CE2 | 1:B:122:CYS:HB3 | 2.43 | 0.54 |
| 1:A:167:LEU:HB3 | 1:A:168:PRO:HD2 | 1.90 | 0.54 |
| 1:P:770:ILE:HD11 | 1:P:1022:GLN:HG2 | 1.88 | 0.54 |
| 1:O:436:MET:HE3 | 1:O:467:ASN:HD22 | 1.69 | 0.53 |
| 1:B:433:LEU:HB3 | 1:B:434:PRO:HD3 | 1.89 | 0.53 |
| 1:H:322:LEU:HD23 | 1:H:323:ILE:N | 2.23 | 0.53 |
| 1:F:322:LEU:HD23 | 1:F:323:ILE:N | 2.23 | 0.53 |
| 1:E:433:LEU:HB3 | 1:E:434:PRO:HD3 | 1.89 | 0.53 |
| 1:F:740:LEU:HD12 | 1:F:741:THR:H | 1.72 | 0.53 |
| 1:K:127:PHE:HE2 | 1:K:184:LEU:HG | 1.73 | 0.53 |
| 1:P:127:PHE:HE2 | 1:P:184:LEU:HG | 1.73 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:73:TRP:CE2 | 1:N:122:CYS:HB3 | 2.43 | 0.53 |
| 1:M:50:GLN:O | 1:M:215:LEU:HA | 2.08 | 0.53 |
| 1:F:37:ARG:NH2 | 1:F:218:PRO:HD3 | 2.23 | 0.53 |
| 1:F:856:TYR:HD2 | 1:F:864:MET:HE2 | 1.73 | 0.53 |
| 1:H:740:LEU:HD12 | 1:H:741:THR:H | 1.72 | 0.53 |
| 1:C:740:LEU:HD12 | 1:C:741:THR:H | 1.73 | 0.53 |
| 1:N:125:LEU:HG | 1:N:126:THR:N | 2.23 | 0.53 |
| 1:A:37:ARG:NH2 | 1:A:218:PRO:HD3 | 2.24 | 0.53 |
| 1:P:50:GLN:O | 1:P:215:LEU:HA | 2.08 | 0.53 |
| 1:D:50:GLN:O | 1:D:215:LEU:HA | 2.08 | 0.53 |
| 1:O:50:GLN:O | 1:O:215:LEU:HA | 2.08 | 0.53 |
| 1:O:37:ARG:NH2 | 1:O:218:PRO:HD3 | 2.23 | 0.53 |
| 1:B:427:THR:HA | 1:B:436:MET:HE2 | 1.86 | 0.53 |
| 1:C:322:LEU:HD23 | 1:C:323:ILE:N | 2.23 | 0.53 |
| 1:O:254:LEU:O | 1:O:255:ARG:HG2 | 2.08 | 0.53 |
| 1:E:254:LEU:O | 1:E:255:ARG:HG2 | 2.08 | 0.53 |
| 1:K:770:ILE:HD11 | 1:K:1022:GLN:HG2 | 1.89 | 0.53 |
| 1:B:127:PHE:HE2 | 1:B:184:LEU:HG | 1.73 | 0.53 |
| 1:G:50:GLN:O | 1:G:215:LEU:HA | 2.08 | 0.53 |
| 1:L:73:TRP:CE2 | 1:L:122:CYS:HB3 | 2.43 | 0.53 |
| 1:N:740:LEU:HD12 | 1:N:741:THR:H | 1.73 | 0.53 |
| 1:M:125:LEU:HG | 1:M:126:THR:N | 2.23 | 0.53 |
| 1:I:282:ARG:HD3 | 1:L:420:MET:O | 2.08 | 0.53 |
| 1:N:37:ARG:NH2 | 1:N:218:PRO:HD3 | 2.23 | 0.53 |
| 1:C:125:LEU:HG | 1:C:126:THR:N | 2.23 | 0.53 |
| 1:F:73:TRP:CE2 | 1:F:122:CYS:HB3 | 2.43 | 0.53 |
| 1:D:322:LEU:HD23 | 1:D:323:ILE:N | 2.23 | 0.53 |
| 1:G:322:LEU:HD23 | 1:G:323:ILE:N | 2.23 | 0.53 |
| 1:A:703:PRO:O | 1:A:711:ALA:HB1 | 2.09 | 0.53 |
| 1:P:703:PRO:O | 1:P:711:ALA:HB1 | 2.09 | 0.53 |
| 1:G:703:PRO:O | 1:G:711:ALA:HB1 | 2.09 | 0.53 |
| 1:N:703:PRO:O | 1:N:711:ALA:HB1 | 2.09 | 0.53 |
| 1:C:63:PHE:CB | 1:C:64:PRO:HD2 | 2.34 | 0.53 |
| 1:H:433:LEU:HB3 | 1:H:434:PRO:HD3 | 1.89 | 0.53 |
| 1:F:422:PRO:HG2 | 1:G:279:ILE:HD11 | 1.90 | 0.53 |
| 1:K:125:LEU:HG | 1:K:126:THR:N | 2.23 | 0.53 |
| 1:E:770:ILE:HD11 | 1:E:1022:GLN:HG2 | 1.88 | 0.53 |
| 1:B:369:GLU:O | 1:B:373:VAL:HG23 | 2.09 | 0.53 |
| 1:J:167:LEU:HB3 | 1:J:168:PRO:HD2 | 1.90 | 0.53 |
| 1:M:770:ILE:HD11 | 1:M:1022:GLN:HG2 | 1.88 | 0.53 |
| 1:I:127:PHE:HE2 | 1:I:184:LEU:HG | 1.73 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:369:GLU:O | 1:J:373:VAL:HG23 | 2.09 | 0.53 |
| 1:L:127:PHE:HE2 | 1:L:184:LEU:HG | 1.73 | 0.53 |
| 1:G:167:LEU:HB3 | 1:G:168:PRO:HD2 | 1.90 | 0.53 |
| 1:D:37:ARG:NH2 | 1:D:218:PRO:HD3 | 2.23 | 0.53 |
| 1:B:703:PRO:O | 1:B:711:ALA:HB1 | 2.09 | 0.53 |
| 1:D:703:PRO:O | 1:D:711:ALA:HB1 | 2.09 | 0.53 |
| 1:H:703:PRO:O | 1:H:711:ALA:HB1 | 2.09 | 0.53 |
| 1:A:673:ALA:HB1 | 1:A:674:PRO:HD2 | 1.91 | 0.53 |
| 1:G:37:ARG:NH2 | 1:G:218:PRO:HD3 | 2.23 | 0.53 |
| 1:P:740:LEU:HD12 | 1:P:741:THR:H | 1.73 | 0.53 |
| 1:G:125:LEU:HG | 1:G:126:THR:N | 2.23 | 0.53 |
| 1:L:369:GLU:O | 1:L:373:VAL:HG23 | 2.09 | 0.53 |
| 1:A:50:GLN:O | 1:A:215:LEU:HA | 2.08 | 0.53 |
| 1:A:436:MET:HE3 | 1:A:467:ASN:HD22 | 1.72 | 0.53 |
| 1:G:369:GLU:O | 1:G:373:VAL:HG23 | 2.09 | 0.53 |
| 1:O:167:LEU:HB3 | 1:O:168:PRO:HD2 | 1.90 | 0.53 |
| 1:I:369:GLU:O | 1:I:373:VAL:HG23 | 2.09 | 0.53 |
| 1:O:673:ALA:HB1 | 1:O:674:PRO:HD2 | 1.91 | 0.53 |
| 1:E:127:PHE:HE2 | 1:E:184:LEU:HG | 1.73 | 0.53 |
| 1:I:856:TYR:HD2 | 1:I:864:MET:HE2 | 1.73 | 0.53 |
| 1:F:127:PHE:HE2 | 1:F:184:LEU:HG | 1.73 | 0.53 |
| 1:P:37:ARG:NH2 | 1:P:218:PRO:HD3 | 2.23 | 0.53 |
| 1:P:322:LEU:HD23 | 1:P:323:ILE:N | 2.24 | 0.53 |
| 1:J:322:LEU:HD23 | 1:J:323:ILE:N | 2.23 | 0.53 |
| 1:O:322:LEU:HD23 | 1:O:323:ILE:N | 2.23 | 0.53 |
| 1:I:703:PRO:O | 1:I:711:ALA:HB1 | 2.09 | 0.53 |
| 1:E:703:PRO:O | 1:E:711:ALA:HB1 | 2.09 | 0.53 |
| 1:B:745:MET:HA | 1:B:745:MET:CE | 2.39 | 0.53 |
| 1:A:43:ARG:NH1 | 1:A:44:THR:HG23 | 2.22 | 0.53 |
| 1:J:745:MET:HA | 1:J:745:MET:CE | 2.39 | 0.53 |
| 1:C:360:HIS:ND1 | 1:C:361:PRO:HD2 | 2.22 | 0.53 |
| 1:A:125:LEU:HG | 1:A:126:THR:N | 2.23 | 0.53 |
| 1:E:69:VAL:HG13 | 1:E:70:PRO:HD2 | 1.91 | 0.53 |
| 1:K:50:GLN:O | 1:K:215:LEU:HA | 2.08 | 0.53 |
| 1:M:740:LEU:HD12 | 1:M:741:THR:H | 1.72 | 0.53 |
| 1:G:673:ALA:HB1 | 1:G:674:PRO:HD2 | 1.91 | 0.53 |
| 1:B:473:ARG:HD2 | 1:C:469:ASP:HB3 | 1.90 | 0.53 |
| 1:O:369:GLU:O | 1:O:373:VAL:HG23 | 2.09 | 0.53 |
| 1:H:37:ARG:NH2 | 1:H:218:PRO:HD3 | 2.24 | 0.53 |
| 1:C:673:ALA:HB1 | 1:C:674:PRO:HD2 | 1.91 | 0.53 |
| 1:N:422:PRO:HG2 | 1:O:279:ILE:HD11 | 1.89 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:282:ARG:NH1 | 1:D:419:GLY:O | 2.41 | 0.53 |
| 1:K:322:LEU:HD23 | 1:K:323:ILE:N | 2.23 | 0.53 |
| 1:M:127:PHE:HE2 | 1:M:184:LEU:HG | 1.73 | 0.53 |
| 1:M:37:ARG:NH2 | 1:M:218:PRO:HD3 | 2.23 | 0.53 |
| 1:M:69:VAL:HG13 | 1:M:70:PRO:HD2 | 1.91 | 0.53 |
| 1:N:673:ALA:HB1 | 1:N:674:PRO:HD2 | 1.91 | 0.53 |
| 1:H:673:ALA:HB1 | 1:H:674:PRO:HD2 | 1.91 | 0.53 |
| 1:E:824:GLN:O | 1:E:838:THR:HA | 2.07 | 0.53 |
| 1:E:740:LEU:HD12 | 1:E:741:THR:H | 1.73 | 0.53 |
| 1:N:322:LEU:HD23 | 1:N:323:ILE:N | 2.23 | 0.53 |
| 1:M:703:PRO:O | 1:M:711:ALA:HB1 | 2.09 | 0.53 |
| 1:J:703:PRO:O | 1:J:711:ALA:HB1 | 2.09 | 0.53 |
| 1:O:703:PRO:O | 1:O:711:ALA:HB1 | 2.09 | 0.53 |
| 1:A:63:PHE:CB | 1:A:64:PRO:HD2 | 2.34 | 0.53 |
| 1:P:745:MET:HA | 1:P:745:MET:CE | 2.39 | 0.53 |
| 1:H:745:MET:HA | 1:H:745:MET:CE | 2.39 | 0.53 |
| 1:E:73:TRP:CE2 | 1:E:122:CYS:HB3 | 2.43 | 0.53 |
| 1:E:37:ARG:NH2 | 1:E:218:PRO:HD3 | 2.24 | 0.53 |
| 1:A:740:LEU:HD12 | 1:A:741:THR:H | 1.73 | 0.53 |
| 1:L:37:ARG:NH2 | 1:L:218:PRO:HD3 | 2.23 | 0.53 |
| 1:M:673:ALA:HB1 | 1:M:674:PRO:HD2 | 1.91 | 0.53 |
| 1:D:167:LEU:HB3 | 1:D:168:PRO:HD2 | 1.90 | 0.53 |
| 1:D:369:GLU:O | 1:D:373:VAL:HG23 | 2.09 | 0.53 |
| 1:I:125:LEU:HG | 1:I:126:THR:N | 2.23 | 0.53 |
| 1:A:322:LEU:HD23 | 1:A:323:ILE:N | 2.23 | 0.53 |
| 1:J:949:HIS:HD2 | 1:J:1020:TRP:HE1 | 1.53 | 0.53 |
| 1:O:745:MET:CE | 1:O:745:MET:HA | 2.39 | 0.53 |
| 1:A:745:MET:CE | 1:A:745:MET:HA | 2.39 | 0.53 |
| 1:G:745:MET:HA | 1:G:745:MET:CE | 2.39 | 0.53 |
| 1:I:651:LEU:CD1 | 1:I:669:PRO:HA | 2.39 | 0.53 |
| 1:B:651:LEU:CD1 | 1:B:669:PRO:HA | 2.39 | 0.53 |
| 1:M:73:TRP:CE2 | 1:M:122:CYS:HB3 | 2.43 | 0.53 |
| 1:M:369:GLU:O | 1:M:373:VAL:HG23 | 2.09 | 0.53 |
| 1:H:369:GLU:O | 1:H:373:VAL:HG23 | 2.09 | 0.53 |
| 1:I:50:GLN:O | 1:I:215:LEU:HA | 2.08 | 0.53 |
| 1:I:73:TRP:CE2 | 1:I:122:CYS:HB3 | 2.43 | 0.53 |
| 1:O:949:HIS:HD2 | 1:O:1020:TRP:HE1 | 1.53 | 0.53 |
| 1:M:7:LEU:HD13 | 1:M:74:LEU:CD1 | 2.39 | 0.53 |
| 1:O:7:LEU:HD13 | 1:O:74:LEU:CD1 | 2.39 | 0.53 |
| 1:L:651:LEU:CD1 | 1:L:669:PRO:HA | 2.39 | 0.53 |
| 1:P:651:LEU:CD1 | 1:P:669:PRO:HA | 2.39 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:279:ILE:CD1 | 1:O:422:PRO:HG2 | 2.39 | 0.53 |
| 1:E:673:ALA:HB1 | 1:E:674:PRO:HD2 | 1.91 | 0.53 |
| 1:J:37:ARG:NH2 | 1:J:218:PRO:HD3 | 2.23 | 0.53 |
| 1:A:369:GLU:O | 1:A:373:VAL:HG23 | 2.09 | 0.53 |
| 1:K:37:ARG:NH2 | 1:K:218:PRO:HD3 | 2.24 | 0.53 |
| 1:P:369:GLU:O | 1:P:373:VAL:HG23 | 2.09 | 0.53 |
| 1:I:673:ALA:HB1 | 1:I:674:PRO:HD2 | 1.91 | 0.53 |
| 1:J:662:PRO:C | 1:J:663:LEU:HD23 | 2.30 | 0.53 |
| 1:D:662:PRO:C | 1:D:663:LEU:HD23 | 2.30 | 0.53 |
| 1:J:69:VAL:HG13 | 1:J:70:PRO:HD2 | 1.91 | 0.53 |
| 1:P:673:ALA:HB1 | 1:P:674:PRO:HD2 | 1.91 | 0.53 |
| 1:D:69:VAL:HG13 | 1:D:70:PRO:HD2 | 1.91 | 0.53 |
| 1:J:673:ALA:HB1 | 1:J:674:PRO:HD2 | 1.91 | 0.53 |
| 1:E:50:GLN:O | 1:E:215:LEU:HA | 2.08 | 0.53 |
| 1:E:322:LEU:HD23 | 1:E:323:ILE:N | 2.23 | 0.52 |
| 1:L:703:PRO:O | 1:L:711:ALA:HB1 | 2.09 | 0.52 |
| 1:P:278:ILE:H | 1:P:278:ILE:CD1 | 2.22 | 0.52 |
| 1:O:856:TYR:CD2 | 1:O:864:MET:HE2 | 2.43 | 0.52 |
| 1:C:682:LEU:CD2 | 1:C:683:PRO:HD2 | 2.39 | 0.52 |
| 1:J:651:LEU:CD1 | 1:J:669:PRO:HA | 2.39 | 0.52 |
| 1:K:651:LEU:CD1 | 1:K:669:PRO:HA | 2.39 | 0.52 |
| 1:L:662:PRO:C | 1:L:663:LEU:HD23 | 2.30 | 0.52 |
| 1:N:369:GLU:O | 1:N:373:VAL:HG23 | 2.09 | 0.52 |
| 1:L:673:ALA:HB1 | 1:L:674:PRO:HD2 | 1.91 | 0.52 |
| 1:F:673:ALA:HB1 | 1:F:674:PRO:HD2 | 1.91 | 0.52 |
| 1:F:210:ARG:HD3 | 3:F:3141:HOH:O | 2.10 | 0.52 |
| 1:E:422:PRO:HG2 | 1:H:279:ILE:HD11 | 1.91 | 0.52 |
| 1:B:69:VAL:HG13 | 1:B:70:PRO:HD2 | 1.91 | 0.52 |
| 1:B:50:GLN:O | 1:B:215:LEU:HA | 2.08 | 0.52 |
| 1:G:127:PHE:HE2 | 1:G:184:LEU:HG | 1.73 | 0.52 |
| 1:F:436:MET:HE3 | 1:F:467:ASN:HD22 | 1.72 | 0.52 |
| 1:N:436:MET:HE3 | 1:N:467:ASN:HD22 | 1.72 | 0.52 |
| 1:M:322:LEU:HD23 | 1:M:323:ILE:N | 2.23 | 0.52 |
| 1:F:703:PRO:O | 1:F:711:ALA:HB1 | 2.09 | 0.52 |
| 1:E:7:LEU:HD13 | 1:E:74:LEU:CD1 | 2.40 | 0.52 |
| 1:I:682:LEU:CD2 | 1:I:683:PRO:HD2 | 2.39 | 0.52 |
| 1:H:651:LEU:CD1 | 1:H:669:PRO:HA | 2.39 | 0.52 |
| 1:M:651:LEU:CD1 | 1:M:669:PRO:HA | 2.39 | 0.52 |
| 1:F:662:PRO:C | 1:F:663:LEU:HD23 | 2.30 | 0.52 |
| 1:E:420:MET:O | 1:H:282:ARG:HD3 | 2.10 | 0.52 |
| 1:J:73:TRP:CE2 | 1:J:122:CYS:HB3 | 2.43 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:127:PHE:HE2 | 1:D:184:LEU:HG | 1.73 | 0.52 |
| 1:C:369:GLU:O | 1:C:373:VAL:HG23 | 2.09 | 0.52 |
| 1:K:369:GLU:O | 1:K:373:VAL:HG23 | 2.09 | 0.52 |
| 1:J:210:ARG:HD3 | 3:J:3142:HOH:O | 2.09 | 0.52 |
| 1:E:662:PRO:C | 1:E:663:LEU:HD23 | 2.30 | 0.52 |
| 1:A:949:HIS:HD2 | 1:A:1020:TRP:HE1 | 1.53 | 0.52 |
| 1:C:7:LEU:HD13 | 1:C:74:LEU:CD1 | 2.39 | 0.52 |
| 1:A:420:MET:O | 1:D:282:ARG:HD3 | 2.09 | 0.52 |
| 1:C:651:LEU:CD1 | 1:C:669:PRO:HA | 2.39 | 0.52 |
| 1:H:251:ARG:HB3 | 1:H:253:TYR:CE2 | 2.45 | 0.52 |
| 1:P:251:ARG:HB3 | 1:P:253:TYR:CE2 | 2.45 | 0.52 |
| 1:K:69:VAL:HG13 | 1:K:70:PRO:HD2 | 1.91 | 0.52 |
| 1:K:167:LEU:HB3 | 1:K:168:PRO:HD2 | 1.90 | 0.52 |
| 1:L:210:ARG:HD3 | 3:L:3145:HOH:O | 2.09 | 0.52 |
| 1:L:125:LEU:HG | 1:L:126:THR:N | 2.23 | 0.52 |
| 1:N:50:GLN:O | 1:N:215:LEU:HA | 2.08 | 0.52 |
| 1:D:740:LEU:HD12 | 1:D:741:THR:H | 1.72 | 0.52 |
| 1:I:434:PRO:HB3 | 1:L:434:PRO:HB3 | 1.90 | 0.52 |
| 1:K:73:TRP:CE2 | 1:K:122:CYS:HB3 | 2.43 | 0.52 |
| 1:B:673:ALA:HB1 | 1:B:674:PRO:HD2 | 1.91 | 0.52 |
| 1:B:37:ARG:NH2 | 1:B:218:PRO:HD3 | 2.24 | 0.52 |
| 1:C:210:ARG:HD3 | 3:C:4035:HOH:O | 2.10 | 0.52 |
| 1:F:7:LEU:HD13 | 1:F:74:LEU:CD1 | 2.39 | 0.52 |
| 1:H:7:LEU:HD13 | 1:H:74:LEU:CD1 | 2.39 | 0.52 |
| 1:A:682:LEU:CD2 | 1:A:683:PRO:HD2 | 2.39 | 0.52 |
| 1:M:682:LEU:CD2 | 1:M:683:PRO:HD2 | 2.39 | 0.52 |
| 1:F:251:ARG:HB3 | 1:F:253:TYR:CE2 | 2.45 | 0.52 |
| 1:I:830:LEU:HD11 | 1:J:830:LEU:HD11 | 1.91 | 0.52 |
| 1:N:662:PRO:C | 1:N:663:LEU:HD23 | 2.30 | 0.52 |
| 1:P:662:PRO:C | 1:P:663:LEU:HD23 | 2.30 | 0.52 |
| 1:N:416:GLU:OE1 | 1:N:418:HIS:HB2 | 2.10 | 0.52 |
| 1:F:369:GLU:O | 1:F:373:VAL:HG23 | 2.09 | 0.52 |
| 1:I:322:LEU:HD23 | 1:I:323:ILE:N | 2.23 | 0.52 |
| 1:K:701:VAL:HG22 | 1:K:714:ILE:CD1 | 2.40 | 0.52 |
| 1:K:703:PRO:O | 1:K:711:ALA:HB1 | 2.09 | 0.52 |
| 1:K:7:LEU:HD13 | 1:K:74:LEU:CD1 | 2.40 | 0.52 |
| 1:K:745:MET:HA | 1:K:745:MET:CE | 2.39 | 0.52 |
| 1:H:682:LEU:CD2 | 1:H:683:PRO:HD2 | 2.39 | 0.52 |
| 1:J:682:LEU:CD2 | 1:J:683:PRO:HD2 | 2.39 | 0.52 |
| 1:D:682:LEU:CD2 | 1:D:683:PRO:HD2 | 2.39 | 0.52 |
| 1:L:251:ARG:HB3 | 1:L:253:TYR:CE2 | 2.45 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:127:PHE:HE2 | 1:O:184:LEU:HG | 1.73 | 0.52 |
| 1:K:251:ARG:HB3 | 1:K:253:TYR:CE2 | 2.45 | 0.52 |
| 1:D:210:ARG:HD3 | 3:D:3148:HOH:O | 2.09 | 0.52 |
| 1:B:701:VAL:HG22 | 1:B:714:ILE:CD1 | 2.40 | 0.52 |
| 1:C:701:VAL:HG22 | 1:C:714:ILE:CD1 | 2.40 | 0.52 |
| 1:C:703:PRO:O | 1:C:711:ALA:HB1 | 2.09 | 0.52 |
| 1:O:701:VAL:HG22 | 1:O:714:ILE:CD1 | 2.40 | 0.52 |
| 1:N:745:MET:CE | 1:N:745:MET:HA | 2.39 | 0.52 |
| 1:F:287:ASP:CG | 1:G:425:ARG:HH22 | 2.12 | 0.52 |
| 1:O:251:ARG:HB3 | 1:O:253:TYR:CE2 | 2.45 | 0.52 |
| 1:G:651:LEU:CD1 | 1:G:669:PRO:HA | 2.39 | 0.52 |
| 1:C:416:GLU:OE1 | 1:C:418:HIS:HB2 | 2.10 | 0.52 |
| 1:M:194:GLY:O | 1:M:198:GLU:HG3 | 2.10 | 0.52 |
| 1:H:662:PRO:C | 1:H:663:LEU:HD23 | 2.30 | 0.52 |
| 1:M:416:GLU:OE1 | 1:M:418:HIS:HB2 | 2.10 | 0.52 |
| 1:B:595:THR:HG23 | 1:B:596:PRO:CA | 2.35 | 0.52 |
| 1:G:701:VAL:HG22 | 1:G:714:ILE:CD1 | 2.40 | 0.52 |
| 1:E:701:VAL:HG22 | 1:E:714:ILE:CD1 | 2.40 | 0.52 |
| 1:I:7:LEU:HD13 | 1:I:74:LEU:CD1 | 2.39 | 0.52 |
| 1:N:651:LEU:CD1 | 1:N:669:PRO:HA | 2.39 | 0.52 |
| 1:K:210:ARG:HD3 | 3:K:4035:HOH:O | 2.09 | 0.52 |
| 1:P:416:GLU:OE1 | 1:P:418:HIS:HB2 | 2.10 | 0.52 |
| 1:L:69:VAL:HG13 | 1:L:70:PRO:HD2 | 1.91 | 0.52 |
| 1:H:194:GLY:O | 1:H:198:GLU:HG3 | 2.10 | 0.52 |
| 1:B:194:GLY:O | 1:B:198:GLU:HG3 | 2.10 | 0.52 |
| 1:I:662:PRO:C | 1:I:663:LEU:HD23 | 2.30 | 0.52 |
| 1:H:210:ARG:HD3 | 3:H:4035:HOH:O | 2.09 | 0.52 |
| 1:C:662:PRO:C | 1:C:663:LEU:HD23 | 2.30 | 0.52 |
| 1:B:125:LEU:HG | 1:B:126:THR:N | 2.23 | 0.52 |
| 1:I:69:VAL:HG13 | 1:I:70:PRO:HD2 | 1.91 | 0.52 |
| 1:D:125:LEU:HG | 1:D:126:THR:N | 2.23 | 0.52 |
| 1:A:7:LEU:HD13 | 1:A:74:LEU:CD1 | 2.39 | 0.52 |
| 1:B:881:ARG:HD3 | 1:B:987:ASP:OD1 | 2.10 | 0.52 |
| 1:A:251:ARG:HB3 | 1:A:253:TYR:CE2 | 2.45 | 0.52 |
| 1:B:251:ARG:HB3 | 1:B:253:TYR:CE2 | 2.45 | 0.52 |
| 1:N:251:ARG:HB3 | 1:N:253:TYR:CE2 | 2.45 | 0.52 |
| 1:E:416:GLU:OE1 | 1:E:418:HIS:HB2 | 2.10 | 0.52 |
| 1:B:747:PHE:HE1 | 1:B:825:CYS:HG | 1.58 | 0.52 |
| 1:H:753:ASN:N | 1:H:753:ASN:OD1 | 2.30 | 0.52 |
| 1:I:194:GLY:O | 1:I:198:GLU:HG3 | 2.10 | 0.52 |
| 1:P:210:ARG:HD3 | 3:P:3147:HOH:O | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:701:VAL:HG22 | 1:F:714:ILE:CD1 | 2.40 | 0.52 |
| 1:H:701:VAL:HG22 | 1:H:714:ILE:CD1 | 2.40 | 0.52 |
| 1:O:682:LEU:CD2 | 1:O:683:PRO:HD2 | 2.39 | 0.52 |
| 1:B:682:LEU:CD2 | 1:B:683:PRO:HD2 | 2.39 | 0.52 |
| 1:E:682:LEU:CD2 | 1:E:683:PRO:HD2 | 2.39 | 0.52 |
| 1:M:881:ARG:HD3 | 1:M:987:ASP:OD1 | 2.10 | 0.52 |
| 1:G:251:ARG:HB3 | 1:G:253:TYR:CE2 | 2.45 | 0.52 |
| 1:O:651:LEU:CD1 | 1:O:669:PRO:HA | 2.39 | 0.52 |
| 1:M:251:ARG:HB3 | 1:M:253:TYR:CE2 | 2.45 | 0.52 |
| 1:J:416:GLU:OE1 | 1:J:418:HIS:HB2 | 2.10 | 0.52 |
| 1:O:210:ARG:HD3 | 3:O:3139:HOH:O | 2.10 | 0.52 |
| 1:J:595:THR:HG23 | 1:J:596:PRO:CA | 2.35 | 0.51 |
| 1:E:949:HIS:HD2 | 1:E:1020:TRP:HE1 | 1.53 | 0.51 |
| 1:D:701:VAL:HG22 | 1:D:714:ILE:CD1 | 2.40 | 0.51 |
| 1:P:701:VAL:HG22 | 1:P:714:ILE:CD1 | 2.40 | 0.51 |
| 1:J:701:VAL:HG22 | 1:J:714:ILE:CD1 | 2.40 | 0.51 |
| 1:E:745:MET:CE | 1:E:745:MET:HA | 2.39 | 0.51 |
| 1:A:416:GLU:OE1 | 1:A:418:HIS:HB2 | 2.10 | 0.51 |
| 1:J:856:TYR:CD2 | 1:J:864:MET:HE2 | 2.45 | 0.51 |
| 1:G:682:LEU:CD2 | 1:G:683:PRO:HD2 | 2.39 | 0.51 |
| 1:E:251:ARG:HB3 | 1:E:253:TYR:CE2 | 2.45 | 0.51 |
| 1:E:651:LEU:CD1 | 1:E:669:PRO:HA | 2.39 | 0.51 |
| 1:I:251:ARG:HB3 | 1:I:253:TYR:CE2 | 2.45 | 0.51 |
| 1:H:69:VAL:HG13 | 1:H:70:PRO:HD2 | 1.91 | 0.51 |
| 1:G:662:PRO:C | 1:G:663:LEU:HD23 | 2.30 | 0.51 |
| 1:A:69:VAL:HG13 | 1:A:70:PRO:HD2 | 1.91 | 0.51 |
| 1:O:662:PRO:C | 1:O:663:LEU:HD23 | 2.30 | 0.51 |
| 1:G:210:ARG:HD3 | 3:G:3139:HOH:O | 2.10 | 0.51 |
| 1:D:673:ALA:HB1 | 1:D:674:PRO:HD2 | 1.91 | 0.51 |
| 1:O:416:GLU:OE1 | 1:O:418:HIS:HB2 | 2.10 | 0.51 |
| 1:N:701:VAL:HG22 | 1:N:714:ILE:CD1 | 2.40 | 0.51 |
| 1:O:43:ARG:HH11 | 1:O:43:ARG:CG | 2.24 | 0.51 |
| 1:N:682:LEU:CD2 | 1:N:683:PRO:HD2 | 2.39 | 0.51 |
| 1:F:682:LEU:CD2 | 1:F:683:PRO:HD2 | 2.39 | 0.51 |
| 1:L:881:ARG:HD3 | 1:L:987:ASP:OD1 | 2.10 | 0.51 |
| 1:I:881:ARG:HD3 | 1:I:987:ASP:OD1 | 2.10 | 0.51 |
| 1:C:251:ARG:HB3 | 1:C:253:TYR:CE2 | 2.45 | 0.51 |
| 1:A:651:LEU:CD1 | 1:A:669:PRO:HA | 2.39 | 0.51 |
| 1:C:69:VAL:HG13 | 1:C:70:PRO:HD2 | 1.91 | 0.51 |
| 1:I:37:ARG:NH2 | 1:I:218:PRO:HD3 | 2.24 | 0.51 |
| 1:B:416:GLU:OE1 | 1:B:418:HIS:HB2 | 2.10 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:416:GLU:OE1 | 1:F:418:HIS:HB2 | 2.10 | 0.51 |
| 1:I:416:GLU:OE1 | 1:I:418:HIS:HB2 | 2.10 | 0.51 |
| 1:F:194:GLY:O | 1:F:198:GLU:HG3 | 2.10 | 0.51 |
| 1:J:427:THR:HA | 1:J:436:MET:HE2 | 1.92 | 0.51 |
| 1:L:701:VAL:HG22 | 1:L:714:ILE:CD1 | 2.40 | 0.51 |
| 1:L:7:LEU:HD13 | 1:L:74:LEU:CD1 | 2.39 | 0.51 |
| 1:D:7:LEU:HD13 | 1:D:74:LEU:CD1 | 2.39 | 0.51 |
| 1:C:43:ARG:HH11 | 1:C:43:ARG:CG | 2.24 | 0.51 |
| 1:C:745:MET:CE | 1:C:745:MET:HA | 2.39 | 0.51 |
| 1:J:251:ARG:HB3 | 1:J:253:TYR:CE2 | 2.45 | 0.51 |
| 1:F:651:LEU:CD1 | 1:F:669:PRO:HA | 2.39 | 0.51 |
| 1:I:660:GLY:O | 1:I:662:PRO:HD3 | 2.11 | 0.51 |
| 1:K:673:ALA:HB1 | 1:K:674:PRO:HD2 | 1.91 | 0.51 |
| 1:F:473:ARG:HD3 | 1:F:473:ARG:O | 2.11 | 0.51 |
| 1:E:210:ARG:HD3 | 3:E:4035:HOH:O | 2.10 | 0.51 |
| 1:M:660:GLY:O | 1:M:662:PRO:HD3 | 2.11 | 0.51 |
| 1:E:473:ARG:HD3 | 1:E:473:ARG:O | 2.11 | 0.51 |
| 1:N:210:ARG:HD3 | 3:N:3142:HOH:O | 2.10 | 0.51 |
| 1:L:610:ASP:OD2 | 1:L:612:THR:HG23 | 2.11 | 0.51 |
| 1:B:210:ARG:HD3 | 3:B:3140:HOH:O | 2.09 | 0.51 |
| 1:O:69:VAL:HG13 | 1:O:70:PRO:HD2 | 1.91 | 0.51 |
| 1:M:278:ILE:CD1 | 1:M:278:ILE:H | 2.22 | 0.51 |
| 1:I:278:ILE:H | 1:I:278:ILE:CD1 | 2.22 | 0.51 |
| 1:A:278:ILE:H | 1:A:278:ILE:CD1 | 2.22 | 0.51 |
| 1:P:952:ARG:HD2 | 3:P:3534:HOH:O | 2.11 | 0.51 |
| 1:L:682:LEU:CD2 | 1:L:683:PRO:HD2 | 2.39 | 0.51 |
| 1:K:682:LEU:CD2 | 1:K:683:PRO:HD2 | 2.39 | 0.51 |
| 1:J:881:ARG:HD3 | 1:J:987:ASP:OD1 | 2.10 | 0.51 |
| 1:O:881:ARG:HD3 | 1:O:987:ASP:OD1 | 2.10 | 0.51 |
| 1:H:881:ARG:HD3 | 1:H:987:ASP:OD1 | 2.10 | 0.51 |
| 1:C:881:ARG:HD3 | 1:C:987:ASP:OD1 | 2.10 | 0.51 |
| 1:M:662:PRO:C | 1:M:663:LEU:HD23 | 2.30 | 0.51 |
| 1:P:610:ASP:OD2 | 1:P:612:THR:HG23 | 2.11 | 0.51 |
| 1:G:69:VAL:HG13 | 1:G:70:PRO:HD2 | 1.91 | 0.51 |
| 1:N:473:ARG:HD3 | 1:N:473:ARG:O | 2.11 | 0.51 |
| 1:I:473:ARG:HD3 | 1:I:473:ARG:O | 2.11 | 0.51 |
| 1:H:473:ARG:O | 1:H:473:ARG:HD3 | 2.11 | 0.51 |
| 1:M:473:ARG:O | 1:M:473:ARG:HD3 | 2.11 | 0.51 |
| 1:G:416:GLU:OE1 | 1:G:418:HIS:HB2 | 2.10 | 0.51 |
| 1:A:610:ASP:OD2 | 1:A:612:THR:HG23 | 2.11 | 0.51 |
| 1:P:767:GLN:HG3 | 1:P:768:MET:N | 2.26 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:662:PRO:C | 1:B:663:LEU:HD23 | 2.30 | 0.51 |
| 1:P:69:VAL:HG13 | 1:P:70:PRO:HD2 | 1.91 | 0.51 |
| 1:N:595:THR:HG23 | 1:N:596:PRO:CA | 2.35 | 0.51 |
| 1:D:416:GLU:OE1 | 1:D:418:HIS:HB2 | 2.10 | 0.51 |
| 1:K:1020:TRP:CD1 | 1:K:1021:CME:N | 2.79 | 0.51 |
| 1:H:949:HIS:HD2 | 1:H:1020:TRP:HE1 | 1.53 | 0.51 |
| 1:G:278:ILE:H | 1:G:278:ILE:CD1 | 2.22 | 0.51 |
| 1:P:7:LEU:HD13 | 1:P:74:LEU:CD1 | 2.39 | 0.51 |
| 1:G:881:ARG:HD3 | 1:G:987:ASP:OD1 | 2.11 | 0.51 |
| 1:D:251:ARG:HB3 | 1:D:253:TYR:CE2 | 2.45 | 0.51 |
| 1:E:767:GLN:HG3 | 1:E:768:MET:N | 2.26 | 0.51 |
| 1:A:194:GLY:O | 1:A:198:GLU:HG3 | 2.10 | 0.51 |
| 1:K:416:GLU:OE1 | 1:K:418:HIS:HB2 | 2.10 | 0.51 |
| 1:M:767:GLN:HG3 | 1:M:768:MET:N | 2.26 | 0.51 |
| 1:P:473:ARG:HD3 | 1:P:473:ARG:O | 2.11 | 0.51 |
| 1:D:473:ARG:HD3 | 1:D:473:ARG:O | 2.11 | 0.51 |
| 1:F:5:ASP:OD2 | 1:F:157:ARG:HA | 2.11 | 0.51 |
| 1:J:194:GLY:O | 1:J:198:GLU:HG3 | 2.10 | 0.51 |
| 1:C:767:GLN:HG3 | 1:C:768:MET:N | 2.26 | 0.51 |
| 1:K:194:GLY:O | 1:K:198:GLU:HG3 | 2.10 | 0.51 |
| 1:E:369:GLU:O | 1:E:373:VAL:HG23 | 2.09 | 0.51 |
| 1:K:660:GLY:O | 1:K:662:PRO:HD3 | 2.11 | 0.51 |
| 1:K:662:PRO:C | 1:K:663:LEU:HD23 | 2.30 | 0.51 |
| 1:N:610:ASP:OD2 | 1:N:612:THR:HG23 | 2.11 | 0.51 |
| 1:J:1020:TRP:CD1 | 1:J:1021:CME:N | 2.79 | 0.51 |
| 1:E:278:ILE:CD1 | 1:E:278:ILE:H | 2.22 | 0.51 |
| 1:L:278:ILE:CD1 | 1:L:278:ILE:H | 2.22 | 0.51 |
| 1:C:952:ARG:HD2 | 3:C:4429:HOH:O | 2.11 | 0.51 |
| 1:N:43:ARG:CG | 1:N:43:ARG:HH11 | 2.24 | 0.51 |
| 1:A:881:ARG:HD3 | 1:A:987:ASP:OD1 | 2.10 | 0.51 |
| 1:J:422:PRO:HG2 | 1:K:279:ILE:CD1 | 2.41 | 0.51 |
| 1:D:651:LEU:CD1 | 1:D:669:PRO:HA | 2.39 | 0.51 |
| 1:J:660:GLY:O | 1:J:662:PRO:HD3 | 2.11 | 0.51 |
| 1:N:194:GLY:O | 1:N:198:GLU:HG3 | 2.10 | 0.51 |
| 1:O:571:VAL:HG13 | 1:O:607:VAL:HG23 | 1.93 | 0.51 |
| 1:O:767:GLN:HG3 | 1:O:768:MET:N | 2.26 | 0.51 |
| 1:M:610:ASP:OD2 | 1:M:612:THR:HG23 | 2.11 | 0.51 |
| 1:K:473:ARG:O | 1:K:473:ARG:HD3 | 2.11 | 0.51 |
| 1:J:767:GLN:HG3 | 1:J:768:MET:N | 2.26 | 0.51 |
| 1:G:427:THR:HA | 1:G:436:MET:HE2 | 1.89 | 0.51 |
| 1:F:745:MET:HA | 1:F:745:MET:CE | 2.39 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:7:LEU:HD13 | 1:N:74:LEU:CD1 | 2.39 | 0.51 |
| 1:L:745:MET:HA | 1:L:745:MET:CE | 2.39 | 0.51 |
| 1:K:952:ARG:HD2 | 3:K:4431:HOH:O | 2.11 | 0.51 |
| 1:N:881:ARG:HD3 | 1:N:987:ASP:OD1 | 2.10 | 0.51 |
| 1:F:987:ASP:OD2 | 1:F:990:HIS:HD2 | 1.94 | 0.51 |
| 1:P:881:ARG:HD3 | 1:P:987:ASP:OD1 | 2.10 | 0.51 |
| 1:P:660:GLY:O | 1:P:662:PRO:HD3 | 2.11 | 0.51 |
| 1:C:5:ASP:OD2 | 1:C:157:ARG:HA | 2.11 | 0.51 |
| 1:O:610:ASP:OD2 | 1:O:612:THR:HG23 | 2.11 | 0.51 |
| 1:C:473:ARG:HD3 | 1:C:473:ARG:O | 2.11 | 0.51 |
| 1:G:767:GLN:HG3 | 1:G:768:MET:N | 2.26 | 0.51 |
| 1:O:753:ASN:OD1 | 1:O:753:ASN:N | 2.30 | 0.51 |
| 1:O:5:ASP:OD2 | 1:O:157:ARG:HA | 2.11 | 0.51 |
| 1:P:194:GLY:O | 1:P:198:GLU:HG3 | 2.10 | 0.51 |
| 1:A:210:ARG:HD3 | 3:A:4035:HOH:O | 2.09 | 0.51 |
| 1:H:610:ASP:OD2 | 1:H:612:THR:HG23 | 2.11 | 0.51 |
| 1:E:595:THR:HG23 | 1:E:596:PRO:CA | 2.35 | 0.51 |
| 1:I:701:VAL:HG22 | 1:I:714:ILE:CD1 | 2.40 | 0.51 |
| 1:M:701:VAL:HG22 | 1:M:714:ILE:CD1 | 2.40 | 0.51 |
| 1:J:952:ARG:HD2 | 3:J:3529:HOH:O | 2.11 | 0.51 |
| 1:P:682:LEU:CD2 | 1:P:683:PRO:HD2 | 2.39 | 0.51 |
| 1:N:987:ASP:OD2 | 1:N:990:HIS:HD2 | 1.94 | 0.51 |
| 1:M:987:ASP:OD2 | 1:M:990:HIS:HD2 | 1.94 | 0.51 |
| 1:E:610:ASP:OD2 | 1:E:612:THR:HG23 | 2.11 | 0.51 |
| 1:B:610:ASP:OD2 | 1:B:612:THR:HG23 | 2.11 | 0.51 |
| 1:A:753:ASN:OD1 | 1:A:753:ASN:N | 2.30 | 0.51 |
| 1:L:416:GLU:OE1 | 1:L:418:HIS:HB2 | 2.10 | 0.51 |
| 1:G:5:ASP:OD2 | 1:G:157:ARG:HA | 2.11 | 0.51 |
| 1:E:194:GLY:O | 1:E:198:GLU:HG3 | 2.10 | 0.51 |
| 1:I:279:ILE:CD1 | 1:L:422:PRO:HG2 | 2.40 | 0.51 |
| 1:P:73:TRP:CZ2 | 1:P:185:ALA:HB1 | 2.46 | 0.51 |
| 1:C:73:TRP:CZ2 | 1:C:185:ALA:HB1 | 2.46 | 0.51 |
| 1:H:660:GLY:O | 1:H:662:PRO:HD3 | 2.10 | 0.51 |
| 1:H:261:TRP:CZ3 | 1:H:266:GLN:HB2 | 2.46 | 0.51 |
| 1:L:767:GLN:HG3 | 1:L:768:MET:N | 2.26 | 0.51 |
| 1:G:571:VAL:HG13 | 1:G:607:VAL:HG23 | 1.93 | 0.51 |
| 1:A:662:PRO:C | 1:A:663:LEU:HD23 | 2.30 | 0.51 |
| 1:B:5:ASP:OD2 | 1:B:157:ARG:HA | 2.11 | 0.51 |
| 1:M:210:ARG:HD3 | 3:M:4035:HOH:O | 2.09 | 0.51 |
| 1:O:473:ARG:HD3 | 1:O:473:ARG:O | 2.11 | 0.51 |
| 1:H:767:GLN:HG3 | 1:H:768:MET:N | 2.26 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:767:GLN:HG3 | 1:B:768:MET:N | 2.26 | 0.51 |
| 1:K:261:TRP:CZ3 | 1:K:266:GLN:HB2 | 2.46 | 0.51 |
| 1:C:571:VAL:HG13 | 1:C:607:VAL:HG23 | 1.93 | 0.51 |
| 1:K:610:ASP:OD2 | 1:K:612:THR:HG23 | 2.11 | 0.51 |
| 1:I:210:ARG:HD3 | 3:I:4035:HOH:O | 2.10 | 0.51 |
| 1:B:571:VAL:HG13 | 1:B:607:VAL:HG23 | 1.93 | 0.51 |
| 1:L:194:GLY:O | 1:L:198:GLU:HG3 | 2.10 | 0.51 |
| 1:A:701:VAL:HG22 | 1:A:714:ILE:CD1 | 2.40 | 0.51 |
| 1:D:278:ILE:H | 1:D:278:ILE:CD1 | 2.22 | 0.51 |
| 1:J:7:LEU:HD13 | 1:J:74:LEU:CD1 | 2.39 | 0.51 |
| 1:B:63:PHE:CB | 1:B:64:PRO:HD2 | 2.34 | 0.51 |
| 1:L:43:ARG:HH11 | 1:L:43:ARG:CG | 2.24 | 0.51 |
| 1:L:741:THR:HG22 | 1:L:741:THR:O | 2.11 | 0.51 |
| 1:G:73:TRP:CZ2 | 1:G:185:ALA:HB1 | 2.46 | 0.51 |
| 1:B:73:TRP:CZ2 | 1:B:185:ALA:HB1 | 2.46 | 0.51 |
| 1:B:473:ARG:HD3 | 1:B:473:ARG:O | 2.11 | 0.51 |
| 1:D:660:GLY:O | 1:D:662:PRO:HD3 | 2.11 | 0.51 |
| 1:G:660:GLY:O | 1:G:662:PRO:HD3 | 2.11 | 0.51 |
| 1:O:660:GLY:O | 1:O:662:PRO:HD3 | 2.11 | 0.51 |
| 1:B:660:GLY:O | 1:B:662:PRO:HD3 | 2.11 | 0.51 |
| 1:L:637:GLU:HA | 1:L:679:LEU:HD23 | 1.93 | 0.51 |
| 1:K:573:GLN:HB2 | 1:K:602:CYS:O | 2.11 | 0.51 |
| 1:D:637:GLU:HA | 1:D:679:LEU:HD23 | 1.93 | 0.51 |
| 1:N:637:GLU:HA | 1:N:679:LEU:HD23 | 1.93 | 0.51 |
| 1:F:610:ASP:OD2 | 1:F:612:THR:HG23 | 2.11 | 0.51 |
| 1:A:261:TRP:CZ3 | 1:A:266:GLN:HB2 | 2.46 | 0.51 |
| 1:D:427:THR:HA | 1:D:436:MET:HE2 | 1.87 | 0.50 |
| 1:G:952:ARG:HD2 | 3:G:3527:HOH:O | 2.11 | 0.50 |
| 1:F:881:ARG:HD3 | 1:F:987:ASP:OD1 | 2.10 | 0.50 |
| 1:K:881:ARG:HD3 | 1:K:987:ASP:OD1 | 2.11 | 0.50 |
| 1:K:987:ASP:OD2 | 1:K:990:HIS:HD2 | 1.94 | 0.50 |
| 1:O:741:THR:O | 1:O:741:THR:HG22 | 2.12 | 0.50 |
| 1:K:73:TRP:CZ2 | 1:K:185:ALA:HB1 | 2.46 | 0.50 |
| 1:I:422:PRO:HG2 | 1:L:279:ILE:HD11 | 1.93 | 0.50 |
| 1:G:747:PHE:HE1 | 1:G:825:CYS:HG | 1.59 | 0.50 |
| 1:F:637:GLU:HA | 1:F:679:LEU:HD23 | 1.94 | 0.50 |
| 1:C:261:TRP:CZ3 | 1:C:266:GLN:HB2 | 2.46 | 0.50 |
| 1:K:5:ASP:OD2 | 1:K:157:ARG:HA | 2.11 | 0.50 |
| 1:A:473:ARG:O | 1:A:473:ARG:HD3 | 2.11 | 0.50 |
| 1:A:573:GLN:HB2 | 1:A:602:CYS:O | 2.12 | 0.50 |
| 1:H:416:GLU:OE1 | 1:H:418:HIS:HB2 | 2.10 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:767:GLN:HG3 | 1:D:768:MET:N | 2.26 | 0.50 |
| 1:M:595:THR:HG23 | 1:M:596:PRO:CA | 2.35 | 0.50 |
| 1:G:595:THR:HG23 | 1:G:596:PRO:CA | 2.35 | 0.50 |
| 1:O:595:THR:CG2 | 1:O:596:PRO:HA | 2.37 | 0.50 |
| 1:M:1020:TRP:CD1 | 1:M:1021:CME:N | 2.79 | 0.50 |
| 1:H:278:ILE:CD1 | 1:H:278:ILE:H | 2.22 | 0.50 |
| 1:B:278:ILE:H | 1:B:278:ILE:CD1 | 2.22 | 0.50 |
| 1:B:7:LEU:HD13 | 1:B:74:LEU:CD1 | 2.39 | 0.50 |
| 1:G:7:LEU:HD13 | 1:G:74:LEU:CD1 | 2.39 | 0.50 |
| 1:L:952:ARG:HD2 | 3:L:3532:HOH:O | 2.11 | 0.50 |
| 1:C:741:THR:HG22 | 1:C:741:THR:O | 2.12 | 0.50 |
| 1:E:73:TRP:CZ2 | 1:E:185:ALA:HB1 | 2.46 | 0.50 |
| 1:L:660:GLY:O | 1:L:662:PRO:HD3 | 2.10 | 0.50 |
| 1:K:767:GLN:HG3 | 1:K:768:MET:N | 2.26 | 0.50 |
| 1:N:261:TRP:CZ3 | 1:N:266:GLN:HB2 | 2.46 | 0.50 |
| 1:O:747:PHE:HE1 | 1:O:825:CYS:HG | 1.59 | 0.50 |
| 1:B:261:TRP:CZ3 | 1:B:266:GLN:HB2 | 2.46 | 0.50 |
| 1:G:194:GLY:O | 1:G:198:GLU:HG3 | 2.10 | 0.50 |
| 1:P:573:GLN:HB2 | 1:P:602:CYS:O | 2.11 | 0.50 |
| 1:O:261:TRP:CZ3 | 1:O:266:GLN:HB2 | 2.46 | 0.50 |
| 1:F:69:VAL:HG13 | 1:F:70:PRO:HD2 | 1.91 | 0.50 |
| 1:C:637:GLU:HA | 1:C:679:LEU:HD23 | 1.93 | 0.50 |
| 1:P:261:TRP:CZ3 | 1:P:266:GLN:HB2 | 2.46 | 0.50 |
| 1:L:473:ARG:HD3 | 1:L:473:ARG:O | 2.11 | 0.50 |
| 1:B:637:GLU:HA | 1:B:679:LEU:HD23 | 1.93 | 0.50 |
| 1:B:85:VAL:HG12 | 1:B:86:VAL:N | 2.26 | 0.50 |
| 1:C:427:THR:HA | 1:C:436:MET:HE2 | 1.90 | 0.50 |
| 1:F:595:THR:HG23 | 1:F:596:PRO:CA | 2.35 | 0.50 |
| 1:P:1020:TRP:CD1 | 1:P:1021:CME:N | 2.79 | 0.50 |
| 1:I:745:MET:HA | 1:I:745:MET:CE | 2.39 | 0.50 |
| 1:K:278:ILE:H | 1:K:278:ILE:CD1 | 2.22 | 0.50 |
| 1:D:856:TYR:CD2 | 1:D:864:MET:HE2 | 2.41 | 0.50 |
| 1:M:63:PHE:CB | 1:M:64:PRO:HD2 | 2.34 | 0.50 |
| 1:E:952:ARG:HD2 | 3:E:4422:HOH:O | 2.11 | 0.50 |
| 1:I:987:ASP:OD2 | 1:I:990:HIS:HD2 | 1.94 | 0.50 |
| 1:N:73:TRP:CZ2 | 1:N:185:ALA:HB1 | 2.46 | 0.50 |
| 1:F:73:TRP:CZ2 | 1:F:185:ALA:HB1 | 2.46 | 0.50 |
| 1:E:741:THR:HG22 | 1:E:741:THR:O | 2.12 | 0.50 |
| 1:L:380:LYS:HE3 | 1:L:406:GLY:O | 2.12 | 0.50 |
| 1:L:571:VAL:HG13 | 1:L:607:VAL:HG23 | 1.93 | 0.50 |
| 1:O:194:GLY:O | 1:O:198:GLU:HG3 | 2.10 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:571:VAL:HG13 | 1:H:607:VAL:HG23 | 1.93 | 0.50 |
| 1:D:573:GLN:HB2 | 1:D:602:CYS:O | 2.12 | 0.50 |
| 1:C:194:GLY:O | 1:C:198:GLU:HG3 | 2.10 | 0.50 |
| 1:A:952:ARG:HD2 | 3:A:4429:HOH:O | 2.11 | 0.50 |
| 1:N:952:ARG:HD2 | 3:N:3528:HOH:O | 2.11 | 0.50 |
| 1:K:856:TYR:CD2 | 1:K:864:MET:HE2 | 2.45 | 0.50 |
| 1:E:881:ARG:HD3 | 1:E:987:ASP:OD1 | 2.10 | 0.50 |
| 1:B:987:ASP:OD2 | 1:B:990:HIS:HD2 | 1.94 | 0.50 |
| 1:L:987:ASP:OD2 | 1:L:990:HIS:HD2 | 1.94 | 0.50 |
| 1:P:987:ASP:OD2 | 1:P:990:HIS:HD2 | 1.94 | 0.50 |
| 1:M:741:THR:O | 1:M:741:THR:HG22 | 2.12 | 0.50 |
| 1:M:73:TRP:CZ2 | 1:M:185:ALA:HB1 | 2.46 | 0.50 |
| 1:F:660:GLY:O | 1:F:662:PRO:HD3 | 2.11 | 0.50 |
| 1:D:127:PHE:CE2 | 1:D:184:LEU:HG | 2.47 | 0.50 |
| 1:E:660:GLY:O | 1:E:662:PRO:HD3 | 2.11 | 0.50 |
| 1:K:249:GLU:OE1 | 1:K:251:ARG:NH1 | 2.35 | 0.50 |
| 1:A:660:GLY:O | 1:A:662:PRO:HD3 | 2.11 | 0.50 |
| 1:C:610:ASP:OD2 | 1:C:612:THR:HG23 | 2.11 | 0.50 |
| 1:J:5:ASP:OD2 | 1:J:157:ARG:HA | 2.11 | 0.50 |
| 1:J:610:ASP:OD2 | 1:J:612:THR:HG23 | 2.11 | 0.50 |
| 1:D:610:ASP:OD2 | 1:D:612:THR:HG23 | 2.11 | 0.50 |
| 1:I:637:GLU:HA | 1:I:679:LEU:HD23 | 1.93 | 0.50 |
| 1:C:830:LEU:HD11 | 1:D:830:LEU:HD11 | 1.94 | 0.50 |
| 1:A:85:VAL:HG12 | 1:A:86:VAL:N | 2.27 | 0.50 |
| 1:L:261:TRP:CZ3 | 1:L:266:GLN:HB2 | 2.46 | 0.50 |
| 1:D:571:VAL:HG13 | 1:D:607:VAL:HG23 | 1.93 | 0.50 |
| 1:N:69:VAL:HG13 | 1:N:70:PRO:HD2 | 1.91 | 0.50 |
| 1:H:573:GLN:HB2 | 1:H:602:CYS:O | 2.12 | 0.50 |
| 1:N:5:ASP:OD2 | 1:N:157:ARG:HA | 2.11 | 0.50 |
| 1:O:595:THR:HG23 | 1:O:596:PRO:CA | 2.35 | 0.50 |
| 1:F:952:ARG:HD2 | 3:F:3528:HOH:O | 2.11 | 0.50 |
| 1:A:987:ASP:OD2 | 1:A:990:HIS:HD2 | 1.94 | 0.50 |
| 1:B:287:ASP:CG | 1:C:425:ARG:HH22 | 2.14 | 0.50 |
| 1:N:127:PHE:CE2 | 1:N:184:LEU:HG | 2.47 | 0.50 |
| 1:G:637:GLU:HA | 1:G:679:LEU:HD23 | 1.93 | 0.50 |
| 1:F:1004:SER:HB2 | 1:F:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:A:1004:SER:HB2 | 1:A:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:I:261:TRP:CZ3 | 1:I:266:GLN:HB2 | 2.46 | 0.50 |
| 1:B:380:LYS:HE3 | 1:B:406:GLY:O | 2.12 | 0.50 |
| 1:F:261:TRP:CZ3 | 1:F:266:GLN:HB2 | 2.46 | 0.50 |
| 1:G:610:ASP:OD2 | 1:G:612:THR:HG23 | 2.11 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:380:LYS:HE3 | 1:I:406:GLY:O | 2.12 | 0.50 |
| 1:C:85:VAL:HG12 | 1:C:86:VAL:N | 2.27 | 0.50 |
| 1:E:571:VAL:HG13 | 1:E:607:VAL:HG23 | 1.93 | 0.50 |
| 1:C:1020:TRP:CD1 | 1:C:1021:CME:N | 2.79 | 0.50 |
| 1:O:278:ILE:H | 1:O:278:ILE:CD1 | 2.22 | 0.50 |
| 1:D:745:MET:HA | 1:D:745:MET:CE | 2.39 | 0.50 |
| 1:O:987:ASP:OD2 | 1:O:990:HIS:HD2 | 1.94 | 0.50 |
| 1:A:73:TRP:CZ2 | 1:A:185:ALA:HB1 | 2.46 | 0.50 |
| 1:D:73:TRP:CZ2 | 1:D:185:ALA:HB1 | 2.46 | 0.50 |
| 1:L:73:TRP:CZ2 | 1:L:185:ALA:HB1 | 2.46 | 0.50 |
| 1:E:127:PHE:CE2 | 1:E:184:LEU:HG | 2.47 | 0.50 |
| 1:D:741:THR:O | 1:D:741:THR:HG22 | 2.11 | 0.50 |
| 1:N:660:GLY:O | 1:N:662:PRO:HD3 | 2.11 | 0.50 |
| 1:J:573:GLN:HB2 | 1:J:602:CYS:O | 2.12 | 0.50 |
| 1:N:571:VAL:HG13 | 1:N:607:VAL:HG23 | 1.93 | 0.50 |
| 1:I:571:VAL:HG13 | 1:I:607:VAL:HG23 | 1.93 | 0.50 |
| 1:O:637:GLU:HA | 1:O:679:LEU:HD23 | 1.94 | 0.50 |
| 1:K:380:LYS:HE3 | 1:K:406:GLY:O | 2.12 | 0.50 |
| 1:O:1004:SER:HB2 | 1:O:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:G:473:ARG:HD3 | 1:G:473:ARG:O | 2.11 | 0.50 |
| 1:K:595:THR:CG2 | 1:K:596:PRO:HA | 2.37 | 0.50 |
| 1:D:1020:TRP:CD1 | 1:D:1021:CME:N | 2.79 | 0.50 |
| 1:H:1020:TRP:CD1 | 1:H:1021:CME:N | 2.79 | 0.50 |
| 1:D:952:ARG:HD2 | 3:D:3534:HOH:O | 2.11 | 0.50 |
| 1:G:987:ASP:OD2 | 1:G:990:HIS:HD2 | 1.94 | 0.50 |
| 1:H:987:ASP:OD2 | 1:H:990:HIS:HD2 | 1.94 | 0.50 |
| 1:C:987:ASP:OD2 | 1:C:990:HIS:HD2 | 1.94 | 0.50 |
| 1:H:73:TRP:CZ2 | 1:H:185:ALA:HB1 | 2.46 | 0.50 |
| 1:A:127:PHE:CE2 | 1:A:184:LEU:HG | 2.47 | 0.50 |
| 1:K:127:PHE:CE2 | 1:K:184:LEU:HG | 2.47 | 0.50 |
| 1:I:73:TRP:CZ2 | 1:I:185:ALA:HB1 | 2.46 | 0.50 |
| 1:J:73:TRP:CZ2 | 1:J:185:ALA:HB1 | 2.46 | 0.50 |
| 1:C:660:GLY:O | 1:C:662:PRO:HD3 | 2.10 | 0.50 |
| 1:J:85:VAL:HG12 | 1:J:86:VAL:N | 2.27 | 0.50 |
| 1:F:380:LYS:HE3 | 1:F:406:GLY:O | 2.12 | 0.50 |
| 1:F:571:VAL:HG13 | 1:F:607:VAL:HG23 | 1.93 | 0.50 |
| 1:A:190:ARG:HG3 | 1:A:206:SER:OG | 2.12 | 0.50 |
| 1:H:1004:SER:HB2 | 1:H:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:N:380:LYS:HE3 | 1:N:406:GLY:O | 2.12 | 0.50 |
| 1:D:261:TRP:CZ3 | 1:D:266:GLN:HB2 | 2.46 | 0.50 |
| 1:H:85:VAL:HG12 | 1:H:86:VAL:N | 2.27 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:573:GLN:HB2 | 1:G:602:CYS:O | 2.12 | 0.50 |
| 1:D:5:ASP:OD2 | 1:D:157:ARG:HA | 2.11 | 0.50 |
| 1:P:571:VAL:HG13 | 1:P:607:VAL:HG23 | 1.93 | 0.50 |
| 1:L:903[A]:GLN:NE2 | 3:L:3424:HOH:O | 2.45 | 0.50 |
| 1:I:741:THR:HG22 | 1:I:741:THR:O | 2.12 | 0.50 |
| 1:P:5:ASP:OD2 | 1:P:157:ARG:HA | 2.11 | 0.50 |
| 1:A:767:GLN:HG3 | 1:A:768:MET:N | 2.26 | 0.50 |
| 1:C:1004:SER:HB2 | 1:C:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:E:5:ASP:OD2 | 1:E:157:ARG:HA | 2.11 | 0.50 |
| 1:F:573:GLN:HB2 | 1:F:602:CYS:O | 2.12 | 0.50 |
| 1:M:5:ASP:OD2 | 1:M:157:ARG:HA | 2.11 | 0.50 |
| 1:L:595:THR:HG23 | 1:L:596:PRO:CA | 2.35 | 0.50 |
| 1:B:1020:TRP:CD1 | 1:B:1021:CME:N | 2.79 | 0.50 |
| 1:E:1020:TRP:CD1 | 1:E:1021:CME:N | 2.79 | 0.50 |
| 1:H:856:TYR:HD2 | 1:H:864:MET:CE | 2.25 | 0.50 |
| 1:J:987:ASP:OD2 | 1:J:990:HIS:HD2 | 1.94 | 0.50 |
| 1:J:127:PHE:CE2 | 1:J:184:LEU:HG | 2.47 | 0.50 |
| 1:H:355:ASN:OD1 | 1:H:388:ARG:HD3 | 2.12 | 0.50 |
| 1:G:190:ARG:HG3 | 1:G:206:SER:OG | 2.12 | 0.50 |
| 1:E:85:VAL:HG12 | 1:E:86:VAL:N | 2.27 | 0.50 |
| 1:N:747:PHE:HE1 | 1:N:825:CYS:HG | 1.58 | 0.50 |
| 1:H:380:LYS:HE3 | 1:H:406:GLY:O | 2.12 | 0.50 |
| 1:E:261:TRP:CZ3 | 1:E:266:GLN:HB2 | 2.46 | 0.50 |
| 1:D:194:GLY:O | 1:D:198:GLU:HG3 | 2.10 | 0.50 |
| 1:J:1004:SER:HB2 | 1:J:1006:GLU:OE2 | 2.12 | 0.50 |
| 1:M:571:VAL:HG13 | 1:M:607:VAL:HG23 | 1.93 | 0.50 |
| 1:E:282:ARG:HD3 | 1:H:420:MET:O | 2.12 | 0.50 |
| 1:P:190:ARG:HG3 | 1:P:206:SER:OG | 2.12 | 0.50 |
| 1:N:573:GLN:HB2 | 1:N:602:CYS:O | 2.12 | 0.50 |
| 1:M:261:TRP:CZ3 | 1:M:266:GLN:HB2 | 2.46 | 0.50 |
| 1:H:5:ASP:OD2 | 1:H:157:ARG:HA | 2.11 | 0.50 |
| 1:N:507:ASP:OD1 | 1:N:521:LYS:HE2 | 2.12 | 0.50 |
| 1:M:903[A]:GLN:NE2 | 3:M:4314:HOH:O | 2.45 | 0.50 |
| 1:N:1020:TRP:CD1 | 1:N:1021:CME:N | 2.79 | 0.49 |
| 1:H:952:ARG:HD2 | 3:H:4432:HOH:O | 2.11 | 0.49 |
| 1:O:856:TYR:HD2 | 1:O:864:MET:CE | 2.25 | 0.49 |
| 1:H:856:TYR:CD2 | 1:H:864:MET:HE2 | 2.47 | 0.49 |
| 1:D:881:ARG:HD3 | 1:D:987:ASP:OD1 | 2.10 | 0.49 |
| 1:D:987:ASP:OD2 | 1:D:990:HIS:HD2 | 1.94 | 0.49 |
| 1:H:127:PHE:CE2 | 1:H:184:LEU:HG | 2.47 | 0.49 |
| 1:N:741:THR:HG22 | 1:N:741:THR:O | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:M:127:PHE:CE2 | 1:M:184:LEU:HG | 2.47 | 0.49 |
| 1:K:37:ARG:NH2 | 1:K:216:HIS:O | 2.45 | 0.49 |
| 1:I:37:ARG:NH2 | 1:I:216:HIS:O | 2.45 | 0.49 |
| 1:I:5:ASP:OD2 | 1:I:157:ARG:HA | 2.11 | 0.49 |
| 1:P:507:ASP:OD1 | 1:P:521:LYS:HE2 | 2.12 | 0.49 |
| 1:M:190:ARG:HG3 | 1:M:206:SER:OG | 2.12 | 0.49 |
| 1:I:610:ASP:OD2 | 1:I:612:THR:HG23 | 2.11 | 0.49 |
| 1:M:380:LYS:HE3 | 1:M:406:GLY:O | 2.12 | 0.49 |
| 1:G:380:LYS:HE3 | 1:G:406:GLY:O | 2.12 | 0.49 |
| 1:A:5:ASP:OD2 | 1:A:157:ARG:HA | 2.11 | 0.49 |
| 1:A:571:VAL:HG13 | 1:A:607:VAL:HG23 | 1.93 | 0.49 |
| 1:N:1004:SER:HB2 | 1:N:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:D:507:ASP:OD1 | 1:D:521:LYS:HE2 | 2.12 | 0.49 |
| 1:C:903[A]:GLN:NE2 | 3:C:4315:HOH:O | 2.45 | 0.49 |
| 1:E:573:GLN:HB2 | 1:E:602:CYS:O | 2.11 | 0.49 |
| 1:P:140:ARG:HB2 | 1:P:171:PHE:O | 2.12 | 0.49 |
| 1:O:190:ARG:HG3 | 1:O:206:SER:OG | 2.12 | 0.49 |
| 1:I:190:ARG:HG3 | 1:I:206:SER:OG | 2.12 | 0.49 |
| 1:D:1004:SER:HB2 | 1:D:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:K:190:ARG:HG3 | 1:K:206:SER:OG | 2.12 | 0.49 |
| 1:F:507:ASP:OD1 | 1:F:521:LYS:HE2 | 2.12 | 0.49 |
| 1:B:507:ASP:OD1 | 1:B:521:LYS:HE2 | 2.12 | 0.49 |
| 1:G:261:TRP:CZ3 | 1:G:266:GLN:HB2 | 2.46 | 0.49 |
| 1:L:190:ARG:HG3 | 1:L:206:SER:OG | 2.12 | 0.49 |
| 1:E:595:THR:CG2 | 1:E:596:PRO:HA | 2.37 | 0.49 |
| 1:O:952:ARG:HD2 | 3:O:3524:HOH:O | 2.11 | 0.49 |
| 1:I:952:ARG:HD2 | 3:I:4420:HOH:O | 2.11 | 0.49 |
| 1:K:43:ARG:HH11 | 1:K:43:ARG:CG | 2.24 | 0.49 |
| 1:O:73:TRP:CZ2 | 1:O:185:ALA:HB1 | 2.46 | 0.49 |
| 1:L:37:ARG:NH2 | 1:L:216:HIS:O | 2.46 | 0.49 |
| 1:C:507:ASP:OD1 | 1:C:521:LYS:HE2 | 2.12 | 0.49 |
| 1:J:140:ARG:HB2 | 1:J:171:PHE:O | 2.13 | 0.49 |
| 1:M:85:VAL:HG12 | 1:M:86:VAL:N | 2.27 | 0.49 |
| 1:G:1004:SER:HB2 | 1:G:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:E:380:LYS:HE3 | 1:E:406:GLY:O | 2.12 | 0.49 |
| 1:A:380:LYS:HE3 | 1:A:406:GLY:O | 2.12 | 0.49 |
| 1:M:573:GLN:HB2 | 1:M:602:CYS:O | 2.12 | 0.49 |
| 1:H:190:ARG:HG3 | 1:H:206:SER:OG | 2.12 | 0.49 |
| 1:O:380:LYS:HE3 | 1:O:406:GLY:O | 2.12 | 0.49 |
| 1:A:637:GLU:HA | 1:A:679:LEU:HD23 | 1.93 | 0.49 |
| 1:J:473:ARG:HD3 | 1:J:473:ARG:O | 2.11 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:573:GLN:HB2 | 1:L:602:CYS:O | 2.12 | 0.49 |
| 1:L:5:ASP:OD2 | 1:L:157:ARG:HA | 2.11 | 0.49 |
| 1:K:355:ASN:OD1 | 1:K:388:ARG:HD3 | 2.12 | 0.49 |
| 1:I:573:GLN:HB2 | 1:I:602:CYS:O | 2.11 | 0.49 |
| 1:I:85:VAL:HG12 | 1:I:86:VAL:N | 2.27 | 0.49 |
| 1:B:573:GLN:HB2 | 1:B:602:CYS:O | 2.12 | 0.49 |
| 1:H:507:ASP:OD1 | 1:H:521:LYS:HE2 | 2.12 | 0.49 |
| 1:F:1020:TRP:CD1 | 1:F:1021:CME:N | 2.79 | 0.49 |
| 1:G:1020:TRP:CD1 | 1:G:1021:CME:N | 2.79 | 0.49 |
| 1:O:1020:TRP:CD1 | 1:O:1021:CME:N | 2.79 | 0.49 |
| 1:M:952:ARG:HD2 | 3:M:4420:HOH:O | 2.11 | 0.49 |
| 1:O:433:LEU:O | 1:O:437:SER:HB3 | 2.13 | 0.49 |
| 1:F:741:THR:HG22 | 1:F:741:THR:O | 2.12 | 0.49 |
| 1:I:127:PHE:CE2 | 1:I:184:LEU:HG | 2.47 | 0.49 |
| 1:G:37:ARG:NH2 | 1:G:216:HIS:O | 2.45 | 0.49 |
| 1:F:127:PHE:CE2 | 1:F:184:LEU:HG | 2.47 | 0.49 |
| 1:M:37:ARG:NH2 | 1:M:216:HIS:O | 2.45 | 0.49 |
| 1:L:355:ASN:OD1 | 1:L:388:ARG:HD3 | 2.12 | 0.49 |
| 1:N:355:ASN:OD1 | 1:N:388:ARG:HD3 | 2.12 | 0.49 |
| 1:E:637:GLU:HA | 1:E:679:LEU:HD23 | 1.93 | 0.49 |
| 1:O:507:ASP:OD1 | 1:O:521:LYS:HE2 | 2.12 | 0.49 |
| 1:F:767:GLN:HG3 | 1:F:768:MET:N | 2.26 | 0.49 |
| 1:C:355:ASN:OD1 | 1:C:388:ARG:HD3 | 2.12 | 0.49 |
| 1:B:1004:SER:HB2 | 1:B:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:J:261:TRP:CZ3 | 1:J:266:GLN:HB2 | 2.46 | 0.49 |
| 1:K:322:LEU:HD23 | 1:K:322:LEU:C | 2.33 | 0.49 |
| 1:L:1020:TRP:CD1 | 1:L:1021:CME:N | 2.79 | 0.49 |
| 1:B:188:VAL:C | 1:B:189:LEU:HD23 | 2.33 | 0.49 |
| 1:A:856:TYR:HD2 | 1:A:864:MET:CE | 2.25 | 0.49 |
| 1:B:952:ARG:HD2 | 3:B:3528:HOH:O | 2.11 | 0.49 |
| 1:M:279:ILE:CD1 | 1:P:422:PRO:HG2 | 2.42 | 0.49 |
| 1:M:433:LEU:O | 1:M:437:SER:HB3 | 2.13 | 0.49 |
| 1:G:741:THR:O | 1:G:741:THR:HG22 | 2.12 | 0.49 |
| 1:C:37:ARG:NH2 | 1:C:216:HIS:O | 2.46 | 0.49 |
| 1:O:37:ARG:NH2 | 1:O:216:HIS:O | 2.46 | 0.49 |
| 1:C:573:GLN:HB2 | 1:C:602:CYS:O | 2.11 | 0.49 |
| 1:J:507:ASP:OD1 | 1:J:521:LYS:HE2 | 2.12 | 0.49 |
| 1:K:85:VAL:HG12 | 1:K:86:VAL:N | 2.27 | 0.49 |
| 1:O:355:ASN:OD1 | 1:O:388:ARG:HD3 | 2.12 | 0.49 |
| 1:I:355:ASN:OD1 | 1:I:388:ARG:HD3 | 2.12 | 0.49 |
| 1:N:190:ARG:HG3 | 1:N:206:SER:OG | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:85:VAL:HG12 | 1:F:86:VAL:N | 2.27 | 0.49 |
| 1:J:190:ARG:HG3 | 1:J:206:SER:OG | 2.12 | 0.49 |
| 1:G:507:ASP:OD1 | 1:G:521:LYS:HE2 | 2.12 | 0.49 |
| 1:J:380:LYS:HE3 | 1:J:406:GLY:O | 2.12 | 0.49 |
| 1:J:571:VAL:HG13 | 1:J:607:VAL:HG23 | 1.93 | 0.49 |
| 1:E:1004:SER:HB2 | 1:E:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:G:355:ASN:OD1 | 1:G:388:ARG:HD3 | 2.12 | 0.49 |
| 1:P:856:TYR:HD2 | 1:P:864:MET:CE | 2.25 | 0.49 |
| 1:G:140:ARG:HB2 | 1:G:171:PHE:O | 2.13 | 0.49 |
| 1:F:190:ARG:HG3 | 1:F:206:SER:OG | 2.12 | 0.49 |
| 1:I:322:LEU:HD23 | 1:I:322:LEU:C | 2.33 | 0.49 |
| 1:D:322:LEU:C | 1:D:322:LEU:HD23 | 2.33 | 0.49 |
| 1:A:1020:TRP:CD1 | 1:A:1021:CME:N | 2.79 | 0.49 |
| 1:N:188:VAL:C | 1:N:189:LEU:HD23 | 2.33 | 0.49 |
| 1:N:278:ILE:CD1 | 1:N:278:ILE:H | 2.22 | 0.49 |
| 1:E:43:ARG:HH11 | 1:E:43:ARG:CG | 2.24 | 0.49 |
| 1:J:433:LEU:O | 1:J:437:SER:HB3 | 2.13 | 0.49 |
| 1:K:433:LEU:O | 1:K:437:SER:HB3 | 2.13 | 0.49 |
| 1:D:433:LEU:O | 1:D:437:SER:HB3 | 2.13 | 0.49 |
| 1:B:741:THR:O | 1:B:741:THR:HG22 | 2.11 | 0.49 |
| 1:A:433:LEU:O | 1:A:437:SER:HB3 | 2.13 | 0.49 |
| 1:J:287:ASP:N | 1:J:287:ASP:OD1 | 2.41 | 0.49 |
| 1:P:127:PHE:CE2 | 1:P:184:LEU:HG | 2.47 | 0.49 |
| 1:F:37:ARG:NH2 | 1:F:216:HIS:O | 2.46 | 0.49 |
| 1:N:37:ARG:NH2 | 1:N:216:HIS:O | 2.46 | 0.49 |
| 1:E:37:ARG:NH2 | 1:E:216:HIS:O | 2.45 | 0.49 |
| 1:G:127:PHE:CE2 | 1:G:184:LEU:HG | 2.47 | 0.49 |
| 1:B:37:ARG:NH2 | 1:B:216:HIS:O | 2.46 | 0.49 |
| 1:O:127:PHE:CE2 | 1:O:184:LEU:HG | 2.47 | 0.49 |
| 1:O:573:GLN:HB2 | 1:O:602:CYS:O | 2.12 | 0.49 |
| 1:B:355:ASN:OD1 | 1:B:388:ARG:HD3 | 2.12 | 0.49 |
| 1:M:140:ARG:HB2 | 1:M:171:PHE:O | 2.13 | 0.49 |
| 1:L:507:ASP:OD1 | 1:L:521:LYS:HE2 | 2.12 | 0.49 |
| 1:E:903[A]:GLN:NE2 | 3:E:4314:HOH:O | 2.45 | 0.49 |
| 1:E:190:ARG:HG3 | 1:E:206:SER:OG | 2.12 | 0.49 |
| 1:J:903[A]:GLN:NE2 | 3:J:3421:HOH:O | 2.45 | 0.49 |
| 1:K:1004:SER:HB2 | 1:K:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:B:140:ARG:HB2 | 1:B:171:PHE:O | 2.12 | 0.49 |
| 1:A:355:ASN:OD1 | 1:A:388:ARG:HD3 | 2.12 | 0.49 |
| 1:B:433:LEU:O | 1:B:437:SER:HB3 | 2.13 | 0.49 |
| 1:F:322:LEU:C | 1:F:322:LEU:HD23 | 2.33 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:987:ASP:OD2 | 1:E:990:HIS:HD2 | 1.94 | 0.49 |
| 1:I:433:LEU:O | 1:I:437:SER:HB3 | 2.13 | 0.49 |
| 1:J:741:THR:HG22 | 1:J:741:THR:O | 2.12 | 0.49 |
| 1:F:856:TYR:HD2 | 1:F:864:MET:CE | 2.25 | 0.49 |
| 1:B:903[A]:GLN:NE2 | 3:B:3418:HOH:O | 2.45 | 0.49 |
| 1:E:140:ARG:HB2 | 1:E:171:PHE:O | 2.13 | 0.49 |
| 1:N:767:GLN:HG3 | 1:N:768:MET:N | 2.26 | 0.49 |
| 1:H:800:ARG:CZ | 1:H:800:ARG:HB3 | 2.43 | 0.49 |
| 1:C:800:ARG:HB3 | 1:C:800:ARG:CZ | 2.43 | 0.49 |
| 1:E:355:ASN:OD1 | 1:E:388:ARG:HD3 | 2.13 | 0.49 |
| 1:C:102:ASN:ND2 | 1:C:201:ASP:HB2 | 2.28 | 0.49 |
| 1:K:507:ASP:OD1 | 1:K:521:LYS:HE2 | 2.12 | 0.49 |
| 1:P:102:ASN:ND2 | 1:P:201:ASP:HB2 | 2.28 | 0.49 |
| 1:D:190:ARG:HG3 | 1:D:206:SER:OG | 2.12 | 0.49 |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:C | 2.33 | 0.49 |
| 1:I:1020:TRP:CD1 | 1:I:1021:CME:N | 2.79 | 0.49 |
| 1:C:856:TYR:HD2 | 1:C:864:MET:CE | 2.25 | 0.49 |
| 1:N:856:TYR:HD2 | 1:N:864:MET:CE | 2.25 | 0.49 |
| 1:E:679:LEU:HA | 1:E:679:LEU:HD23 | 1.40 | 0.49 |
| 1:P:856:TYR:HD2 | 1:P:864:MET:HE2 | 1.77 | 0.49 |
| 1:I:903[A]:GLN:NE2 | 3:I:4313:HOH:O | 2.45 | 0.49 |
| 1:B:190:ARG:HG3 | 1:B:206:SER:OG | 2.12 | 0.49 |
| 1:F:800:ARG:CZ | 1:F:800:ARG:HB3 | 2.43 | 0.49 |
| 1:P:800:ARG:CZ | 1:P:800:ARG:HB3 | 2.43 | 0.49 |
| 1:A:507:ASP:OD1 | 1:A:521:LYS:HE2 | 2.12 | 0.49 |
| 1:A:140:ARG:HB2 | 1:A:171:PHE:O | 2.12 | 0.49 |
| 1:I:767:GLN:HG3 | 1:I:768:MET:N | 2.26 | 0.49 |
| 1:L:140:ARG:HB2 | 1:L:171:PHE:O | 2.13 | 0.49 |
| 1:H:102:ASN:ND2 | 1:H:201:ASP:HB2 | 2.28 | 0.49 |
| 1:K:571:VAL:HG13 | 1:K:607:VAL:HG23 | 1.93 | 0.49 |
| 1:N:57:GLU:HG2 | 1:N:83:THR:HG22 | 1.95 | 0.49 |
| 1:G:188:VAL:C | 1:G:189:LEU:HD23 | 2.33 | 0.49 |
| 1:G:433:LEU:O | 1:G:437:SER:HB3 | 2.13 | 0.49 |
| 1:G:65:ALA:HB1 | 1:G:66:PRO:HD2 | 1.95 | 0.49 |
| 1:C:127:PHE:CE2 | 1:C:184:LEU:HG | 2.47 | 0.49 |
| 1:L:127:PHE:CE2 | 1:L:184:LEU:HG | 2.47 | 0.49 |
| 1:M:637:GLU:HA | 1:M:679:LEU:HD23 | 1.93 | 0.49 |
| 1:F:747:PHE:HE1 | 1:F:825:CYS:HG | 1.59 | 0.49 |
| 1:L:102:ASN:ND2 | 1:L:201:ASP:HB2 | 2.28 | 0.49 |
| 1:J:637:GLU:HA | 1:J:679:LEU:HD23 | 1.93 | 0.49 |
| 1:M:102:ASN:ND2 | 1:M:201:ASP:HB2 | 2.28 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:N:102:ASN:ND2 | 1:N:201:ASP:HB2 | 2.28 | 0.49 |
| 1:N:800:ARG:CZ | 1:N:800:ARG:HB3 | 2.43 | 0.49 |
| 1:C:380:LYS:HE3 | 1:C:406:GLY:O | 2.12 | 0.49 |
| 1:D:380:LYS:HE3 | 1:D:406:GLY:O | 2.12 | 0.49 |
| 1:K:595:THR:HG23 | 1:K:596:PRO:CA | 2.35 | 0.49 |
| 1:C:322:LEU:C | 1:C:322:LEU:HD23 | 2.33 | 0.49 |
| 1:L:322:LEU:HD23 | 1:L:322:LEU:C | 2.33 | 0.49 |
| 1:M:285:TYR:CB | 1:M:288:ARG:HG3 | 2.42 | 0.49 |
| 1:L:188:VAL:C | 1:L:189:LEU:HD23 | 2.33 | 0.49 |
| 1:O:188:VAL:C | 1:O:189:LEU:HD23 | 2.33 | 0.49 |
| 1:A:419:GLY:O | 1:D:282:ARG:NH1 | 2.46 | 0.49 |
| 1:D:43:ARG:HH11 | 1:D:43:ARG:CG | 2.24 | 0.49 |
| 1:O:65:ALA:HB1 | 1:O:66:PRO:HD2 | 1.95 | 0.49 |
| 1:H:741:THR:O | 1:H:741:THR:HG22 | 2.12 | 0.49 |
| 1:B:127:PHE:CE2 | 1:B:184:LEU:HG | 2.47 | 0.49 |
| 1:I:856:TYR:HD2 | 1:I:864:MET:CE | 2.26 | 0.49 |
| 1:H:140:ARG:HB2 | 1:H:171:PHE:O | 2.13 | 0.49 |
| 1:M:1004:SER:HB2 | 1:M:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:F:102:ASN:ND2 | 1:F:201:ASP:HB2 | 2.28 | 0.49 |
| 1:I:102:ASN:ND2 | 1:I:201:ASP:HB2 | 2.28 | 0.49 |
| 1:K:637:GLU:HA | 1:K:679:LEU:HD23 | 1.93 | 0.49 |
| 1:C:190:ARG:HG3 | 1:C:206:SER:OG | 2.12 | 0.49 |
| 1:E:102:ASN:ND2 | 1:E:201:ASP:HB2 | 2.28 | 0.49 |
| 1:O:140:ARG:HB2 | 1:O:171:PHE:O | 2.12 | 0.49 |
| 1:I:188:VAL:C | 1:I:189:LEU:HD23 | 2.33 | 0.49 |
| 1:D:65:ALA:HB1 | 1:D:66:PRO:HD2 | 1.95 | 0.49 |
| 1:N:73:TRP:CZ2 | 1:N:122:CYS:HB3 | 2.48 | 0.49 |
| 1:F:73:TRP:CZ2 | 1:F:122:CYS:HB3 | 2.48 | 0.49 |
| 1:D:37:ARG:NH2 | 1:D:216:HIS:O | 2.45 | 0.49 |
| 1:L:1004:SER:HB2 | 1:L:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:M:355:ASN:OD1 | 1:M:388:ARG:HD3 | 2.12 | 0.49 |
| 1:P:429:ASP:OD1 | 1:P:430:PRO:HD2 | 2.13 | 0.49 |
| 1:E:507:ASP:OD1 | 1:E:521:LYS:HE2 | 2.12 | 0.49 |
| 1:J:355:ASN:OD1 | 1:J:388:ARG:HD3 | 2.12 | 0.49 |
| 1:G:85:VAL:HG12 | 1:G:86:VAL:N | 2.27 | 0.49 |
| 1:M:800:ARG:CZ | 1:M:800:ARG:HB3 | 2.43 | 0.49 |
| 1:P:1004:SER:HB2 | 1:P:1006:GLU:OE2 | 2.12 | 0.49 |
| 1:P:380:LYS:HE3 | 1:P:406:GLY:O | 2.12 | 0.49 |
| 1:D:102:ASN:ND2 | 1:D:201:ASP:HB2 | 2.28 | 0.49 |
| 1:F:903[A]:GLN:NE2 | 3:F:3420:HOH:O | 2.45 | 0.49 |
| 1:K:102:ASN:ND2 | 1:K:201:ASP:HB2 | 2.28 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:J:285:TYR:CB | 1:J:288:ARG:HG3 | 2.42 | 0.48 |
| 1:I:949:HIS:HD2 | 1:I:1020:TRP:HE1 | 1.53 | 0.48 |
| 1:M:949:HIS:HD2 | 1:M:1020:TRP:HE1 | 1.53 | 0.48 |
| 1:P:188:VAL:C | 1:P:189:LEU:HD23 | 2.33 | 0.48 |
| 1:B:65:ALA:HB1 | 1:B:66:PRO:HD2 | 1.95 | 0.48 |
| 1:G:73:TRP:CZ2 | 1:G:122:CYS:HB3 | 2.48 | 0.48 |
| 1:J:37:ARG:NH2 | 1:J:216:HIS:O | 2.45 | 0.48 |
| 1:P:85:VAL:HG12 | 1:P:86:VAL:N | 2.27 | 0.48 |
| 1:G:903[A]:GLN:NE2 | 3:G:3418:HOH:O | 2.45 | 0.48 |
| 1:B:429:ASP:OD1 | 1:B:430:PRO:HD2 | 2.13 | 0.48 |
| 1:A:102:ASN:ND2 | 1:A:201:ASP:HB2 | 2.28 | 0.48 |
| 1:I:1004:SER:HB2 | 1:I:1006:GLU:OE2 | 2.12 | 0.48 |
| 1:L:85:VAL:HG12 | 1:L:86:VAL:N | 2.27 | 0.48 |
| 1:E:800:ARG:CZ | 1:E:800:ARG:HB3 | 2.43 | 0.48 |
| 1:I:800:ARG:HB3 | 1:I:800:ARG:CZ | 2.43 | 0.48 |
| 1:B:102:ASN:ND2 | 1:B:201:ASP:HB2 | 2.28 | 0.48 |
| 1:F:9:VAL:O | 1:F:12:GLN:HB3 | 2.13 | 0.48 |
| 1:K:429:ASP:OD1 | 1:K:430:PRO:HD2 | 2.13 | 0.48 |
| 1:P:595:THR:CG2 | 1:P:596:PRO:HA | 2.37 | 0.48 |
| 1:J:322:LEU:HD23 | 1:J:322:LEU:C | 2.33 | 0.48 |
| 1:P:57:GLU:HG2 | 1:P:83:THR:HG22 | 1.95 | 0.48 |
| 1:B:653[A]:HIS:HD2 | 1:B:666:GLY:O | 1.97 | 0.48 |
| 1:H:653[A]:HIS:HD2 | 1:H:666:GLY:O | 1.96 | 0.48 |
| 1:E:653[A]:HIS:HD2 | 1:E:666:GLY:O | 1.96 | 0.48 |
| 1:O:73:TRP:CZ2 | 1:O:122:CYS:HB3 | 2.48 | 0.48 |
| 1:B:73:TRP:CZ2 | 1:B:122:CYS:HB3 | 2.48 | 0.48 |
| 1:L:73:TRP:CZ2 | 1:L:122:CYS:HB3 | 2.48 | 0.48 |
| 1:J:73:TRP:CZ2 | 1:J:122:CYS:HB3 | 2.48 | 0.48 |
| 1:L:9:VAL:O | 1:L:12:GLN:HB3 | 2.13 | 0.48 |
| 1:I:429:ASP:OD1 | 1:I:430:PRO:HD2 | 2.13 | 0.48 |
| 1:J:9:VAL:O | 1:J:12:GLN:HB3 | 2.13 | 0.48 |
| 1:D:134:LEU:HD23 | 1:D:134:LEU:HA | 1.68 | 0.48 |
| 1:L:429:ASP:OD1 | 1:L:430:PRO:HD2 | 2.13 | 0.48 |
| 1:M:507:ASP:OD1 | 1:M:521:LYS:HE2 | 2.12 | 0.48 |
| 1:O:85:VAL:HG12 | 1:O:86:VAL:N | 2.27 | 0.48 |
| 1:N:429:ASP:OD1 | 1:N:430:PRO:HD2 | 2.13 | 0.48 |
| 1:I:507:ASP:OD1 | 1:I:521:LYS:HE2 | 2.12 | 0.48 |
| 1:C:433:LEU:O | 1:C:437:SER:HB3 | 2.13 | 0.48 |
| 1:O:78:LEU:HB3 | 1:O:79:PRO:CD | 2.43 | 0.48 |
| 1:E:65:ALA:HB1 | 1:E:66:PRO:HD2 | 1.95 | 0.48 |
| 1:C:65:ALA:HB1 | 1:C:66:PRO:HD2 | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:65:ALA:HB1 | 1:K:66:PRO:HD2 | 1.95 | 0.48 |
| 1:M:653[A]:HIS:HD2 | 1:M:666:GLY:O | 1.97 | 0.48 |
| 1:C:73:TRP:CZ2 | 1:C:122:CYS:HB3 | 2.48 | 0.48 |
| 1:A:741:THR:HG22 | 1:A:741:THR:O | 2.12 | 0.48 |
| 1:J:469:ASP:HB3 | 1:K:473:ARG:HD2 | 1.94 | 0.48 |
| 1:O:429:ASP:OD1 | 1:O:430:PRO:HD2 | 2.13 | 0.48 |
| 1:H:637:GLU:HA | 1:H:679:LEU:HD23 | 1.93 | 0.48 |
| 1:C:9:VAL:O | 1:C:12:GLN:HB3 | 2.13 | 0.48 |
| 1:O:903[A]:GLN:NE2 | 3:O:3418:HOH:O | 2.45 | 0.48 |
| 1:L:800:ARG:CZ | 1:L:800:ARG:HB3 | 2.43 | 0.48 |
| 1:B:800:ARG:HB3 | 1:B:800:ARG:CZ | 2.43 | 0.48 |
| 1:P:637:GLU:HA | 1:P:679:LEU:HD23 | 1.93 | 0.48 |
| 1:O:322:LEU:HD23 | 1:O:322:LEU:C | 2.33 | 0.48 |
| 1:N:322:LEU:HD23 | 1:N:322:LEU:C | 2.33 | 0.48 |
| 1:H:78:LEU:HB3 | 1:H:79:PRO:CD | 2.43 | 0.48 |
| 1:I:78:LEU:HB3 | 1:I:79:PRO:CD | 2.43 | 0.48 |
| 1:H:433:LEU:O | 1:H:437:SER:HB3 | 2.13 | 0.48 |
| 1:F:653[A]:HIS:HD2 | 1:F:666:GLY:O | 1.97 | 0.48 |
| 1:M:856:TYR:HD2 | 1:M:864:MET:CE | 2.25 | 0.48 |
| 1:P:217:LYS:HG2 | 1:P:218:PRO:HD2 | 1.96 | 0.48 |
| 1:I:73:TRP:CZ2 | 1:I:122:CYS:HB3 | 2.48 | 0.48 |
| 1:J:73:TRP:CH2 | 1:J:185:ALA:HB1 | 2.49 | 0.48 |
| 1:J:429:ASP:OD1 | 1:J:430:PRO:HD2 | 2.13 | 0.48 |
| 1:A:830:LEU:HD11 | 1:B:830:LEU:HD11 | 1.95 | 0.48 |
| 1:H:9:VAL:O | 1:H:12:GLN:HB3 | 2.13 | 0.48 |
| 1:D:355:ASN:OD1 | 1:D:388:ARG:HD3 | 2.12 | 0.48 |
| 1:I:287:ASP:N | 1:I:287:ASP:OD1 | 2.41 | 0.48 |
| 1:P:903[A]:GLN:NE2 | 3:P:3426:HOH:O | 2.45 | 0.48 |
| 1:A:429:ASP:OD1 | 1:A:430:PRO:HD2 | 2.13 | 0.48 |
| 1:D:595:THR:CG2 | 1:D:596:PRO:HA | 2.37 | 0.48 |
| 1:G:322:LEU:C | 1:G:322:LEU:HD23 | 2.33 | 0.48 |
| 1:J:188:VAL:C | 1:J:189:LEU:HD23 | 2.33 | 0.48 |
| 1:F:78:LEU:HB3 | 1:F:79:PRO:CD | 2.43 | 0.48 |
| 1:C:278:ILE:H | 1:C:278:ILE:CD1 | 2.22 | 0.48 |
| 1:J:278:ILE:CD1 | 1:J:278:ILE:H | 2.22 | 0.48 |
| 1:J:65:ALA:HB1 | 1:J:66:PRO:HD2 | 1.95 | 0.48 |
| 1:N:433:LEU:O | 1:N:437:SER:HB3 | 2.13 | 0.48 |
| 1:A:73:TRP:CZ2 | 1:A:122:CYS:HB3 | 2.48 | 0.48 |
| 1:J:35:SER:O | 1:J:50:GLN:HG3 | 2.14 | 0.48 |
| 1:C:35:SER:O | 1:C:50:GLN:HG3 | 2.14 | 0.48 |
| 1:A:37:ARG:NH2 | 1:A:216:HIS:O | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:O:35:SER:O | 1:O:50:GLN:HG3 | 2.14 | 0.48 |
| 1:G:35:SER:O | 1:G:50:GLN:HG3 | 2.14 | 0.48 |
| 1:H:217:LYS:HG2 | 1:H:218:PRO:HD2 | 1.96 | 0.48 |
| 1:I:35:SER:O | 1:I:50:GLN:HG3 | 2.14 | 0.48 |
| 1:F:420:MET:O | 1:G:282:ARG:HD3 | 2.14 | 0.48 |
| 1:B:9:VAL:O | 1:B:12:GLN:HB3 | 2.14 | 0.48 |
| 1:O:800:ARG:CZ | 1:O:800:ARG:HB3 | 2.43 | 0.48 |
| 1:J:800:ARG:CZ | 1:J:800:ARG:HB3 | 2.43 | 0.48 |
| 1:K:903[A]:GLN:NE2 | 3:K:4315:HOH:O | 2.45 | 0.48 |
| 1:N:85:VAL:HG12 | 1:N:86:VAL:N | 2.27 | 0.48 |
| 1:P:355:ASN:OD1 | 1:P:388:ARG:HD3 | 2.12 | 0.48 |
| 1:P:9:VAL:O | 1:P:12:GLN:HB3 | 2.14 | 0.48 |
| 1:E:322:LEU:HD23 | 1:E:322:LEU:C | 2.33 | 0.48 |
| 1:M:322:LEU:C | 1:M:322:LEU:HD23 | 2.33 | 0.48 |
| 1:H:57:GLU:HG2 | 1:H:83:THR:HG22 | 1.95 | 0.48 |
| 1:K:188:VAL:C | 1:K:189:LEU:HD23 | 2.33 | 0.48 |
| 1:E:433:LEU:O | 1:E:437:SER:HB3 | 2.13 | 0.48 |
| 1:G:653[A]:HIS:HD2 | 1:G:666:GLY:O | 1.97 | 0.48 |
| 1:H:35:SER:O | 1:H:50:GLN:HG3 | 2.14 | 0.48 |
| 1:N:73:TRP:CH2 | 1:N:185:ALA:HB1 | 2.49 | 0.48 |
| 1:A:217:LYS:HG2 | 1:A:218:PRO:HD2 | 1.96 | 0.48 |
| 1:L:73:TRP:CH2 | 1:L:185:ALA:HB1 | 2.49 | 0.48 |
| 1:E:73:TRP:CH2 | 1:E:185:ALA:HB1 | 2.49 | 0.48 |
| 1:M:73:TRP:CH2 | 1:M:185:ALA:HB1 | 2.49 | 0.48 |
| 1:I:73:TRP:CH2 | 1:I:185:ALA:HB1 | 2.49 | 0.48 |
| 1:K:73:TRP:CZ2 | 1:K:122:CYS:HB3 | 2.48 | 0.48 |
| 1:H:261:TRP:CH2 | 1:H:266:GLN:HB2 | 2.49 | 0.48 |
| 1:A:903[A]:GLN:NE2 | 3:A:4315:HOH:O | 2.45 | 0.48 |
| 1:K:800:ARG:CZ | 1:K:800:ARG:HB3 | 2.43 | 0.48 |
| 1:O:9:VAL:O | 1:O:12:GLN:HB3 | 2.13 | 0.48 |
| 1:A:595:THR:CG2 | 1:A:596:PRO:HA | 2.37 | 0.48 |
| 1:B:322:LEU:C | 1:B:322:LEU:HD23 | 2.33 | 0.48 |
| 1:N:78:LEU:HB3 | 1:N:79:PRO:CD | 2.43 | 0.48 |
| 1:F:188:VAL:C | 1:F:189:LEU:HD23 | 2.33 | 0.48 |
| 1:M:65:ALA:HB1 | 1:M:66:PRO:HD2 | 1.95 | 0.48 |
| 1:L:433:LEU:O | 1:L:437:SER:HB3 | 2.13 | 0.48 |
| 1:P:73:TRP:CH2 | 1:P:185:ALA:HB1 | 2.49 | 0.48 |
| 1:P:35:SER:O | 1:P:50:GLN:HG3 | 2.14 | 0.48 |
| 1:P:741:THR:HG22 | 1:P:741:THR:O | 2.12 | 0.48 |
| 1:M:73:TRP:CZ2 | 1:M:122:CYS:HB3 | 2.48 | 0.48 |
| 1:K:73:TRP:CH2 | 1:K:185:ALA:HB1 | 2.49 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:261:TRP:CH2 | 1:K:266:GLN:HB2 | 2.49 | 0.48 |
| 1:P:261:TRP:CH2 | 1:P:266:GLN:HB2 | 2.49 | 0.48 |
| 1:I:147:ASN:HA | 1:I:148:SER:HA | 1.57 | 0.48 |
| 1:N:140:ARG:HB2 | 1:N:171:PHE:O | 2.13 | 0.48 |
| 1:E:429:ASP:OD1 | 1:E:430:PRO:HD2 | 2.13 | 0.48 |
| 1:D:903[A]:GLN:NE2 | 3:D:3427:HOH:O | 2.45 | 0.48 |
| 1:A:9:VAL:O | 1:A:12:GLN:HB3 | 2.13 | 0.48 |
| 1:C:140:ARG:HB2 | 1:C:171:PHE:O | 2.12 | 0.48 |
| 1:G:800:ARG:CZ | 1:G:800:ARG:HB3 | 2.43 | 0.48 |
| 1:C:581:ASN:O | 1:J:581:ASN:O | 2.30 | 0.48 |
| 1:I:140:ARG:HB2 | 1:I:171:PHE:O | 2.13 | 0.48 |
| 1:P:322:LEU:HD23 | 1:P:322:LEU:C | 2.33 | 0.48 |
| 1:B:57:GLU:HG2 | 1:B:83:THR:HG22 | 1.95 | 0.48 |
| 1:O:285:TYR:CB | 1:O:288:ARG:HG3 | 2.42 | 0.48 |
| 1:G:856:TYR:HD2 | 1:G:864:MET:CE | 2.26 | 0.48 |
| 1:B:856:TYR:HD2 | 1:B:864:MET:CE | 2.25 | 0.48 |
| 1:P:433:LEU:O | 1:P:437:SER:HB3 | 2.13 | 0.48 |
| 1:L:856:TYR:HD2 | 1:L:864:MET:CE | 2.26 | 0.48 |
| 1:K:741:THR:O | 1:K:741:THR:HG22 | 2.12 | 0.48 |
| 1:D:73:TRP:CH2 | 1:D:185:ALA:HB1 | 2.49 | 0.48 |
| 1:D:35:SER:O | 1:D:50:GLN:HG3 | 2.14 | 0.48 |
| 1:N:261:TRP:CH2 | 1:N:266:GLN:HB2 | 2.49 | 0.48 |
| 1:D:85:VAL:HG12 | 1:D:86:VAL:N | 2.27 | 0.48 |
| 1:M:9:VAL:O | 1:M:12:GLN:HB3 | 2.13 | 0.48 |
| 1:K:140:ARG:HB2 | 1:K:171:PHE:O | 2.13 | 0.48 |
| 1:G:102:ASN:ND2 | 1:G:201:ASP:HB2 | 2.28 | 0.48 |
| 1:G:80:GLU:H | 1:G:80:GLU:HG3 | 1.29 | 0.48 |
| 1:D:800:ARG:CZ | 1:D:800:ARG:HB3 | 2.43 | 0.48 |
| 1:O:102:ASN:ND2 | 1:O:201:ASP:HB2 | 2.28 | 0.48 |
| 1:M:429:ASP:OD1 | 1:M:430:PRO:HD2 | 2.13 | 0.48 |
| 1:G:429:ASP:OD1 | 1:G:430:PRO:HD2 | 2.13 | 0.48 |
| 1:N:147:ASN:HA | 1:N:148:SER:HA | 1.58 | 0.48 |
| 1:C:595:THR:CG2 | 1:C:596:PRO:HA | 2.37 | 0.48 |
| 1:G:285:TYR:CB | 1:G:288:ARG:HG3 | 2.42 | 0.48 |
| 1:E:78:LEU:HB3 | 1:E:79:PRO:CD | 2.43 | 0.48 |
| 1:F:65:ALA:HB1 | 1:F:66:PRO:HD2 | 1.95 | 0.48 |
| 1:N:65:ALA:HB1 | 1:N:66:PRO:HD2 | 1.95 | 0.48 |
| 1:A:653[A]:HIS:HD2 | 1:A:666:GLY:O | 1.97 | 0.48 |
| 1:D:217:LYS:HG2 | 1:D:218:PRO:HD2 | 1.96 | 0.48 |
| 1:P:37:ARG:NH2 | 1:P:216:HIS:O | 2.45 | 0.48 |
| 1:H:37:ARG:NH2 | 1:H:216:HIS:O | 2.45 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:J:217:LYS:HG2 | 1:J:218:PRO:HD2 | 1.96 | 0.48 |
| 1:B:35:SER:O | 1:B:50:GLN:HG3 | 2.14 | 0.48 |
| 1:I:261:TRP:CH2 | 1:I:266:GLN:HB2 | 2.49 | 0.48 |
| 1:F:261:TRP:CH2 | 1:F:266:GLN:HB2 | 2.49 | 0.48 |
| 1:H:903[A]:GLN:NE2 | 3:H:4315:HOH:O | 2.45 | 0.48 |
| 1:F:147:ASN:HA | 1:F:148:SER:HA | 1.57 | 0.48 |
| 1:C:80:GLU:H | 1:C:80:GLU:HG3 | 1.29 | 0.48 |
| 1:A:800:ARG:CZ | 1:A:800:ARG:HB3 | 2.43 | 0.48 |
| 1:D:140:ARG:HB2 | 1:D:171:PHE:O | 2.13 | 0.48 |
| 1:F:355:ASN:OD1 | 1:F:388:ARG:HD3 | 2.12 | 0.48 |
| 1:J:425:ARG:NH2 | 1:K:287:ASP:OD2 | 2.47 | 0.48 |
| 1:J:102:ASN:ND2 | 1:J:201:ASP:HB2 | 2.28 | 0.48 |
| 1:E:9:VAL:O | 1:E:12:GLN:HB3 | 2.13 | 0.48 |
| 1:H:322:LEU:HD23 | 1:H:322:LEU:C | 2.33 | 0.48 |
| 1:A:188:VAL:C | 1:A:189:LEU:HD23 | 2.33 | 0.48 |
| 1:H:188:VAL:C | 1:H:189:LEU:HD23 | 2.33 | 0.48 |
| 1:P:65:ALA:HB1 | 1:P:66:PRO:HD2 | 1.95 | 0.48 |
| 1:C:653[A]:HIS:HD2 | 1:C:666:GLY:O | 1.97 | 0.48 |
| 1:A:279:ILE:CD1 | 1:D:422:PRO:HG2 | 2.43 | 0.48 |
| 1:K:653[A]:HIS:HD2 | 1:K:666:GLY:O | 1.97 | 0.48 |
| 1:A:73:TRP:CH2 | 1:A:185:ALA:HB1 | 2.49 | 0.48 |
| 1:E:73:TRP:CZ2 | 1:E:122:CYS:HB3 | 2.48 | 0.48 |
| 1:K:217:LYS:HG2 | 1:K:218:PRO:HD2 | 1.96 | 0.48 |
| 1:N:35:SER:O | 1:N:50:GLN:HG3 | 2.14 | 0.48 |
| 1:E:261:TRP:CH2 | 1:E:266:GLN:HB2 | 2.49 | 0.48 |
| 1:J:261:TRP:CH2 | 1:J:266:GLN:HB2 | 2.49 | 0.48 |
| 1:N:903[A]:GLN:NE2 | 3:N:3421:HOH:O | 2.45 | 0.48 |
| 1:I:914:CME:HE2 | 1:I:914:CME:HB3 | 1.74 | 0.48 |
| 1:P:595:THR:HG23 | 1:P:596:PRO:CA | 2.35 | 0.47 |
| 1:M:745:MET:CE | 1:M:745:MET:HA | 2.39 | 0.47 |
| 1:C:188:VAL:C | 1:C:189:LEU:HD23 | 2.33 | 0.47 |
| 1:F:278:ILE:CD1 | 1:F:278:ILE:H | 2.22 | 0.47 |
| 1:H:65:ALA:HB1 | 1:H:66:PRO:HD2 | 1.95 | 0.47 |
| 1:I:65:ALA:HB1 | 1:I:66:PRO:HD2 | 1.95 | 0.47 |
| 1:D:73:TRP:CZ2 | 1:D:122:CYS:HB3 | 2.48 | 0.47 |
| 1:F:35:SER:O | 1:F:50:GLN:HG3 | 2.14 | 0.47 |
| 1:L:35:SER:O | 1:L:50:GLN:HG3 | 2.14 | 0.47 |
| 1:F:217:LYS:HG2 | 1:F:218:PRO:HD2 | 1.96 | 0.47 |
| 1:N:217:LYS:HG2 | 1:N:218:PRO:HD2 | 1.96 | 0.47 |
| 1:L:217:LYS:HG2 | 1:L:218:PRO:HD2 | 1.96 | 0.47 |
| 1:D:261:TRP:CH2 | 1:D:266:GLN:HB2 | 2.49 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:M:261:TRP:CH2 | 1:M:266:GLN:HB2 | 2.49 | 0.47 |
| 1:K:910:LEU:C | 1:K:910:LEU:HD12 | 2.35 | 0.47 |
| 1:E:279:ILE:HD11 | 1:H:422:PRO:HG2 | 1.95 | 0.47 |
| 1:H:429:ASP:OD1 | 1:H:430:PRO:HD2 | 2.13 | 0.47 |
| 1:G:57:GLU:HG2 | 1:G:83:THR:HG22 | 1.95 | 0.47 |
| 1:K:856:TYR:HD2 | 1:K:864:MET:CE | 2.25 | 0.47 |
| 1:D:653[A]:HIS:HD2 | 1:D:666:GLY:O | 1.96 | 0.47 |
| 1:G:73:TRP:CH2 | 1:G:185:ALA:HB1 | 2.49 | 0.47 |
| 1:O:73:TRP:CH2 | 1:O:185:ALA:HB1 | 2.49 | 0.47 |
| 1:A:35:SER:O | 1:A:50:GLN:HG3 | 2.14 | 0.47 |
| 1:B:261:TRP:CH2 | 1:B:266:GLN:HB2 | 2.49 | 0.47 |
| 1:A:3:ILE:HG13 | 1:A:4:THR:N | 2.25 | 0.47 |
| 1:D:18:ASN:ND2 | 1:D:21:VAL:HG23 | 2.29 | 0.47 |
| 1:D:910:LEU:HD12 | 1:D:910:LEU:C | 2.35 | 0.47 |
| 1:N:914:CME:HB3 | 1:N:914:CME:HE2 | 1.74 | 0.47 |
| 1:I:595:THR:HG23 | 1:I:596:PRO:CA | 2.35 | 0.47 |
| 1:L:65:ALA:HB1 | 1:L:66:PRO:HD2 | 1.95 | 0.47 |
| 1:N:653[A]:HIS:HD2 | 1:N:666:GLY:O | 1.97 | 0.47 |
| 1:C:217:LYS:HG2 | 1:C:218:PRO:HD2 | 1.96 | 0.47 |
| 1:B:217:LYS:HG2 | 1:B:218:PRO:HD2 | 1.96 | 0.47 |
| 1:D:429:ASP:OD1 | 1:D:430:PRO:HD2 | 2.13 | 0.47 |
| 1:F:429:ASP:OD1 | 1:F:430:PRO:HD2 | 2.13 | 0.47 |
| 1:G:9:VAL:O | 1:G:12:GLN:HB3 | 2.13 | 0.47 |
| 1:L:257:THR:OG1 | 1:L:316:HIS:HE1 | 1.98 | 0.47 |
| 1:G:257:THR:OG1 | 1:G:316:HIS:HE1 | 1.98 | 0.47 |
| 1:M:257:THR:OG1 | 1:M:316:HIS:HE1 | 1.98 | 0.47 |
| 1:M:188:VAL:C | 1:M:189:LEU:HD23 | 2.33 | 0.47 |
| 1:F:433:LEU:O | 1:F:437:SER:HB3 | 2.13 | 0.47 |
| 1:A:43:ARG:HH11 | 1:A:43:ARG:CG | 2.24 | 0.47 |
| 1:F:254:LEU:HD23 | 1:F:254:LEU:HA | 1.71 | 0.47 |
| 1:L:653[A]:HIS:HD2 | 1:L:666:GLY:O | 1.96 | 0.47 |
| 1:F:645:ARG:HH22 | 1:F:650:GLU:CD | 2.18 | 0.47 |
| 1:C:645:ARG:HH22 | 1:C:650:GLU:CD | 2.18 | 0.47 |
| 1:C:73:TRP:CH2 | 1:C:185:ALA:HB1 | 2.49 | 0.47 |
| 1:I:18:ASN:ND2 | 1:I:21:VAL:HG23 | 2.29 | 0.47 |
| 1:E:910:LEU:HD12 | 1:E:910:LEU:C | 2.35 | 0.47 |
| 1:L:910:LEU:C | 1:L:910:LEU:HD12 | 2.35 | 0.47 |
| 1:D:9:VAL:O | 1:D:12:GLN:HB3 | 2.13 | 0.47 |
| 1:E:188:VAL:C | 1:E:189:LEU:HD23 | 2.33 | 0.47 |
| 1:P:254:LEU:HD23 | 1:P:254:LEU:HA | 1.71 | 0.47 |
| 1:J:856:TYR:HD2 | 1:J:864:MET:CE | 2.26 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:645:ARG:HH22 | 1:E:650:GLU:CD | 2.18 | 0.47 |
| 1:O:645:ARG:HH22 | 1:O:650:GLU:CD | 2.18 | 0.47 |
| 1:O:261:TRP:CH2 | 1:O:266:GLN:HB2 | 2.49 | 0.47 |
| 1:J:3:ILE:HG13 | 1:J:4:THR:N | 2.25 | 0.47 |
| 1:C:429:ASP:OD1 | 1:C:430:PRO:HD2 | 2.13 | 0.47 |
| 1:P:18:ASN:ND2 | 1:P:21:VAL:HG23 | 2.29 | 0.47 |
| 1:P:910:LEU:HD12 | 1:P:910:LEU:C | 2.35 | 0.47 |
| 1:P:257:THR:OG1 | 1:P:316:HIS:HE1 | 1.98 | 0.47 |
| 1:C:78:LEU:HB3 | 1:C:79:PRO:CD | 2.43 | 0.47 |
| 1:A:419:GLY:C | 1:D:282:ARG:HH11 | 2.16 | 0.47 |
| 1:P:653[A]:HIS:HD2 | 1:P:666:GLY:O | 1.96 | 0.47 |
| 1:P:73:TRP:CZ2 | 1:P:122:CYS:HB3 | 2.48 | 0.47 |
| 1:H:73:TRP:CH2 | 1:H:185:ALA:HB1 | 2.49 | 0.47 |
| 1:F:73:TRP:CH2 | 1:F:185:ALA:HB1 | 2.49 | 0.47 |
| 1:I:287:ASP:OD2 | 1:L:425:ARG:NH2 | 2.47 | 0.47 |
| 1:H:910:LEU:C | 1:H:910:LEU:HD12 | 2.35 | 0.47 |
| 1:O:910:LEU:HD12 | 1:O:910:LEU:C | 2.35 | 0.47 |
| 1:F:595:THR:CG2 | 1:F:596:PRO:HA | 2.37 | 0.47 |
| 1:D:188:VAL:C | 1:D:189:LEU:HD23 | 2.33 | 0.47 |
| 1:B:43:ARG:CG | 1:B:43:ARG:HH11 | 2.24 | 0.47 |
| 1:F:43:ARG:CG | 1:F:43:ARG:HH11 | 2.24 | 0.47 |
| 1:O:653[A]:HIS:HD2 | 1:O:666:GLY:O | 1.97 | 0.47 |
| 1:P:645:ARG:HH22 | 1:P:650:GLU:CD | 2.18 | 0.47 |
| 1:J:645:ARG:HH22 | 1:J:650:GLU:CD | 2.18 | 0.47 |
| 1:J:653[A]:HIS:HD2 | 1:J:666:GLY:O | 1.97 | 0.47 |
| 1:B:645:ARG:HH22 | 1:B:650:GLU:CD | 2.18 | 0.47 |
| 1:H:73:TRP:CZ2 | 1:H:122:CYS:HB3 | 2.48 | 0.47 |
| 1:B:73:TRP:CH2 | 1:B:185:ALA:HB1 | 2.49 | 0.47 |
| 1:M:35:SER:O | 1:M:50:GLN:HG3 | 2.14 | 0.47 |
| 1:K:35:SER:O | 1:K:50:GLN:HG3 | 2.14 | 0.47 |
| 1:A:261:TRP:CH2 | 1:A:266:GLN:HB2 | 2.49 | 0.47 |
| 1:P:679:LEU:HD23 | 1:P:679:LEU:HA | 1.40 | 0.47 |
| 1:N:9:VAL:O | 1:N:12:GLN:HB3 | 2.13 | 0.47 |
| 1:C:910:LEU:HD12 | 1:C:910:LEU:C | 2.35 | 0.47 |
| 1:E:18:ASN:ND2 | 1:E:21:VAL:HG23 | 2.29 | 0.47 |
| 1:K:9:VAL:O | 1:K:12:GLN:HB3 | 2.13 | 0.47 |
| 1:A:910:LEU:HD12 | 1:A:910:LEU:C | 2.35 | 0.47 |
| 1:G:237:ARG:HE | 1:G:237:ARG:HB2 | 1.35 | 0.47 |
| 1:M:910:LEU:HD12 | 1:M:910:LEU:C | 2.35 | 0.47 |
| 1:G:910:LEU:C | 1:G:910:LEU:HD12 | 2.35 | 0.47 |
| 1:B:910:LEU:C | 1:B:910:LEU:HD12 | 2.35 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:9:VAL:O | 1:I:12:GLN:HB3 | 2.13 | 0.47 |
| 1:F:257:THR:OG1 | 1:F:316:HIS:HE1 | 1.98 | 0.47 |
| 1:O:362:LEU:HD23 | 1:O:362:LEU:HA | 1.70 | 0.47 |
| 1:L:645:ARG:HH22 | 1:L:650:GLU:CD | 2.18 | 0.47 |
| 1:K:645:ARG:HH22 | 1:K:650:GLU:CD | 2.18 | 0.47 |
| 1:H:645:ARG:HH22 | 1:H:650:GLU:CD | 2.18 | 0.47 |
| 1:G:217:LYS:HG2 | 1:G:218:PRO:HD2 | 1.96 | 0.47 |
| 1:E:35:SER:O | 1:E:50:GLN:HG3 | 2.14 | 0.47 |
| 1:O:658:LEU:N | 1:O:661:LYS:O | 2.40 | 0.47 |
| 1:C:261:TRP:CH2 | 1:C:266:GLN:HB2 | 2.49 | 0.47 |
| 1:A:679:LEU:HD23 | 1:A:679:LEU:HA | 1.40 | 0.47 |
| 1:F:140:ARG:HB2 | 1:F:171:PHE:O | 2.13 | 0.47 |
| 1:P:36:TRP:CE2 | 1:P:42:ALA:HA | 2.50 | 0.47 |
| 1:J:134:LEU:HD23 | 1:J:134:LEU:HA | 1.68 | 0.47 |
| 1:B:914:CME:HB3 | 1:B:914:CME:HE2 | 1.74 | 0.47 |
| 1:A:18:ASN:ND2 | 1:A:21:VAL:HG23 | 2.29 | 0.47 |
| 1:I:257:THR:OG1 | 1:I:316:HIS:HE1 | 1.98 | 0.47 |
| 1:B:257:THR:OG1 | 1:B:316:HIS:HE1 | 1.98 | 0.47 |
| 1:M:78:LEU:HB3 | 1:M:79:PRO:CD | 2.43 | 0.47 |
| 1:A:183:ARG:HD3 | 1:A:183:ARG:HH11 | 1.62 | 0.47 |
| 1:C:856:TYR:CD2 | 1:C:864:MET:HE2 | 2.48 | 0.47 |
| 1:O:217:LYS:HG2 | 1:O:218:PRO:HD2 | 1.96 | 0.47 |
| 1:G:261:TRP:CH2 | 1:G:266:GLN:HB2 | 2.49 | 0.47 |
| 1:C:36:TRP:CE2 | 1:C:42:ALA:HA | 2.50 | 0.47 |
| 1:H:18:ASN:ND2 | 1:H:21:VAL:HG23 | 2.29 | 0.47 |
| 1:B:18:ASN:ND2 | 1:B:21:VAL:HG23 | 2.29 | 0.47 |
| 1:B:202:MET:HB3 | 1:B:202:MET:HE3 | 1.82 | 0.47 |
| 1:P:134:LEU:HD23 | 1:P:134:LEU:HA | 1.68 | 0.47 |
| 1:K:134:LEU:HD23 | 1:K:134:LEU:HA | 1.68 | 0.47 |
| 1:F:18:ASN:ND2 | 1:F:21:VAL:HG23 | 2.29 | 0.47 |
| 1:H:595:THR:HG23 | 1:H:596:PRO:CA | 2.35 | 0.47 |
| 1:K:78:LEU:HB3 | 1:K:79:PRO:CD | 2.43 | 0.47 |
| 1:K:949:HIS:HD2 | 1:K:1020:TRP:HE1 | 1.53 | 0.47 |
| 1:I:7:LEU:HD12 | 1:I:74:LEU:HD11 | 1.97 | 0.47 |
| 1:H:43:ARG:CG | 1:H:43:ARG:HH11 | 2.24 | 0.47 |
| 1:F:952:ARG:CG | 1:F:952:ARG:HH11 | 2.28 | 0.47 |
| 1:K:668:VAL:CG1 | 1:K:669:PRO:HD2 | 2.45 | 0.47 |
| 1:L:261:TRP:CH2 | 1:L:266:GLN:HB2 | 2.49 | 0.47 |
| 1:I:287:ASP:CG | 1:L:425:ARG:HH22 | 2.17 | 0.47 |
| 1:N:18:ASN:ND2 | 1:N:21:VAL:HG23 | 2.29 | 0.47 |
| 1:O:18:ASN:ND2 | 1:O:21:VAL:HG23 | 2.29 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:N:910:LEU:HD12 | 1:N:910:LEU:C | 2.35 | 0.47 |
| 1:F:134:LEU:HD23 | 1:F:134:LEU:HA | 1.68 | 0.47 |
| 1:G:18:ASN:ND2 | 1:G:21:VAL:HG23 | 2.29 | 0.47 |
| 1:L:63:PHE:CB | 1:L:64:PRO:HD2 | 2.34 | 0.46 |
| 1:D:952:ARG:HH11 | 1:D:952:ARG:CG | 2.28 | 0.46 |
| 1:A:65:ALA:HB1 | 1:A:66:PRO:HD2 | 1.95 | 0.46 |
| 1:I:653[A]:HIS:HD2 | 1:I:666:GLY:O | 1.97 | 0.46 |
| 1:F:668:VAL:CG1 | 1:F:669:PRO:HD2 | 2.45 | 0.46 |
| 1:N:645:ARG:HH22 | 1:N:650:GLU:CD | 2.18 | 0.46 |
| 1:G:645:ARG:HH22 | 1:G:650:GLU:CD | 2.18 | 0.46 |
| 1:B:612:THR:HB | 1:B:613:PRO:HD2 | 1.98 | 0.46 |
| 1:J:429:ASP:HA | 1:J:430:PRO:HD3 | 1.73 | 0.46 |
| 1:C:429:ASP:HA | 1:C:430:PRO:HD3 | 1.73 | 0.46 |
| 1:P:147:ASN:HA | 1:P:148:SER:HA | 1.57 | 0.46 |
| 1:C:18:ASN:ND2 | 1:C:21:VAL:HG23 | 2.29 | 0.46 |
| 1:K:18:ASN:ND2 | 1:K:21:VAL:HG23 | 2.29 | 0.46 |
| 1:I:378:LEU:HA | 1:I:378:LEU:HD23 | 1.74 | 0.46 |
| 1:A:914:CME:HB3 | 1:A:914:CME:HE2 | 1.74 | 0.46 |
| 1:G:753:ASN:OD1 | 1:G:753:ASN:N | 2.30 | 0.46 |
| 1:L:134:LEU:HD23 | 1:L:134:LEU:HA | 1.68 | 0.46 |
| 1:J:910:LEU:HD12 | 1:J:910:LEU:C | 2.35 | 0.46 |
| 1:E:830:LEU:HD11 | 1:F:830:LEU:HD11 | 1.97 | 0.46 |
| 1:M:18:ASN:ND2 | 1:M:21:VAL:HG23 | 2.29 | 0.46 |
| 1:A:57:GLU:HG2 | 1:A:83:THR:HG22 | 1.95 | 0.46 |
| 1:F:57:GLU:HG2 | 1:F:83:THR:HG22 | 1.95 | 0.46 |
| 1:O:7:LEU:HD12 | 1:O:74:LEU:HD11 | 1.97 | 0.46 |
| 1:I:645:ARG:HH22 | 1:I:650:GLU:CD | 2.18 | 0.46 |
| 1:M:856:TYR:CD2 | 1:M:864:MET:HE2 | 2.50 | 0.46 |
| 1:A:100:TYR:CE1 | 1:A:602:CYS:HB3 | 2.51 | 0.46 |
| 1:H:100:TYR:CE1 | 1:H:602:CYS:HB3 | 2.51 | 0.46 |
| 1:D:36:TRP:CE2 | 1:D:42:ALA:HA | 2.50 | 0.46 |
| 1:A:36:TRP:CE2 | 1:A:42:ALA:HA | 2.50 | 0.46 |
| 1:I:910:LEU:C | 1:I:910:LEU:HD12 | 2.35 | 0.46 |
| 1:H:114:VAL:HG22 | 1:H:191:TRP:HB3 | 1.98 | 0.46 |
| 1:G:91:GLN:HG3 | 1:G:96:ASP:OD1 | 2.15 | 0.46 |
| 1:N:91:GLN:HG3 | 1:N:96:ASP:OD1 | 2.16 | 0.46 |
| 1:I:91:GLN:HG3 | 1:I:96:ASP:OD1 | 2.16 | 0.46 |
| 1:J:257:THR:OG1 | 1:J:316:HIS:HE1 | 1.98 | 0.46 |
| 1:D:57:GLU:HG2 | 1:D:83:THR:HG22 | 1.95 | 0.46 |
| 1:I:57:GLU:HG2 | 1:I:83:THR:HG22 | 1.95 | 0.46 |
| 1:K:952:ARG:CG | 1:K:952:ARG:HH11 | 2.28 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:362:LEU:HD23 | 1:E:362:LEU:HA | 1.70 | 0.46 |
| 1:C:668:VAL:CG1 | 1:C:669:PRO:HD2 | 2.45 | 0.46 |
| 1:D:645:ARG:HH22 | 1:D:650:GLU:CD | 2.18 | 0.46 |
| 1:D:100:TYR:CE1 | 1:D:602:CYS:HB3 | 2.51 | 0.46 |
| 1:B:429:ASP:HA | 1:B:430:PRO:HD3 | 1.73 | 0.46 |
| 1:G:36:TRP:CE2 | 1:G:42:ALA:HA | 2.50 | 0.46 |
| 1:B:753:ASN:OD1 | 1:B:753:ASN:N | 2.30 | 0.46 |
| 1:O:80:GLU:HG3 | 1:O:80:GLU:H | 1.28 | 0.46 |
| 1:P:114:VAL:HG22 | 1:P:191:TRP:HB3 | 1.98 | 0.46 |
| 1:A:91:GLN:HG3 | 1:A:96:ASP:OD1 | 2.16 | 0.46 |
| 1:I:36:TRP:CE2 | 1:I:42:ALA:HA | 2.50 | 0.46 |
| 1:L:18:ASN:ND2 | 1:L:21:VAL:HG23 | 2.29 | 0.46 |
| 1:L:36:TRP:CE2 | 1:L:42:ALA:HA | 2.50 | 0.46 |
| 1:L:595:THR:CG2 | 1:L:596:PRO:HA | 2.37 | 0.46 |
| 1:I:595:THR:CG2 | 1:I:596:PRO:HA | 2.37 | 0.46 |
| 1:E:257:THR:OG1 | 1:E:316:HIS:HE1 | 1.98 | 0.46 |
| 1:C:952:ARG:HH11 | 1:C:952:ARG:CG | 2.28 | 0.46 |
| 1:I:43:ARG:CG | 1:I:43:ARG:HH11 | 2.24 | 0.46 |
| 1:A:362:LEU:HD23 | 1:A:362:LEU:HA | 1.70 | 0.46 |
| 1:L:668:VAL:CG1 | 1:L:669:PRO:HD2 | 2.45 | 0.46 |
| 1:A:645:ARG:HH22 | 1:A:650:GLU:CD | 2.18 | 0.46 |
| 1:G:657:ALA:HA | 1:G:661:LYS:O | 2.16 | 0.46 |
| 1:I:217:LYS:HG2 | 1:I:218:PRO:HD2 | 1.96 | 0.46 |
| 1:B:100:TYR:CE1 | 1:B:602:CYS:HB3 | 2.51 | 0.46 |
| 1:K:3:ILE:HG13 | 1:K:4:THR:N | 2.25 | 0.46 |
| 1:M:546:LEU:HA | 3:M:4124:HOH:O | 2.16 | 0.46 |
| 1:D:91:GLN:HG3 | 1:D:96:ASP:OD1 | 2.16 | 0.46 |
| 1:A:658:LEU:N | 1:A:661:LYS:O | 2.40 | 0.46 |
| 1:J:395:HIS:HA | 1:J:396:PRO:HD3 | 1.69 | 0.46 |
| 1:B:91:GLN:HG3 | 1:B:96:ASP:OD1 | 2.16 | 0.46 |
| 1:C:257:THR:OG1 | 1:C:316:HIS:HE1 | 1.98 | 0.46 |
| 1:O:257:THR:OG1 | 1:O:316:HIS:HE1 | 1.98 | 0.46 |
| 1:L:285:TYR:CB | 1:L:288:ARG:HG3 | 2.42 | 0.46 |
| 1:D:78:LEU:HB3 | 1:D:79:PRO:CD | 2.43 | 0.46 |
| 1:P:952:ARG:HH11 | 1:P:952:ARG:CG | 2.28 | 0.46 |
| 1:M:43:ARG:HH11 | 1:M:43:ARG:CG | 2.24 | 0.46 |
| 1:O:668:VAL:CG1 | 1:O:669:PRO:HD2 | 2.45 | 0.46 |
| 1:E:272:ALA:HA | 1:E:273:PRO:HD3 | 1.78 | 0.46 |
| 1:L:612:THR:HB | 1:L:613:PRO:HD2 | 1.98 | 0.46 |
| 1:N:612:THR:HB | 1:N:613:PRO:HD2 | 1.98 | 0.46 |
| 1:N:679:LEU:HD23 | 1:N:679:LEU:HA | 1.40 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:612:THR:HB | 1:G:613:PRO:HD2 | 1.98 | 0.46 |
| 1:A:657:ALA:HA | 1:A:661:LYS:O | 2.16 | 0.46 |
| 1:O:36:TRP:CE2 | 1:O:42:ALA:HA | 2.50 | 0.46 |
| 1:A:114:VAL:HG22 | 1:A:191:TRP:HB3 | 1.98 | 0.46 |
| 1:F:910:LEU:C | 1:F:910:LEU:HD12 | 2.35 | 0.46 |
| 1:P:772:ASP:N | 1:P:772:ASP:OD1 | 2.48 | 0.46 |
| 1:E:36:TRP:CE2 | 1:E:42:ALA:HA | 2.50 | 0.46 |
| 1:L:427:THR:HA | 1:L:436:MET:HE2 | 1.93 | 0.46 |
| 1:K:57:GLU:HG2 | 1:K:83:THR:HG22 | 1.95 | 0.46 |
| 1:B:579:ASP:HB2 | 1:B:580:GLU:OE2 | 2.16 | 0.46 |
| 1:O:952:ARG:CG | 1:O:952:ARG:HH11 | 2.28 | 0.46 |
| 1:H:254:LEU:HD23 | 1:H:254:LEU:HA | 1.71 | 0.46 |
| 1:B:856:TYR:CD2 | 1:B:864:MET:HE2 | 2.48 | 0.46 |
| 1:A:422:PRO:HG3 | 1:D:284:GLY:C | 2.35 | 0.46 |
| 1:E:217:LYS:HG2 | 1:E:218:PRO:HD2 | 1.96 | 0.46 |
| 1:E:657:ALA:HA | 1:E:661:LYS:O | 2.16 | 0.46 |
| 1:O:657:ALA:HA | 1:O:661:LYS:O | 2.16 | 0.46 |
| 1:F:612:THR:HB | 1:F:613:PRO:HD2 | 1.98 | 0.46 |
| 1:E:100:TYR:CE1 | 1:E:602:CYS:HB3 | 2.51 | 0.46 |
| 1:L:657:ALA:HA | 1:L:661:LYS:O | 2.16 | 0.46 |
| 1:J:91:GLN:HG3 | 1:J:96:ASP:OD1 | 2.15 | 0.46 |
| 1:B:36:TRP:CE2 | 1:B:42:ALA:HA | 2.50 | 0.46 |
| 1:M:134:LEU:HA | 1:M:134:LEU:HD23 | 1.68 | 0.46 |
| 1:K:114:VAL:HG22 | 1:K:191:TRP:HB3 | 1.98 | 0.46 |
| 1:D:657:ALA:HA | 1:D:661:LYS:O | 2.16 | 0.46 |
| 1:F:36:TRP:CE2 | 1:F:42:ALA:HA | 2.50 | 0.46 |
| 1:F:920:LEU:HB3 | 1:F:921:PRO:CD | 2.46 | 0.46 |
| 1:I:579:ASP:HB2 | 1:I:580:GLU:OE2 | 2.16 | 0.46 |
| 1:D:579:ASP:HB2 | 1:D:580:GLU:OE2 | 2.16 | 0.46 |
| 1:M:254:LEU:HD23 | 1:M:254:LEU:HA | 1.71 | 0.46 |
| 1:A:668:VAL:CG1 | 1:A:669:PRO:HD2 | 2.45 | 0.46 |
| 1:J:287:ASP:CG | 1:K:425:ARG:HH22 | 2.18 | 0.46 |
| 1:O:612:THR:HB | 1:O:613:PRO:HD2 | 1.98 | 0.46 |
| 1:D:612:THR:HB | 1:D:613:PRO:HD2 | 1.98 | 0.46 |
| 1:J:100:TYR:CE1 | 1:J:602:CYS:HB3 | 2.51 | 0.46 |
| 1:F:469:ASP:HB3 | 1:G:473:ARG:HD2 | 1.97 | 0.46 |
| 1:I:612:THR:HB | 1:I:613:PRO:HD2 | 1.98 | 0.46 |
| 1:I:767:GLN:CG | 1:I:768:MET:N | 2.79 | 0.46 |
| 1:H:3:ILE:HG13 | 1:H:4:THR:N | 2.25 | 0.46 |
| 1:J:425:ARG:HH22 | 1:K:287:ASP:CG | 2.19 | 0.46 |
| 1:J:147:ASN:HA | 1:J:148:SER:HA | 1.57 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:657:ALA:HA | 1:H:661:LYS:O | 2.16 | 0.46 |
| 1:O:237:ARG:HE | 1:O:237:ARG:HB2 | 1.35 | 0.46 |
| 1:N:36:TRP:CE2 | 1:N:42:ALA:HA | 2.50 | 0.46 |
| 1:H:91:GLN:HG3 | 1:H:96:ASP:OD1 | 2.16 | 0.46 |
| 1:B:657:ALA:HA | 1:B:661:LYS:O | 2.16 | 0.46 |
| 1:N:257:THR:OG1 | 1:N:316:HIS:HE1 | 1.98 | 0.46 |
| 1:H:285:TYR:CB | 1:H:288:ARG:HG3 | 2.42 | 0.46 |
| 1:J:78:LEU:HB3 | 1:J:79:PRO:CD | 2.43 | 0.46 |
| 1:N:920:LEU:HB3 | 1:N:921:PRO:CD | 2.46 | 0.46 |
| 1:N:579:ASP:HB2 | 1:N:580:GLU:OE2 | 2.16 | 0.46 |
| 1:H:952:ARG:HH11 | 1:H:952:ARG:CG | 2.28 | 0.46 |
| 1:G:952:ARG:HH11 | 1:G:952:ARG:CG | 2.28 | 0.46 |
| 1:J:668:VAL:CG1 | 1:J:669:PRO:HD2 | 2.45 | 0.46 |
| 1:M:217:LYS:HG2 | 1:M:218:PRO:HD2 | 1.96 | 0.46 |
| 1:N:282:ARG:HD2 | 1:O:418:HIS:O | 2.15 | 0.46 |
| 1:P:612:THR:HB | 1:P:613:PRO:HD2 | 1.98 | 0.46 |
| 1:D:767:GLN:CG | 1:D:768:MET:N | 2.79 | 0.46 |
| 1:C:100:TYR:CE1 | 1:C:602:CYS:HB3 | 2.51 | 0.46 |
| 1:M:679:LEU:HA | 1:M:679:LEU:HD23 | 1.40 | 0.46 |
| 1:B:279:ILE:HD11 | 1:C:422:PRO:HG2 | 1.96 | 0.46 |
| 1:M:36:TRP:CE2 | 1:M:42:ALA:HA | 2.50 | 0.46 |
| 1:B:114:VAL:HG22 | 1:B:191:TRP:HB3 | 1.98 | 0.46 |
| 1:A:685:LEU:HA | 1:A:686:PRO:HD3 | 1.83 | 0.46 |
| 1:L:91:GLN:HG3 | 1:L:96:ASP:OD1 | 2.16 | 0.46 |
| 1:J:986:ILE:HG23 | 1:J:986:ILE:HD13 | 1.67 | 0.46 |
| 1:M:91:GLN:HG3 | 1:M:96:ASP:OD1 | 2.15 | 0.46 |
| 1:C:118:ASN:HA | 1:C:119:PRO:HD2 | 1.62 | 0.46 |
| 1:P:657:ALA:HA | 1:P:661:LYS:O | 2.16 | 0.46 |
| 1:J:18:ASN:ND2 | 1:J:21:VAL:HG23 | 2.29 | 0.46 |
| 1:P:118:ASN:HA | 1:P:119:PRO:HD2 | 1.62 | 0.46 |
| 1:O:57:GLU:HG2 | 1:O:83:THR:HG22 | 1.95 | 0.46 |
| 1:K:701:VAL:HG12 | 1:K:702:GLN:N | 2.31 | 0.46 |
| 1:P:701:VAL:HG12 | 1:P:702:GLN:N | 2.31 | 0.46 |
| 1:L:7:LEU:HD12 | 1:L:74:LEU:HD11 | 1.97 | 0.46 |
| 1:G:579:ASP:HB2 | 1:G:580:GLU:OE2 | 2.16 | 0.46 |
| 1:O:579:ASP:HB2 | 1:O:580:GLU:OE2 | 2.16 | 0.46 |
| 1:G:254:LEU:HA | 1:G:254:LEU:HD23 | 1.71 | 0.46 |
| 1:B:668:VAL:CG1 | 1:B:669:PRO:HD2 | 2.45 | 0.46 |
| 1:E:668:VAL:CG1 | 1:E:669:PRO:HD2 | 2.45 | 0.46 |
| 1:E:767:GLN:CG | 1:E:768:MET:N | 2.79 | 0.46 |
| 1:O:767:GLN:CG | 1:O:768:MET:N | 2.79 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------|--------------------------|-------------------|
| 1:M:85:VAL:CG1 | 1:M:86:VAL:N | 2.79 | 0.46 |
| 1:G:429:ASP:HA | 1:G:430:PRO:HD3 | 1.74 | 0.46 |
| 1:L:42:ALA:O | 1:L:310:ARG:NH1 | 2.49 | 0.46 |
| 1:D:658:LEU:N | 1:D:661:LYS:O | 2.40 | 0.46 |
| 1:K:42:ALA:O | 1:K:310:ARG:NH1 | 2.49 | 0.46 |
| 1:H:237:ARG:HB2 | 1:H:237:ARG:HE | 1.35 | 0.46 |
| 1:P:730:LEU:HA | 1:P:731:PRO:HD3 | 1.80 | 0.46 |
| 1:B:111:PRO:HA | 1:B:112:PRO:HA | 1.66 | 0.46 |
| 1:I:657:ALA:HA | 1:I:661:LYS:O | 2.16 | 0.46 |
| 1:C:395:HIS:CG | 1:C:396:PRO:HD2 | 2.51 | 0.46 |
| 1:K:546:LEU:HA | 3:K:4124:HOH:O | 2.16 | 0.46 |
| 1:B:285:TYR:CB | 1:B:288:ARG:HG3 | 2.42 | 0.46 |
| 1:C:57:GLU:HG2 | 1:C:83:THR:HG22 | 1.95 | 0.46 |
| 1:D:701:VAL:HG12 | 1:D:702:GLN:N | 2.31 | 0.46 |
| 1:M:701:VAL:HG12 | 1:M:702:GLN:N | 2.31 | 0.46 |
| 1:N:701:VAL:HG12 | 1:N:702:GLN:N | 2.31 | 0.46 |
| 1:J:701:VAL:HG12 | 1:J:702:GLN:N | 2.31 | 0.46 |
| 1:E:701:VAL:HG12 | 1:E:702:GLN:N | 2.31 | 0.46 |
| 1:O:920:LEU:HB3 | 1:O:921:PRO:CD | 2.46 | 0.46 |
| 1:J:579:ASP:HB2 | 1:J:580:GLU:OE2 | 2.16 | 0.46 |
| 1:J:43:ARG:HH11 | 1:J:43:ARG:CG | 2.24 | 0.46 |
| 1:M:653[B]:HIS:CD2 | 1:M:667:GLU:HG2 | 2.51 | 0.46 |
| 1:P:767:GLN:CG | 1:P:768:MET:N | 2.79 | 0.46 |
| 1:G:767:GLN:CG | 1:G:768:MET:N | 2.79 | 0.46 |
| 1:K:100:TYR:CE1 | 1:K:602:CYS:HB3 | 2.51 | 0.46 |
| 1:K:767:GLN:CG | 1:K:768:MET:N | 2.79 | 0.46 |
| 1:P:100:TYR:CE1 | 1:P:602:CYS:HB3 | 2.51 | 0.46 |
| 1:B:85:VAL:CG1 | 1:B:86:VAL:N | 2.79 | 0.46 |
| 1:E:85:VAL:CG1 | 1:E:86:VAL:N | 2.79 | 0.46 |
| 1:N:3:ILE:HG13 | 1:N:4:THR:N | 2.25 | 0.46 |
| 1:G:546:LEU:HA | 3:G:3228:HOH:O | 2.16 | 0.46 |
| 1:J:546:LEU:HA | 3:J:3231:HOH:O | 2.16 | 0.46 |
| 1:O:546:LEU:HA | 3:O:3228:HOH:O | 2.16 | 0.46 |
| 1:A:395:HIS:HA | 1:A:396:PRO:HD3 | 1.69 | 0.46 |
| 1:I:546:LEU:HA | 3:I:4123:HOH:O | 2.16 | 0.46 |
| 1:E:655:MET:HE3 | 1:E:655:MET:HB2 | 1.73 | 0.46 |
| 1:N:778:THR:HG23 | 1:N:779:PRO:HD2 | 1.98 | 0.46 |
| 1:J:36:TRP:CE2 | 1:J:42:ALA:HA | 2.50 | 0.46 |
| 1:H:595:THR:CG2 | 1:H:596:PRO:HA | 2.37 | 0.45 |
| 1:M:595:THR:CG2 | 1:M:596:PRO:HA | 2.37 | 0.45 |
| 1:F:701:VAL:HG12 | 1:F:702:GLN:N | 2.31 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:M:920:LEU:HB3 | 1:M:921:PRO:CD | 2.46 | 0.45 |
| 1:P:579:ASP:HB2 | 1:P:580:GLU:OE2 | 2.16 | 0.45 |
| 1:F:579:ASP:HB2 | 1:F:580:GLU:OE2 | 2.16 | 0.45 |
| 1:H:579:ASP:HB2 | 1:H:580:GLU:OE2 | 2.16 | 0.45 |
| 1:I:653[B]:HIS:CD2 | 1:I:667:GLU:HG2 | 2.51 | 0.45 |
| 1:A:433:LEU:N | 1:A:434:PRO:CD | 2.80 | 0.45 |
| 1:A:612:THR:HB | 1:A:613:PRO:HD2 | 1.98 | 0.45 |
| 1:J:42:ALA:O | 1:J:310:ARG:NH1 | 2.49 | 0.45 |
| 1:B:395:HIS:HA | 1:B:396:PRO:HD3 | 1.69 | 0.45 |
| 1:K:914:CME:HB3 | 1:K:914:CME:HE2 | 1.74 | 0.45 |
| 1:O:118:ASN:HA | 1:O:119:PRO:HD2 | 1.62 | 0.45 |
| 1:M:687:GLN:HA | 1:M:688:PRO:HD3 | 1.73 | 0.45 |
| 1:H:36:TRP:CE2 | 1:H:42:ALA:HA | 2.50 | 0.45 |
| 1:P:395:HIS:CG | 1:P:396:PRO:HD2 | 2.51 | 0.45 |
| 1:L:114:VAL:HG22 | 1:L:191:TRP:HB3 | 1.98 | 0.45 |
| 1:O:147:ASN:HA | 1:O:148:SER:HA | 1.57 | 0.45 |
| 1:E:285:TYR:CB | 1:E:288:ARG:HG3 | 2.42 | 0.45 |
| 1:E:920:LEU:HB3 | 1:E:921:PRO:CD | 2.46 | 0.45 |
| 1:C:7:LEU:HD12 | 1:C:74:LEU:HD11 | 1.97 | 0.45 |
| 1:E:43:ARG:NH1 | 1:E:44:THR:CG2 | 2.80 | 0.45 |
| 1:K:433:LEU:N | 1:K:434:PRO:CD | 2.80 | 0.45 |
| 1:B:362:LEU:HD23 | 1:B:362:LEU:HA | 1.70 | 0.45 |
| 1:O:653[B]:HIS:CD2 | 1:O:667:GLU:HG2 | 2.51 | 0.45 |
| 1:L:653[B]:HIS:CD2 | 1:L:667:GLU:HG2 | 2.51 | 0.45 |
| 1:C:653[B]:HIS:CD2 | 1:C:667:GLU:HG2 | 2.51 | 0.45 |
| 1:D:668:VAL:CG1 | 1:D:669:PRO:HD2 | 2.45 | 0.45 |
| 1:J:653[B]:HIS:CD2 | 1:J:667:GLU:HG2 | 2.51 | 0.45 |
| 1:M:668:VAL:CG1 | 1:M:669:PRO:HD2 | 2.45 | 0.45 |
| 1:E:653[B]:HIS:CD2 | 1:E:667:GLU:HG2 | 2.51 | 0.45 |
| 1:C:657:ALA:HA | 1:C:661:LYS:O | 2.16 | 0.45 |
| 1:M:767:GLN:CG | 1:M:768:MET:N | 2.79 | 0.45 |
| 1:H:612:THR:HB | 1:H:613:PRO:HD2 | 1.98 | 0.45 |
| 1:L:767:GLN:CG | 1:L:768:MET:N | 2.79 | 0.45 |
| 1:C:679:LEU:HA | 1:C:679:LEU:HD23 | 1.40 | 0.45 |
| 1:G:100:TYR:CE1 | 1:G:602:CYS:HB3 | 2.51 | 0.45 |
| 1:L:85:VAL:CG1 | 1:L:86:VAL:N | 2.79 | 0.45 |
| 1:P:3:ILE:HG13 | 1:P:4:THR:N | 2.25 | 0.45 |
| 1:K:36:TRP:CE2 | 1:K:42:ALA:HA | 2.50 | 0.45 |
| 1:H:42:ALA:O | 1:H:310:ARG:NH1 | 2.49 | 0.45 |
| 1:D:778:THR:HG23 | 1:D:779:PRO:HD2 | 1.98 | 0.45 |
| 1:J:878:HIS:HA | 1:J:879:PRO:HD3 | 1.83 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:395:HIS:CG | 1:F:396:PRO:HD2 | 2.51 | 0.45 |
| 1:P:13:ARG:O | 1:P:14:ARG:HB2 | 2.17 | 0.45 |
| 1:F:778:THR:HG23 | 1:F:779:PRO:HD2 | 1.98 | 0.45 |
| 1:M:114:VAL:HG22 | 1:M:191:TRP:HB3 | 1.98 | 0.45 |
| 1:G:118:ASN:HA | 1:G:119:PRO:HD2 | 1.62 | 0.45 |
| 1:I:211:ASP:OD1 | 1:I:211:ASP:N | 2.50 | 0.45 |
| 1:P:986:ILE:HD13 | 1:P:986:ILE:HG23 | 1.67 | 0.45 |
| 1:O:395:HIS:CG | 1:O:396:PRO:HD2 | 2.51 | 0.45 |
| 1:I:114:VAL:HG22 | 1:I:191:TRP:HB3 | 1.98 | 0.45 |
| 1:C:947:GLY:HA3 | 1:C:948:PRO:HD2 | 1.82 | 0.45 |
| 1:D:257:THR:OG1 | 1:D:316:HIS:HE1 | 1.98 | 0.45 |
| 1:J:322:LEU:CD2 | 1:J:324:GLU:N | 2.80 | 0.45 |
| 1:H:257:THR:OG1 | 1:H:316:HIS:HE1 | 1.98 | 0.45 |
| 1:C:701:VAL:HG12 | 1:C:702:GLN:N | 2.31 | 0.45 |
| 1:H:920:LEU:HB3 | 1:H:921:PRO:CD | 2.46 | 0.45 |
| 1:C:579:ASP:HB2 | 1:C:580:GLU:OE2 | 2.16 | 0.45 |
| 1:A:579:ASP:HB2 | 1:A:580:GLU:OE2 | 2.16 | 0.45 |
| 1:L:579:ASP:HB2 | 1:L:580:GLU:OE2 | 2.16 | 0.45 |
| 1:J:43:ARG:NH1 | 1:J:44:THR:CG2 | 2.80 | 0.45 |
| 1:M:43:ARG:NH1 | 1:M:44:THR:CG2 | 2.80 | 0.45 |
| 1:N:43:ARG:HH12 | 1:N:44:THR:CG2 | 2.30 | 0.45 |
| 1:J:129:VAL:CG2 | 1:J:182:ASN:ND2 | 2.80 | 0.45 |
| 1:K:254:LEU:HA | 1:K:254:LEU:HD23 | 1.71 | 0.45 |
| 1:D:129:VAL:CG2 | 1:D:182:ASN:ND2 | 2.80 | 0.45 |
| 1:B:129:VAL:CG2 | 1:B:182:ASN:ND2 | 2.80 | 0.45 |
| 1:C:362:LEU:HD23 | 1:C:362:LEU:HA | 1.70 | 0.45 |
| 1:N:847:LYS:HG3 | 1:N:848:THR:N | 2.32 | 0.45 |
| 1:E:433:LEU:N | 1:E:434:PRO:CD | 2.80 | 0.45 |
| 1:N:668:VAL:CG1 | 1:N:669:PRO:HD2 | 2.45 | 0.45 |
| 1:F:653[B]:HIS:CD2 | 1:F:667:GLU:HG2 | 2.51 | 0.45 |
| 1:H:668:VAL:CG1 | 1:H:669:PRO:HD2 | 2.45 | 0.45 |
| 1:M:645:ARG:HH22 | 1:M:650:GLU:CD | 2.18 | 0.45 |
| 1:E:612:THR:HA | 1:E:613:PRO:HD3 | 1.59 | 0.45 |
| 1:F:100:TYR:CE1 | 1:F:602:CYS:HB3 | 2.51 | 0.45 |
| 1:I:100:TYR:CE1 | 1:I:602:CYS:HB3 | 2.51 | 0.45 |
| 1:F:767:GLN:CG | 1:F:768:MET:N | 2.79 | 0.45 |
| 1:O:100:TYR:CE1 | 1:O:602:CYS:HB3 | 2.51 | 0.45 |
| 1:P:42:ALA:O | 1:P:310:ARG:NH1 | 2.49 | 0.45 |
| 1:F:847:LYS:HG3 | 1:F:848:THR:N | 2.32 | 0.45 |
| 1:L:395:HIS:CG | 1:L:396:PRO:HD2 | 2.51 | 0.45 |
| 1:K:91:GLN:HG3 | 1:K:96:ASP:OD1 | 2.15 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-----------------|--------------------------|-------------------|
| 1:G:847:LYS:HG3 | 1:G:848:THR:N | 2.32 | 0.45 |
| 1:E:91:GLN:HG3 | 1:E:96:ASP:OD1 | 2.16 | 0.45 |
| 1:N:114:VAL:HG22 | 1:N:191:TRP:HB3 | 1.98 | 0.45 |
| 1:G:395:HIS:CG | 1:G:396:PRO:HD2 | 2.51 | 0.45 |
| 1:L:914:CME:HB3 | 1:L:914:CME:HE2 | 1.74 | 0.45 |
| 1:J:211:ASP:OD1 | 1:J:211:ASP:N | 2.50 | 0.45 |
| 1:H:914:CME:HE2 | 1:H:914:CME:HB3 | 1.74 | 0.45 |
| 1:A:202:MET:HE3 | 1:A:202:MET:HB3 | 1.84 | 0.45 |
| 1:N:395:HIS:CG | 1:N:396:PRO:HD2 | 2.51 | 0.45 |
| 1:B:778:THR:HG23 | 1:B:779:PRO:HD2 | 1.98 | 0.45 |
| 1:B:425:ARG:NH2 | 1:C:287:ASP:OD2 | 2.50 | 0.45 |
| 1:C:91:GLN:HG3 | 1:C:96:ASP:OD1 | 2.16 | 0.45 |
| 1:J:778:THR:HG23 | 1:J:779:PRO:HD2 | 1.98 | 0.45 |
| 1:J:595:THR:CG2 | 1:J:596:PRO:HA | 2.37 | 0.45 |
| 1:P:78:LEU:HB3 | 1:P:79:PRO:CD | 2.43 | 0.45 |
| 1:N:7:LEU:HD12 | 1:N:74:LEU:HD11 | 1.97 | 0.45 |
| 1:I:920:LEU:HB3 | 1:I:921:PRO:CD | 2.46 | 0.45 |
| 1:H:43:ARG:NH1 | 1:H:44:THR:CG2 | 2.80 | 0.45 |
| 1:G:43:ARG:NH1 | 1:G:44:THR:CG2 | 2.80 | 0.45 |
| 1:D:43:ARG:NH1 | 1:D:44:THR:CG2 | 2.80 | 0.45 |
| 1:J:433:LEU:N | 1:J:434:PRO:CD | 2.80 | 0.45 |
| 1:H:653[B]:HIS:CD2 | 1:H:667:GLU:HG2 | 2.51 | 0.45 |
| 1:P:668:VAL:CG1 | 1:P:669:PRO:HD2 | 2.45 | 0.45 |
| 1:M:657:ALA:HA | 1:M:661:LYS:O | 2.16 | 0.45 |
| 1:C:767:GLN:CG | 1:C:768:MET:N | 2.79 | 0.45 |
| 1:A:85:VAL:CG1 | 1:A:86:VAL:N | 2.79 | 0.45 |
| 1:H:85:VAL:CG1 | 1:H:86:VAL:N | 2.79 | 0.45 |
| 1:N:100:TYR:CE1 | 1:N:602:CYS:HB3 | 2.51 | 0.45 |
| 1:I:85:VAL:CG1 | 1:I:86:VAL:N | 2.79 | 0.45 |
| 1:N:767:GLN:CG | 1:N:768:MET:N | 2.79 | 0.45 |
| 1:F:3:ILE:HD12 | 1:F:3:ILE:O | 2.17 | 0.45 |
| 1:P:3:ILE:HD12 | 1:P:3:ILE:O | 2.17 | 0.45 |
| 1:N:3:ILE:HD12 | 1:N:3:ILE:O | 2.17 | 0.45 |
| 1:G:42:ALA:O | 1:G:310:ARG:NH1 | 2.49 | 0.45 |
| 1:O:42:ALA:O | 1:O:310:ARG:NH1 | 2.49 | 0.45 |
| 1:F:657:ALA:HA | 1:F:661:LYS:O | 2.16 | 0.45 |
| 1:N:546:LEU:HA | 3:N:3231:HOH:O | 2.16 | 0.45 |
| 1:E:687:GLN:HA | 1:E:688:PRO:HD3 | 1.73 | 0.45 |
| 1:O:114:VAL:HG22 | 1:O:191:TRP:HB3 | 1.98 | 0.45 |
| 1:A:211:ASP:OD1 | 1:A:211:ASP:N | 2.50 | 0.45 |
| 1:F:237:ARG:HE | 1:F:237:ARG:HB2 | 1.35 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:D:211:ASP:N | 1:D:211:ASP:OD1 | 2.50 | 0.45 |
| 1:L:546:LEU:HA | 3:L:3234:HOH:O | 2.16 | 0.45 |
| 1:C:778:THR:HG23 | 1:C:779:PRO:HD2 | 1.98 | 0.45 |
| 1:L:778:THR:HG23 | 1:L:779:PRO:HD2 | 1.98 | 0.45 |
| 1:P:546:LEU:HA | 3:P:3236:HOH:O | 2.16 | 0.45 |
| 1:O:91:GLN:HG3 | 1:O:96:ASP:OD1 | 2.16 | 0.45 |
| 1:K:257:THR:OG1 | 1:K:316:HIS:HE1 | 1.98 | 0.45 |
| 1:D:920:LEU:HB3 | 1:D:921:PRO:CD | 2.46 | 0.45 |
| 1:D:278:ILE:N | 1:D:278:ILE:CD1 | 2.80 | 0.45 |
| 1:F:7:LEU:HD12 | 1:F:74:LEU:HD11 | 1.97 | 0.45 |
| 1:H:183:ARG:HD3 | 1:H:183:ARG:HH11 | 1.62 | 0.45 |
| 1:O:43:ARG:HH12 | 1:O:44:THR:CG2 | 2.30 | 0.45 |
| 1:B:952:ARG:HH11 | 1:B:952:ARG:CG | 2.28 | 0.45 |
| 1:A:653[B]:HIS:CD2 | 1:A:667:GLU:HG2 | 2.51 | 0.45 |
| 1:B:599:ARG:HB2 | 1:B:600:GLN:H | 1.63 | 0.45 |
| 1:M:433:LEU:N | 1:M:434:PRO:CD | 2.80 | 0.45 |
| 1:D:433:LEU:N | 1:D:434:PRO:CD | 2.80 | 0.45 |
| 1:J:767:GLN:CG | 1:J:768:MET:N | 2.79 | 0.45 |
| 1:K:612:THR:HB | 1:K:613:PRO:HD2 | 1.98 | 0.45 |
| 1:J:612:THR:HB | 1:J:613:PRO:HD2 | 1.98 | 0.45 |
| 1:J:85:VAL:CG1 | 1:J:86:VAL:N | 2.79 | 0.45 |
| 1:L:100:TYR:CE1 | 1:L:602:CYS:HB3 | 2.51 | 0.45 |
| 1:K:3:ILE:O | 1:K:3:ILE:HD12 | 2.17 | 0.45 |
| 1:N:42:ALA:O | 1:N:310:ARG:NH1 | 2.49 | 0.45 |
| 1:M:42:ALA:O | 1:M:310:ARG:NH1 | 2.49 | 0.45 |
| 1:L:991:MET:HE2 | 1:L:1003:VAL:HG21 | 1.98 | 0.45 |
| 1:H:13:ARG:O | 1:H:14:ARG:HB2 | 2.17 | 0.45 |
| 1:I:425:ARG:NH2 | 1:L:287:ASP:OD2 | 2.50 | 0.45 |
| 1:G:114:VAL:HG22 | 1:G:191:TRP:HB3 | 1.98 | 0.45 |
| 1:D:147:ASN:HA | 1:D:148:SER:HA | 1.57 | 0.45 |
| 1:M:847:LYS:HG3 | 1:M:848:THR:N | 2.32 | 0.45 |
| 1:N:657:ALA:HA | 1:N:661:LYS:O | 2.16 | 0.45 |
| 1:M:80:GLU:HG3 | 1:M:80:GLU:H | 1.29 | 0.45 |
| 1:D:237:ARG:HB2 | 1:D:237:ARG:HE | 1.35 | 0.45 |
| 1:M:670:LEU:HD23 | 1:M:670:LEU:HA | 1.75 | 0.45 |
| 1:K:657:ALA:HA | 1:K:661:LYS:O | 2.16 | 0.45 |
| 1:F:279:ILE:HD12 | 1:F:279:ILE:HG21 | 1.77 | 0.45 |
| 1:D:947:GLY:HA3 | 1:D:948:PRO:HD2 | 1.82 | 0.45 |
| 1:G:778:THR:HG23 | 1:G:779:PRO:HD2 | 1.98 | 0.45 |
| 1:K:395:HIS:CG | 1:K:396:PRO:HD2 | 2.51 | 0.45 |
| 1:F:114:VAL:HG22 | 1:F:191:TRP:HB3 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:701:VAL:HG12 | 1:I:702:GLN:N | 2.31 | 0.45 |
| 1:P:183:ARG:HH11 | 1:P:183:ARG:HD3 | 1.62 | 0.45 |
| 1:M:579:ASP:HB2 | 1:M:580:GLU:OE2 | 2.16 | 0.45 |
| 1:E:43:ARG:HH12 | 1:E:44:THR:CG2 | 2.30 | 0.45 |
| 1:E:952:ARG:CG | 1:E:952:ARG:HH11 | 2.28 | 0.45 |
| 1:A:43:ARG:HH12 | 1:A:44:THR:CG2 | 2.30 | 0.45 |
| 1:L:43:ARG:NH1 | 1:L:44:THR:CG2 | 2.80 | 0.45 |
| 1:J:576:ILE:CG2 | 1:J:577:LYS:N | 2.79 | 0.45 |
| 1:M:418:HIS:O | 1:P:282:ARG:HD2 | 2.17 | 0.45 |
| 1:D:85:VAL:CG1 | 1:D:86:VAL:N | 2.79 | 0.45 |
| 1:M:3:ILE:O | 1:M:3:ILE:HD12 | 2.17 | 0.45 |
| 1:J:395:HIS:CG | 1:J:396:PRO:HD2 | 2.51 | 0.45 |
| 1:F:42:ALA:O | 1:F:310:ARG:NH1 | 2.49 | 0.45 |
| 1:K:395:HIS:HA | 1:K:396:PRO:HD3 | 1.69 | 0.45 |
| 1:E:395:HIS:CG | 1:E:396:PRO:HD2 | 2.52 | 0.45 |
| 1:A:546:LEU:HA | 3:A:4124:HOH:O | 2.16 | 0.45 |
| 1:A:847:LYS:HG3 | 1:A:848:THR:N | 2.32 | 0.45 |
| 1:K:147:ASN:HA | 1:K:148:SER:HA | 1.57 | 0.45 |
| 1:J:13:ARG:O | 1:J:14:ARG:HB2 | 2.17 | 0.45 |
| 1:G:134:LEU:HA | 1:G:134:LEU:HD23 | 1.68 | 0.45 |
| 1:A:237:ARG:HE | 1:A:237:ARG:HB2 | 1.35 | 0.45 |
| 1:H:134:LEU:HA | 1:H:134:LEU:HD23 | 1.68 | 0.45 |
| 1:O:134:LEU:HD23 | 1:O:134:LEU:HA | 1.68 | 0.45 |
| 1:I:395:HIS:CG | 1:I:396:PRO:HD2 | 2.51 | 0.45 |
| 1:O:778:THR:HG23 | 1:O:779:PRO:HD2 | 1.98 | 0.45 |
| 1:B:847:LYS:HG3 | 1:B:848:THR:N | 2.32 | 0.45 |
| 1:E:114:VAL:HG22 | 1:E:191:TRP:HB3 | 1.98 | 0.45 |
| 1:H:395:HIS:CG | 1:H:396:PRO:HD2 | 2.51 | 0.45 |
| 1:P:111:PRO:HA | 1:P:112:PRO:HA | 1.66 | 0.45 |
| 1:C:114:VAL:HG22 | 1:C:191:TRP:HB3 | 1.98 | 0.45 |
| 1:C:322:LEU:CD2 | 1:C:324:GLU:N | 2.80 | 0.45 |
| 1:N:322:LEU:CD2 | 1:N:324:GLU:N | 2.80 | 0.45 |
| 1:A:701:VAL:HG12 | 1:A:702:GLN:N | 2.31 | 0.45 |
| 1:B:701:VAL:HG12 | 1:B:702:GLN:N | 2.31 | 0.45 |
| 1:C:285:TYR:CB | 1:C:288:ARG:HG3 | 2.42 | 0.45 |
| 1:H:278:ILE:CD1 | 1:H:278:ILE:N | 2.80 | 0.45 |
| 1:P:278:ILE:CD1 | 1:P:278:ILE:N | 2.80 | 0.45 |
| 1:A:7:LEU:HD12 | 1:A:74:LEU:HD11 | 1.97 | 0.45 |
| 1:K:63:PHE:CB | 1:K:64:PRO:HD2 | 2.34 | 0.45 |
| 1:P:43:ARG:NH1 | 1:P:44:THR:CG2 | 2.80 | 0.45 |
| 1:M:43:ARG:HH12 | 1:M:44:THR:CG2 | 2.30 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:129:VAL:CG2 | 1:L:182:ASN:ND2 | 2.80 | 0.45 |
| 1:G:129:VAL:CG2 | 1:G:182:ASN:ND2 | 2.80 | 0.45 |
| 1:J:856:TYR:CD2 | 1:J:864:MET:CE | 3.00 | 0.45 |
| 1:D:362:LEU:HD23 | 1:D:362:LEU:HA | 1.70 | 0.45 |
| 1:N:473:ARG:HD2 | 1:O:469:ASP:HB3 | 1.98 | 0.45 |
| 1:F:679:LEU:HD23 | 1:F:679:LEU:HA | 1.40 | 0.45 |
| 1:P:85:VAL:CG1 | 1:P:86:VAL:N | 2.79 | 0.45 |
| 1:F:3:ILE:HG13 | 1:F:4:THR:N | 2.25 | 0.45 |
| 1:G:3:ILE:O | 1:G:3:ILE:HD12 | 2.17 | 0.45 |
| 1:A:42:ALA:O | 1:A:310:ARG:NH1 | 2.49 | 0.45 |
| 1:E:42:ALA:O | 1:E:310:ARG:NH1 | 2.49 | 0.45 |
| 1:K:778:THR:HG23 | 1:K:779:PRO:HD2 | 1.98 | 0.45 |
| 1:M:479:ASP:HA | 1:M:480:PRO:HD2 | 1.77 | 0.45 |
| 1:L:687:GLN:HA | 1:L:688:PRO:HD3 | 1.73 | 0.45 |
| 1:B:211:ASP:OD1 | 1:B:211:ASP:N | 2.50 | 0.45 |
| 1:I:847:LYS:HG3 | 1:I:848:THR:N | 2.32 | 0.45 |
| 1:F:91:GLN:HG3 | 1:F:96:ASP:OD1 | 2.15 | 0.45 |
| 1:D:395:HIS:CG | 1:D:396:PRO:HD2 | 2.51 | 0.45 |
| 1:P:947:GLY:HA3 | 1:P:948:PRO:HD2 | 1.82 | 0.45 |
| 1:L:322:LEU:CD2 | 1:L:324:GLU:N | 2.80 | 0.45 |
| 1:O:322:LEU:CD2 | 1:O:324:GLU:N | 2.80 | 0.45 |
| 1:D:285:TYR:CB | 1:D:288:ARG:HG3 | 2.42 | 0.45 |
| 1:C:920:LEU:HB3 | 1:C:921:PRO:CD | 2.46 | 0.45 |
| 1:E:579:ASP:HB2 | 1:E:580:GLU:OE2 | 2.16 | 0.45 |
| 1:J:254:LEU:HA | 1:J:254:LEU:HD23 | 1.71 | 0.45 |
| 1:G:668:VAL:CG1 | 1:G:669:PRO:HD2 | 2.45 | 0.45 |
| 1:M:668:VAL:HA | 1:M:669:PRO:HD3 | 1.83 | 0.45 |
| 1:I:433:LEU:N | 1:I:434:PRO:CD | 2.80 | 0.45 |
| 1:M:612:THR:HB | 1:M:613:PRO:HD2 | 1.98 | 0.45 |
| 1:O:3:ILE:O | 1:O:3:ILE:HD12 | 2.17 | 0.45 |
| 1:C:42:ALA:O | 1:C:310:ARG:NH1 | 2.49 | 0.45 |
| 1:N:111:PRO:HA | 1:N:112:PRO:HA | 1.66 | 0.45 |
| 1:C:546:LEU:HA | 3:C:4124:HOH:O | 2.16 | 0.45 |
| 1:H:211:ASP:N | 1:H:211:ASP:OD1 | 2.50 | 0.45 |
| 1:M:482:ARG:HH11 | 1:M:482:ARG:HD2 | 1.63 | 0.45 |
| 1:L:80:GLU:HG3 | 1:L:80:GLU:H | 1.29 | 0.45 |
| 1:M:211:ASP:N | 1:M:211:ASP:OD1 | 2.50 | 0.45 |
| 1:M:778:THR:HG23 | 1:M:779:PRO:HD2 | 1.98 | 0.45 |
| 1:E:546:LEU:HA | 3:E:4124:HOH:O | 2.16 | 0.45 |
| 1:P:847:LYS:HG3 | 1:P:848:THR:N | 2.32 | 0.45 |
| 1:D:847:LYS:HG3 | 1:D:848:THR:N | 2.32 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:J:114:VAL:HG22 | 1:J:191:TRP:HB3 | 1.98 | 0.45 |
| 1:B:433:LEU:N | 1:B:434:PRO:CD | 2.80 | 0.45 |
| 1:B:322:LEU:CD2 | 1:B:324:GLU:N | 2.80 | 0.45 |
| 1:G:701:VAL:HG12 | 1:G:702:GLN:N | 2.31 | 0.45 |
| 1:E:278:ILE:CD1 | 1:E:278:ILE:N | 2.80 | 0.45 |
| 1:O:701:VAL:HG12 | 1:O:702:GLN:N | 2.31 | 0.45 |
| 1:C:43:ARG:NH1 | 1:C:44:THR:CG2 | 2.80 | 0.45 |
| 1:N:43:ARG:NH1 | 1:N:44:THR:CG2 | 2.80 | 0.45 |
| 1:F:43:ARG:NH1 | 1:F:44:THR:CG2 | 2.80 | 0.45 |
| 1:F:43:ARG:HH12 | 1:F:44:THR:CG2 | 2.30 | 0.45 |
| 1:K:43:ARG:NH1 | 1:K:44:THR:CG2 | 2.80 | 0.45 |
| 1:K:43:ARG:HH12 | 1:K:44:THR:CG2 | 2.30 | 0.45 |
| 1:I:254:LEU:HD23 | 1:I:254:LEU:HA | 1.71 | 0.45 |
| 1:H:856:TYR:CD2 | 1:H:864:MET:CE | 3.00 | 0.45 |
| 1:G:653[B]:HIS:CD2 | 1:G:667:GLU:HG2 | 2.51 | 0.45 |
| 1:P:653[B]:HIS:CD2 | 1:P:667:GLU:HG2 | 2.51 | 0.45 |
| 1:M:100:TYR:CE1 | 1:M:602:CYS:HB3 | 2.51 | 0.45 |
| 1:C:102:ASN:C | 1:C:102:ASN:HD22 | 2.21 | 0.45 |
| 1:B:102:ASN:C | 1:B:102:ASN:HD22 | 2.21 | 0.45 |
| 1:L:3:ILE:HD12 | 1:L:3:ILE:O | 2.17 | 0.45 |
| 1:A:395:HIS:CG | 1:A:396:PRO:HD2 | 2.51 | 0.45 |
| 1:B:395:HIS:CG | 1:B:396:PRO:HD2 | 2.51 | 0.45 |
| 1:C:246:MET:HG2 | 1:C:274:PHE:CE2 | 2.52 | 0.45 |
| 1:H:546:LEU:HA | 3:H:4124:HOH:O | 2.16 | 0.45 |
| 1:M:395:HIS:CG | 1:M:396:PRO:HD2 | 2.51 | 0.45 |
| 1:O:246:MET:HG2 | 1:O:274:PHE:CE2 | 2.52 | 0.45 |
| 1:G:111:PRO:HA | 1:G:112:PRO:HA | 1.66 | 0.45 |
| 1:O:211:ASP:OD1 | 1:O:211:ASP:N | 2.50 | 0.45 |
| 1:I:772:ASP:N | 1:I:772:ASP:OD1 | 2.48 | 0.45 |
| 1:N:378:LEU:HD23 | 1:N:378:LEU:HA | 1.74 | 0.45 |
| 1:M:867:THR:HG22 | 3:M:4298:HOH:O | 2.17 | 0.45 |
| 1:D:114:VAL:HG22 | 1:D:191:TRP:HB3 | 1.98 | 0.45 |
| 1:P:778:THR:HG23 | 1:P:779:PRO:HD2 | 1.98 | 0.45 |
| 1:M:322:LEU:CD2 | 1:M:324:GLU:N | 2.80 | 0.45 |
| 1:J:57:GLU:HG2 | 1:J:83:THR:HG22 | 1.95 | 0.45 |
| 1:B:78:LEU:HB3 | 1:B:79:PRO:CD | 2.43 | 0.45 |
| 1:G:78:LEU:HB3 | 1:G:79:PRO:CD | 2.43 | 0.45 |
| 1:B:567:VAL:HG12 | 1:B:568:TRP:N | 2.32 | 0.45 |
| 1:K:579:ASP:HB2 | 1:K:580:GLU:OE2 | 2.16 | 0.45 |
| 1:A:952:ARG:CG | 1:A:952:ARG:HH11 | 2.28 | 0.45 |
| 1:P:129:VAL:CG2 | 1:P:182:ASN:ND2 | 2.80 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:K:362:LEU:HD23 | 1:K:362:LEU:HA | 1.70 | 0.45 |
| 1:B:856:TYR:CD2 | 1:B:864:MET:CE | 3.00 | 0.45 |
| 1:H:433:LEU:N | 1:H:434:PRO:CD | 2.80 | 0.45 |
| 1:B:653[B]:HIS:CD2 | 1:B:667:GLU:HG2 | 2.51 | 0.45 |
| 1:M:856:TYR:CD2 | 1:M:864:MET:CE | 3.00 | 0.45 |
| 1:K:653[B]:HIS:CD2 | 1:K:667:GLU:HG2 | 2.51 | 0.45 |
| 1:L:856:TYR:CD2 | 1:L:864:MET:HE2 | 2.51 | 0.45 |
| 1:I:856:TYR:CD2 | 1:I:864:MET:CE | 3.00 | 0.45 |
| 1:A:612:THR:HA | 1:A:613:PRO:HD3 | 1.59 | 0.45 |
| 1:N:612:THR:HA | 1:N:613:PRO:HD3 | 1.59 | 0.45 |
| 1:B:767:GLN:CG | 1:B:768:MET:N | 2.79 | 0.45 |
| 1:A:767:GLN:CG | 1:A:768:MET:N | 2.79 | 0.45 |
| 1:P:856:TYR:CD2 | 1:P:864:MET:CE | 3.00 | 0.45 |
| 1:J:679:LEU:HA | 1:J:679:LEU:HD23 | 1.40 | 0.45 |
| 1:D:42:ALA:O | 1:D:310:ARG:NH1 | 2.49 | 0.45 |
| 1:M:246:MET:HG2 | 1:M:274:PHE:CE2 | 2.52 | 0.45 |
| 1:E:867:THR:HG22 | 3:E:4298:HOH:O | 2.17 | 0.45 |
| 1:I:13:ARG:O | 1:I:14:ARG:HB2 | 2.16 | 0.45 |
| 1:C:3:ILE:O | 1:C:3:ILE:HD12 | 2.17 | 0.45 |
| 1:F:378:LEU:HA | 1:F:378:LEU:HD23 | 1.74 | 0.45 |
| 1:D:80:GLU:H | 1:D:80:GLU:HG3 | 1.29 | 0.45 |
| 1:M:13:ARG:O | 1:M:14:ARG:HB2 | 2.17 | 0.45 |
| 1:C:433:LEU:N | 1:C:434:PRO:CD | 2.80 | 0.44 |
| 1:J:567:VAL:HG12 | 1:J:568:TRP:N | 2.32 | 0.44 |
| 1:H:7:LEU:HD12 | 1:H:74:LEU:HD11 | 1.97 | 0.44 |
| 1:J:63:PHE:CB | 1:J:64:PRO:HD2 | 2.34 | 0.44 |
| 1:D:856:TYR:HD2 | 1:D:864:MET:CE | 2.25 | 0.44 |
| 1:B:43:ARG:HH12 | 1:B:44:THR:CG2 | 2.30 | 0.44 |
| 1:L:43:ARG:HH12 | 1:L:44:THR:CG2 | 2.30 | 0.44 |
| 1:I:43:ARG:HH12 | 1:I:44:THR:CG2 | 2.30 | 0.44 |
| 1:G:362:LEU:HD23 | 1:G:362:LEU:HA | 1.70 | 0.44 |
| 1:O:433:LEU:N | 1:O:434:PRO:CD | 2.80 | 0.44 |
| 1:N:653[B]:HIS:CD2 | 1:N:667:GLU:HG2 | 2.51 | 0.44 |
| 1:E:612:THR:HB | 1:E:613:PRO:HD2 | 1.98 | 0.44 |
| 1:C:612:THR:HB | 1:C:613:PRO:HD2 | 1.98 | 0.44 |
| 1:K:85:VAL:CG1 | 1:K:86:VAL:N | 2.79 | 0.44 |
| 1:P:102:ASN:HD22 | 1:P:102:ASN:C | 2.21 | 0.44 |
| 1:F:102:ASN:HD22 | 1:F:102:ASN:C | 2.21 | 0.44 |
| 1:K:102:ASN:C | 1:K:102:ASN:HD22 | 2.21 | 0.44 |
| 1:E:3:ILE:O | 1:E:3:ILE:HD12 | 2.17 | 0.44 |
| 1:G:395:HIS:HA | 1:G:396:PRO:HD3 | 1.69 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:991:MET:HE2 | 1:B:1003:VAL:HG21 | 1.99 | 0.44 |
| 1:K:13:ARG:O | 1:K:14:ARG:HB2 | 2.17 | 0.44 |
| 1:I:991:MET:HE2 | 1:I:1003:VAL:HG21 | 1.99 | 0.44 |
| 1:F:687:GLN:HA | 1:F:688:PRO:HD3 | 1.73 | 0.44 |
| 1:J:246:MET:HG2 | 1:J:274:PHE:CE2 | 2.52 | 0.44 |
| 1:G:694:LEU:HD12 | 1:G:694:LEU:HA | 1.84 | 0.44 |
| 1:D:546:LEU:HA | 3:D:3237:HOH:O | 2.16 | 0.44 |
| 1:E:246:MET:HG2 | 1:E:274:PHE:CE2 | 2.52 | 0.44 |
| 1:K:991:MET:HE2 | 1:K:1003:VAL:HG21 | 2.00 | 0.44 |
| 1:H:246:MET:HG2 | 1:H:274:PHE:CE2 | 2.52 | 0.44 |
| 1:B:595:THR:CG2 | 1:B:596:PRO:HA | 2.37 | 0.44 |
| 1:G:595:THR:CG2 | 1:G:596:PRO:HA | 2.37 | 0.44 |
| 1:G:322:LEU:CD2 | 1:G:324:GLU:N | 2.80 | 0.44 |
| 1:A:257:THR:OG1 | 1:A:316:HIS:HE1 | 1.98 | 0.44 |
| 1:H:701:VAL:HG12 | 1:H:702:GLN:N | 2.31 | 0.44 |
| 1:K:7:LEU:HD12 | 1:K:74:LEU:HD11 | 1.97 | 0.44 |
| 1:E:856:TYR:CD2 | 1:E:864:MET:CE | 3.00 | 0.44 |
| 1:P:43:ARG:HH12 | 1:P:44:THR:CG2 | 2.30 | 0.44 |
| 1:G:43:ARG:CG | 1:G:43:ARG:HH11 | 2.24 | 0.44 |
| 1:G:43:ARG:HH12 | 1:G:44:THR:CG2 | 2.30 | 0.44 |
| 1:L:272:ALA:HA | 1:L:273:PRO:HD3 | 1.78 | 0.44 |
| 1:I:668:VAL:CG1 | 1:I:669:PRO:HD2 | 2.45 | 0.44 |
| 1:L:433:LEU:N | 1:L:434:PRO:CD | 2.80 | 0.44 |
| 1:N:856:TYR:CD2 | 1:N:864:MET:HE2 | 2.52 | 0.44 |
| 1:C:85:VAL:CG1 | 1:C:86:VAL:N | 2.79 | 0.44 |
| 1:G:85:VAL:CG1 | 1:G:86:VAL:N | 2.79 | 0.44 |
| 1:N:85:VAL:CG1 | 1:N:86:VAL:N | 2.79 | 0.44 |
| 1:D:3:ILE:HD12 | 1:D:3:ILE:O | 2.17 | 0.44 |
| 1:B:42:ALA:O | 1:B:310:ARG:NH1 | 2.49 | 0.44 |
| 1:G:246:MET:HG2 | 1:G:274:PHE:CE2 | 2.52 | 0.44 |
| 1:B:13:ARG:O | 1:B:14:ARG:HB2 | 2.17 | 0.44 |
| 1:A:246:MET:HG2 | 1:A:274:PHE:CE2 | 2.52 | 0.44 |
| 1:P:246:MET:HG2 | 1:P:274:PHE:CE2 | 2.52 | 0.44 |
| 1:P:914:CME:HE2 | 1:P:914:CME:HB3 | 1.74 | 0.44 |
| 1:K:246:MET:HG2 | 1:K:274:PHE:CE2 | 2.52 | 0.44 |
| 1:E:730:LEU:HA | 1:E:731:PRO:HD3 | 1.80 | 0.44 |
| 1:G:867:THR:HG22 | 3:G:3402:HOH:O | 2.17 | 0.44 |
| 1:F:638:VAL:O | 1:F:677:LYS:HA | 2.18 | 0.44 |
| 1:E:322:LEU:CD2 | 1:E:324:GLU:N | 2.80 | 0.44 |
| 1:P:702:GLN:O | 1:P:712:GLY:N | 2.47 | 0.44 |
| 1:A:920:LEU:HB3 | 1:A:921:PRO:CD | 2.46 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:567:VAL:HG12 | 1:N:568:TRP:N | 2.32 | 0.44 |
| 1:F:567:VAL:HG12 | 1:F:568:TRP:N | 2.32 | 0.44 |
| 1:O:63:PHE:CB | 1:O:64:PRO:HD2 | 2.34 | 0.44 |
| 1:G:433:LEU:N | 1:G:434:PRO:CD | 2.80 | 0.44 |
| 1:J:43:ARG:HH12 | 1:J:44:THR:CG2 | 2.30 | 0.44 |
| 1:G:856:TYR:CD2 | 1:G:864:MET:CE | 3.00 | 0.44 |
| 1:E:254:LEU:HD23 | 1:E:254:LEU:HA | 1.71 | 0.44 |
| 1:E:129:VAL:CG2 | 1:E:182:ASN:ND2 | 2.80 | 0.44 |
| 1:K:129:VAL:CG2 | 1:K:182:ASN:ND2 | 2.80 | 0.44 |
| 1:F:129:VAL:CG2 | 1:F:182:ASN:ND2 | 2.80 | 0.44 |
| 1:K:856:TYR:CD2 | 1:K:864:MET:CE | 3.00 | 0.44 |
| 1:N:433:LEU:N | 1:N:434:PRO:CD | 2.80 | 0.44 |
| 1:H:767:GLN:CG | 1:H:768:MET:N | 2.79 | 0.44 |
| 1:M:102:ASN:C | 1:M:102:ASN:HD22 | 2.21 | 0.44 |
| 1:E:102:ASN:C | 1:E:102:ASN:HD22 | 2.21 | 0.44 |
| 1:D:102:ASN:HD22 | 1:D:102:ASN:C | 2.21 | 0.44 |
| 1:O:85:VAL:CG1 | 1:O:86:VAL:N | 2.80 | 0.44 |
| 1:B:3:ILE:HD12 | 1:B:3:ILE:O | 2.17 | 0.44 |
| 1:A:3:ILE:HD12 | 1:A:3:ILE:O | 2.17 | 0.44 |
| 1:H:638:VAL:O | 1:H:677:LYS:HA | 2.18 | 0.44 |
| 1:G:991:MET:HE2 | 1:G:1003:VAL:HG21 | 1.99 | 0.44 |
| 1:B:546:LEU:HA | 3:B:3228:HOH:O | 2.16 | 0.44 |
| 1:C:13:ARG:O | 1:C:14:ARG:HB2 | 2.17 | 0.44 |
| 1:A:80:GLU:H | 1:A:80:GLU:HG3 | 1.29 | 0.44 |
| 1:M:986:ILE:HD13 | 1:M:986:ILE:HG23 | 1.67 | 0.44 |
| 1:O:694:LEU:HA | 1:O:694:LEU:HD12 | 1.84 | 0.44 |
| 1:A:670:LEU:HA | 1:A:670:LEU:HD23 | 1.75 | 0.44 |
| 1:B:638:VAL:O | 1:B:677:LYS:HA | 2.18 | 0.44 |
| 1:I:778:THR:HG23 | 1:I:779:PRO:HD2 | 1.98 | 0.44 |
| 1:P:638:VAL:O | 1:P:677:LYS:HA | 2.18 | 0.44 |
| 1:O:991:MET:HE2 | 1:O:1003:VAL:HG21 | 1.99 | 0.44 |
| 1:N:702:GLN:O | 1:N:712:GLY:N | 2.47 | 0.44 |
| 1:M:567:VAL:HG12 | 1:M:568:TRP:N | 2.32 | 0.44 |
| 1:E:567:VAL:HG12 | 1:E:568:TRP:N | 2.32 | 0.44 |
| 1:G:7:LEU:O | 1:G:11:LEU:HG | 2.18 | 0.44 |
| 1:D:567:VAL:HG12 | 1:D:568:TRP:N | 2.32 | 0.44 |
| 1:E:856:TYR:HD2 | 1:E:864:MET:CE | 2.25 | 0.44 |
| 1:F:433:LEU:N | 1:F:434:PRO:CD | 2.80 | 0.44 |
| 1:B:43:ARG:NH1 | 1:B:44:THR:CG2 | 2.80 | 0.44 |
| 1:C:43:ARG:HH12 | 1:C:44:THR:CG2 | 2.30 | 0.44 |
| 1:O:129:VAL:CG2 | 1:O:182:ASN:ND2 | 2.80 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:C:129:VAL:CG2 | 1:C:182:ASN:ND2 | 2.80 | 0.44 |
| 1:D:653[B]:HIS:CD2 | 1:D:667:GLU:HG2 | 2.51 | 0.44 |
| 1:H:102:ASN:C | 1:H:102:ASN:HD22 | 2.21 | 0.44 |
| 1:I:102:ASN:C | 1:I:102:ASN:HD22 | 2.21 | 0.44 |
| 1:H:3:ILE:O | 1:H:3:ILE:HD12 | 2.17 | 0.44 |
| 1:F:658:LEU:N | 1:F:661:LYS:O | 2.40 | 0.44 |
| 1:P:91:GLN:HG3 | 1:P:96:ASP:OD1 | 2.16 | 0.44 |
| 1:J:420:MET:O | 1:K:282:ARG:HD3 | 2.18 | 0.44 |
| 1:I:638:VAL:O | 1:I:677:LYS:HA | 2.18 | 0.44 |
| 1:E:778:THR:HG23 | 1:E:779:PRO:HD2 | 1.98 | 0.44 |
| 1:M:221:GLN:H | 1:M:221:GLN:HG2 | 1.63 | 0.44 |
| 1:O:202:MET:HE3 | 1:O:202:MET:HB3 | 1.84 | 0.44 |
| 1:G:202:MET:HE3 | 1:G:202:MET:HB3 | 1.84 | 0.44 |
| 1:C:847:LYS:HG3 | 1:C:848:THR:N | 2.32 | 0.44 |
| 1:I:867:THR:HG22 | 3:I:4297:HOH:O | 2.17 | 0.44 |
| 1:H:778:THR:HG23 | 1:H:779:PRO:HD2 | 1.98 | 0.44 |
| 1:G:13:ARG:O | 1:G:14:ARG:HB2 | 2.17 | 0.44 |
| 1:K:285:TYR:CB | 1:K:288:ARG:HG3 | 2.42 | 0.44 |
| 1:K:567:VAL:HG12 | 1:K:568:TRP:N | 2.32 | 0.44 |
| 1:B:7:LEU:O | 1:B:11:LEU:HG | 2.18 | 0.44 |
| 1:P:7:LEU:O | 1:P:11:LEU:HG | 2.18 | 0.44 |
| 1:G:183:ARG:HD3 | 1:G:183:ARG:HH11 | 1.62 | 0.44 |
| 1:H:43:ARG:HH12 | 1:H:44:THR:CG2 | 2.30 | 0.44 |
| 1:O:43:ARG:NH1 | 1:O:44:THR:CG2 | 2.80 | 0.44 |
| 1:A:43:ARG:NH1 | 1:A:44:THR:CG2 | 2.80 | 0.44 |
| 1:I:43:ARG:NH1 | 1:I:44:THR:CG2 | 2.80 | 0.44 |
| 1:G:599:ARG:HB2 | 1:G:600:GLN:H | 1.64 | 0.44 |
| 1:L:856:TYR:CD2 | 1:L:864:MET:CE | 3.00 | 0.44 |
| 1:M:658:LEU:N | 1:M:661:LYS:O | 2.40 | 0.44 |
| 1:L:279:ILE:HD12 | 1:L:279:ILE:HG21 | 1.77 | 0.44 |
| 1:G:102:ASN:HD22 | 1:G:102:ASN:C | 2.21 | 0.44 |
| 1:K:658:LEU:N | 1:K:661:LYS:O | 2.40 | 0.44 |
| 1:G:638:VAL:O | 1:G:677:LYS:HA | 2.18 | 0.44 |
| 1:A:867:THR:HG22 | 3:A:4299:HOH:O | 2.17 | 0.44 |
| 1:J:638:VAL:O | 1:J:677:LYS:HA | 2.18 | 0.44 |
| 1:F:111:PRO:HA | 1:F:112:PRO:HA | 1.66 | 0.44 |
| 1:D:13:ARG:O | 1:D:14:ARG:HB2 | 2.17 | 0.44 |
| 1:H:772:ASP:OD1 | 1:H:772:ASP:N | 2.48 | 0.44 |
| 1:D:638:VAL:O | 1:D:677:LYS:HA | 2.18 | 0.44 |
| 1:P:80:GLU:HG3 | 1:P:80:GLU:H | 1.29 | 0.44 |
| 1:H:847:LYS:HG3 | 1:H:848:THR:N | 2.32 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:847:LYS:HG3 | 1:O:848:THR:N | 2.32 | 0.44 |
| 1:L:13:ARG:O | 1:L:14:ARG:HB2 | 2.17 | 0.44 |
| 1:J:657:ALA:HA | 1:J:661:LYS:O | 2.16 | 0.44 |
| 1:E:847:LYS:HG3 | 1:E:848:THR:N | 2.32 | 0.44 |
| 1:P:322:LEU:CD2 | 1:P:324:GLU:N | 2.80 | 0.44 |
| 1:K:322:LEU:CD2 | 1:K:324:GLU:N | 2.80 | 0.44 |
| 1:F:322:LEU:CD2 | 1:F:324:GLU:N | 2.80 | 0.44 |
| 1:K:702:GLN:O | 1:K:712:GLY:N | 2.47 | 0.44 |
| 1:D:702:GLN:O | 1:D:712:GLY:N | 2.47 | 0.44 |
| 1:L:701:VAL:HG12 | 1:L:702:GLN:N | 2.31 | 0.44 |
| 1:K:7:LEU:O | 1:K:11:LEU:HG | 2.18 | 0.44 |
| 1:I:7:LEU:O | 1:I:11:LEU:HG | 2.18 | 0.44 |
| 1:H:7:LEU:O | 1:H:11:LEU:HG | 2.18 | 0.44 |
| 1:O:567:VAL:HG12 | 1:O:568:TRP:N | 2.32 | 0.44 |
| 1:D:43:ARG:HH12 | 1:D:44:THR:CG2 | 2.30 | 0.44 |
| 1:A:129:VAL:CG2 | 1:A:182:ASN:ND2 | 2.80 | 0.44 |
| 1:P:599:ARG:HB2 | 1:P:600:GLN:H | 1.64 | 0.44 |
| 1:P:433:LEU:N | 1:P:434:PRO:CD | 2.80 | 0.44 |
| 1:F:856:TYR:CD2 | 1:F:864:MET:CE | 3.00 | 0.44 |
| 1:I:42:ALA:O | 1:I:310:ARG:NH1 | 2.49 | 0.44 |
| 1:M:638:VAL:O | 1:M:677:LYS:HA | 2.18 | 0.44 |
| 1:K:867:THR:HG22 | 3:K:4299:HOH:O | 2.17 | 0.44 |
| 1:F:685:LEU:HA | 1:F:686:PRO:HD3 | 1.83 | 0.44 |
| 1:C:211:ASP:OD1 | 1:C:211:ASP:N | 2.50 | 0.44 |
| 1:N:687:GLN:HA | 1:N:688:PRO:HD3 | 1.73 | 0.44 |
| 1:F:546:LEU:HA | 3:F:3230:HOH:O | 2.16 | 0.44 |
| 1:J:111:PRO:HA | 1:J:112:PRO:HA | 1.65 | 0.44 |
| 1:B:479:ASP:HA | 1:B:480:PRO:HD2 | 1.77 | 0.44 |
| 1:D:322:LEU:CD2 | 1:D:324:GLU:N | 2.80 | 0.44 |
| 1:O:702:GLN:O | 1:O:712:GLY:N | 2.47 | 0.44 |
| 1:A:7:LEU:O | 1:A:11:LEU:HG | 2.18 | 0.44 |
| 1:O:183:ARG:HD3 | 1:O:183:ARG:HH11 | 1.62 | 0.44 |
| 1:D:856:TYR:CD2 | 1:D:864:MET:CE | 3.00 | 0.44 |
| 1:A:856:TYR:CD2 | 1:A:864:MET:CE | 3.00 | 0.44 |
| 1:N:254:LEU:HD23 | 1:N:254:LEU:HA | 1.71 | 0.44 |
| 1:P:362:LEU:HA | 1:P:362:LEU:HD23 | 1.70 | 0.44 |
| 1:B:612:THR:HA | 1:B:613:PRO:HD3 | 1.59 | 0.44 |
| 1:B:679:LEU:HD23 | 1:B:679:LEU:HA | 1.40 | 0.44 |
| 1:D:612:THR:HA | 1:D:613:PRO:HD3 | 1.59 | 0.44 |
| 1:F:85:VAL:CG1 | 1:F:86:VAL:N | 2.79 | 0.44 |
| 1:E:3:ILE:HG13 | 1:E:4:THR:N | 2.25 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:147:ASN:HA | 1:E:148:SER:HA | 1.57 | 0.44 |
| 1:I:836:ILE:HG23 | 1:I:836:ILE:HD12 | 1.73 | 0.44 |
| 1:D:378:LEU:HD23 | 1:D:378:LEU:HA | 1.74 | 0.44 |
| 1:O:772:ASP:N | 1:O:772:ASP:OD1 | 2.48 | 0.44 |
| 1:P:857:ARG:HH11 | 1:P:857:ARG:HG2 | 1.83 | 0.44 |
| 1:G:836:ILE:HD12 | 1:G:836:ILE:HG23 | 1.73 | 0.44 |
| 1:A:655:MET:HB2 | 1:A:655:MET:HE3 | 1.78 | 0.44 |
| 1:J:991:MET:HE2 | 1:J:1003:VAL:HG21 | 1.99 | 0.44 |
| 1:F:13:ARG:O | 1:F:14:ARG:HB2 | 2.16 | 0.44 |
| 1:C:111:PRO:HA | 1:C:112:PRO:HA | 1.66 | 0.44 |
| 1:F:246:MET:HG2 | 1:F:274:PHE:CE2 | 2.52 | 0.44 |
| 1:A:13:ARG:O | 1:A:14:ARG:HB2 | 2.17 | 0.44 |
| 1:K:847:LYS:HG3 | 1:K:848:THR:N | 2.32 | 0.44 |
| 1:F:285:TYR:CB | 1:F:288:ARG:HG3 | 2.42 | 0.44 |
| 1:L:78:LEU:HB3 | 1:L:79:PRO:CD | 2.43 | 0.44 |
| 1:B:278:ILE:N | 1:B:278:ILE:CD1 | 2.80 | 0.44 |
| 1:M:7:LEU:O | 1:M:11:LEU:HG | 2.18 | 0.44 |
| 1:J:7:LEU:HD12 | 1:J:74:LEU:HD11 | 1.97 | 0.44 |
| 1:D:7:LEU:HD12 | 1:D:74:LEU:HD11 | 1.97 | 0.44 |
| 1:F:682:LEU:HD23 | 1:F:682:LEU:HA | 1.85 | 0.44 |
| 1:K:599:ARG:HB2 | 1:K:600:GLN:H | 1.64 | 0.44 |
| 1:N:856:TYR:CD2 | 1:N:864:MET:CE | 3.00 | 0.44 |
| 1:F:473:ARG:HD2 | 1:G:469:ASP:HB3 | 1.99 | 0.44 |
| 1:D:679:LEU:HD23 | 1:D:679:LEU:HA | 1.40 | 0.44 |
| 1:B:3:ILE:HG13 | 1:B:4:THR:N | 2.25 | 0.44 |
| 1:D:867:THR:HG22 | 3:D:3411:HOH:O | 2.17 | 0.44 |
| 1:O:638:VAL:O | 1:O:677:LYS:HA | 2.18 | 0.44 |
| 1:C:638:VAL:O | 1:C:677:LYS:HA | 2.18 | 0.44 |
| 1:I:3:ILE:HD12 | 1:I:3:ILE:O | 2.17 | 0.44 |
| 1:D:914:CME:HE2 | 1:D:914:CME:HB3 | 1.74 | 0.44 |
| 1:I:80:GLU:H | 1:I:80:GLU:HG3 | 1.29 | 0.44 |
| 1:K:237:ARG:HB2 | 1:K:237:ARG:HE | 1.35 | 0.44 |
| 1:N:479:ASP:HA | 1:N:480:PRO:HD2 | 1.77 | 0.44 |
| 1:A:322:LEU:CD2 | 1:A:324:GLU:N | 2.80 | 0.44 |
| 1:I:567:VAL:HG12 | 1:I:568:TRP:N | 2.32 | 0.44 |
| 1:C:567:VAL:HG12 | 1:C:568:TRP:N | 2.32 | 0.44 |
| 1:C:7:LEU:O | 1:C:11:LEU:HG | 2.18 | 0.44 |
| 1:G:567:VAL:HG12 | 1:G:568:TRP:N | 2.32 | 0.44 |
| 1:A:419:GLY:HA2 | 1:D:282:ARG:NH1 | 2.32 | 0.44 |
| 1:N:129:VAL:CG2 | 1:N:182:ASN:ND2 | 2.80 | 0.44 |
| 1:J:682:LEU:HD23 | 1:J:682:LEU:HA | 1.85 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:856:TYR:CD2 | 1:C:864:MET:CE | 3.00 | 0.44 |
| 1:E:599:ARG:HB2 | 1:E:600:GLN:OE1 | 2.18 | 0.44 |
| 1:H:599:ARG:HB2 | 1:H:600:GLN:OE1 | 2.18 | 0.44 |
| 1:C:599:ARG:HB2 | 1:C:600:GLN:OE1 | 2.18 | 0.44 |
| 1:F:856:TYR:CD2 | 1:F:864:MET:HE2 | 2.53 | 0.44 |
| 1:I:612:THR:HA | 1:I:613:PRO:HD3 | 1.59 | 0.44 |
| 1:J:3:ILE:HD12 | 1:J:3:ILE:O | 2.17 | 0.44 |
| 1:N:13:ARG:O | 1:N:14:ARG:HB2 | 2.16 | 0.44 |
| 1:N:246:MET:HG2 | 1:N:274:PHE:CE2 | 2.52 | 0.44 |
| 1:A:638:VAL:O | 1:A:677:LYS:HA | 2.18 | 0.44 |
| 1:H:857:ARG:HH11 | 1:H:857:ARG:HG2 | 1.83 | 0.44 |
| 1:L:211:ASP:N | 1:L:211:ASP:OD1 | 2.50 | 0.44 |
| 1:K:638:VAL:O | 1:K:677:LYS:HA | 2.18 | 0.44 |
| 1:B:867:THR:HG22 | 3:B:3402:HOH:O | 2.17 | 0.44 |
| 1:I:322:LEU:CD2 | 1:I:324:GLU:N | 2.80 | 0.43 |
| 1:L:57:GLU:HG2 | 1:L:83:THR:HG22 | 1.95 | 0.43 |
| 1:N:285:TYR:CB | 1:N:288:ARG:HG3 | 2.42 | 0.43 |
| 1:L:567:VAL:HG12 | 1:L:568:TRP:N | 2.32 | 0.43 |
| 1:J:7:LEU:O | 1:J:11:LEU:HG | 2.18 | 0.43 |
| 1:D:599:ARG:HB2 | 1:D:600:GLN:OE1 | 2.18 | 0.43 |
| 1:J:599:ARG:HB2 | 1:J:600:GLN:OE1 | 2.18 | 0.43 |
| 1:P:612:THR:HA | 1:P:613:PRO:HD3 | 1.59 | 0.43 |
| 1:L:102:ASN:C | 1:L:102:ASN:HD22 | 2.21 | 0.43 |
| 1:O:102:ASN:C | 1:O:102:ASN:HD22 | 2.21 | 0.43 |
| 1:D:3:ILE:HG13 | 1:D:4:THR:N | 2.24 | 0.43 |
| 1:N:658:LEU:N | 1:N:661:LYS:O | 2.40 | 0.43 |
| 1:D:246:MET:HG2 | 1:D:274:PHE:CE2 | 2.52 | 0.43 |
| 1:M:772:ASP:N | 1:M:772:ASP:OD1 | 2.48 | 0.43 |
| 1:D:173:LEU:HD23 | 1:D:173:LEU:HA | 1.85 | 0.43 |
| 1:J:378:LEU:HD23 | 1:J:378:LEU:HA | 1.74 | 0.43 |
| 1:N:836:ILE:HD12 | 1:N:836:ILE:HG23 | 1.73 | 0.43 |
| 1:A:778:THR:HG23 | 1:A:779:PRO:HD2 | 1.98 | 0.43 |
| 1:I:111:PRO:HA | 1:I:112:PRO:HA | 1.65 | 0.43 |
| 1:H:322:LEU:CD2 | 1:H:324:GLU:N | 2.80 | 0.43 |
| 1:C:702:GLN:O | 1:C:712:GLY:N | 2.47 | 0.43 |
| 1:P:567:VAL:HG12 | 1:P:568:TRP:N | 2.32 | 0.43 |
| 1:J:278:ILE:N | 1:J:278:ILE:CD1 | 2.80 | 0.43 |
| 1:O:856:TYR:CD2 | 1:O:864:MET:CE | 3.00 | 0.43 |
| 1:L:576:ILE:CG2 | 1:L:577:LYS:N | 2.79 | 0.43 |
| 1:P:599:ARG:HB2 | 1:P:600:GLN:OE1 | 2.18 | 0.43 |
| 1:A:599:ARG:HB2 | 1:A:600:GLN:H | 1.63 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:127:PHE:CD2 | 1:L:127:PHE:N | 2.87 | 0.43 |
| 1:K:679:LEU:HA | 1:K:679:LEU:HD23 | 1.40 | 0.43 |
| 1:M:3:ILE:HG13 | 1:M:4:THR:N | 2.25 | 0.43 |
| 1:M:991:MET:HE2 | 1:M:1003:VAL:HG21 | 1.99 | 0.43 |
| 1:N:857:ARG:HH11 | 1:N:857:ARG:HG2 | 1.83 | 0.43 |
| 1:I:857:ARG:HH11 | 1:I:857:ARG:HG2 | 1.83 | 0.43 |
| 1:G:986:ILE:HD13 | 1:G:986:ILE:HG23 | 1.67 | 0.43 |
| 1:K:378:LEU:HD23 | 1:K:378:LEU:HA | 1.74 | 0.43 |
| 1:E:378:LEU:HD23 | 1:E:378:LEU:HA | 1.74 | 0.43 |
| 1:E:482:ARG:HD2 | 1:E:482:ARG:HH11 | 1.63 | 0.43 |
| 1:L:246:MET:HG2 | 1:L:274:PHE:CE2 | 2.52 | 0.43 |
| 1:C:685:LEU:HA | 1:C:686:PRO:HD3 | 1.83 | 0.43 |
| 1:P:687:GLN:HA | 1:P:688:PRO:HD3 | 1.73 | 0.43 |
| 1:J:867:THR:HG22 | 3:J:3405:HOH:O | 2.18 | 0.43 |
| 1:L:920:LEU:HB3 | 1:L:921:PRO:CD | 2.46 | 0.43 |
| 1:F:7:LEU:O | 1:F:11:LEU:HG | 2.18 | 0.43 |
| 1:C:576:ILE:CG2 | 1:C:577:LYS:N | 2.79 | 0.43 |
| 1:D:576:ILE:CG2 | 1:D:577:LYS:N | 2.79 | 0.43 |
| 1:J:127:PHE:CD2 | 1:J:127:PHE:N | 2.87 | 0.43 |
| 1:G:127:PHE:N | 1:G:127:PHE:CD2 | 2.87 | 0.43 |
| 1:O:127:PHE:CD2 | 1:O:127:PHE:N | 2.86 | 0.43 |
| 1:L:612:THR:HA | 1:L:613:PRO:HD3 | 1.59 | 0.43 |
| 1:N:102:ASN:C | 1:N:102:ASN:HD22 | 2.21 | 0.43 |
| 1:A:102:ASN:C | 1:A:102:ASN:HD22 | 2.21 | 0.43 |
| 1:L:847:LYS:HG3 | 1:L:848:THR:N | 2.32 | 0.43 |
| 1:N:638:VAL:O | 1:N:677:LYS:HA | 2.18 | 0.43 |
| 1:B:80:GLU:HG3 | 1:B:80:GLU:H | 1.29 | 0.43 |
| 1:E:857:ARG:HG2 | 1:E:857:ARG:HH11 | 1.83 | 0.43 |
| 1:D:221:GLN:H | 1:D:221:GLN:HG2 | 1.63 | 0.43 |
| 1:L:857:ARG:HG2 | 1:L:857:ARG:HH11 | 1.83 | 0.43 |
| 1:M:857:ARG:HH11 | 1:M:857:ARG:HG2 | 1.83 | 0.43 |
| 1:A:857:ARG:HG2 | 1:A:857:ARG:HH11 | 1.83 | 0.43 |
| 1:H:947:GLY:HA3 | 1:H:948:PRO:HD2 | 1.82 | 0.43 |
| 1:E:638:VAL:O | 1:E:677:LYS:HA | 2.18 | 0.43 |
| 1:J:847:LYS:HG3 | 1:J:848:THR:N | 2.32 | 0.43 |
| 1:A:991:MET:HE2 | 1:A:1003:VAL:HG21 | 2.00 | 0.43 |
| 1:B:246:MET:HG2 | 1:B:274:PHE:CE2 | 2.52 | 0.43 |
| 1:P:189:LEU:CD2 | 1:P:189:LEU:N | 2.79 | 0.43 |
| 1:O:7:LEU:O | 1:O:11:LEU:HG | 2.18 | 0.43 |
| 1:L:183:ARG:HD3 | 1:L:183:ARG:HH11 | 1.62 | 0.43 |
| 1:B:183:ARG:HD3 | 1:B:183:ARG:HH11 | 1.62 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:7:LEU:O | 1:D:11:LEU:HG | 2.18 | 0.43 |
| 1:J:952:ARG:HH11 | 1:J:952:ARG:CG | 2.28 | 0.43 |
| 1:M:279:ILE:HD12 | 1:M:279:ILE:HG21 | 1.77 | 0.43 |
| 1:I:129:VAL:CG2 | 1:I:182:ASN:ND2 | 2.80 | 0.43 |
| 1:B:599:ARG:HB2 | 1:B:600:GLN:OE1 | 2.18 | 0.43 |
| 1:A:599:ARG:HB2 | 1:A:600:GLN:OE1 | 2.18 | 0.43 |
| 1:H:599:ARG:HB2 | 1:H:600:GLN:H | 1.64 | 0.43 |
| 1:C:599:ARG:HB2 | 1:C:600:GLN:H | 1.63 | 0.43 |
| 1:A:127:PHE:CD2 | 1:A:127:PHE:N | 2.87 | 0.43 |
| 1:G:3:ILE:HG13 | 1:G:4:THR:N | 2.25 | 0.43 |
| 1:I:425:ARG:HH22 | 1:L:287:ASP:CG | 2.22 | 0.43 |
| 1:F:279:ILE:HD11 | 1:G:422:PRO:HG2 | 2.01 | 0.43 |
| 1:B:730:LEU:HA | 1:B:731:PRO:HD3 | 1.80 | 0.43 |
| 1:F:867:THR:HG22 | 3:F:3404:HOH:O | 2.17 | 0.43 |
| 1:I:246:MET:HG2 | 1:I:274:PHE:CE2 | 2.52 | 0.43 |
| 1:J:914:CME:HB3 | 1:J:914:CME:HE2 | 1.74 | 0.43 |
| 1:N:772:ASP:N | 1:N:772:ASP:OD1 | 2.48 | 0.43 |
| 1:O:857:ARG:HG2 | 1:O:857:ARG:HH11 | 1.83 | 0.43 |
| 1:H:655:MET:HE3 | 1:H:655:MET:HB2 | 1.73 | 0.43 |
| 1:G:670:LEU:HA | 1:G:670:LEU:HD23 | 1.75 | 0.43 |
| 1:I:947:GLY:HA3 | 1:I:948:PRO:HD2 | 1.82 | 0.43 |
| 1:L:638:VAL:O | 1:L:677:LYS:HA | 2.18 | 0.43 |
| 1:I:285:TYR:CB | 1:I:288:ARG:HG3 | 2.42 | 0.43 |
| 1:H:702:GLN:O | 1:H:712:GLY:N | 2.47 | 0.43 |
| 1:N:702:GLN:HA | 1:N:703:PRO:HD2 | 1.88 | 0.43 |
| 1:K:920:LEU:HB3 | 1:K:921:PRO:CD | 2.46 | 0.43 |
| 1:K:278:ILE:N | 1:K:278:ILE:CD1 | 2.80 | 0.43 |
| 1:G:7:LEU:HD12 | 1:G:74:LEU:HD11 | 1.97 | 0.43 |
| 1:A:254:LEU:HD23 | 1:A:254:LEU:HA | 1.71 | 0.43 |
| 1:O:599:ARG:HB2 | 1:O:600:GLN:OE1 | 2.18 | 0.43 |
| 1:G:599:ARG:HB2 | 1:G:600:GLN:OE1 | 2.18 | 0.43 |
| 1:N:279:ILE:CD1 | 1:O:422:PRO:CG | 2.95 | 0.43 |
| 1:I:127:PHE:CD2 | 1:I:127:PHE:N | 2.87 | 0.43 |
| 1:N:986:ILE:HD12 | 1:N:986:ILE:HG21 | 1.75 | 0.43 |
| 1:F:836:ILE:HD12 | 1:F:836:ILE:HG23 | 1.73 | 0.43 |
| 1:G:914:CME:HE2 | 1:G:914:CME:HB3 | 1.74 | 0.43 |
| 1:F:694:LEU:HA | 1:F:694:LEU:HD12 | 1.84 | 0.43 |
| 1:I:685:LEU:HA | 1:I:686:PRO:HD3 | 1.83 | 0.43 |
| 1:P:867:THR:HG22 | 3:P:3410:HOH:O | 2.17 | 0.43 |
| 1:E:702:GLN:O | 1:E:712:GLY:N | 2.47 | 0.43 |
| 1:A:567:VAL:HG12 | 1:A:568:TRP:N | 2.32 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:7:LEU:O | 1:N:11:LEU:HG | 2.18 | 0.43 |
| 1:G:278:ILE:N | 1:G:278:ILE:CD1 | 2.80 | 0.43 |
| 1:H:567:VAL:HG12 | 1:H:568:TRP:N | 2.32 | 0.43 |
| 1:M:183:ARG:HH11 | 1:M:183:ARG:HD3 | 1.62 | 0.43 |
| 1:L:7:LEU:O | 1:L:11:LEU:HG | 2.18 | 0.43 |
| 1:F:183:ARG:HD3 | 1:F:183:ARG:HH11 | 1.62 | 0.43 |
| 1:M:129:VAL:CG2 | 1:M:182:ASN:ND2 | 2.80 | 0.43 |
| 1:K:576:ILE:CG2 | 1:K:577:LYS:N | 2.79 | 0.43 |
| 1:K:599:ARG:HB2 | 1:K:600:GLN:OE1 | 2.18 | 0.43 |
| 1:M:599:ARG:HB2 | 1:M:600:GLN:H | 1.63 | 0.43 |
| 1:M:429:ASP:HA | 1:M:430:PRO:HD3 | 1.73 | 0.43 |
| 1:K:287:ASP:N | 1:K:287:ASP:OD1 | 2.41 | 0.43 |
| 1:L:658:LEU:N | 1:L:661:LYS:O | 2.40 | 0.43 |
| 1:D:778:THR:HB | 1:D:887:GLN:H | 1.84 | 0.43 |
| 1:N:1017:GLN:HB3 | 3:N:3513:HOH:O | 2.19 | 0.43 |
| 1:E:13:ARG:O | 1:E:14:ARG:HB2 | 2.17 | 0.43 |
| 1:F:857:ARG:HH11 | 1:F:857:ARG:HG2 | 1.83 | 0.43 |
| 1:F:670:LEU:HA | 1:F:670:LEU:HD23 | 1.75 | 0.43 |
| 1:F:80:GLU:H | 1:F:80:GLU:HG3 | 1.28 | 0.43 |
| 1:O:1017:GLN:HB3 | 3:O:3509:HOH:O | 2.19 | 0.43 |
| 1:O:685:LEU:HA | 1:O:686:PRO:HD3 | 1.83 | 0.43 |
| 1:E:316:HIS:HA | 1:E:323:ILE:HD13 | 2.01 | 0.43 |
| 1:E:57:GLU:HG2 | 1:E:83:THR:HG22 | 1.95 | 0.43 |
| 1:I:702:GLN:O | 1:I:712:GLY:N | 2.47 | 0.43 |
| 1:E:702:GLN:HA | 1:E:703:PRO:HD2 | 1.88 | 0.43 |
| 1:B:7:LEU:HD12 | 1:B:74:LEU:HD11 | 1.97 | 0.43 |
| 1:H:129:VAL:CG2 | 1:H:182:ASN:ND2 | 2.80 | 0.43 |
| 1:N:599:ARG:HB2 | 1:N:600:GLN:OE1 | 2.18 | 0.43 |
| 1:F:127:PHE:CD2 | 1:F:127:PHE:N | 2.87 | 0.43 |
| 1:M:127:PHE:N | 1:M:127:PHE:CD2 | 2.87 | 0.43 |
| 1:I:679:LEU:HA | 1:I:679:LEU:HD23 | 1.40 | 0.43 |
| 1:L:3:ILE:HG13 | 1:L:4:THR:N | 2.24 | 0.43 |
| 1:G:778:THR:HB | 1:G:887:GLN:H | 1.84 | 0.43 |
| 1:O:778:THR:HB | 1:O:887:GLN:H | 1.84 | 0.43 |
| 1:G:1017:GLN:HB3 | 3:G:3512:HOH:O | 2.19 | 0.43 |
| 1:P:237:ARG:HB2 | 1:P:237:ARG:HE | 1.35 | 0.43 |
| 1:A:482:ARG:HD2 | 1:A:482:ARG:HH11 | 1.63 | 0.43 |
| 1:F:221:GLN:H | 1:F:221:GLN:HG2 | 1.63 | 0.43 |
| 1:B:1017:GLN:HB3 | 3:B:3513:HOH:O | 2.19 | 0.43 |
| 1:O:867:THR:HG22 | 3:O:3402:HOH:O | 2.17 | 0.43 |
| 1:K:1017:GLN:HB3 | 3:K:4414:HOH:O | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:278:ILE:N | 1:L:278:ILE:CD1 | 2.80 | 0.43 |
| 1:A:78:LEU:HB3 | 1:A:79:PRO:CD | 2.43 | 0.43 |
| 1:E:7:LEU:O | 1:E:11:LEU:HG | 2.18 | 0.43 |
| 1:M:952:ARG:CG | 1:M:952:ARG:HH11 | 2.28 | 0.43 |
| 1:L:254:LEU:HD23 | 1:L:254:LEU:HA | 1.71 | 0.43 |
| 1:N:279:ILE:HD11 | 1:O:422:PRO:HB2 | 1.99 | 0.43 |
| 1:E:127:PHE:CD2 | 1:E:127:PHE:N | 2.87 | 0.43 |
| 1:L:679:LEU:HD23 | 1:L:679:LEU:HA | 1.40 | 0.43 |
| 1:G:612:THR:HA | 1:G:613:PRO:HD3 | 1.59 | 0.43 |
| 1:B:279:ILE:HD11 | 1:C:422:PRO:HB2 | 2.01 | 0.43 |
| 1:O:13:ARG:O | 1:O:14:ARG:HB2 | 2.17 | 0.43 |
| 1:D:836:ILE:HD12 | 1:D:836:ILE:HG23 | 1.73 | 0.43 |
| 1:B:986:ILE:HD13 | 1:B:986:ILE:HG23 | 1.67 | 0.43 |
| 1:E:772:ASP:OD1 | 1:E:772:ASP:N | 2.48 | 0.43 |
| 1:H:867:THR:HG22 | 3:H:4299:HOH:O | 2.17 | 0.43 |
| 1:L:147:ASN:HA | 1:L:148:SER:HA | 1.57 | 0.43 |
| 1:G:682:LEU:HA | 1:G:682:LEU:HD23 | 1.85 | 0.43 |
| 1:N:778:THR:HB | 1:N:887:GLN:H | 1.84 | 0.43 |
| 1:K:778:THR:HB | 1:K:887:GLN:H | 1.84 | 0.43 |
| 1:P:778:THR:HB | 1:P:887:GLN:H | 1.83 | 0.43 |
| 1:P:878:HIS:HA | 1:P:879:PRO:HD3 | 1.83 | 0.43 |
| 1:B:670:LEU:HD23 | 1:B:670:LEU:HA | 1.75 | 0.43 |
| 1:A:221:GLN:HG2 | 1:A:221:GLN:H | 1.63 | 0.43 |
| 1:N:134:LEU:HA | 1:N:134:LEU:HD23 | 1.68 | 0.43 |
| 1:I:237:ARG:HE | 1:I:237:ARG:HB2 | 1.35 | 0.43 |
| 1:K:857:ARG:HG2 | 1:K:857:ARG:HH11 | 1.83 | 0.43 |
| 1:C:1000:SER:HA | 1:C:1001:PRO:HD3 | 1.88 | 0.43 |
| 1:J:237:ARG:HB2 | 1:J:237:ARG:HE | 1.35 | 0.43 |
| 1:G:857:ARG:HG2 | 1:G:857:ARG:HH11 | 1.83 | 0.43 |
| 1:F:991:MET:HE2 | 1:F:1003:VAL:HG21 | 2.00 | 0.43 |
| 1:J:118:ASN:HA | 1:J:119:PRO:HD2 | 1.62 | 0.43 |
| 1:G:685:LEU:HA | 1:G:686:PRO:HD3 | 1.83 | 0.43 |
| 1:G:702:GLN:HA | 1:G:703:PRO:HD2 | 1.88 | 0.43 |
| 1:O:682:LEU:HD23 | 1:O:682:LEU:HA | 1.85 | 0.43 |
| 1:M:599:ARG:HB2 | 1:M:600:GLN:OE1 | 2.18 | 0.43 |
| 1:F:599:ARG:HB2 | 1:F:600:GLN:OE1 | 2.19 | 0.43 |
| 1:N:127:PHE:CD2 | 1:N:127:PHE:N | 2.87 | 0.43 |
| 1:C:127:PHE:N | 1:C:127:PHE:CD2 | 2.86 | 0.43 |
| 1:J:217:LYS:NZ | 1:J:326:GLU:OE2 | 2.52 | 0.43 |
| 1:O:612:THR:HA | 1:O:613:PRO:HD3 | 1.59 | 0.43 |
| 1:J:102:ASN:C | 1:J:102:ASN:HD22 | 2.21 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:778:THR:HB | 1:B:887:GLN:H | 1.84 | 0.43 |
| 1:H:778:THR:HB | 1:H:887:GLN:H | 1.84 | 0.43 |
| 1:A:778:THR:HB | 1:A:887:GLN:H | 1.84 | 0.43 |
| 1:K:118:ASN:HA | 1:K:119:PRO:HD2 | 1.62 | 0.43 |
| 1:F:1017:GLN:HB3 | 3:F:3513:HOH:O | 2.19 | 0.43 |
| 1:L:867:THR:HG22 | 3:L:3408:HOH:O | 2.17 | 0.43 |
| 1:N:991:MET:HE2 | 1:N:1003:VAL:HG21 | 2.00 | 0.43 |
| 1:N:694:LEU:HD12 | 1:N:694:LEU:HA | 1.84 | 0.43 |
| 1:L:836:ILE:HD12 | 1:L:836:ILE:HG23 | 1.73 | 0.43 |
| 1:D:1017:GLN:HB3 | 3:D:3519:HOH:O | 2.19 | 0.43 |
| 1:H:189:LEU:N | 1:H:189:LEU:CD2 | 2.79 | 0.42 |
| 1:O:702:GLN:HA | 1:O:703:PRO:HD2 | 1.88 | 0.42 |
| 1:F:271:THR:HG22 | 1:F:272:ALA:N | 2.34 | 0.42 |
| 1:K:271:THR:HG22 | 1:K:272:ALA:N | 2.35 | 0.42 |
| 1:I:599:ARG:HB2 | 1:I:600:GLN:H | 1.63 | 0.42 |
| 1:M:217:LYS:NZ | 1:M:326:GLU:OE2 | 2.52 | 0.42 |
| 1:K:4:THR:HA | 1:K:9:VAL:HG11 | 2.01 | 0.42 |
| 1:I:395:HIS:HA | 1:I:396:PRO:HD3 | 1.69 | 0.42 |
| 1:B:857:ARG:HH11 | 1:B:857:ARG:HG2 | 1.83 | 0.42 |
| 1:P:378:LEU:HD23 | 1:P:378:LEU:HA | 1.74 | 0.42 |
| 1:C:857:ARG:HG2 | 1:C:857:ARG:HH11 | 1.83 | 0.42 |
| 1:C:134:LEU:HA | 1:C:134:LEU:HD23 | 1.68 | 0.42 |
| 1:P:316:HIS:HA | 1:P:323:ILE:HD13 | 2.01 | 0.42 |
| 1:B:287:ASP:OD1 | 1:B:287:ASP:N | 2.41 | 0.42 |
| 1:M:271:THR:HG22 | 1:M:272:ALA:N | 2.34 | 0.42 |
| 1:H:271:THR:HG22 | 1:H:272:ALA:N | 2.34 | 0.42 |
| 1:A:217:LYS:NZ | 1:A:326:GLU:OE2 | 2.52 | 0.42 |
| 1:H:217:LYS:NZ | 1:H:326:GLU:OE2 | 2.52 | 0.42 |
| 1:E:217:LYS:NZ | 1:E:326:GLU:OE2 | 2.52 | 0.42 |
| 1:K:217:LYS:NZ | 1:K:326:GLU:OE2 | 2.52 | 0.42 |
| 1:A:380:LYS:HE2 | 3:A:4075:HOH:O | 2.19 | 0.42 |
| 1:D:429:ASP:HA | 1:D:430:PRO:HD3 | 1.73 | 0.42 |
| 1:J:778:THR:HB | 1:J:887:GLN:H | 1.84 | 0.42 |
| 1:C:778:THR:HB | 1:C:887:GLN:H | 1.84 | 0.42 |
| 1:G:479:ASP:HA | 1:G:480:PRO:HD2 | 1.77 | 0.42 |
| 1:G:378:LEU:HA | 1:G:378:LEU:HD23 | 1.74 | 0.42 |
| 1:N:867:THR:HG22 | 3:N:3405:HOH:O | 2.17 | 0.42 |
| 1:J:1017:GLN:HB3 | 3:J:3514:HOH:O | 2.18 | 0.42 |
| 1:D:702:GLN:HA | 1:D:703:PRO:HD2 | 1.88 | 0.42 |
| 1:M:917:ARG:HD2 | 3:M:4341:HOH:O | 2.19 | 0.42 |
| 1:P:576:ILE:CG2 | 1:P:577:LYS:N | 2.79 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:576:ILE:CG2 | 1:M:577:LYS:N | 2.79 | 0.42 |
| 1:J:271:THR:HG22 | 1:J:272:ALA:N | 2.35 | 0.42 |
| 1:D:271:THR:HG22 | 1:D:272:ALA:N | 2.34 | 0.42 |
| 1:H:127:PHE:N | 1:H:127:PHE:CD2 | 2.87 | 0.42 |
| 1:P:127:PHE:CD2 | 1:P:127:PHE:N | 2.87 | 0.42 |
| 1:F:217:LYS:NZ | 1:F:326:GLU:OE2 | 2.52 | 0.42 |
| 1:N:422:PRO:HG2 | 1:O:279:ILE:CD1 | 2.49 | 0.42 |
| 1:H:679:LEU:HA | 1:H:679:LEU:HD23 | 1.40 | 0.42 |
| 1:H:4:THR:HA | 1:H:9:VAL:HG11 | 2.02 | 0.42 |
| 1:P:4:THR:HA | 1:P:9:VAL:HG11 | 2.02 | 0.42 |
| 1:L:778:THR:HB | 1:L:887:GLN:H | 1.84 | 0.42 |
| 1:N:80:GLU:H | 1:N:80:GLU:HG3 | 1.29 | 0.42 |
| 1:D:772:ASP:N | 1:D:772:ASP:OD1 | 2.48 | 0.42 |
| 1:L:772:ASP:N | 1:L:772:ASP:OD1 | 2.48 | 0.42 |
| 1:J:173:LEU:HA | 1:J:173:LEU:HD23 | 1.85 | 0.42 |
| 1:I:118:ASN:HA | 1:I:119:PRO:HD2 | 1.62 | 0.42 |
| 1:F:278:ILE:CD1 | 1:F:278:ILE:N | 2.80 | 0.42 |
| 1:C:254:LEU:HD23 | 1:C:254:LEU:HA | 1.71 | 0.42 |
| 1:B:599:ARG:HD2 | 1:B:600:GLN:OE1 | 2.20 | 0.42 |
| 1:B:127:PHE:N | 1:B:127:PHE:CD2 | 2.87 | 0.42 |
| 1:B:469:ASP:HB3 | 1:C:473:ARG:HD2 | 2.01 | 0.42 |
| 1:H:380:LYS:HE2 | 3:H:4075:HOH:O | 2.19 | 0.42 |
| 1:M:380:LYS:HE2 | 3:M:4075:HOH:O | 2.19 | 0.42 |
| 1:E:380:LYS:HE2 | 3:E:4075:HOH:O | 2.19 | 0.42 |
| 1:P:380:LYS:HE2 | 3:P:3187:HOH:O | 2.19 | 0.42 |
| 1:L:429:ASP:HA | 1:L:430:PRO:HD3 | 1.73 | 0.42 |
| 1:C:4:THR:HA | 1:C:9:VAL:HG11 | 2.01 | 0.42 |
| 1:E:4:THR:HA | 1:E:9:VAL:HG11 | 2.02 | 0.42 |
| 1:F:778:THR:HB | 1:F:887:GLN:H | 1.84 | 0.42 |
| 1:K:111:PRO:HA | 1:K:112:PRO:HA | 1.66 | 0.42 |
| 1:E:234:ASP:O | 1:E:235:PHE:HB2 | 2.20 | 0.42 |
| 1:P:836:ILE:HG23 | 1:P:836:ILE:HD12 | 1.73 | 0.42 |
| 1:D:857:ARG:HH11 | 1:D:857:ARG:HG2 | 1.83 | 0.42 |
| 1:A:173:LEU:HD23 | 1:A:173:LEU:HA | 1.86 | 0.42 |
| 1:K:80:GLU:H | 1:K:80:GLU:HG3 | 1.29 | 0.42 |
| 1:L:670:LEU:HA | 1:L:670:LEU:HD23 | 1.75 | 0.42 |
| 1:P:173:LEU:HD23 | 1:P:173:LEU:HA | 1.85 | 0.42 |
| 1:A:130:ASP:OD1 | 1:A:131:GLU:N | 2.53 | 0.42 |
| 1:B:685:LEU:HA | 1:B:686:PRO:HD3 | 1.83 | 0.42 |
| 1:P:1017:GLN:HB3 | 3:P:3519:HOH:O | 2.19 | 0.42 |
| 1:I:687:GLN:HA | 1:I:688:PRO:HD3 | 1.73 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:427:THR:HA | 1:M:436:MET:HE2 | 1.93 | 0.42 |
| 1:B:920:LEU:HB3 | 1:B:921:PRO:CD | 2.46 | 0.42 |
| 1:F:917:ARG:HD2 | 3:F:3447:HOH:O | 2.19 | 0.42 |
| 1:B:917:ARG:HD2 | 3:B:3446:HOH:O | 2.19 | 0.42 |
| 1:O:576:ILE:CG2 | 1:O:577:LYS:N | 2.79 | 0.42 |
| 1:E:576:ILE:CG2 | 1:E:577:LYS:N | 2.79 | 0.42 |
| 1:D:599:ARG:HD2 | 1:D:600:GLN:OE1 | 2.20 | 0.42 |
| 1:M:599:ARG:HD2 | 1:M:600:GLN:OE1 | 2.20 | 0.42 |
| 1:A:599:ARG:HD2 | 1:A:600:GLN:OE1 | 2.20 | 0.42 |
| 1:F:599:ARG:HD2 | 1:F:600:GLN:OE1 | 2.20 | 0.42 |
| 1:K:668:VAL:HA | 1:K:669:PRO:HD3 | 1.83 | 0.42 |
| 1:K:127:PHE:N | 1:K:127:PHE:CD2 | 2.87 | 0.42 |
| 1:B:217:LYS:NZ | 1:B:326:GLU:OE2 | 2.52 | 0.42 |
| 1:N:380:LYS:HE2 | 3:N:3182:HOH:O | 2.19 | 0.42 |
| 1:M:4:THR:HA | 1:M:9:VAL:HG11 | 2.02 | 0.42 |
| 1:B:658:LEU:N | 1:B:661:LYS:O | 2.40 | 0.42 |
| 1:P:130:ASP:OD1 | 1:P:131:GLU:N | 2.53 | 0.42 |
| 1:L:1017:GLN:HB3 | 3:L:3517:HOH:O | 2.19 | 0.42 |
| 1:C:914:CME:HE2 | 1:C:914:CME:HB3 | 1.74 | 0.42 |
| 1:K:562:LEU:HD23 | 1:K:562:LEU:HA | 1.90 | 0.42 |
| 1:J:857:ARG:HH11 | 1:J:857:ARG:HG2 | 1.83 | 0.42 |
| 1:G:176:PHE:CD1 | 1:G:176:PHE:N | 2.88 | 0.42 |
| 1:F:772:ASP:N | 1:F:772:ASP:OD1 | 2.48 | 0.42 |
| 1:O:479:ASP:HA | 1:O:480:PRO:HD2 | 1.77 | 0.42 |
| 1:C:867:THR:HG22 | 3:C:4299:HOH:O | 2.17 | 0.42 |
| 1:F:702:GLN:O | 1:F:712:GLY:N | 2.47 | 0.42 |
| 1:P:920:LEU:HB3 | 1:P:921:PRO:CD | 2.46 | 0.42 |
| 1:E:917:ARG:HD2 | 3:E:4342:HOH:O | 2.19 | 0.42 |
| 1:L:599:ARG:HB2 | 1:L:600:GLN:OE1 | 2.18 | 0.42 |
| 1:O:667:GLU:C | 1:O:668:VAL:HG23 | 2.40 | 0.42 |
| 1:C:271:THR:HG22 | 1:C:272:ALA:N | 2.35 | 0.42 |
| 1:N:667:GLU:C | 1:N:668:VAL:HG23 | 2.40 | 0.42 |
| 1:F:667:GLU:C | 1:F:668:VAL:HG23 | 2.40 | 0.42 |
| 1:M:667:GLU:C | 1:M:668:VAL:HG23 | 2.40 | 0.42 |
| 1:I:599:ARG:HB2 | 1:I:600:GLN:OE1 | 2.18 | 0.42 |
| 1:L:217:LYS:NZ | 1:L:326:GLU:OE2 | 2.52 | 0.42 |
| 1:K:130:ASP:OD1 | 1:K:131:GLU:N | 2.53 | 0.42 |
| 1:L:130:ASP:OD1 | 1:L:131:GLU:N | 2.53 | 0.42 |
| 1:J:176:PHE:CD1 | 1:J:176:PHE:N | 2.88 | 0.42 |
| 1:C:670:LEU:HD23 | 1:C:670:LEU:HA | 1.75 | 0.42 |
| 1:J:482:ARG:HD2 | 1:J:482:ARG:HH11 | 1.63 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:237:ARG:HE | 1:B:237:ARG:HB2 | 1.35 | 0.42 |
| 1:E:836:ILE:HD12 | 1:E:836:ILE:HG23 | 1.73 | 0.42 |
| 1:M:176:PHE:CD1 | 1:M:176:PHE:N | 2.88 | 0.42 |
| 1:E:202:MET:HE3 | 1:E:202:MET:HB3 | 1.90 | 0.42 |
| 1:H:173:LEU:HA | 1:H:173:LEU:HD23 | 1.85 | 0.42 |
| 1:H:111:PRO:HA | 1:H:112:PRO:HA | 1.66 | 0.42 |
| 1:M:130:ASP:OD1 | 1:M:131:GLU:N | 2.53 | 0.42 |
| 1:C:176:PHE:CD1 | 1:C:176:PHE:N | 2.88 | 0.42 |
| 1:C:1017:GLN:HB3 | 3:C:4412:HOH:O | 2.19 | 0.42 |
| 1:A:285:TYR:CB | 1:A:288:ARG:HG3 | 2.42 | 0.42 |
| 1:I:272:ALA:HA | 1:I:273:PRO:HD3 | 1.78 | 0.42 |
| 1:N:217:LYS:NZ | 1:N:326:GLU:OE2 | 2.52 | 0.42 |
| 1:O:679:LEU:HD23 | 1:O:679:LEU:HA | 1.40 | 0.42 |
| 1:F:380:LYS:HE2 | 3:F:3181:HOH:O | 2.19 | 0.42 |
| 1:C:380:LYS:HE2 | 3:C:4075:HOH:O | 2.19 | 0.42 |
| 1:F:4:THR:HA | 1:F:9:VAL:HG11 | 2.02 | 0.42 |
| 1:N:4:THR:HA | 1:N:9:VAL:HG11 | 2.02 | 0.42 |
| 1:H:395:HIS:HA | 1:H:396:PRO:HD3 | 1.69 | 0.42 |
| 1:E:778:THR:HB | 1:E:887:GLN:H | 1.84 | 0.42 |
| 1:F:234:ASP:O | 1:F:235:PHE:HB2 | 2.20 | 0.42 |
| 1:C:147:ASN:HA | 1:C:148:SER:HA | 1.57 | 0.42 |
| 1:K:687:GLN:HA | 1:K:688:PRO:HD3 | 1.73 | 0.42 |
| 1:J:279:ILE:HD11 | 1:K:422:PRO:HG2 | 2.02 | 0.42 |
| 1:C:378:LEU:HA | 1:C:378:LEU:HD23 | 1.74 | 0.42 |
| 1:E:176:PHE:CD1 | 1:E:176:PHE:N | 2.88 | 0.42 |
| 1:L:378:LEU:HA | 1:L:378:LEU:HD23 | 1.74 | 0.42 |
| 1:N:176:PHE:CD1 | 1:N:176:PHE:N | 2.88 | 0.42 |
| 1:M:755:ARG:HD2 | 1:M:755:ARG:HH11 | 1.74 | 0.42 |
| 1:F:211:ASP:N | 1:F:211:ASP:OD1 | 2.50 | 0.42 |
| 1:G:147:ASN:HA | 1:G:148:SER:HA | 1.57 | 0.42 |
| 1:E:287:ASP:OD2 | 1:H:425:ARG:NH2 | 2.53 | 0.42 |
| 1:M:7:LEU:HD12 | 1:M:74:LEU:HD11 | 1.97 | 0.42 |
| 1:P:7:LEU:HD12 | 1:P:74:LEU:HD11 | 1.97 | 0.42 |
| 1:O:917:ARG:HD2 | 3:O:3445:HOH:O | 2.19 | 0.42 |
| 1:G:917:ARG:HD2 | 3:G:3446:HOH:O | 2.19 | 0.42 |
| 1:I:917:ARG:HD2 | 3:I:4340:HOH:O | 2.19 | 0.42 |
| 1:I:668:VAL:HA | 1:I:669:PRO:HD3 | 1.83 | 0.42 |
| 1:N:599:ARG:HD2 | 1:N:600:GLN:OE1 | 2.20 | 0.42 |
| 1:J:667:GLU:C | 1:J:668:VAL:HG23 | 2.40 | 0.42 |
| 1:D:127:PHE:N | 1:D:127:PHE:CD2 | 2.87 | 0.42 |
| 1:M:778:THR:HG22 | 1:M:779:PRO:O | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:778:THR:HB | 1:I:887:GLN:H | 1.84 | 0.42 |
| 1:N:986:ILE:HG23 | 1:N:986:ILE:HD13 | 1.67 | 0.42 |
| 1:I:670:LEU:HA | 1:I:670:LEU:HD23 | 1.75 | 0.42 |
| 1:C:772:ASP:OD1 | 1:C:772:ASP:N | 2.48 | 0.42 |
| 1:A:176:PHE:CD1 | 1:A:176:PHE:N | 2.88 | 0.42 |
| 1:E:670:LEU:HA | 1:E:670:LEU:HD23 | 1.75 | 0.42 |
| 1:B:176:PHE:N | 1:B:176:PHE:CD1 | 2.88 | 0.42 |
| 1:B:726:LEU:HD23 | 1:B:726:LEU:HA | 1.76 | 0.42 |
| 1:A:755:ARG:HH11 | 1:A:755:ARG:HD2 | 1.74 | 0.42 |
| 1:G:130:ASP:OD1 | 1:G:131:GLU:N | 2.53 | 0.42 |
| 1:G:878:HIS:HA | 1:G:879:PRO:HD3 | 1.83 | 0.42 |
| 1:G:513:PRO:O | 1:G:514:ALA:HB3 | 2.20 | 0.42 |
| 1:O:878:HIS:HA | 1:O:879:PRO:HD3 | 1.83 | 0.42 |
| 1:E:1017:GLN:HB3 | 3:E:4407:HOH:O | 2.19 | 0.42 |
| 1:N:595:THR:CG2 | 1:N:596:PRO:HA | 2.37 | 0.42 |
| 1:K:917:ARG:HD2 | 3:K:4343:HOH:O | 2.19 | 0.42 |
| 1:J:362:LEU:HA | 1:J:362:LEU:HD23 | 1.70 | 0.42 |
| 1:L:599:ARG:HD2 | 1:L:600:GLN:OE1 | 2.20 | 0.42 |
| 1:E:599:ARG:HD2 | 1:E:600:GLN:OE1 | 2.20 | 0.42 |
| 1:K:272:ALA:HA | 1:K:273:PRO:HD3 | 1.78 | 0.42 |
| 1:H:667:GLU:C | 1:H:668:VAL:HG23 | 2.40 | 0.42 |
| 1:D:667:GLU:C | 1:D:668:VAL:HG23 | 2.40 | 0.42 |
| 1:D:217:LYS:NZ | 1:D:326:GLU:OE2 | 2.52 | 0.42 |
| 1:I:856:TYR:CD2 | 1:I:864:MET:HE2 | 2.53 | 0.42 |
| 1:B:4:THR:HA | 1:B:9:VAL:HG11 | 2.02 | 0.42 |
| 1:D:4:THR:HA | 1:D:9:VAL:HG11 | 2.01 | 0.42 |
| 1:C:778:THR:HG22 | 1:C:779:PRO:O | 2.20 | 0.42 |
| 1:K:778:THR:HG22 | 1:K:779:PRO:O | 2.20 | 0.42 |
| 1:M:395:HIS:HA | 1:M:396:PRO:HD3 | 1.69 | 0.42 |
| 1:J:658:LEU:N | 1:J:661:LYS:O | 2.40 | 0.42 |
| 1:E:991:MET:HE2 | 1:E:1003:VAL:HG21 | 2.01 | 0.42 |
| 1:K:513:PRO:O | 1:K:514:ALA:HB3 | 2.20 | 0.42 |
| 1:H:482:ARG:HD2 | 1:H:482:ARG:HH11 | 1.63 | 0.42 |
| 1:N:211:ASP:N | 1:N:211:ASP:OD1 | 2.50 | 0.42 |
| 1:M:378:LEU:HA | 1:M:378:LEU:HD23 | 1.74 | 0.42 |
| 1:B:655:MET:O | 1:B:655:MET:HG3 | 2.20 | 0.42 |
| 1:L:513:PRO:O | 1:L:514:ALA:HB3 | 2.20 | 0.42 |
| 1:N:130:ASP:OD1 | 1:N:131:GLU:N | 2.53 | 0.42 |
| 1:M:422:PRO:HB2 | 1:P:279:ILE:HD11 | 2.02 | 0.42 |
| 1:B:234:ASP:O | 1:B:235:PHE:HB2 | 2.20 | 0.42 |
| 1:C:130:ASP:OD1 | 1:C:131:GLU:N | 2.53 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:316:HIS:HA | 1:K:323:ILE:HD13 | 2.01 | 0.42 |
| 1:P:702:GLN:HA | 1:P:703:PRO:HD2 | 1.88 | 0.42 |
| 1:N:183:ARG:HD3 | 1:N:183:ARG:HH11 | 1.62 | 0.42 |
| 1:H:917:ARG:HD2 | 3:H:4343:HOH:O | 2.19 | 0.42 |
| 1:F:576:ILE:CG2 | 1:F:577:LYS:N | 2.79 | 0.42 |
| 1:K:599:ARG:HD2 | 1:K:600:GLN:OE1 | 2.20 | 0.42 |
| 1:C:667:GLU:C | 1:C:668:VAL:HG23 | 2.40 | 0.42 |
| 1:G:599:ARG:HD2 | 1:G:600:GLN:OE1 | 2.20 | 0.42 |
| 1:A:422:PRO:CG | 1:D:279:ILE:CD1 | 2.97 | 0.42 |
| 1:E:667:GLU:C | 1:E:668:VAL:HG23 | 2.40 | 0.42 |
| 1:I:217:LYS:NZ | 1:I:326:GLU:OE2 | 2.52 | 0.42 |
| 1:A:4:THR:HA | 1:A:9:VAL:HG11 | 2.01 | 0.42 |
| 1:J:778:THR:HG22 | 1:J:779:PRO:O | 2.20 | 0.42 |
| 1:P:279:ILE:HD12 | 1:P:279:ILE:HG21 | 1.77 | 0.42 |
| 1:K:234:ASP:O | 1:K:235:PHE:HB2 | 2.20 | 0.42 |
| 1:G:211:ASP:OD1 | 1:G:211:ASP:N | 2.50 | 0.42 |
| 1:E:173:LEU:HD23 | 1:E:173:LEU:HA | 1.85 | 0.42 |
| 1:F:176:PHE:CD1 | 1:F:176:PHE:N | 2.88 | 0.42 |
| 1:K:655:MET:O | 1:K:655:MET:HG3 | 2.20 | 0.42 |
| 1:K:221:GLN:HG2 | 1:K:221:GLN:H | 1.62 | 0.42 |
| 1:E:694:LEU:HD12 | 1:E:694:LEU:HA | 1.84 | 0.42 |
| 1:O:53:SER:C | 1:O:54:LEU:HD23 | 2.41 | 0.42 |
| 1:H:130:ASP:OD1 | 1:H:131:GLU:N | 2.53 | 0.42 |
| 1:O:687:GLN:HA | 1:O:688:PRO:HD3 | 1.73 | 0.42 |
| 1:N:513:PRO:O | 1:N:514:ALA:HB3 | 2.20 | 0.42 |
| 1:H:513:PRO:O | 1:H:514:ALA:HB3 | 2.20 | 0.42 |
| 1:B:513:PRO:O | 1:B:514:ALA:HB3 | 2.20 | 0.42 |
| 1:D:917:ARG:HD2 | 3:D:3454:HOH:O | 2.19 | 0.41 |
| 1:H:576:ILE:CG2 | 1:H:577:LYS:N | 2.79 | 0.41 |
| 1:J:599:ARG:HB2 | 1:J:600:GLN:H | 1.64 | 0.41 |
| 1:H:599:ARG:HD2 | 1:H:600:GLN:OE1 | 2.20 | 0.41 |
| 1:C:599:ARG:HD2 | 1:C:600:GLN:OE1 | 2.20 | 0.41 |
| 1:C:217:LYS:NZ | 1:C:326:GLU:OE2 | 2.52 | 0.41 |
| 1:O:217:LYS:NZ | 1:O:326:GLU:OE2 | 2.52 | 0.41 |
| 1:P:217:LYS:NZ | 1:P:326:GLU:OE2 | 2.52 | 0.41 |
| 1:I:422:PRO:HG2 | 1:L:279:ILE:CD1 | 2.50 | 0.41 |
| 1:B:778:THR:HG22 | 1:B:779:PRO:O | 2.20 | 0.41 |
| 1:F:130:ASP:OD1 | 1:F:131:GLU:N | 2.53 | 0.41 |
| 1:A:118:ASN:HA | 1:A:119:PRO:HD2 | 1.62 | 0.41 |
| 1:I:655:MET:HE3 | 1:I:655:MET:HB2 | 1.81 | 0.41 |
| 1:H:670:LEU:HD23 | 1:H:670:LEU:HA | 1.75 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:176:PHE:N | 1:K:176:PHE:CD1 | 2.88 | 0.41 |
| 1:K:726:LEU:HD23 | 1:K:726:LEU:HA | 1.76 | 0.41 |
| 1:O:130:ASP:OD1 | 1:O:131:GLU:N | 2.53 | 0.41 |
| 1:F:74:LEU:HA | 1:F:74:LEU:HD23 | 1.92 | 0.41 |
| 1:B:254:LEU:HD23 | 1:B:254:LEU:HA | 1.71 | 0.41 |
| 1:N:576:ILE:CG2 | 1:N:577:LYS:N | 2.79 | 0.41 |
| 1:B:271:THR:HG22 | 1:B:272:ALA:N | 2.35 | 0.41 |
| 1:A:667:GLU:C | 1:A:668:VAL:HG23 | 2.40 | 0.41 |
| 1:I:667:GLU:C | 1:I:668:VAL:HG23 | 2.40 | 0.41 |
| 1:O:599:ARG:HD2 | 1:O:600:GLN:OE1 | 2.20 | 0.41 |
| 1:G:217:LYS:NZ | 1:G:326:GLU:OE2 | 2.52 | 0.41 |
| 1:H:662:PRO:O | 1:H:663:LEU:HD23 | 2.20 | 0.41 |
| 1:I:69:VAL:CG1 | 1:I:70:PRO:HD2 | 2.51 | 0.41 |
| 1:M:661:LYS:HA | 1:M:662:PRO:HD3 | 1.74 | 0.41 |
| 1:M:662:PRO:O | 1:M:663:LEU:HD23 | 2.20 | 0.41 |
| 1:D:234:ASP:O | 1:D:235:PHE:HB2 | 2.20 | 0.41 |
| 1:M:1017:GLN:HB3 | 3:M:4405:HOH:O | 2.19 | 0.41 |
| 1:O:836:ILE:HG23 | 1:O:836:ILE:HD12 | 1.73 | 0.41 |
| 1:C:836:ILE:HG23 | 1:C:836:ILE:HD12 | 1.73 | 0.41 |
| 1:L:176:PHE:N | 1:L:176:PHE:CD1 | 2.88 | 0.41 |
| 1:F:482:ARG:HH11 | 1:F:482:ARG:HD2 | 1.63 | 0.41 |
| 1:M:655:MET:O | 1:M:655:MET:HG3 | 2.20 | 0.41 |
| 1:D:986:ILE:HD13 | 1:D:986:ILE:HG23 | 1.67 | 0.41 |
| 1:I:726:LEU:HA | 1:I:726:LEU:HD23 | 1.76 | 0.41 |
| 1:N:655:MET:HG3 | 1:N:655:MET:O | 2.20 | 0.41 |
| 1:E:802:ASP:HA | 1:E:803:PRO:HD3 | 1.83 | 0.41 |
| 1:M:234:ASP:O | 1:M:235:PHE:HB2 | 2.20 | 0.41 |
| 1:P:53:SER:C | 1:P:54:LEU:HD23 | 2.41 | 0.41 |
| 1:H:234:ASP:O | 1:H:235:PHE:HB2 | 2.20 | 0.41 |
| 1:A:917:ARG:HD2 | 3:A:4343:HOH:O | 2.20 | 0.41 |
| 1:P:599:ARG:HD2 | 1:P:600:GLN:OE1 | 2.20 | 0.41 |
| 1:A:69:VAL:CG1 | 1:A:70:PRO:HD2 | 2.50 | 0.41 |
| 1:B:380:LYS:HE2 | 3:B:3180:HOH:O | 2.19 | 0.41 |
| 1:J:4:THR:HA | 1:J:9:VAL:HG11 | 2.02 | 0.41 |
| 1:O:4:THR:HA | 1:O:9:VAL:HG11 | 2.01 | 0.41 |
| 1:N:778:THR:HG22 | 1:N:779:PRO:O | 2.20 | 0.41 |
| 1:D:395:HIS:HA | 1:D:396:PRO:HD3 | 1.69 | 0.41 |
| 1:F:947:GLY:HA3 | 1:F:948:PRO:HD2 | 1.82 | 0.41 |
| 1:A:772:ASP:OD1 | 1:A:772:ASP:N | 2.48 | 0.41 |
| 1:J:694:LEU:HD12 | 1:J:694:LEU:HA | 1.84 | 0.41 |
| 1:M:287:ASP:N | 1:M:287:ASP:OD1 | 2.41 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:914:CME:HE2 | 1:O:914:CME:HB3 | 1.74 | 0.41 |
| 1:D:53:SER:C | 1:D:54:LEU:HD23 | 2.41 | 0.41 |
| 1:A:513:PRO:O | 1:A:514:ALA:HB3 | 2.20 | 0.41 |
| 1:P:285:TYR:CB | 1:P:288:ARG:HG3 | 2.42 | 0.41 |
| 1:E:7:LEU:HD12 | 1:E:74:LEU:HD11 | 1.97 | 0.41 |
| 1:I:183:ARG:HH11 | 1:I:183:ARG:HD3 | 1.62 | 0.41 |
| 1:A:576:ILE:CG2 | 1:A:577:LYS:N | 2.79 | 0.41 |
| 1:L:271:THR:HG22 | 1:L:272:ALA:N | 2.35 | 0.41 |
| 1:P:667:GLU:C | 1:P:668:VAL:HG23 | 2.40 | 0.41 |
| 1:J:662:PRO:O | 1:J:663:LEU:HD23 | 2.20 | 0.41 |
| 1:L:69:VAL:CG1 | 1:L:70:PRO:HD2 | 2.50 | 0.41 |
| 1:C:662:PRO:O | 1:C:663:LEU:HD23 | 2.20 | 0.41 |
| 1:G:69:VAL:CG1 | 1:G:70:PRO:HD2 | 2.51 | 0.41 |
| 1:L:380:LYS:HE2 | 3:L:3185:HOH:O | 2.19 | 0.41 |
| 1:G:4:THR:HA | 1:G:9:VAL:HG11 | 2.02 | 0.41 |
| 1:I:4:THR:HA | 1:I:9:VAL:HG11 | 2.01 | 0.41 |
| 1:F:778:THR:HG22 | 1:F:779:PRO:O | 2.20 | 0.41 |
| 1:L:778:THR:HG22 | 1:L:779:PRO:O | 2.20 | 0.41 |
| 1:H:778:THR:HG22 | 1:H:779:PRO:O | 2.20 | 0.41 |
| 1:F:53:SER:C | 1:F:54:LEU:HD23 | 2.41 | 0.41 |
| 1:L:118:ASN:HA | 1:L:119:PRO:HD2 | 1.62 | 0.41 |
| 1:J:513:PRO:O | 1:J:514:ALA:HB3 | 2.20 | 0.41 |
| 1:D:513:PRO:O | 1:D:514:ALA:HB3 | 2.20 | 0.41 |
| 1:M:118:ASN:HA | 1:M:119:PRO:HD2 | 1.62 | 0.41 |
| 1:L:258:VAL:HA | 1:L:312:VAL:O | 2.21 | 0.41 |
| 1:E:258:VAL:HA | 1:E:312:VAL:O | 2.21 | 0.41 |
| 1:C:482:ARG:HH11 | 1:C:482:ARG:HD2 | 1.63 | 0.41 |
| 1:B:134:LEU:HA | 1:B:134:LEU:HD23 | 1.68 | 0.41 |
| 1:M:836:ILE:HG23 | 1:M:836:ILE:HD12 | 1.73 | 0.41 |
| 1:J:730:LEU:HA | 1:J:731:PRO:HD3 | 1.80 | 0.41 |
| 1:I:1017:GLN:HB3 | 3:I:4405:HOH:O | 2.19 | 0.41 |
| 1:M:513:PRO:O | 1:M:514:ALA:HB3 | 2.20 | 0.41 |
| 1:M:258:VAL:HA | 1:M:312:VAL:O | 2.21 | 0.41 |
| 1:F:702:GLN:HA | 1:F:703:PRO:HD2 | 1.88 | 0.41 |
| 1:H:702:GLN:HA | 1:H:703:PRO:HD2 | 1.88 | 0.41 |
| 1:A:418:HIS:O | 1:D:282:ARG:CD | 2.67 | 0.41 |
| 1:L:917:ARG:HD2 | 3:L:3452:HOH:O | 2.19 | 0.41 |
| 1:J:367:MET:HB3 | 1:J:372:MET:CE | 2.50 | 0.41 |
| 1:D:682:LEU:HD23 | 1:D:682:LEU:HA | 1.85 | 0.41 |
| 1:O:651:LEU:HA | 1:O:651:LEU:HD13 | 1.64 | 0.41 |
| 1:B:667:GLU:C | 1:B:668:VAL:HG23 | 2.40 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:668:VAL:HA | 1:N:669:PRO:HD3 | 1.83 | 0.41 |
| 1:E:271:THR:HG22 | 1:E:272:ALA:N | 2.35 | 0.41 |
| 1:K:667:GLU:C | 1:K:668:VAL:HG23 | 2.40 | 0.41 |
| 1:M:69:VAL:CG1 | 1:M:70:PRO:HD2 | 2.50 | 0.41 |
| 1:O:661:LYS:HA | 1:O:662:PRO:HD3 | 1.74 | 0.41 |
| 1:M:473:ARG:HD2 | 1:P:469:ASP:HB3 | 2.02 | 0.41 |
| 1:K:429:ASP:HA | 1:K:430:PRO:HD3 | 1.73 | 0.41 |
| 1:L:4:THR:HA | 1:L:9:VAL:HG11 | 2.01 | 0.41 |
| 1:H:429:ASP:HA | 1:H:430:PRO:HD3 | 1.73 | 0.41 |
| 1:M:778:THR:HB | 1:M:887:GLN:H | 1.84 | 0.41 |
| 1:C:234:ASP:O | 1:C:235:PHE:HB2 | 2.20 | 0.41 |
| 1:J:130:ASP:OD1 | 1:J:131:GLU:N | 2.53 | 0.41 |
| 1:L:53:SER:C | 1:L:54:LEU:HD23 | 2.41 | 0.41 |
| 1:C:513:PRO:O | 1:C:514:ALA:HB3 | 2.20 | 0.41 |
| 1:J:234:ASP:O | 1:J:235:PHE:HB2 | 2.20 | 0.41 |
| 1:E:130:ASP:OD1 | 1:E:131:GLU:N | 2.53 | 0.41 |
| 1:N:53:SER:C | 1:N:54:LEU:HD23 | 2.41 | 0.41 |
| 1:P:726:LEU:HA | 1:P:726:LEU:HD23 | 1.76 | 0.41 |
| 1:I:176:PHE:CD1 | 1:I:176:PHE:N | 2.88 | 0.41 |
| 1:O:726:LEU:HD23 | 1:O:726:LEU:HA | 1.76 | 0.41 |
| 1:E:986:ILE:HG21 | 1:E:986:ILE:HD12 | 1.74 | 0.41 |
| 1:I:53:SER:C | 1:I:54:LEU:HD23 | 2.41 | 0.41 |
| 1:M:807:VAL:HG13 | 1:M:808:GLU:N | 2.36 | 0.41 |
| 1:C:258:VAL:HA | 1:C:312:VAL:O | 2.21 | 0.41 |
| 1:E:53:SER:C | 1:E:54:LEU:HD23 | 2.41 | 0.41 |
| 1:O:234:ASP:O | 1:O:235:PHE:HB2 | 2.20 | 0.41 |
| 1:N:74:LEU:HA | 1:N:74:LEU:HD23 | 1.92 | 0.41 |
| 1:M:682:LEU:HA | 1:M:682:LEU:HD23 | 1.85 | 0.41 |
| 1:O:271:THR:HG22 | 1:O:272:ALA:N | 2.34 | 0.41 |
| 1:I:271:THR:HG22 | 1:I:272:ALA:N | 2.34 | 0.41 |
| 1:A:271:THR:HG22 | 1:A:272:ALA:N | 2.35 | 0.41 |
| 1:N:271:THR:HG22 | 1:N:272:ALA:N | 2.34 | 0.41 |
| 1:G:667:GLU:C | 1:G:668:VAL:HG23 | 2.40 | 0.41 |
| 1:B:654:TRP:CE2 | 1:B:666:GLY:HA3 | 2.56 | 0.41 |
| 1:N:654:TRP:CE2 | 1:N:666:GLY:HA3 | 2.56 | 0.41 |
| 1:P:654:TRP:CE2 | 1:P:666:GLY:HA3 | 2.56 | 0.41 |
| 1:E:654:TRP:CE2 | 1:E:666:GLY:HA3 | 2.56 | 0.41 |
| 1:D:662:PRO:O | 1:D:663:LEU:HD23 | 2.20 | 0.41 |
| 1:G:661:LYS:HA | 1:G:662:PRO:HD3 | 1.74 | 0.41 |
| 1:O:662:PRO:O | 1:O:663:LEU:HD23 | 2.20 | 0.41 |
| 1:K:380:LYS:HE2 | 3:K:4075:HOH:O | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:380:LYS:HE2 | 3:J:3182:HOH:O | 2.19 | 0.41 |
| 1:P:234:ASP:O | 1:P:235:PHE:HB2 | 2.20 | 0.41 |
| 1:O:258:VAL:HA | 1:O:312:VAL:O | 2.21 | 0.41 |
| 1:M:53:SER:C | 1:M:54:LEU:HD23 | 2.41 | 0.41 |
| 1:G:53:SER:C | 1:G:54:LEU:HD23 | 2.41 | 0.41 |
| 1:P:258:VAL:HA | 1:P:312:VAL:O | 2.21 | 0.41 |
| 1:D:258:VAL:HA | 1:D:312:VAL:O | 2.21 | 0.41 |
| 1:I:557:ARG:HD2 | 1:I:557:ARG:HH11 | 1.73 | 0.41 |
| 1:N:482:ARG:HH11 | 1:N:482:ARG:HD2 | 1.63 | 0.41 |
| 1:A:694:LEU:HA | 1:A:694:LEU:HD12 | 1.84 | 0.41 |
| 1:L:173:LEU:HA | 1:L:173:LEU:HD23 | 1.86 | 0.41 |
| 1:H:986:ILE:HG23 | 1:H:986:ILE:HD13 | 1.67 | 0.41 |
| 1:E:755:ARG:HD2 | 1:E:755:ARG:HH11 | 1.74 | 0.41 |
| 1:C:991:MET:HE2 | 1:C:1003:VAL:HG21 | 2.01 | 0.41 |
| 1:C:53:SER:C | 1:C:54:LEU:HD23 | 2.41 | 0.41 |
| 1:B:130:ASP:OD1 | 1:B:131:GLU:N | 2.53 | 0.41 |
| 1:G:807:VAL:HG13 | 1:G:808:GLU:N | 2.36 | 0.41 |
| 1:M:57:GLU:HG2 | 1:M:83:THR:HG22 | 1.95 | 0.41 |
| 1:G:271:THR:HG22 | 1:G:272:ALA:N | 2.35 | 0.41 |
| 1:E:599:ARG:HB2 | 1:E:600:GLN:H | 1.63 | 0.41 |
| 1:O:654:TRP:CE2 | 1:O:666:GLY:HA3 | 2.56 | 0.41 |
| 1:J:422:PRO:CG | 1:K:279:ILE:CD1 | 2.98 | 0.41 |
| 1:F:422:PRO:HG2 | 1:G:279:ILE:CD1 | 2.50 | 0.41 |
| 1:H:69:VAL:CG1 | 1:H:70:PRO:HD2 | 2.51 | 0.41 |
| 1:P:69:VAL:CG1 | 1:P:70:PRO:HD2 | 2.51 | 0.41 |
| 1:G:679:LEU:HA | 1:G:679:LEU:HD23 | 1.40 | 0.41 |
| 1:H:258:VAL:HA | 1:H:312:VAL:O | 2.21 | 0.41 |
| 1:B:807:VAL:CG1 | 1:B:808:GLU:N | 2.84 | 0.41 |
| 1:A:730:LEU:HA | 1:A:731:PRO:HD3 | 1.80 | 0.41 |
| 1:K:499:ILE:HG22 | 1:K:501:PRO:HD3 | 2.03 | 0.41 |
| 1:H:53:SER:C | 1:H:54:LEU:HD23 | 2.41 | 0.41 |
| 1:E:425:ARG:NH2 | 1:H:287:ASP:OD2 | 2.54 | 0.41 |
| 1:D:807:VAL:HG13 | 1:D:808:GLU:N | 2.36 | 0.41 |
| 1:D:176:PHE:CD1 | 1:D:176:PHE:N | 2.88 | 0.41 |
| 1:I:694:LEU:HD12 | 1:I:694:LEU:HA | 1.84 | 0.41 |
| 1:O:176:PHE:CD1 | 1:O:176:PHE:N | 2.88 | 0.41 |
| 1:G:287:ASP:N | 1:G:287:ASP:OD1 | 2.41 | 0.41 |
| 1:D:730:LEU:HA | 1:D:731:PRO:HD3 | 1.80 | 0.41 |
| 1:A:234:ASP:O | 1:A:235:PHE:HB2 | 2.20 | 0.41 |
| 1:D:991:MET:HE2 | 1:D:1003:VAL:HG21 | 2.02 | 0.41 |
| 1:K:1000:SER:HA | 1:K:1001:PRO:HD3 | 1.88 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:130:ASP:OD1 | 1:I:131:GLU:N | 2.53 | 0.41 |
| 1:L:952:ARG:CG | 1:L:952:ARG:HH11 | 2.28 | 0.41 |
| 1:J:917:ARG:HD2 | 3:J:3449:HOH:O | 2.19 | 0.41 |
| 1:C:917:ARG:HD2 | 3:C:4343:HOH:O | 2.19 | 0.41 |
| 1:N:917:ARG:HD2 | 3:N:3447:HOH:O | 2.19 | 0.41 |
| 1:P:917:ARG:HD2 | 3:P:3453:HOH:O | 2.19 | 0.41 |
| 1:P:271:THR:HG22 | 1:P:272:ALA:N | 2.35 | 0.41 |
| 1:A:422:PRO:CG | 1:D:279:ILE:HD13 | 2.50 | 0.41 |
| 1:B:662:PRO:O | 1:B:663:LEU:HD23 | 2.20 | 0.41 |
| 1:J:612:THR:HA | 1:J:613:PRO:HD3 | 1.59 | 0.41 |
| 1:I:380:LYS:HE2 | 3:I:4074:HOH:O | 2.19 | 0.41 |
| 1:D:380:LYS:HE2 | 3:D:3188:HOH:O | 2.19 | 0.41 |
| 1:C:36:TRP:CD2 | 1:C:42:ALA:HA | 2.56 | 0.41 |
| 1:D:807:VAL:CG1 | 1:D:808:GLU:N | 2.84 | 0.41 |
| 1:L:927:THR:HA | 1:L:928:PRO:HD3 | 1.82 | 0.41 |
| 1:O:513:PRO:O | 1:O:514:ALA:HB3 | 2.20 | 0.41 |
| 1:N:807:VAL:CG1 | 1:N:808:GLU:N | 2.84 | 0.41 |
| 1:D:130:ASP:OD1 | 1:D:131:GLU:N | 2.53 | 0.41 |
| 1:L:950:GLN:HB2 | 1:L:1023:LYS:HE2 | 2.03 | 0.41 |
| 1:P:991:MET:HE2 | 1:P:1003:VAL:HG21 | 2.01 | 0.41 |
| 1:L:234:ASP:O | 1:L:235:PHE:HB2 | 2.20 | 0.41 |
| 1:B:258:VAL:HA | 1:B:312:VAL:O | 2.21 | 0.41 |
| 1:B:147:ASN:HA | 1:B:148:SER:HA | 1.57 | 0.41 |
| 1:A:258:VAL:HA | 1:A:312:VAL:O | 2.21 | 0.41 |
| 1:P:714:ILE:HA | 1:P:714:ILE:HD13 | 1.78 | 0.41 |
| 1:D:63:PHE:CB | 1:D:64:PRO:HD2 | 2.34 | 0.41 |
| 1:P:682:LEU:HD23 | 1:P:682:LEU:HA | 1.85 | 0.41 |
| 1:G:272:ALA:HA | 1:G:273:PRO:HD3 | 1.78 | 0.41 |
| 1:B:272:ALA:HA | 1:B:273:PRO:HD3 | 1.78 | 0.41 |
| 1:G:654:TRP:CE2 | 1:G:666:GLY:HA3 | 2.56 | 0.41 |
| 1:I:654:TRP:CE2 | 1:I:666:GLY:HA3 | 2.56 | 0.41 |
| 1:H:654:TRP:CE2 | 1:H:666:GLY:HA3 | 2.56 | 0.41 |
| 1:J:668:VAL:HA | 1:J:669:PRO:HD3 | 1.83 | 0.41 |
| 1:I:599:ARG:HD2 | 1:I:600:GLN:OE1 | 2.20 | 0.41 |
| 1:J:69:VAL:CG1 | 1:J:70:PRO:HD2 | 2.51 | 0.41 |
| 1:E:422:PRO:HG2 | 1:H:279:ILE:CD1 | 2.50 | 0.41 |
| 1:E:662:PRO:O | 1:E:663:LEU:HD23 | 2.20 | 0.41 |
| 1:C:661:LYS:HA | 1:C:662:PRO:HD3 | 1.74 | 0.41 |
| 1:O:69:VAL:CG1 | 1:O:70:PRO:HD2 | 2.51 | 0.41 |
| 1:K:662:PRO:O | 1:K:663:LEU:HD23 | 2.20 | 0.41 |
| 1:F:69:VAL:CG1 | 1:F:70:PRO:HD2 | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:O:36:TRP:CD2 | 1:O:42:ALA:HA | 2.56 | 0.41 |
| 1:F:36:TRP:CD2 | 1:F:42:ALA:HA | 2.56 | 0.41 |
| 1:N:36:TRP:CD2 | 1:N:42:ALA:HA | 2.56 | 0.41 |
| 1:M:36:TRP:CD2 | 1:M:42:ALA:HA | 2.56 | 0.41 |
| 1:P:395:HIS:HA | 1:P:396:PRO:HD3 | 1.69 | 0.41 |
| 1:D:778:THR:HG22 | 1:D:779:PRO:O | 2.20 | 0.41 |
| 1:G:778:THR:HG22 | 1:G:779:PRO:O | 2.20 | 0.41 |
| 1:O:778:THR:HA | 1:O:779:PRO:HD3 | 1.95 | 0.41 |
| 1:I:778:THR:HG22 | 1:I:779:PRO:O | 2.20 | 0.41 |
| 1:E:778:THR:HG22 | 1:E:779:PRO:O | 2.20 | 0.41 |
| 1:J:1017:GLN:HB2 | 1:J:1017:GLN:HE21 | 1.65 | 0.41 |
| 1:M:807:VAL:CG1 | 1:M:808:GLU:N | 2.84 | 0.41 |
| 1:B:807:VAL:HG13 | 1:B:808:GLU:N | 2.36 | 0.41 |
| 1:K:258:VAL:HA | 1:K:312:VAL:O | 2.21 | 0.41 |
| 1:I:258:VAL:HA | 1:I:312:VAL:O | 2.21 | 0.41 |
| 1:A:1017:GLN:HB3 | 3:A:4412:HOH:O | 2.19 | 0.41 |
| 1:H:991:MET:HE2 | 1:H:1003:VAL:HG21 | 2.02 | 0.41 |
| 1:H:305:ILE:HG21 | 1:H:305:ILE:HD13 | 1.84 | 0.41 |
| 1:K:836:ILE:HD12 | 1:K:836:ILE:HG23 | 1.73 | 0.41 |
| 1:O:221:GLN:HG2 | 1:O:221:GLN:H | 1.63 | 0.41 |
| 1:I:986:ILE:HG23 | 1:I:986:ILE:HD13 | 1.67 | 0.41 |
| 1:P:176:PHE:N | 1:P:176:PHE:CD1 | 2.88 | 0.41 |
| 1:H:1017:GLN:HB3 | 3:H:4415:HOH:O | 2.19 | 0.41 |
| 1:I:499:ILE:HG22 | 1:I:501:PRO:HD3 | 2.03 | 0.41 |
| 1:J:499:ILE:HG22 | 1:J:501:PRO:HD3 | 2.03 | 0.41 |
| 1:A:53:SER:C | 1:A:54:LEU:HD23 | 2.41 | 0.41 |
| 1:B:53:SER:C | 1:B:54:LEU:HD23 | 2.41 | 0.41 |
| 1:A:748:CME:HB3 | 1:A:748:CME:HE2 | 1.15 | 0.41 |
| 1:F:807:VAL:CG1 | 1:F:808:GLU:N | 2.84 | 0.41 |
| 1:F:807:VAL:HG13 | 1:F:808:GLU:N | 2.36 | 0.41 |
| 1:A:367:MET:HB3 | 1:A:372:MET:CE | 2.50 | 0.41 |
| 1:C:654:TRP:CE2 | 1:C:666:GLY:HA3 | 2.56 | 0.41 |
| 1:J:599:ARG:HD2 | 1:J:600:GLN:OE1 | 2.20 | 0.41 |
| 1:M:654:TRP:CE2 | 1:M:666:GLY:HA3 | 2.56 | 0.41 |
| 1:K:654:TRP:CE2 | 1:K:666:GLY:HA3 | 2.56 | 0.41 |
| 1:D:69:VAL:CG1 | 1:D:70:PRO:HD2 | 2.51 | 0.41 |
| 1:P:662:PRO:O | 1:P:663:LEU:HD23 | 2.20 | 0.41 |
| 1:C:69:VAL:CG1 | 1:C:70:PRO:HD2 | 2.51 | 0.41 |
| 1:K:5:ASP:OD2 | 1:K:157:ARG:HG2 | 2.21 | 0.41 |
| 1:N:69:VAL:CG1 | 1:N:70:PRO:HD2 | 2.51 | 0.41 |
| 1:E:5:ASP:OD2 | 1:E:157:ARG:HG2 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:5:ASP:OD2 | 1:I:157:ARG:HG2 | 2.21 | 0.41 |
| 1:A:5:ASP:OD2 | 1:A:157:ARG:HG2 | 2.21 | 0.41 |
| 1:O:380:LYS:HE2 | 3:O:3179:HOH:O | 2.19 | 0.41 |
| 1:K:905:ASN:HB2 | 1:K:910:LEU:HB3 | 2.03 | 0.41 |
| 1:J:905:ASN:HB2 | 1:J:910:LEU:HB3 | 2.03 | 0.41 |
| 1:K:36:TRP:CD2 | 1:K:42:ALA:HA | 2.56 | 0.41 |
| 1:H:36:TRP:CD2 | 1:H:42:ALA:HA | 2.56 | 0.41 |
| 1:O:778:THR:HG22 | 1:O:779:PRO:O | 2.20 | 0.41 |
| 1:N:807:VAL:HG13 | 1:N:808:GLU:N | 2.36 | 0.41 |
| 1:H:807:VAL:CG1 | 1:H:808:GLU:N | 2.84 | 0.41 |
| 1:E:874:SER:HB3 | 1:F:724:GLU:OE1 | 2.21 | 0.41 |
| 1:I:928:PRO:HB2 | 1:I:973:ARG:HH11 | 1.86 | 0.41 |
| 1:P:807:VAL:CG1 | 1:P:808:GLU:N | 2.84 | 0.41 |
| 1:C:655:MET:O | 1:C:655:MET:HG3 | 2.20 | 0.41 |
| 1:G:221:GLN:HG2 | 1:G:221:GLN:H | 1.63 | 0.41 |
| 1:D:748:CME:HE2 | 1:D:748:CME:HB3 | 1.15 | 0.41 |
| 1:D:202:MET:HE3 | 1:D:202:MET:HB3 | 1.87 | 0.41 |
| 1:H:176:PHE:N | 1:H:176:PHE:CD1 | 2.88 | 0.41 |
| 1:E:807:VAL:CG1 | 1:E:808:GLU:N | 2.84 | 0.41 |
| 1:B:499:ILE:HG22 | 1:B:501:PRO:HD3 | 2.03 | 0.41 |
| 1:L:807:VAL:CG1 | 1:L:808:GLU:N | 2.84 | 0.41 |
| 1:G:153:TRP:CD1 | 1:G:158:TRP:HA | 2.56 | 0.41 |
| 1:J:901:GLY:HA3 | 1:J:902:PRO:HA | 1.89 | 0.41 |
| 1:B:928:PRO:HB2 | 1:B:973:ARG:HH11 | 1.86 | 0.41 |
| 1:B:153:TRP:CD1 | 1:B:158:TRP:HA | 2.56 | 0.41 |
| 1:A:282:ARG:HD2 | 1:D:418:HIS:O | 2.21 | 0.40 |
| 1:B:682:LEU:HA | 1:B:682:LEU:HD23 | 1.85 | 0.40 |
| 1:D:599:ARG:HB2 | 1:D:600:GLN:H | 1.64 | 0.40 |
| 1:L:654:TRP:CE2 | 1:L:666:GLY:HA3 | 2.56 | 0.40 |
| 1:J:422:PRO:CG | 1:K:279:ILE:HD11 | 2.50 | 0.40 |
| 1:D:654:TRP:CE2 | 1:D:666:GLY:HA3 | 2.56 | 0.40 |
| 1:I:253:TYR:O | 1:I:318:ALA:N | 2.55 | 0.40 |
| 1:F:662:PRO:O | 1:F:663:LEU:HD23 | 2.20 | 0.40 |
| 1:N:662:PRO:O | 1:N:663:LEU:HD23 | 2.20 | 0.40 |
| 1:G:662:PRO:O | 1:G:663:LEU:HD23 | 2.20 | 0.40 |
| 1:F:5:ASP:OD2 | 1:F:157:ARG:HG2 | 2.21 | 0.40 |
| 1:N:5:ASP:OD2 | 1:N:157:ARG:HG2 | 2.21 | 0.40 |
| 1:G:380:LYS:HE2 | 3:G:3179:HOH:O | 2.19 | 0.40 |
| 1:H:905:ASN:HB2 | 1:H:910:LEU:HB3 | 2.04 | 0.40 |
| 1:A:905:ASN:HB2 | 1:A:910:LEU:HB3 | 2.03 | 0.40 |
| 1:P:778:THR:HG22 | 1:P:779:PRO:O | 2.20 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:M:1017:GLN:HE21 | 1:M:1017:GLN:HB2 | 1.65 | 0.40 |
| 1:E:807:VAL:HG13 | 1:E:808:GLU:N | 2.36 | 0.40 |
| 1:C:153:TRP:CD1 | 1:C:158:TRP:HA | 2.56 | 0.40 |
| 1:K:685:LEU:HA | 1:K:686:PRO:HD3 | 1.83 | 0.40 |
| 1:O:807:VAL:CG1 | 1:O:808:GLU:N | 2.84 | 0.40 |
| 1:L:499:ILE:HG22 | 1:L:501:PRO:HD3 | 2.03 | 0.40 |
| 1:J:258:VAL:HA | 1:J:312:VAL:O | 2.21 | 0.40 |
| 1:E:520:ILE:HG21 | 1:E:520:ILE:HD13 | 1.79 | 0.40 |
| 1:I:134:LEU:HA | 1:I:134:LEU:HD23 | 1.68 | 0.40 |
| 1:M:173:LEU:HD23 | 1:M:173:LEU:HA | 1.85 | 0.40 |
| 1:P:211:ASP:N | 1:P:211:ASP:OD1 | 2.50 | 0.40 |
| 1:K:772:ASP:OD1 | 1:K:772:ASP:N | 2.48 | 0.40 |
| 1:K:901:GLY:HA3 | 1:K:902:PRO:HA | 1.89 | 0.40 |
| 1:C:950:GLN:HB2 | 1:C:1023:LYS:HE2 | 2.03 | 0.40 |
| 1:K:53:SER:C | 1:K:54:LEU:HD23 | 2.41 | 0.40 |
| 1:H:153:TRP:CD1 | 1:H:158:TRP:HA | 2.56 | 0.40 |
| 1:A:807:VAL:CG1 | 1:A:808:GLU:N | 2.84 | 0.40 |
| 1:A:807:VAL:HG13 | 1:A:808:GLU:N | 2.36 | 0.40 |
| 1:L:256:VAL:HG12 | 1:L:257:THR:N | 2.37 | 0.40 |
| 1:J:316:HIS:HA | 1:J:323:ILE:HD13 | 2.01 | 0.40 |
| 1:M:278:ILE:CD1 | 1:M:278:ILE:N | 2.80 | 0.40 |
| 1:M:74:LEU:HA | 1:M:74:LEU:HD23 | 1.92 | 0.40 |
| 1:B:63:PHE:CD1 | 1:B:63:PHE:N | 2.90 | 0.40 |
| 1:J:63:PHE:CD1 | 1:J:63:PHE:N | 2.90 | 0.40 |
| 1:O:367:MET:HB3 | 1:O:372:MET:CE | 2.50 | 0.40 |
| 1:B:253:TYR:O | 1:B:318:ALA:N | 2.54 | 0.40 |
| 1:F:253:TYR:O | 1:F:318:ALA:N | 2.54 | 0.40 |
| 1:E:661:LYS:HA | 1:E:662:PRO:HD3 | 1.74 | 0.40 |
| 1:G:658:LEU:N | 1:G:661:LYS:O | 2.40 | 0.40 |
| 1:H:5:ASP:OD2 | 1:H:157:ARG:HG2 | 2.21 | 0.40 |
| 1:E:521:LYS:HB2 | 1:F:559:TYR:OH | 2.21 | 0.40 |
| 1:O:3:ILE:HG13 | 1:O:4:THR:N | 2.25 | 0.40 |
| 1:E:429:ASP:HA | 1:E:430:PRO:HD3 | 1.74 | 0.40 |
| 1:L:36:TRP:CD2 | 1:L:42:ALA:HA | 2.56 | 0.40 |
| 1:G:807:VAL:CG1 | 1:G:808:GLU:N | 2.84 | 0.40 |
| 1:L:928:PRO:HB2 | 1:L:973:ARG:HH11 | 1.86 | 0.40 |
| 1:P:499:ILE:HG22 | 1:P:501:PRO:HD3 | 2.03 | 0.40 |
| 1:L:685:LEU:HA | 1:L:686:PRO:HD3 | 1.83 | 0.40 |
| 1:E:513:PRO:O | 1:E:514:ALA:HB3 | 2.20 | 0.40 |
| 1:O:670:LEU:HD23 | 1:O:670:LEU:HA | 1.75 | 0.40 |
| 1:J:772:ASP:OD1 | 1:J:772:ASP:N | 2.48 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:726:LEU:HA | 1:N:726:LEU:HD23 | 1.76 | 0.40 |
| 1:E:134:LEU:HA | 1:E:134:LEU:HD23 | 1.68 | 0.40 |
| 1:K:807:VAL:CG1 | 1:K:808:GLU:N | 2.84 | 0.40 |
| 1:H:878:HIS:HA | 1:H:879:PRO:HD3 | 1.83 | 0.40 |
| 1:N:234:ASP:O | 1:N:235:PHE:HB2 | 2.20 | 0.40 |
| 1:D:479:ASP:HA | 1:D:480:PRO:HD2 | 1.77 | 0.40 |
| 1:O:928:PRO:HB2 | 1:O:973:ARG:HH11 | 1.86 | 0.40 |
| 1:N:256:VAL:HG12 | 1:N:257:THR:N | 2.37 | 0.40 |
| 1:B:702:GLN:HA | 1:B:703:PRO:HD2 | 1.88 | 0.40 |
| 1:B:78:LEU:CB | 1:B:79:PRO:CD | 3.00 | 0.40 |
| 1:F:78:LEU:CB | 1:F:79:PRO:CD | 3.00 | 0.40 |
| 1:I:745:MET:CA | 1:I:745:MET:CE | 3.00 | 0.40 |
| 1:L:667:GLU:C | 1:L:668:VAL:HG23 | 2.40 | 0.40 |
| 1:J:654:TRP:CE2 | 1:J:666:GLY:HA3 | 2.56 | 0.40 |
| 1:K:69:VAL:CG1 | 1:K:70:PRO:HD2 | 2.50 | 0.40 |
| 1:C:5:ASP:OD2 | 1:C:157:ARG:HG2 | 2.22 | 0.40 |
| 1:O:5:ASP:OD2 | 1:O:157:ARG:HG2 | 2.21 | 0.40 |
| 1:G:5:ASP:OD2 | 1:G:157:ARG:HG2 | 2.21 | 0.40 |
| 1:F:612:THR:HA | 1:F:613:PRO:HD3 | 1.59 | 0.40 |
| 1:P:905:ASN:HB2 | 1:P:910:LEU:HB3 | 2.03 | 0.40 |
| 1:E:36:TRP:CD2 | 1:E:42:ALA:HA | 2.56 | 0.40 |
| 1:A:778:THR:HG22 | 1:A:779:PRO:O | 2.20 | 0.40 |
| 1:I:655:MET:HG3 | 1:I:655:MET:O | 2.20 | 0.40 |
| 1:I:513:PRO:O | 1:I:514:ALA:HB3 | 2.20 | 0.40 |
| 1:I:807:VAL:CG1 | 1:I:808:GLU:N | 2.84 | 0.40 |
| 1:E:153:TRP:CD1 | 1:E:158:TRP:HA | 2.56 | 0.40 |
| 1:K:748:CME:HE2 | 1:K:748:CME:HB3 | 1.14 | 0.40 |
| 1:C:928:PRO:HB2 | 1:C:973:ARG:HH11 | 1.86 | 0.40 |
| 1:M:928:PRO:HB2 | 1:M:973:ARG:HH11 | 1.86 | 0.40 |
| 1:M:802:ASP:HA | 1:M:803:PRO:HD3 | 1.83 | 0.40 |
| 1:N:153:TRP:CD1 | 1:N:158:TRP:HA | 2.56 | 0.40 |
| 1:K:256:VAL:HG12 | 1:K:257:THR:N | 2.37 | 0.40 |
| 1:K:714:ILE:HD13 | 1:K:714:ILE:HA | 1.78 | 0.40 |
| 1:D:78:LEU:CB | 1:D:79:PRO:CD | 3.00 | 0.40 |
| 1:N:78:LEU:CB | 1:N:79:PRO:CD | 3.00 | 0.40 |
| 1:J:920:LEU:CB | 1:J:921:PRO:CD | 2.99 | 0.40 |
| 1:I:189:LEU:CD2 | 1:I:189:LEU:N | 2.79 | 0.40 |
| 1:A:31:PRO:CB | 1:A:32:PRO:CD | 3.00 | 0.40 |
| 1:F:654:TRP:CE2 | 1:F:666:GLY:HA3 | 2.56 | 0.40 |
| 1:N:279:ILE:HD13 | 1:O:422:PRO:CG | 2.52 | 0.40 |
| 1:C:658:LEU:N | 1:C:661:LYS:O | 2.40 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:5:ASP:OD2 | 1:L:157:ARG:HG2 | 2.21 | 0.40 |
| 1:P:36:TRP:CD2 | 1:P:42:ALA:HA | 2.56 | 0.40 |
| 1:I:36:TRP:CD2 | 1:I:42:ALA:HA | 2.56 | 0.40 |
| 1:J:36:TRP:CD2 | 1:J:42:ALA:HA | 2.56 | 0.40 |
| 1:M:422:PRO:HG2 | 1:P:279:ILE:HD11 | 2.03 | 0.40 |
| 1:E:986:ILE:HG23 | 1:E:986:ILE:HD13 | 1.67 | 0.40 |
| 1:F:425:ARG:NH2 | 1:G:287:ASP:OD2 | 2.55 | 0.40 |
| 1:K:947:GLY:HA3 | 1:K:948:PRO:HD2 | 1.82 | 0.40 |
| 1:P:928:PRO:HB2 | 1:P:973:ARG:HH11 | 1.86 | 0.40 |
| 1:D:655:MET:O | 1:D:655:MET:HG3 | 2.20 | 0.40 |
| 1:K:211:ASP:N | 1:K:211:ASP:OD1 | 2.50 | 0.40 |
| 1:M:305:ILE:HG21 | 1:M:305:ILE:HD13 | 1.85 | 0.40 |
| 1:F:513:PRO:O | 1:F:514:ALA:HB3 | 2.20 | 0.40 |
| 1:L:153:TRP:CD1 | 1:L:158:TRP:HA | 2.56 | 0.40 |
| 1:F:153:TRP:CD1 | 1:F:158:TRP:HA | 2.56 | 0.40 |
| 1:M:147:ASN:HA | 1:M:148:SER:HA | 1.57 | 0.40 |
| 1:F:499:ILE:HG22 | 1:F:501:PRO:HD3 | 2.03 | 0.40 |
| 1:N:499:ILE:HG22 | 1:N:501:PRO:HD3 | 2.03 | 0.40 |
| 1:A:153:TRP:CD1 | 1:A:158:TRP:HA | 2.56 | 0.40 |
| 1:H:499:ILE:HG22 | 1:H:501:PRO:HD3 | 2.03 | 0.40 |
| 1:C:499:ILE:HG22 | 1:C:501:PRO:HD3 | 2.03 | 0.40 |
| 1:G:316:HIS:HA | 1:G:323:ILE:HD13 | 2.01 | 0.40 |
| 1:D:74:LEU:HD23 | 1:D:74:LEU:HA | 1.92 | 0.40 |
| 1:I:63:PHE:CD1 | 1:I:63:PHE:N | 2.90 | 0.40 |
| 1:D:745:MET:CE | 1:D:745:MET:CA | 3.00 | 0.40 |
| 1:H:63:PHE:CD1 | 1:H:63:PHE:N | 2.90 | 0.40 |
| 1:O:254:LEU:HA | 1:O:254:LEU:HD23 | 1.71 | 0.40 |
| 1:K:745:MET:CE | 1:K:745:MET:CA | 3.00 | 0.40 |
| 1:C:253:TYR:O | 1:C:318:ALA:N | 2.55 | 0.40 |
| 1:O:253:TYR:O | 1:O:318:ALA:N | 2.55 | 0.40 |
| 1:L:662:PRO:O | 1:L:663:LEU:HD23 | 2.20 | 0.40 |
| 1:K:253:TYR:O | 1:K:318:ALA:N | 2.55 | 0.40 |
| 1:J:5:ASP:OD2 | 1:J:157:ARG:HG2 | 2.22 | 0.40 |
| 1:P:5:ASP:OD2 | 1:P:157:ARG:HG2 | 2.21 | 0.40 |
| 1:I:521:LYS:HB2 | 1:J:559:TYR:OH | 2.22 | 0.40 |
| 1:B:36:TRP:CD2 | 1:B:42:ALA:HA | 2.56 | 0.40 |
| 1:E:395:HIS:HA | 1:E:396:PRO:HD3 | 1.69 | 0.40 |
| 1:P:807:VAL:HG13 | 1:P:808:GLU:N | 2.36 | 0.40 |
| 1:P:141:ILE:HG12 | 1:P:142:ILE:N | 2.37 | 0.40 |
| 1:L:111:PRO:HA | 1:L:112:PRO:HA | 1.66 | 0.40 |
| 1:C:807:VAL:HG13 | 1:C:808:GLU:N | 2.36 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:807:VAL:CG1 | 1:J:808:GLU:N | 2.84 | 0.40 |
| 1:K:694:LEU:HA | 1:K:694:LEU:HD12 | 1.84 | 0.40 |
| 1:G:141:ILE:HG12 | 1:G:142:ILE:N | 2.37 | 0.40 |
| 1:G:928:PRO:HB2 | 1:G:973:ARG:HH11 | 1.86 | 0.40 |
| 1:H:141:ILE:HG12 | 1:H:142:ILE:N | 2.37 | 0.40 |
| 1:P:950:GLN:HB2 | 1:P:1023:LYS:HE2 | 2.03 | 0.40 |
| 1:J:128:ASN:ND2 | 1:J:180:GLY:HA2 | 2.37 | 0.40 |
| 1:J:685:LEU:HA | 1:J:686:PRO:HD3 | 1.83 | 0.40 |

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:580:GLU:O | 1:B:578:TYR:CB[2_555] | 1.77 | 0.43 |
| 1:A:580:GLU:O | 1:B:578:TYR:CG[2_555] | 1.85 | 0.35 |
| 1:A:580:GLU:O | 1:B:578:TYR:CD1[2_555] | 2.10 | 0.10 |
| 1:B:739:HIS:NE2 | 1:P:738:PRO:O[1_354] | 2.10 | 0.10 |
| 1:C:739:HIS:ND1 | 1:I:734:SER:O[1_655] | 2.15 | 0.05 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|-----------|---------|----------|-------------|----|
| 1 | A | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | B | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | C | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | D | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | E | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | F | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | G | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|----------|----------|-------------|----|
| 1 | H | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | I | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | J | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | K | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | L | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | M | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | N | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | O | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| 1 | P | 1021/1023 (100%) | 976 (96%) | 42 (4%) | 3 (0%) | 46 | 68 |
| All | All | 16336/16368 (100%) | 15616 (96%) | 672 (4%) | 48 (0%) | 46 | 68 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 174 | SER |
| 1 | B | 174 | SER |
| 1 | C | 174 | SER |
| 1 | D | 174 | SER |
| 1 | E | 174 | SER |
| 1 | F | 174 | SER |
| 1 | G | 174 | SER |
| 1 | H | 174 | SER |
| 1 | I | 174 | SER |
| 1 | J | 174 | SER |
| 1 | K | 174 | SER |
| 1 | L | 174 | SER |
| 1 | M | 174 | SER |
| 1 | N | 174 | SER |
| 1 | O | 174 | SER |
| 1 | P | 174 | SER |
| 1 | A | 164 | ASP |
| 1 | B | 164 | ASP |
| 1 | C | 164 | ASP |
| 1 | D | 164 | ASP |
| 1 | E | 164 | ASP |
| 1 | F | 164 | ASP |
| 1 | G | 164 | ASP |
| 1 | H | 164 | ASP |
| 1 | I | 164 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 164 | ASP |
| 1 | K | 164 | ASP |
| 1 | L | 164 | ASP |
| 1 | M | 164 | ASP |
| 1 | N | 164 | ASP |
| 1 | O | 164 | ASP |
| 1 | P | 164 | ASP |
| 1 | A | 119 | PRO |
| 1 | B | 119 | PRO |
| 1 | C | 119 | PRO |
| 1 | D | 119 | PRO |
| 1 | E | 119 | PRO |
| 1 | F | 119 | PRO |
| 1 | G | 119 | PRO |
| 1 | H | 119 | PRO |
| 1 | I | 119 | PRO |
| 1 | J | 119 | PRO |
| 1 | K | 119 | PRO |
| 1 | L | 119 | PRO |
| 1 | M | 119 | PRO |
| 1 | N | 119 | PRO |
| 1 | O | 119 | PRO |
| 1 | P | 119 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | B | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | C | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | D | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | E | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | F | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|------------|-------------|----|
| 1 | G | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | H | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | I | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | J | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | K | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | L | 875/872 (100%) | 777 (89%) | 98 (11%) | 7 | 14 |
| 1 | M | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | N | 875/872 (100%) | 777 (89%) | 98 (11%) | 7 | 14 |
| 1 | O | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| 1 | P | 875/872 (100%) | 776 (89%) | 99 (11%) | 7 | 13 |
| All | All | 14000/13952 (100%) | 12418 (89%) | 1582 (11%) | 7 | 13 |

All (1582) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ILE |
| 1 | A | 14 | ARG |
| 1 | A | 37 | ARG |
| 1 | A | 39 | SER |
| 1 | A | 46 | ARG |
| 1 | A | 48 | SER |
| 1 | A | 49 | GLN |
| 1 | A | 50 | GLN |
| 1 | A | 52 | ARG |
| 1 | A | 59 | ARG |
| 1 | A | 71 | GLU |
| 1 | A | 72 | SER |
| 1 | A | 80 | GLU |
| 1 | A | 84 | VAL |
| 1 | A | 90 | TRP |
| 1 | A | 102 | ASN |
| 1 | A | 116 | THR |
| 1 | A | 125 | LEU |
| 1 | A | 128 | ASN |
| 1 | A | 132 | SER |
| 1 | A | 136 | GLU |
| 1 | A | 165 | SER |
| 1 | A | 166 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 171 | PHE |
| 1 | A | 189 | LEU |
| 1 | A | 202 | MET |
| 1 | A | 210 | ARG |
| 1 | A | 211 | ASP |
| 1 | A | 217 | LYS |
| 1 | A | 219 | THR |
| 1 | A | 246 | MET |
| 1 | A | 247 | CYS |
| 1 | A | 249 | GLU |
| 1 | A | 250 | LEU |
| 1 | A | 259 | SER |
| 1 | A | 262 | GLN |
| 1 | A | 264 | GLU |
| 1 | A | 279 | ILE |
| 1 | A | 299 | LYS |
| 1 | A | 310 | ARG |
| 1 | A | 314 | GLU |
| 1 | A | 319 | ASP |
| 1 | A | 333 | ARG |
| 1 | A | 344 | LEU |
| 1 | A | 347 | LYS |
| 1 | A | 370 | GLN |
| 1 | A | 377 | LEU |
| 1 | A | 394 | ASN |
| 1 | A | 425 | ARG |
| 1 | A | 437 | SER |
| 1 | A | 448 | ARG |
| 1 | A | 473 | ARG |
| 1 | A | 519 | SER |
| 1 | A | 521 | LYS |
| 1 | A | 532 | PRO |
| 1 | A | 546 | LEU |
| 1 | A | 554 | GLN |
| 1 | A | 571 | VAL |
| 1 | A | 580 | GLU |
| 1 | A | 599 | ARG |
| 1 | A | 600 | GLN |
| 1 | A | 630 | ARG |
| 1 | A | 632 | SER |
| 1 | A | 645 | ARG |
| 1 | A | 651 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 655 | MET |
| 1 | A | 665 | SER |
| 1 | A | 672 | VAL |
| 1 | A | 684 | GLU |
| 1 | A | 687 | GLN |
| 1 | A | 690 | SER |
| 1 | A | 710 | GLU |
| 1 | A | 719 | GLN |
| 1 | A | 730 | LEU |
| 1 | A | 734 | SER |
| 1 | A | 741 | THR |
| 1 | A | 743 | SER |
| 1 | A | 751 | LEU |
| 1 | A | 753 | ASN |
| 1 | A | 755 | ARG |
| 1 | A | 768 | MET |
| 1 | A | 778 | THR |
| 1 | A | 781 | ARG |
| 1 | A | 797 | GLU |
| 1 | A | 799 | THR |
| 1 | A | 800 | ARG |
| 1 | A | 824 | GLN |
| 1 | A | 829 | THR |
| 1 | A | 832 | ASP |
| 1 | A | 881 | ARG |
| 1 | A | 893 | GLU |
| 1 | A | 903[A] | GLN |
| 1 | A | 903[B] | GLN |
| 1 | A | 917 | ARG |
| 1 | A | 938 | ARG |
| 1 | A | 952 | ARG |
| 1 | A | 956 | GLN |
| 1 | A | 1006 | GLU |
| 1 | A | 1017 | GLN |
| 1 | B | 3 | ILE |
| 1 | B | 14 | ARG |
| 1 | B | 37 | ARG |
| 1 | B | 39 | SER |
| 1 | B | 46 | ARG |
| 1 | B | 48 | SER |
| 1 | B | 49 | GLN |
| 1 | B | 50 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 52 | ARG |
| 1 | B | 59 | ARG |
| 1 | B | 71 | GLU |
| 1 | B | 72 | SER |
| 1 | B | 80 | GLU |
| 1 | B | 84 | VAL |
| 1 | B | 90 | TRP |
| 1 | B | 102 | ASN |
| 1 | B | 116 | THR |
| 1 | B | 125 | LEU |
| 1 | B | 128 | ASN |
| 1 | B | 132 | SER |
| 1 | B | 136 | GLU |
| 1 | B | 165 | SER |
| 1 | B | 166 | ARG |
| 1 | B | 171 | PHE |
| 1 | B | 189 | LEU |
| 1 | B | 202 | MET |
| 1 | B | 210 | ARG |
| 1 | B | 211 | ASP |
| 1 | B | 217 | LYS |
| 1 | B | 219 | THR |
| 1 | B | 246 | MET |
| 1 | B | 247 | CYS |
| 1 | B | 249 | GLU |
| 1 | B | 250 | LEU |
| 1 | B | 259 | SER |
| 1 | B | 262 | GLN |
| 1 | B | 264 | GLU |
| 1 | B | 279 | ILE |
| 1 | B | 299 | LYS |
| 1 | B | 310 | ARG |
| 1 | B | 314 | GLU |
| 1 | B | 319 | ASP |
| 1 | B | 333 | ARG |
| 1 | B | 344 | LEU |
| 1 | B | 347 | LYS |
| 1 | B | 370 | GLN |
| 1 | B | 377 | LEU |
| 1 | B | 394 | ASN |
| 1 | B | 425 | ARG |
| 1 | B | 437 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | B | 448 | ARG |
| 1 | B | 473 | ARG |
| 1 | B | 519 | SER |
| 1 | B | 521 | LYS |
| 1 | B | 532 | PRO |
| 1 | B | 546 | LEU |
| 1 | B | 554 | GLN |
| 1 | B | 571 | VAL |
| 1 | B | 580 | GLU |
| 1 | B | 599 | ARG |
| 1 | B | 600 | GLN |
| 1 | B | 630 | ARG |
| 1 | B | 632 | SER |
| 1 | B | 645 | ARG |
| 1 | B | 651 | LEU |
| 1 | B | 655 | MET |
| 1 | B | 665 | SER |
| 1 | B | 672 | VAL |
| 1 | B | 684 | GLU |
| 1 | B | 687 | GLN |
| 1 | B | 690 | SER |
| 1 | B | 710 | GLU |
| 1 | B | 719 | GLN |
| 1 | B | 730 | LEU |
| 1 | B | 734 | SER |
| 1 | B | 741 | THR |
| 1 | B | 743 | SER |
| 1 | B | 751 | LEU |
| 1 | B | 753 | ASN |
| 1 | B | 755 | ARG |
| 1 | B | 768 | MET |
| 1 | B | 778 | THR |
| 1 | B | 781 | ARG |
| 1 | B | 797 | GLU |
| 1 | B | 799 | THR |
| 1 | B | 800 | ARG |
| 1 | B | 824 | GLN |
| 1 | B | 829 | THR |
| 1 | B | 832 | ASP |
| 1 | B | 881 | ARG |
| 1 | B | 893 | GLU |
| 1 | B | 903[A] | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | B | 903[B] | GLN |
| 1 | B | 917 | ARG |
| 1 | B | 938 | ARG |
| 1 | B | 952 | ARG |
| 1 | B | 956 | GLN |
| 1 | B | 1006 | GLU |
| 1 | B | 1017 | GLN |
| 1 | C | 3 | ILE |
| 1 | C | 14 | ARG |
| 1 | C | 37 | ARG |
| 1 | C | 39 | SER |
| 1 | C | 46 | ARG |
| 1 | C | 48 | SER |
| 1 | C | 49 | GLN |
| 1 | C | 50 | GLN |
| 1 | C | 52 | ARG |
| 1 | C | 59 | ARG |
| 1 | C | 71 | GLU |
| 1 | C | 72 | SER |
| 1 | C | 80 | GLU |
| 1 | C | 84 | VAL |
| 1 | C | 90 | TRP |
| 1 | C | 102 | ASN |
| 1 | C | 116 | THR |
| 1 | C | 125 | LEU |
| 1 | C | 128 | ASN |
| 1 | C | 132 | SER |
| 1 | C | 136 | GLU |
| 1 | C | 165 | SER |
| 1 | C | 166 | ARG |
| 1 | C | 171 | PHE |
| 1 | C | 189 | LEU |
| 1 | C | 202 | MET |
| 1 | C | 210 | ARG |
| 1 | C | 211 | ASP |
| 1 | C | 217 | LYS |
| 1 | C | 219 | THR |
| 1 | C | 246 | MET |
| 1 | C | 247 | CYS |
| 1 | C | 249 | GLU |
| 1 | C | 250 | LEU |
| 1 | C | 259 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 262 | GLN |
| 1 | C | 264 | GLU |
| 1 | C | 279 | ILE |
| 1 | C | 299 | LYS |
| 1 | C | 310 | ARG |
| 1 | C | 314 | GLU |
| 1 | C | 319 | ASP |
| 1 | C | 333 | ARG |
| 1 | C | 344 | LEU |
| 1 | C | 347 | LYS |
| 1 | C | 370 | GLN |
| 1 | C | 377 | LEU |
| 1 | C | 394 | ASN |
| 1 | C | 425 | ARG |
| 1 | C | 437 | SER |
| 1 | C | 448 | ARG |
| 1 | C | 473 | ARG |
| 1 | C | 519 | SER |
| 1 | C | 521 | LYS |
| 1 | C | 532 | PRO |
| 1 | C | 546 | LEU |
| 1 | C | 554 | GLN |
| 1 | C | 571 | VAL |
| 1 | C | 580 | GLU |
| 1 | C | 599 | ARG |
| 1 | C | 600 | GLN |
| 1 | C | 630 | ARG |
| 1 | C | 632 | SER |
| 1 | C | 645 | ARG |
| 1 | C | 651 | LEU |
| 1 | C | 655 | MET |
| 1 | C | 665 | SER |
| 1 | C | 672 | VAL |
| 1 | C | 684 | GLU |
| 1 | C | 687 | GLN |
| 1 | C | 690 | SER |
| 1 | C | 710 | GLU |
| 1 | C | 719 | GLN |
| 1 | C | 730 | LEU |
| 1 | C | 734 | SER |
| 1 | C | 741 | THR |
| 1 | C | 743 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | C | 751 | LEU |
| 1 | C | 753 | ASN |
| 1 | C | 755 | ARG |
| 1 | C | 768 | MET |
| 1 | C | 778 | THR |
| 1 | C | 781 | ARG |
| 1 | C | 797 | GLU |
| 1 | C | 799 | THR |
| 1 | C | 800 | ARG |
| 1 | C | 824 | GLN |
| 1 | C | 829 | THR |
| 1 | C | 832 | ASP |
| 1 | C | 881 | ARG |
| 1 | C | 893 | GLU |
| 1 | C | 903[A] | GLN |
| 1 | C | 903[B] | GLN |
| 1 | C | 917 | ARG |
| 1 | C | 938 | ARG |
| 1 | C | 952 | ARG |
| 1 | C | 956 | GLN |
| 1 | C | 1006 | GLU |
| 1 | C | 1017 | GLN |
| 1 | D | 3 | ILE |
| 1 | D | 14 | ARG |
| 1 | D | 37 | ARG |
| 1 | D | 39 | SER |
| 1 | D | 46 | ARG |
| 1 | D | 48 | SER |
| 1 | D | 49 | GLN |
| 1 | D | 50 | GLN |
| 1 | D | 52 | ARG |
| 1 | D | 59 | ARG |
| 1 | D | 71 | GLU |
| 1 | D | 72 | SER |
| 1 | D | 80 | GLU |
| 1 | D | 84 | VAL |
| 1 | D | 90 | TRP |
| 1 | D | 102 | ASN |
| 1 | D | 116 | THR |
| 1 | D | 125 | LEU |
| 1 | D | 128 | ASN |
| 1 | D | 132 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 136 | GLU |
| 1 | D | 165 | SER |
| 1 | D | 166 | ARG |
| 1 | D | 171 | PHE |
| 1 | D | 189 | LEU |
| 1 | D | 202 | MET |
| 1 | D | 210 | ARG |
| 1 | D | 211 | ASP |
| 1 | D | 217 | LYS |
| 1 | D | 219 | THR |
| 1 | D | 246 | MET |
| 1 | D | 247 | CYS |
| 1 | D | 249 | GLU |
| 1 | D | 250 | LEU |
| 1 | D | 259 | SER |
| 1 | D | 262 | GLN |
| 1 | D | 264 | GLU |
| 1 | D | 279 | ILE |
| 1 | D | 299 | LYS |
| 1 | D | 310 | ARG |
| 1 | D | 314 | GLU |
| 1 | D | 319 | ASP |
| 1 | D | 333 | ARG |
| 1 | D | 344 | LEU |
| 1 | D | 347 | LYS |
| 1 | D | 370 | GLN |
| 1 | D | 377 | LEU |
| 1 | D | 394 | ASN |
| 1 | D | 425 | ARG |
| 1 | D | 437 | SER |
| 1 | D | 448 | ARG |
| 1 | D | 473 | ARG |
| 1 | D | 519 | SER |
| 1 | D | 521 | LYS |
| 1 | D | 532 | PRO |
| 1 | D | 546 | LEU |
| 1 | D | 554 | GLN |
| 1 | D | 571 | VAL |
| 1 | D | 580 | GLU |
| 1 | D | 599 | ARG |
| 1 | D | 600 | GLN |
| 1 | D | 630 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | D | 632 | SER |
| 1 | D | 645 | ARG |
| 1 | D | 651 | LEU |
| 1 | D | 655 | MET |
| 1 | D | 665 | SER |
| 1 | D | 672 | VAL |
| 1 | D | 684 | GLU |
| 1 | D | 687 | GLN |
| 1 | D | 690 | SER |
| 1 | D | 710 | GLU |
| 1 | D | 719 | GLN |
| 1 | D | 730 | LEU |
| 1 | D | 734 | SER |
| 1 | D | 741 | THR |
| 1 | D | 743 | SER |
| 1 | D | 751 | LEU |
| 1 | D | 753 | ASN |
| 1 | D | 755 | ARG |
| 1 | D | 768 | MET |
| 1 | D | 778 | THR |
| 1 | D | 781 | ARG |
| 1 | D | 797 | GLU |
| 1 | D | 799 | THR |
| 1 | D | 800 | ARG |
| 1 | D | 824 | GLN |
| 1 | D | 829 | THR |
| 1 | D | 832 | ASP |
| 1 | D | 881 | ARG |
| 1 | D | 893 | GLU |
| 1 | D | 903[A] | GLN |
| 1 | D | 903[B] | GLN |
| 1 | D | 917 | ARG |
| 1 | D | 938 | ARG |
| 1 | D | 952 | ARG |
| 1 | D | 956 | GLN |
| 1 | D | 1006 | GLU |
| 1 | D | 1017 | GLN |
| 1 | E | 3 | ILE |
| 1 | E | 14 | ARG |
| 1 | E | 37 | ARG |
| 1 | E | 39 | SER |
| 1 | E | 46 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 48 | SER |
| 1 | E | 49 | GLN |
| 1 | E | 50 | GLN |
| 1 | E | 52 | ARG |
| 1 | E | 59 | ARG |
| 1 | E | 71 | GLU |
| 1 | E | 72 | SER |
| 1 | E | 80 | GLU |
| 1 | E | 84 | VAL |
| 1 | E | 90 | TRP |
| 1 | E | 102 | ASN |
| 1 | E | 116 | THR |
| 1 | E | 125 | LEU |
| 1 | E | 128 | ASN |
| 1 | E | 132 | SER |
| 1 | E | 136 | GLU |
| 1 | E | 165 | SER |
| 1 | E | 166 | ARG |
| 1 | E | 171 | PHE |
| 1 | E | 189 | LEU |
| 1 | E | 202 | MET |
| 1 | E | 210 | ARG |
| 1 | E | 211 | ASP |
| 1 | E | 217 | LYS |
| 1 | E | 219 | THR |
| 1 | E | 246 | MET |
| 1 | E | 247 | CYS |
| 1 | E | 249 | GLU |
| 1 | E | 250 | LEU |
| 1 | E | 259 | SER |
| 1 | E | 262 | GLN |
| 1 | E | 264 | GLU |
| 1 | E | 279 | ILE |
| 1 | E | 299 | LYS |
| 1 | E | 310 | ARG |
| 1 | E | 314 | GLU |
| 1 | E | 319 | ASP |
| 1 | E | 333 | ARG |
| 1 | E | 344 | LEU |
| 1 | E | 347 | LYS |
| 1 | E | 370 | GLN |
| 1 | E | 377 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 394 | ASN |
| 1 | E | 425 | ARG |
| 1 | E | 437 | SER |
| 1 | E | 448 | ARG |
| 1 | E | 473 | ARG |
| 1 | E | 519 | SER |
| 1 | E | 521 | LYS |
| 1 | E | 532 | PRO |
| 1 | E | 546 | LEU |
| 1 | E | 554 | GLN |
| 1 | E | 571 | VAL |
| 1 | E | 580 | GLU |
| 1 | E | 599 | ARG |
| 1 | E | 600 | GLN |
| 1 | E | 630 | ARG |
| 1 | E | 632 | SER |
| 1 | E | 645 | ARG |
| 1 | E | 651 | LEU |
| 1 | E | 655 | MET |
| 1 | E | 665 | SER |
| 1 | E | 672 | VAL |
| 1 | E | 684 | GLU |
| 1 | E | 687 | GLN |
| 1 | E | 690 | SER |
| 1 | E | 710 | GLU |
| 1 | E | 719 | GLN |
| 1 | E | 730 | LEU |
| 1 | E | 734 | SER |
| 1 | E | 741 | THR |
| 1 | E | 743 | SER |
| 1 | E | 751 | LEU |
| 1 | E | 753 | ASN |
| 1 | E | 755 | ARG |
| 1 | E | 768 | MET |
| 1 | E | 778 | THR |
| 1 | E | 781 | ARG |
| 1 | E | 797 | GLU |
| 1 | E | 799 | THR |
| 1 | E | 800 | ARG |
| 1 | E | 824 | GLN |
| 1 | E | 829 | THR |
| 1 | E | 832 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | E | 881 | ARG |
| 1 | E | 893 | GLU |
| 1 | E | 903[A] | GLN |
| 1 | E | 903[B] | GLN |
| 1 | E | 917 | ARG |
| 1 | E | 938 | ARG |
| 1 | E | 952 | ARG |
| 1 | E | 956 | GLN |
| 1 | E | 1006 | GLU |
| 1 | E | 1017 | GLN |
| 1 | F | 3 | ILE |
| 1 | F | 14 | ARG |
| 1 | F | 37 | ARG |
| 1 | F | 39 | SER |
| 1 | F | 46 | ARG |
| 1 | F | 48 | SER |
| 1 | F | 49 | GLN |
| 1 | F | 50 | GLN |
| 1 | F | 52 | ARG |
| 1 | F | 59 | ARG |
| 1 | F | 71 | GLU |
| 1 | F | 72 | SER |
| 1 | F | 80 | GLU |
| 1 | F | 84 | VAL |
| 1 | F | 90 | TRP |
| 1 | F | 102 | ASN |
| 1 | F | 116 | THR |
| 1 | F | 125 | LEU |
| 1 | F | 128 | ASN |
| 1 | F | 132 | SER |
| 1 | F | 136 | GLU |
| 1 | F | 165 | SER |
| 1 | F | 166 | ARG |
| 1 | F | 171 | PHE |
| 1 | F | 189 | LEU |
| 1 | F | 202 | MET |
| 1 | F | 210 | ARG |
| 1 | F | 211 | ASP |
| 1 | F | 217 | LYS |
| 1 | F | 219 | THR |
| 1 | F | 246 | MET |
| 1 | F | 247 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 249 | GLU |
| 1 | F | 250 | LEU |
| 1 | F | 259 | SER |
| 1 | F | 262 | GLN |
| 1 | F | 264 | GLU |
| 1 | F | 279 | ILE |
| 1 | F | 299 | LYS |
| 1 | F | 310 | ARG |
| 1 | F | 314 | GLU |
| 1 | F | 319 | ASP |
| 1 | F | 333 | ARG |
| 1 | F | 344 | LEU |
| 1 | F | 347 | LYS |
| 1 | F | 370 | GLN |
| 1 | F | 377 | LEU |
| 1 | F | 394 | ASN |
| 1 | F | 425 | ARG |
| 1 | F | 437 | SER |
| 1 | F | 448 | ARG |
| 1 | F | 473 | ARG |
| 1 | F | 519 | SER |
| 1 | F | 521 | LYS |
| 1 | F | 532 | PRO |
| 1 | F | 546 | LEU |
| 1 | F | 554 | GLN |
| 1 | F | 571 | VAL |
| 1 | F | 580 | GLU |
| 1 | F | 599 | ARG |
| 1 | F | 600 | GLN |
| 1 | F | 630 | ARG |
| 1 | F | 632 | SER |
| 1 | F | 645 | ARG |
| 1 | F | 651 | LEU |
| 1 | F | 655 | MET |
| 1 | F | 665 | SER |
| 1 | F | 672 | VAL |
| 1 | F | 684 | GLU |
| 1 | F | 687 | GLN |
| 1 | F | 690 | SER |
| 1 | F | 710 | GLU |
| 1 | F | 719 | GLN |
| 1 | F | 730 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | F | 734 | SER |
| 1 | F | 741 | THR |
| 1 | F | 743 | SER |
| 1 | F | 751 | LEU |
| 1 | F | 753 | ASN |
| 1 | F | 755 | ARG |
| 1 | F | 768 | MET |
| 1 | F | 778 | THR |
| 1 | F | 781 | ARG |
| 1 | F | 797 | GLU |
| 1 | F | 799 | THR |
| 1 | F | 800 | ARG |
| 1 | F | 824 | GLN |
| 1 | F | 829 | THR |
| 1 | F | 832 | ASP |
| 1 | F | 881 | ARG |
| 1 | F | 893 | GLU |
| 1 | F | 903[A] | GLN |
| 1 | F | 903[B] | GLN |
| 1 | F | 917 | ARG |
| 1 | F | 938 | ARG |
| 1 | F | 952 | ARG |
| 1 | F | 956 | GLN |
| 1 | F | 1006 | GLU |
| 1 | F | 1017 | GLN |
| 1 | G | 3 | ILE |
| 1 | G | 14 | ARG |
| 1 | G | 37 | ARG |
| 1 | G | 39 | SER |
| 1 | G | 46 | ARG |
| 1 | G | 48 | SER |
| 1 | G | 49 | GLN |
| 1 | G | 50 | GLN |
| 1 | G | 52 | ARG |
| 1 | G | 59 | ARG |
| 1 | G | 71 | GLU |
| 1 | G | 72 | SER |
| 1 | G | 80 | GLU |
| 1 | G | 84 | VAL |
| 1 | G | 90 | TRP |
| 1 | G | 102 | ASN |
| 1 | G | 116 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 125 | LEU |
| 1 | G | 128 | ASN |
| 1 | G | 132 | SER |
| 1 | G | 136 | GLU |
| 1 | G | 165 | SER |
| 1 | G | 166 | ARG |
| 1 | G | 171 | PHE |
| 1 | G | 189 | LEU |
| 1 | G | 202 | MET |
| 1 | G | 210 | ARG |
| 1 | G | 211 | ASP |
| 1 | G | 217 | LYS |
| 1 | G | 219 | THR |
| 1 | G | 246 | MET |
| 1 | G | 247 | CYS |
| 1 | G | 249 | GLU |
| 1 | G | 250 | LEU |
| 1 | G | 259 | SER |
| 1 | G | 262 | GLN |
| 1 | G | 264 | GLU |
| 1 | G | 279 | ILE |
| 1 | G | 299 | LYS |
| 1 | G | 310 | ARG |
| 1 | G | 314 | GLU |
| 1 | G | 319 | ASP |
| 1 | G | 333 | ARG |
| 1 | G | 344 | LEU |
| 1 | G | 347 | LYS |
| 1 | G | 370 | GLN |
| 1 | G | 377 | LEU |
| 1 | G | 394 | ASN |
| 1 | G | 425 | ARG |
| 1 | G | 437 | SER |
| 1 | G | 448 | ARG |
| 1 | G | 473 | ARG |
| 1 | G | 519 | SER |
| 1 | G | 521 | LYS |
| 1 | G | 532 | PRO |
| 1 | G | 546 | LEU |
| 1 | G | 554 | GLN |
| 1 | G | 571 | VAL |
| 1 | G | 580 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | G | 599 | ARG |
| 1 | G | 600 | GLN |
| 1 | G | 630 | ARG |
| 1 | G | 632 | SER |
| 1 | G | 645 | ARG |
| 1 | G | 651 | LEU |
| 1 | G | 655 | MET |
| 1 | G | 665 | SER |
| 1 | G | 672 | VAL |
| 1 | G | 684 | GLU |
| 1 | G | 687 | GLN |
| 1 | G | 690 | SER |
| 1 | G | 710 | GLU |
| 1 | G | 719 | GLN |
| 1 | G | 730 | LEU |
| 1 | G | 734 | SER |
| 1 | G | 741 | THR |
| 1 | G | 743 | SER |
| 1 | G | 751 | LEU |
| 1 | G | 753 | ASN |
| 1 | G | 755 | ARG |
| 1 | G | 768 | MET |
| 1 | G | 778 | THR |
| 1 | G | 781 | ARG |
| 1 | G | 797 | GLU |
| 1 | G | 799 | THR |
| 1 | G | 800 | ARG |
| 1 | G | 824 | GLN |
| 1 | G | 829 | THR |
| 1 | G | 832 | ASP |
| 1 | G | 881 | ARG |
| 1 | G | 893 | GLU |
| 1 | G | 903[A] | GLN |
| 1 | G | 903[B] | GLN |
| 1 | G | 917 | ARG |
| 1 | G | 938 | ARG |
| 1 | G | 952 | ARG |
| 1 | G | 956 | GLN |
| 1 | G | 1006 | GLU |
| 1 | G | 1017 | GLN |
| 1 | H | 3 | ILE |
| 1 | H | 14 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 37 | ARG |
| 1 | H | 39 | SER |
| 1 | H | 46 | ARG |
| 1 | H | 48 | SER |
| 1 | H | 49 | GLN |
| 1 | H | 50 | GLN |
| 1 | H | 52 | ARG |
| 1 | H | 59 | ARG |
| 1 | H | 71 | GLU |
| 1 | H | 72 | SER |
| 1 | H | 80 | GLU |
| 1 | H | 84 | VAL |
| 1 | H | 90 | TRP |
| 1 | H | 102 | ASN |
| 1 | H | 116 | THR |
| 1 | H | 125 | LEU |
| 1 | H | 128 | ASN |
| 1 | H | 132 | SER |
| 1 | H | 136 | GLU |
| 1 | H | 165 | SER |
| 1 | H | 166 | ARG |
| 1 | H | 171 | PHE |
| 1 | H | 189 | LEU |
| 1 | H | 202 | MET |
| 1 | H | 210 | ARG |
| 1 | H | 211 | ASP |
| 1 | H | 217 | LYS |
| 1 | H | 219 | THR |
| 1 | H | 246 | MET |
| 1 | H | 247 | CYS |
| 1 | H | 249 | GLU |
| 1 | H | 250 | LEU |
| 1 | H | 259 | SER |
| 1 | H | 262 | GLN |
| 1 | H | 264 | GLU |
| 1 | H | 279 | ILE |
| 1 | H | 299 | LYS |
| 1 | H | 310 | ARG |
| 1 | H | 314 | GLU |
| 1 | H | 319 | ASP |
| 1 | H | 333 | ARG |
| 1 | H | 344 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 347 | LYS |
| 1 | H | 370 | GLN |
| 1 | H | 377 | LEU |
| 1 | H | 394 | ASN |
| 1 | H | 425 | ARG |
| 1 | H | 437 | SER |
| 1 | H | 448 | ARG |
| 1 | H | 473 | ARG |
| 1 | H | 519 | SER |
| 1 | H | 521 | LYS |
| 1 | H | 532 | PRO |
| 1 | H | 546 | LEU |
| 1 | H | 554 | GLN |
| 1 | H | 571 | VAL |
| 1 | H | 580 | GLU |
| 1 | H | 599 | ARG |
| 1 | H | 600 | GLN |
| 1 | H | 630 | ARG |
| 1 | H | 632 | SER |
| 1 | H | 645 | ARG |
| 1 | H | 651 | LEU |
| 1 | H | 655 | MET |
| 1 | H | 665 | SER |
| 1 | H | 672 | VAL |
| 1 | H | 684 | GLU |
| 1 | H | 687 | GLN |
| 1 | H | 690 | SER |
| 1 | H | 710 | GLU |
| 1 | H | 719 | GLN |
| 1 | H | 730 | LEU |
| 1 | H | 734 | SER |
| 1 | H | 741 | THR |
| 1 | H | 743 | SER |
| 1 | H | 751 | LEU |
| 1 | H | 753 | ASN |
| 1 | H | 755 | ARG |
| 1 | H | 768 | MET |
| 1 | H | 778 | THR |
| 1 | H | 781 | ARG |
| 1 | H | 797 | GLU |
| 1 | H | 799 | THR |
| 1 | H | 800 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | H | 824 | GLN |
| 1 | H | 829 | THR |
| 1 | H | 832 | ASP |
| 1 | H | 881 | ARG |
| 1 | H | 893 | GLU |
| 1 | H | 903[A] | GLN |
| 1 | H | 903[B] | GLN |
| 1 | H | 917 | ARG |
| 1 | H | 938 | ARG |
| 1 | H | 952 | ARG |
| 1 | H | 956 | GLN |
| 1 | H | 1006 | GLU |
| 1 | H | 1017 | GLN |
| 1 | I | 3 | ILE |
| 1 | I | 14 | ARG |
| 1 | I | 37 | ARG |
| 1 | I | 39 | SER |
| 1 | I | 46 | ARG |
| 1 | I | 48 | SER |
| 1 | I | 49 | GLN |
| 1 | I | 50 | GLN |
| 1 | I | 52 | ARG |
| 1 | I | 59 | ARG |
| 1 | I | 71 | GLU |
| 1 | I | 72 | SER |
| 1 | I | 80 | GLU |
| 1 | I | 84 | VAL |
| 1 | I | 90 | TRP |
| 1 | I | 102 | ASN |
| 1 | I | 116 | THR |
| 1 | I | 125 | LEU |
| 1 | I | 128 | ASN |
| 1 | I | 132 | SER |
| 1 | I | 136 | GLU |
| 1 | I | 165 | SER |
| 1 | I | 166 | ARG |
| 1 | I | 171 | PHE |
| 1 | I | 189 | LEU |
| 1 | I | 202 | MET |
| 1 | I | 210 | ARG |
| 1 | I | 211 | ASP |
| 1 | I | 217 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 219 | THR |
| 1 | I | 246 | MET |
| 1 | I | 247 | CYS |
| 1 | I | 249 | GLU |
| 1 | I | 250 | LEU |
| 1 | I | 259 | SER |
| 1 | I | 262 | GLN |
| 1 | I | 264 | GLU |
| 1 | I | 279 | ILE |
| 1 | I | 299 | LYS |
| 1 | I | 310 | ARG |
| 1 | I | 314 | GLU |
| 1 | I | 319 | ASP |
| 1 | I | 333 | ARG |
| 1 | I | 344 | LEU |
| 1 | I | 347 | LYS |
| 1 | I | 370 | GLN |
| 1 | I | 377 | LEU |
| 1 | I | 394 | ASN |
| 1 | I | 425 | ARG |
| 1 | I | 437 | SER |
| 1 | I | 448 | ARG |
| 1 | I | 473 | ARG |
| 1 | I | 519 | SER |
| 1 | I | 521 | LYS |
| 1 | I | 532 | PRO |
| 1 | I | 546 | LEU |
| 1 | I | 554 | GLN |
| 1 | I | 571 | VAL |
| 1 | I | 580 | GLU |
| 1 | I | 599 | ARG |
| 1 | I | 600 | GLN |
| 1 | I | 630 | ARG |
| 1 | I | 632 | SER |
| 1 | I | 645 | ARG |
| 1 | I | 651 | LEU |
| 1 | I | 655 | MET |
| 1 | I | 665 | SER |
| 1 | I | 672 | VAL |
| 1 | I | 684 | GLU |
| 1 | I | 687 | GLN |
| 1 | I | 690 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | I | 710 | GLU |
| 1 | I | 719 | GLN |
| 1 | I | 730 | LEU |
| 1 | I | 734 | SER |
| 1 | I | 741 | THR |
| 1 | I | 743 | SER |
| 1 | I | 751 | LEU |
| 1 | I | 753 | ASN |
| 1 | I | 755 | ARG |
| 1 | I | 768 | MET |
| 1 | I | 778 | THR |
| 1 | I | 781 | ARG |
| 1 | I | 797 | GLU |
| 1 | I | 799 | THR |
| 1 | I | 800 | ARG |
| 1 | I | 824 | GLN |
| 1 | I | 829 | THR |
| 1 | I | 832 | ASP |
| 1 | I | 881 | ARG |
| 1 | I | 893 | GLU |
| 1 | I | 903[A] | GLN |
| 1 | I | 903[B] | GLN |
| 1 | I | 917 | ARG |
| 1 | I | 938 | ARG |
| 1 | I | 952 | ARG |
| 1 | I | 956 | GLN |
| 1 | I | 1006 | GLU |
| 1 | I | 1017 | GLN |
| 1 | J | 3 | ILE |
| 1 | J | 14 | ARG |
| 1 | J | 37 | ARG |
| 1 | J | 39 | SER |
| 1 | J | 46 | ARG |
| 1 | J | 48 | SER |
| 1 | J | 49 | GLN |
| 1 | J | 50 | GLN |
| 1 | J | 52 | ARG |
| 1 | J | 59 | ARG |
| 1 | J | 71 | GLU |
| 1 | J | 72 | SER |
| 1 | J | 80 | GLU |
| 1 | J | 84 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 90 | TRP |
| 1 | J | 102 | ASN |
| 1 | J | 116 | THR |
| 1 | J | 125 | LEU |
| 1 | J | 128 | ASN |
| 1 | J | 132 | SER |
| 1 | J | 136 | GLU |
| 1 | J | 165 | SER |
| 1 | J | 166 | ARG |
| 1 | J | 171 | PHE |
| 1 | J | 189 | LEU |
| 1 | J | 202 | MET |
| 1 | J | 210 | ARG |
| 1 | J | 211 | ASP |
| 1 | J | 217 | LYS |
| 1 | J | 219 | THR |
| 1 | J | 246 | MET |
| 1 | J | 247 | CYS |
| 1 | J | 249 | GLU |
| 1 | J | 250 | LEU |
| 1 | J | 259 | SER |
| 1 | J | 262 | GLN |
| 1 | J | 264 | GLU |
| 1 | J | 279 | ILE |
| 1 | J | 299 | LYS |
| 1 | J | 310 | ARG |
| 1 | J | 314 | GLU |
| 1 | J | 319 | ASP |
| 1 | J | 333 | ARG |
| 1 | J | 344 | LEU |
| 1 | J | 347 | LYS |
| 1 | J | 370 | GLN |
| 1 | J | 377 | LEU |
| 1 | J | 394 | ASN |
| 1 | J | 425 | ARG |
| 1 | J | 437 | SER |
| 1 | J | 448 | ARG |
| 1 | J | 473 | ARG |
| 1 | J | 519 | SER |
| 1 | J | 521 | LYS |
| 1 | J | 532 | PRO |
| 1 | J | 546 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | J | 554 | GLN |
| 1 | J | 571 | VAL |
| 1 | J | 580 | GLU |
| 1 | J | 599 | ARG |
| 1 | J | 600 | GLN |
| 1 | J | 630 | ARG |
| 1 | J | 632 | SER |
| 1 | J | 645 | ARG |
| 1 | J | 651 | LEU |
| 1 | J | 655 | MET |
| 1 | J | 665 | SER |
| 1 | J | 672 | VAL |
| 1 | J | 684 | GLU |
| 1 | J | 687 | GLN |
| 1 | J | 690 | SER |
| 1 | J | 710 | GLU |
| 1 | J | 719 | GLN |
| 1 | J | 730 | LEU |
| 1 | J | 734 | SER |
| 1 | J | 741 | THR |
| 1 | J | 743 | SER |
| 1 | J | 751 | LEU |
| 1 | J | 753 | ASN |
| 1 | J | 755 | ARG |
| 1 | J | 768 | MET |
| 1 | J | 778 | THR |
| 1 | J | 781 | ARG |
| 1 | J | 797 | GLU |
| 1 | J | 799 | THR |
| 1 | J | 800 | ARG |
| 1 | J | 824 | GLN |
| 1 | J | 829 | THR |
| 1 | J | 832 | ASP |
| 1 | J | 881 | ARG |
| 1 | J | 893 | GLU |
| 1 | J | 903[A] | GLN |
| 1 | J | 903[B] | GLN |
| 1 | J | 917 | ARG |
| 1 | J | 938 | ARG |
| 1 | J | 952 | ARG |
| 1 | J | 956 | GLN |
| 1 | J | 1006 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | J | 1017 | GLN |
| 1 | K | 3 | ILE |
| 1 | K | 14 | ARG |
| 1 | K | 37 | ARG |
| 1 | K | 39 | SER |
| 1 | K | 46 | ARG |
| 1 | K | 48 | SER |
| 1 | K | 49 | GLN |
| 1 | K | 50 | GLN |
| 1 | K | 52 | ARG |
| 1 | K | 59 | ARG |
| 1 | K | 71 | GLU |
| 1 | K | 72 | SER |
| 1 | K | 80 | GLU |
| 1 | K | 84 | VAL |
| 1 | K | 90 | TRP |
| 1 | K | 102 | ASN |
| 1 | K | 116 | THR |
| 1 | K | 125 | LEU |
| 1 | K | 128 | ASN |
| 1 | K | 132 | SER |
| 1 | K | 136 | GLU |
| 1 | K | 165 | SER |
| 1 | K | 166 | ARG |
| 1 | K | 171 | PHE |
| 1 | K | 189 | LEU |
| 1 | K | 202 | MET |
| 1 | K | 210 | ARG |
| 1 | K | 211 | ASP |
| 1 | K | 217 | LYS |
| 1 | K | 219 | THR |
| 1 | K | 246 | MET |
| 1 | K | 247 | CYS |
| 1 | K | 249 | GLU |
| 1 | K | 250 | LEU |
| 1 | K | 259 | SER |
| 1 | K | 262 | GLN |
| 1 | K | 264 | GLU |
| 1 | K | 279 | ILE |
| 1 | K | 299 | LYS |
| 1 | K | 310 | ARG |
| 1 | K | 314 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 319 | ASP |
| 1 | K | 333 | ARG |
| 1 | K | 344 | LEU |
| 1 | K | 347 | LYS |
| 1 | K | 370 | GLN |
| 1 | K | 377 | LEU |
| 1 | K | 394 | ASN |
| 1 | K | 425 | ARG |
| 1 | K | 437 | SER |
| 1 | K | 448 | ARG |
| 1 | K | 473 | ARG |
| 1 | K | 519 | SER |
| 1 | K | 521 | LYS |
| 1 | K | 532 | PRO |
| 1 | K | 546 | LEU |
| 1 | K | 554 | GLN |
| 1 | K | 571 | VAL |
| 1 | K | 580 | GLU |
| 1 | K | 599 | ARG |
| 1 | K | 600 | GLN |
| 1 | K | 630 | ARG |
| 1 | K | 632 | SER |
| 1 | K | 645 | ARG |
| 1 | K | 651 | LEU |
| 1 | K | 655 | MET |
| 1 | K | 665 | SER |
| 1 | K | 672 | VAL |
| 1 | K | 684 | GLU |
| 1 | K | 687 | GLN |
| 1 | K | 690 | SER |
| 1 | K | 710 | GLU |
| 1 | K | 719 | GLN |
| 1 | K | 730 | LEU |
| 1 | K | 734 | SER |
| 1 | K | 741 | THR |
| 1 | K | 743 | SER |
| 1 | K | 751 | LEU |
| 1 | K | 753 | ASN |
| 1 | K | 755 | ARG |
| 1 | K | 768 | MET |
| 1 | K | 778 | THR |
| 1 | K | 781 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | K | 797 | GLU |
| 1 | K | 799 | THR |
| 1 | K | 800 | ARG |
| 1 | K | 824 | GLN |
| 1 | K | 829 | THR |
| 1 | K | 832 | ASP |
| 1 | K | 881 | ARG |
| 1 | K | 893 | GLU |
| 1 | K | 903[A] | GLN |
| 1 | K | 903[B] | GLN |
| 1 | K | 917 | ARG |
| 1 | K | 938 | ARG |
| 1 | K | 952 | ARG |
| 1 | K | 956 | GLN |
| 1 | K | 1006 | GLU |
| 1 | K | 1017 | GLN |
| 1 | L | 3 | ILE |
| 1 | L | 14 | ARG |
| 1 | L | 37 | ARG |
| 1 | L | 39 | SER |
| 1 | L | 46 | ARG |
| 1 | L | 48 | SER |
| 1 | L | 49 | GLN |
| 1 | L | 50 | GLN |
| 1 | L | 52 | ARG |
| 1 | L | 59 | ARG |
| 1 | L | 71 | GLU |
| 1 | L | 72 | SER |
| 1 | L | 80 | GLU |
| 1 | L | 84 | VAL |
| 1 | L | 90 | TRP |
| 1 | L | 102 | ASN |
| 1 | L | 116 | THR |
| 1 | L | 125 | LEU |
| 1 | L | 128 | ASN |
| 1 | L | 136 | GLU |
| 1 | L | 165 | SER |
| 1 | L | 166 | ARG |
| 1 | L | 171 | PHE |
| 1 | L | 189 | LEU |
| 1 | L | 202 | MET |
| 1 | L | 210 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 211 | ASP |
| 1 | L | 217 | LYS |
| 1 | L | 219 | THR |
| 1 | L | 246 | MET |
| 1 | L | 247 | CYS |
| 1 | L | 249 | GLU |
| 1 | L | 250 | LEU |
| 1 | L | 259 | SER |
| 1 | L | 262 | GLN |
| 1 | L | 264 | GLU |
| 1 | L | 279 | ILE |
| 1 | L | 299 | LYS |
| 1 | L | 310 | ARG |
| 1 | L | 314 | GLU |
| 1 | L | 319 | ASP |
| 1 | L | 333 | ARG |
| 1 | L | 344 | LEU |
| 1 | L | 347 | LYS |
| 1 | L | 370 | GLN |
| 1 | L | 377 | LEU |
| 1 | L | 394 | ASN |
| 1 | L | 425 | ARG |
| 1 | L | 437 | SER |
| 1 | L | 448 | ARG |
| 1 | L | 473 | ARG |
| 1 | L | 519 | SER |
| 1 | L | 521 | LYS |
| 1 | L | 532 | PRO |
| 1 | L | 546 | LEU |
| 1 | L | 554 | GLN |
| 1 | L | 571 | VAL |
| 1 | L | 580 | GLU |
| 1 | L | 599 | ARG |
| 1 | L | 600 | GLN |
| 1 | L | 630 | ARG |
| 1 | L | 632 | SER |
| 1 | L | 645 | ARG |
| 1 | L | 651 | LEU |
| 1 | L | 655 | MET |
| 1 | L | 665 | SER |
| 1 | L | 672 | VAL |
| 1 | L | 684 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | L | 687 | GLN |
| 1 | L | 690 | SER |
| 1 | L | 710 | GLU |
| 1 | L | 719 | GLN |
| 1 | L | 730 | LEU |
| 1 | L | 734 | SER |
| 1 | L | 741 | THR |
| 1 | L | 743 | SER |
| 1 | L | 751 | LEU |
| 1 | L | 753 | ASN |
| 1 | L | 755 | ARG |
| 1 | L | 768 | MET |
| 1 | L | 778 | THR |
| 1 | L | 781 | ARG |
| 1 | L | 797 | GLU |
| 1 | L | 799 | THR |
| 1 | L | 800 | ARG |
| 1 | L | 824 | GLN |
| 1 | L | 829 | THR |
| 1 | L | 832 | ASP |
| 1 | L | 881 | ARG |
| 1 | L | 893 | GLU |
| 1 | L | 903[A] | GLN |
| 1 | L | 903[B] | GLN |
| 1 | L | 917 | ARG |
| 1 | L | 938 | ARG |
| 1 | L | 952 | ARG |
| 1 | L | 956 | GLN |
| 1 | L | 1006 | GLU |
| 1 | L | 1017 | GLN |
| 1 | M | 3 | ILE |
| 1 | M | 14 | ARG |
| 1 | M | 37 | ARG |
| 1 | M | 39 | SER |
| 1 | M | 46 | ARG |
| 1 | M | 48 | SER |
| 1 | M | 49 | GLN |
| 1 | M | 50 | GLN |
| 1 | M | 52 | ARG |
| 1 | M | 59 | ARG |
| 1 | M | 71 | GLU |
| 1 | M | 72 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 80 | GLU |
| 1 | M | 84 | VAL |
| 1 | M | 90 | TRP |
| 1 | M | 102 | ASN |
| 1 | M | 116 | THR |
| 1 | M | 125 | LEU |
| 1 | M | 128 | ASN |
| 1 | M | 132 | SER |
| 1 | M | 136 | GLU |
| 1 | M | 165 | SER |
| 1 | M | 166 | ARG |
| 1 | M | 171 | PHE |
| 1 | M | 189 | LEU |
| 1 | M | 202 | MET |
| 1 | M | 210 | ARG |
| 1 | M | 211 | ASP |
| 1 | M | 217 | LYS |
| 1 | M | 219 | THR |
| 1 | M | 246 | MET |
| 1 | M | 247 | CYS |
| 1 | M | 249 | GLU |
| 1 | M | 250 | LEU |
| 1 | M | 259 | SER |
| 1 | M | 262 | GLN |
| 1 | M | 264 | GLU |
| 1 | M | 279 | ILE |
| 1 | M | 299 | LYS |
| 1 | M | 310 | ARG |
| 1 | M | 314 | GLU |
| 1 | M | 319 | ASP |
| 1 | M | 333 | ARG |
| 1 | M | 344 | LEU |
| 1 | M | 347 | LYS |
| 1 | M | 370 | GLN |
| 1 | M | 377 | LEU |
| 1 | M | 394 | ASN |
| 1 | M | 425 | ARG |
| 1 | M | 437 | SER |
| 1 | M | 448 | ARG |
| 1 | M | 473 | ARG |
| 1 | M | 519 | SER |
| 1 | M | 521 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | M | 532 | PRO |
| 1 | M | 546 | LEU |
| 1 | M | 554 | GLN |
| 1 | M | 571 | VAL |
| 1 | M | 580 | GLU |
| 1 | M | 599 | ARG |
| 1 | M | 600 | GLN |
| 1 | M | 630 | ARG |
| 1 | M | 632 | SER |
| 1 | M | 645 | ARG |
| 1 | M | 651 | LEU |
| 1 | M | 655 | MET |
| 1 | M | 665 | SER |
| 1 | M | 672 | VAL |
| 1 | M | 684 | GLU |
| 1 | M | 687 | GLN |
| 1 | M | 690 | SER |
| 1 | M | 710 | GLU |
| 1 | M | 719 | GLN |
| 1 | M | 730 | LEU |
| 1 | M | 734 | SER |
| 1 | M | 741 | THR |
| 1 | M | 743 | SER |
| 1 | M | 751 | LEU |
| 1 | M | 753 | ASN |
| 1 | M | 755 | ARG |
| 1 | M | 768 | MET |
| 1 | M | 778 | THR |
| 1 | M | 781 | ARG |
| 1 | M | 797 | GLU |
| 1 | M | 799 | THR |
| 1 | M | 800 | ARG |
| 1 | M | 824 | GLN |
| 1 | M | 829 | THR |
| 1 | M | 832 | ASP |
| 1 | M | 881 | ARG |
| 1 | M | 893 | GLU |
| 1 | M | 903[A] | GLN |
| 1 | M | 903[B] | GLN |
| 1 | M | 917 | ARG |
| 1 | M | 938 | ARG |
| 1 | M | 952 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | M | 956 | GLN |
| 1 | M | 1006 | GLU |
| 1 | M | 1017 | GLN |
| 1 | N | 3 | ILE |
| 1 | N | 14 | ARG |
| 1 | N | 37 | ARG |
| 1 | N | 39 | SER |
| 1 | N | 46 | ARG |
| 1 | N | 48 | SER |
| 1 | N | 49 | GLN |
| 1 | N | 50 | GLN |
| 1 | N | 52 | ARG |
| 1 | N | 59 | ARG |
| 1 | N | 71 | GLU |
| 1 | N | 72 | SER |
| 1 | N | 80 | GLU |
| 1 | N | 84 | VAL |
| 1 | N | 90 | TRP |
| 1 | N | 102 | ASN |
| 1 | N | 116 | THR |
| 1 | N | 125 | LEU |
| 1 | N | 128 | ASN |
| 1 | N | 132 | SER |
| 1 | N | 136 | GLU |
| 1 | N | 165 | SER |
| 1 | N | 166 | ARG |
| 1 | N | 171 | PHE |
| 1 | N | 189 | LEU |
| 1 | N | 202 | MET |
| 1 | N | 210 | ARG |
| 1 | N | 211 | ASP |
| 1 | N | 217 | LYS |
| 1 | N | 219 | THR |
| 1 | N | 246 | MET |
| 1 | N | 247 | CYS |
| 1 | N | 249 | GLU |
| 1 | N | 250 | LEU |
| 1 | N | 259 | SER |
| 1 | N | 262 | GLN |
| 1 | N | 264 | GLU |
| 1 | N | 279 | ILE |
| 1 | N | 299 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 310 | ARG |
| 1 | N | 314 | GLU |
| 1 | N | 319 | ASP |
| 1 | N | 333 | ARG |
| 1 | N | 344 | LEU |
| 1 | N | 347 | LYS |
| 1 | N | 370 | GLN |
| 1 | N | 377 | LEU |
| 1 | N | 394 | ASN |
| 1 | N | 425 | ARG |
| 1 | N | 437 | SER |
| 1 | N | 448 | ARG |
| 1 | N | 473 | ARG |
| 1 | N | 519 | SER |
| 1 | N | 521 | LYS |
| 1 | N | 546 | LEU |
| 1 | N | 554 | GLN |
| 1 | N | 571 | VAL |
| 1 | N | 580 | GLU |
| 1 | N | 599 | ARG |
| 1 | N | 600 | GLN |
| 1 | N | 630 | ARG |
| 1 | N | 632 | SER |
| 1 | N | 645 | ARG |
| 1 | N | 651 | LEU |
| 1 | N | 655 | MET |
| 1 | N | 665 | SER |
| 1 | N | 672 | VAL |
| 1 | N | 684 | GLU |
| 1 | N | 687 | GLN |
| 1 | N | 690 | SER |
| 1 | N | 710 | GLU |
| 1 | N | 719 | GLN |
| 1 | N | 730 | LEU |
| 1 | N | 734 | SER |
| 1 | N | 741 | THR |
| 1 | N | 743 | SER |
| 1 | N | 751 | LEU |
| 1 | N | 753 | ASN |
| 1 | N | 755 | ARG |
| 1 | N | 768 | MET |
| 1 | N | 778 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | N | 781 | ARG |
| 1 | N | 797 | GLU |
| 1 | N | 799 | THR |
| 1 | N | 800 | ARG |
| 1 | N | 824 | GLN |
| 1 | N | 829 | THR |
| 1 | N | 832 | ASP |
| 1 | N | 881 | ARG |
| 1 | N | 893 | GLU |
| 1 | N | 903[A] | GLN |
| 1 | N | 903[B] | GLN |
| 1 | N | 917 | ARG |
| 1 | N | 938 | ARG |
| 1 | N | 952 | ARG |
| 1 | N | 956 | GLN |
| 1 | N | 1006 | GLU |
| 1 | N | 1017 | GLN |
| 1 | O | 3 | ILE |
| 1 | O | 14 | ARG |
| 1 | O | 37 | ARG |
| 1 | O | 39 | SER |
| 1 | O | 46 | ARG |
| 1 | O | 48 | SER |
| 1 | O | 49 | GLN |
| 1 | O | 50 | GLN |
| 1 | O | 52 | ARG |
| 1 | O | 59 | ARG |
| 1 | O | 71 | GLU |
| 1 | O | 72 | SER |
| 1 | O | 80 | GLU |
| 1 | O | 84 | VAL |
| 1 | O | 90 | TRP |
| 1 | O | 102 | ASN |
| 1 | O | 116 | THR |
| 1 | O | 125 | LEU |
| 1 | O | 128 | ASN |
| 1 | O | 132 | SER |
| 1 | O | 136 | GLU |
| 1 | O | 165 | SER |
| 1 | O | 166 | ARG |
| 1 | O | 171 | PHE |
| 1 | O | 189 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 202 | MET |
| 1 | O | 210 | ARG |
| 1 | O | 211 | ASP |
| 1 | O | 217 | LYS |
| 1 | O | 219 | THR |
| 1 | O | 246 | MET |
| 1 | O | 247 | CYS |
| 1 | O | 249 | GLU |
| 1 | O | 250 | LEU |
| 1 | O | 259 | SER |
| 1 | O | 262 | GLN |
| 1 | O | 264 | GLU |
| 1 | O | 279 | ILE |
| 1 | O | 299 | LYS |
| 1 | O | 310 | ARG |
| 1 | O | 314 | GLU |
| 1 | O | 319 | ASP |
| 1 | O | 333 | ARG |
| 1 | O | 344 | LEU |
| 1 | O | 347 | LYS |
| 1 | O | 370 | GLN |
| 1 | O | 377 | LEU |
| 1 | O | 394 | ASN |
| 1 | O | 425 | ARG |
| 1 | O | 437 | SER |
| 1 | O | 448 | ARG |
| 1 | O | 473 | ARG |
| 1 | O | 519 | SER |
| 1 | O | 521 | LYS |
| 1 | O | 532 | PRO |
| 1 | O | 546 | LEU |
| 1 | O | 554 | GLN |
| 1 | O | 571 | VAL |
| 1 | O | 580 | GLU |
| 1 | O | 599 | ARG |
| 1 | O | 600 | GLN |
| 1 | O | 630 | ARG |
| 1 | O | 632 | SER |
| 1 | O | 645 | ARG |
| 1 | O | 651 | LEU |
| 1 | O | 655 | MET |
| 1 | O | 665 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | O | 672 | VAL |
| 1 | O | 684 | GLU |
| 1 | O | 687 | GLN |
| 1 | O | 690 | SER |
| 1 | O | 710 | GLU |
| 1 | O | 719 | GLN |
| 1 | O | 730 | LEU |
| 1 | O | 734 | SER |
| 1 | O | 741 | THR |
| 1 | O | 743 | SER |
| 1 | O | 751 | LEU |
| 1 | O | 753 | ASN |
| 1 | O | 755 | ARG |
| 1 | O | 768 | MET |
| 1 | O | 778 | THR |
| 1 | O | 781 | ARG |
| 1 | O | 797 | GLU |
| 1 | O | 799 | THR |
| 1 | O | 800 | ARG |
| 1 | O | 824 | GLN |
| 1 | O | 829 | THR |
| 1 | O | 832 | ASP |
| 1 | O | 881 | ARG |
| 1 | O | 893 | GLU |
| 1 | O | 903[A] | GLN |
| 1 | O | 903[B] | GLN |
| 1 | O | 917 | ARG |
| 1 | O | 938 | ARG |
| 1 | O | 952 | ARG |
| 1 | O | 956 | GLN |
| 1 | O | 1006 | GLU |
| 1 | O | 1017 | GLN |
| 1 | P | 3 | ILE |
| 1 | P | 14 | ARG |
| 1 | P | 37 | ARG |
| 1 | P | 39 | SER |
| 1 | P | 46 | ARG |
| 1 | P | 48 | SER |
| 1 | P | 49 | GLN |
| 1 | P | 50 | GLN |
| 1 | P | 52 | ARG |
| 1 | P | 59 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 71 | GLU |
| 1 | P | 72 | SER |
| 1 | P | 80 | GLU |
| 1 | P | 84 | VAL |
| 1 | P | 90 | TRP |
| 1 | P | 102 | ASN |
| 1 | P | 116 | THR |
| 1 | P | 125 | LEU |
| 1 | P | 128 | ASN |
| 1 | P | 132 | SER |
| 1 | P | 136 | GLU |
| 1 | P | 165 | SER |
| 1 | P | 166 | ARG |
| 1 | P | 171 | PHE |
| 1 | P | 189 | LEU |
| 1 | P | 202 | MET |
| 1 | P | 210 | ARG |
| 1 | P | 211 | ASP |
| 1 | P | 217 | LYS |
| 1 | P | 219 | THR |
| 1 | P | 246 | MET |
| 1 | P | 247 | CYS |
| 1 | P | 249 | GLU |
| 1 | P | 250 | LEU |
| 1 | P | 259 | SER |
| 1 | P | 262 | GLN |
| 1 | P | 264 | GLU |
| 1 | P | 279 | ILE |
| 1 | P | 299 | LYS |
| 1 | P | 310 | ARG |
| 1 | P | 314 | GLU |
| 1 | P | 319 | ASP |
| 1 | P | 333 | ARG |
| 1 | P | 344 | LEU |
| 1 | P | 347 | LYS |
| 1 | P | 370 | GLN |
| 1 | P | 377 | LEU |
| 1 | P | 394 | ASN |
| 1 | P | 425 | ARG |
| 1 | P | 437 | SER |
| 1 | P | 448 | ARG |
| 1 | P | 473 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | P | 519 | SER |
| 1 | P | 521 | LYS |
| 1 | P | 532 | PRO |
| 1 | P | 546 | LEU |
| 1 | P | 554 | GLN |
| 1 | P | 571 | VAL |
| 1 | P | 580 | GLU |
| 1 | P | 599 | ARG |
| 1 | P | 600 | GLN |
| 1 | P | 630 | ARG |
| 1 | P | 632 | SER |
| 1 | P | 645 | ARG |
| 1 | P | 651 | LEU |
| 1 | P | 655 | MET |
| 1 | P | 665 | SER |
| 1 | P | 672 | VAL |
| 1 | P | 684 | GLU |
| 1 | P | 687 | GLN |
| 1 | P | 690 | SER |
| 1 | P | 710 | GLU |
| 1 | P | 719 | GLN |
| 1 | P | 730 | LEU |
| 1 | P | 734 | SER |
| 1 | P | 741 | THR |
| 1 | P | 743 | SER |
| 1 | P | 751 | LEU |
| 1 | P | 753 | ASN |
| 1 | P | 755 | ARG |
| 1 | P | 768 | MET |
| 1 | P | 778 | THR |
| 1 | P | 781 | ARG |
| 1 | P | 797 | GLU |
| 1 | P | 799 | THR |
| 1 | P | 800 | ARG |
| 1 | P | 824 | GLN |
| 1 | P | 829 | THR |
| 1 | P | 832 | ASP |
| 1 | P | 881 | ARG |
| 1 | P | 893 | GLU |
| 1 | P | 903[A] | GLN |
| 1 | P | 903[B] | GLN |
| 1 | P | 917 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | P | 938 | ARG |
| 1 | P | 952 | ARG |
| 1 | P | 956 | GLN |
| 1 | P | 1006 | GLU |
| 1 | P | 1017 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 102 | ASN |
| 1 | A | 128 | ASN |
| 1 | A | 226 | HIS |
| 1 | A | 316 | HIS |
| 1 | A | 467 | ASN |
| 1 | A | 597 | ASN |
| 1 | A | 604 | ASN |
| 1 | A | 624 | GLN |
| 1 | A | 761 | GLN |
| 1 | A | 817 | GLN |
| 1 | A | 824 | GLN |
| 1 | A | 949 | HIS |
| 1 | A | 990 | HIS |
| 1 | A | 1017 | GLN |
| 1 | B | 102 | ASN |
| 1 | B | 128 | ASN |
| 1 | B | 226 | HIS |
| 1 | B | 316 | HIS |
| 1 | B | 467 | ASN |
| 1 | B | 597 | ASN |
| 1 | B | 604 | ASN |
| 1 | B | 624 | GLN |
| 1 | B | 739 | HIS |
| 1 | B | 761 | GLN |
| 1 | B | 817 | GLN |
| 1 | B | 824 | GLN |
| 1 | B | 949 | HIS |
| 1 | B | 990 | HIS |
| 1 | B | 1017 | GLN |
| 1 | C | 102 | ASN |
| 1 | C | 128 | ASN |
| 1 | C | 226 | HIS |
| 1 | C | 316 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 467 | ASN |
| 1 | C | 597 | ASN |
| 1 | C | 604 | ASN |
| 1 | C | 624 | GLN |
| 1 | C | 739 | HIS |
| 1 | C | 761 | GLN |
| 1 | C | 817 | GLN |
| 1 | C | 824 | GLN |
| 1 | C | 949 | HIS |
| 1 | C | 990 | HIS |
| 1 | C | 1017 | GLN |
| 1 | D | 102 | ASN |
| 1 | D | 128 | ASN |
| 1 | D | 226 | HIS |
| 1 | D | 316 | HIS |
| 1 | D | 467 | ASN |
| 1 | D | 597 | ASN |
| 1 | D | 604 | ASN |
| 1 | D | 624 | GLN |
| 1 | D | 739 | HIS |
| 1 | D | 761 | GLN |
| 1 | D | 817 | GLN |
| 1 | D | 824 | GLN |
| 1 | D | 949 | HIS |
| 1 | D | 990 | HIS |
| 1 | D | 1017 | GLN |
| 1 | E | 102 | ASN |
| 1 | E | 128 | ASN |
| 1 | E | 226 | HIS |
| 1 | E | 316 | HIS |
| 1 | E | 467 | ASN |
| 1 | E | 597 | ASN |
| 1 | E | 604 | ASN |
| 1 | E | 624 | GLN |
| 1 | E | 761 | GLN |
| 1 | E | 817 | GLN |
| 1 | E | 824 | GLN |
| 1 | E | 949 | HIS |
| 1 | E | 990 | HIS |
| 1 | E | 1017 | GLN |
| 1 | F | 102 | ASN |
| 1 | F | 128 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | F | 226 | HIS |
| 1 | F | 316 | HIS |
| 1 | F | 467 | ASN |
| 1 | F | 597 | ASN |
| 1 | F | 604 | ASN |
| 1 | F | 624 | GLN |
| 1 | F | 761 | GLN |
| 1 | F | 817 | GLN |
| 1 | F | 824 | GLN |
| 1 | F | 949 | HIS |
| 1 | F | 990 | HIS |
| 1 | F | 1017 | GLN |
| 1 | G | 102 | ASN |
| 1 | G | 128 | ASN |
| 1 | G | 226 | HIS |
| 1 | G | 316 | HIS |
| 1 | G | 467 | ASN |
| 1 | G | 597 | ASN |
| 1 | G | 604 | ASN |
| 1 | G | 624 | GLN |
| 1 | G | 739 | HIS |
| 1 | G | 761 | GLN |
| 1 | G | 817 | GLN |
| 1 | G | 824 | GLN |
| 1 | G | 949 | HIS |
| 1 | G | 990 | HIS |
| 1 | G | 1017 | GLN |
| 1 | H | 102 | ASN |
| 1 | H | 128 | ASN |
| 1 | H | 226 | HIS |
| 1 | H | 316 | HIS |
| 1 | H | 467 | ASN |
| 1 | H | 597 | ASN |
| 1 | H | 604 | ASN |
| 1 | H | 624 | GLN |
| 1 | H | 761 | GLN |
| 1 | H | 817 | GLN |
| 1 | H | 824 | GLN |
| 1 | H | 949 | HIS |
| 1 | H | 990 | HIS |
| 1 | H | 1017 | GLN |
| 1 | I | 102 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | I | 128 | ASN |
| 1 | I | 226 | HIS |
| 1 | I | 316 | HIS |
| 1 | I | 467 | ASN |
| 1 | I | 597 | ASN |
| 1 | I | 604 | ASN |
| 1 | I | 624 | GLN |
| 1 | I | 739 | HIS |
| 1 | I | 761 | GLN |
| 1 | I | 817 | GLN |
| 1 | I | 824 | GLN |
| 1 | I | 949 | HIS |
| 1 | I | 990 | HIS |
| 1 | I | 1017 | GLN |
| 1 | J | 102 | ASN |
| 1 | J | 128 | ASN |
| 1 | J | 226 | HIS |
| 1 | J | 316 | HIS |
| 1 | J | 467 | ASN |
| 1 | J | 597 | ASN |
| 1 | J | 604 | ASN |
| 1 | J | 624 | GLN |
| 1 | J | 739 | HIS |
| 1 | J | 761 | GLN |
| 1 | J | 817 | GLN |
| 1 | J | 824 | GLN |
| 1 | J | 949 | HIS |
| 1 | J | 990 | HIS |
| 1 | J | 1017 | GLN |
| 1 | K | 102 | ASN |
| 1 | K | 128 | ASN |
| 1 | K | 226 | HIS |
| 1 | K | 316 | HIS |
| 1 | K | 467 | ASN |
| 1 | K | 597 | ASN |
| 1 | K | 604 | ASN |
| 1 | K | 624 | GLN |
| 1 | K | 739 | HIS |
| 1 | K | 761 | GLN |
| 1 | K | 817 | GLN |
| 1 | K | 824 | GLN |
| 1 | K | 949 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | K | 990 | HIS |
| 1 | K | 1017 | GLN |
| 1 | L | 102 | ASN |
| 1 | L | 128 | ASN |
| 1 | L | 226 | HIS |
| 1 | L | 316 | HIS |
| 1 | L | 467 | ASN |
| 1 | L | 597 | ASN |
| 1 | L | 604 | ASN |
| 1 | L | 624 | GLN |
| 1 | L | 739 | HIS |
| 1 | L | 761 | GLN |
| 1 | L | 817 | GLN |
| 1 | L | 824 | GLN |
| 1 | L | 949 | HIS |
| 1 | L | 990 | HIS |
| 1 | L | 1017 | GLN |
| 1 | M | 102 | ASN |
| 1 | M | 128 | ASN |
| 1 | M | 226 | HIS |
| 1 | M | 316 | HIS |
| 1 | M | 467 | ASN |
| 1 | M | 597 | ASN |
| 1 | M | 604 | ASN |
| 1 | M | 624 | GLN |
| 1 | M | 739 | HIS |
| 1 | M | 761 | GLN |
| 1 | M | 817 | GLN |
| 1 | M | 824 | GLN |
| 1 | M | 949 | HIS |
| 1 | M | 990 | HIS |
| 1 | M | 1017 | GLN |
| 1 | N | 102 | ASN |
| 1 | N | 128 | ASN |
| 1 | N | 226 | HIS |
| 1 | N | 316 | HIS |
| 1 | N | 467 | ASN |
| 1 | N | 597 | ASN |
| 1 | N | 604 | ASN |
| 1 | N | 624 | GLN |
| 1 | N | 739 | HIS |
| 1 | N | 761 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | N | 817 | GLN |
| 1 | N | 824 | GLN |
| 1 | N | 949 | HIS |
| 1 | N | 990 | HIS |
| 1 | N | 1017 | GLN |
| 1 | O | 102 | ASN |
| 1 | O | 128 | ASN |
| 1 | O | 226 | HIS |
| 1 | O | 316 | HIS |
| 1 | O | 467 | ASN |
| 1 | O | 597 | ASN |
| 1 | O | 604 | ASN |
| 1 | O | 624 | GLN |
| 1 | O | 761 | GLN |
| 1 | O | 817 | GLN |
| 1 | O | 824 | GLN |
| 1 | O | 949 | HIS |
| 1 | O | 990 | HIS |
| 1 | O | 1017 | GLN |
| 1 | P | 102 | ASN |
| 1 | P | 128 | ASN |
| 1 | P | 226 | HIS |
| 1 | P | 316 | HIS |
| 1 | P | 467 | ASN |
| 1 | P | 597 | ASN |
| 1 | P | 604 | ASN |
| 1 | P | 624 | GLN |
| 1 | P | 761 | GLN |
| 1 | P | 817 | GLN |
| 1 | P | 824 | GLN |
| 1 | P | 949 | HIS |
| 1 | P | 990 | HIS |
| 1 | P | 1017 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | CME | A | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | A | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | A | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | B | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | B | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | B | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | C | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | C | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | C | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | D | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | D | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | D | 914 | 1 | 8,9,10 | 0.74 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | E | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | E | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | E | 914 | 1 | 8,9,10 | 0.74 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | F | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | F | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | F | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | G | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | G | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | G | 914 | 1 | 8,9,10 | 0.74 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | H | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | H | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | H | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | I | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | I | 748 | 1 | 8,9,10 | 0.78 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | I | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | J | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | J | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | CME | J | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | K | 1021 | 1 | 8,9,10 | 1.12 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | K | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | K | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | L | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | L | 748 | 1 | 8,9,10 | 0.80 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | L | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | M | 1021 | 1 | 8,9,10 | 1.14 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | M | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | M | 914 | 1 | 8,9,10 | 0.76 | 0 | 6,9,11 | 2.29 | 1 (16%) |
| 1 | CME | N | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | N | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | N | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | O | 1021 | 1 | 8,9,10 | 1.14 | 0 | 6,9,11 | 4.47 | 1 (16%) |
| 1 | CME | O | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | O | 914 | 1 | 8,9,10 | 0.75 | 0 | 6,9,11 | 2.28 | 1 (16%) |
| 1 | CME | P | 1021 | 1 | 8,9,10 | 1.13 | 0 | 6,9,11 | 4.48 | 1 (16%) |
| 1 | CME | P | 748 | 1 | 8,9,10 | 0.79 | 1 (12%) | 6,9,11 | 1.02 | 0 |
| 1 | CME | P | 914 | 1 | 8,9,10 | 0.74 | 0 | 6,9,11 | 2.28 | 1 (16%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 1 | CME | A | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | A | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | A | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | B | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | B | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | B | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | C | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | C | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | C | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | D | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | D | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | D | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 1 | CME | E | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | E | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | E | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | F | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | F | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | F | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | G | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | G | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | G | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | H | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | H | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | H | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | I | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | I | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | I | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | J | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | J | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | J | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | K | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | K | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | K | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | L | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | L | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | L | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | M | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | M | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | M | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | N | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | N | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | N | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | O | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | O | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | O | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | P | 1021 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | P | 748 | 1 | - | 0/5/8/10 | 0/0/0/0 |
| 1 | CME | P | 914 | 1 | - | 0/5/8/10 | 0/0/0/0 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | J | 748 | CME | CA-N | -2.11 | 1.41 | 1.47 |
| 1 | H | 748 | CME | CA-N | -2.11 | 1.41 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | K | 748 | CME | CA-N | -2.11 | 1.41 | 1.47 |
| 1 | F | 748 | CME | CA-N | -2.10 | 1.41 | 1.47 |
| 1 | G | 748 | CME | CA-N | -2.10 | 1.41 | 1.47 |
| 1 | L | 748 | CME | CA-N | -2.10 | 1.41 | 1.47 |
| 1 | E | 748 | CME | CA-N | -2.10 | 1.41 | 1.47 |
| 1 | O | 748 | CME | CA-N | -2.09 | 1.41 | 1.47 |
| 1 | B | 748 | CME | CA-N | -2.09 | 1.41 | 1.47 |
| 1 | A | 748 | CME | CA-N | -2.09 | 1.41 | 1.47 |
| 1 | C | 748 | CME | CA-N | -2.09 | 1.41 | 1.47 |
| 1 | D | 748 | CME | CA-N | -2.09 | 1.41 | 1.47 |
| 1 | N | 748 | CME | CA-N | -2.08 | 1.41 | 1.47 |
| 1 | M | 748 | CME | CA-N | -2.08 | 1.41 | 1.47 |
| 1 | P | 748 | CME | CA-N | -2.07 | 1.41 | 1.47 |
| 1 | I | 748 | CME | CA-N | -2.07 | 1.41 | 1.47 |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | D | 1021 | CME | CB-SG-SD | -10.72 | 83.06 | 103.95 |
| 1 | K | 1021 | CME | CB-SG-SD | -10.72 | 83.07 | 103.95 |
| 1 | P | 1021 | CME | CB-SG-SD | -10.71 | 83.08 | 103.95 |
| 1 | N | 1021 | CME | CB-SG-SD | -10.71 | 83.09 | 103.95 |
| 1 | I | 1021 | CME | CB-SG-SD | -10.70 | 83.10 | 103.95 |
| 1 | L | 1021 | CME | CB-SG-SD | -10.70 | 83.10 | 103.95 |
| 1 | E | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | A | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | F | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | J | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | H | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | G | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | B | 1021 | CME | CB-SG-SD | -10.70 | 83.11 | 103.95 |
| 1 | M | 1021 | CME | CB-SG-SD | -10.69 | 83.12 | 103.95 |
| 1 | C | 1021 | CME | CB-SG-SD | -10.69 | 83.12 | 103.95 |
| 1 | O | 1021 | CME | CB-SG-SD | -10.68 | 83.15 | 103.95 |
| 1 | C | 914 | CME | CB-SG-SD | -5.50 | 93.23 | 103.95 |
| 1 | L | 914 | CME | CB-SG-SD | -5.50 | 93.24 | 103.95 |
| 1 | B | 914 | CME | CB-SG-SD | -5.49 | 93.25 | 103.95 |
| 1 | H | 914 | CME | CB-SG-SD | -5.49 | 93.26 | 103.95 |
| 1 | E | 914 | CME | CB-SG-SD | -5.49 | 93.26 | 103.95 |
| 1 | I | 914 | CME | CB-SG-SD | -5.49 | 93.26 | 103.95 |
| 1 | M | 914 | CME | CB-SG-SD | -5.48 | 93.27 | 103.95 |
| 1 | K | 914 | CME | CB-SG-SD | -5.48 | 93.27 | 103.95 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | J | 914 | CME | CB-SG-SD | -5.48 | 93.27 | 103.95 |
| 1 | F | 914 | CME | CB-SG-SD | -5.48 | 93.27 | 103.95 |
| 1 | N | 914 | CME | CB-SG-SD | -5.48 | 93.27 | 103.95 |
| 1 | D | 914 | CME | CB-SG-SD | -5.48 | 93.28 | 103.95 |
| 1 | G | 914 | CME | CB-SG-SD | -5.48 | 93.28 | 103.95 |
| 1 | A | 914 | CME | CB-SG-SD | -5.48 | 93.28 | 103.95 |
| 1 | O | 914 | CME | CB-SG-SD | -5.47 | 93.28 | 103.95 |
| 1 | P | 914 | CME | CB-SG-SD | -5.47 | 93.29 | 103.95 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 64 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | A | 1021 | CME | 3 | 0 |
| 1 | A | 748 | CME | 1 | 0 |
| 1 | A | 914 | CME | 1 | 0 |
| 1 | B | 1021 | CME | 3 | 0 |
| 1 | B | 914 | CME | 1 | 0 |
| 1 | C | 1021 | CME | 3 | 0 |
| 1 | C | 914 | CME | 1 | 0 |
| 1 | D | 1021 | CME | 3 | 0 |
| 1 | D | 748 | CME | 1 | 0 |
| 1 | D | 914 | CME | 1 | 0 |
| 1 | E | 1021 | CME | 3 | 0 |
| 1 | F | 1021 | CME | 3 | 0 |
| 1 | G | 1021 | CME | 3 | 0 |
| 1 | G | 914 | CME | 1 | 0 |
| 1 | H | 1021 | CME | 3 | 0 |
| 1 | H | 914 | CME | 1 | 0 |
| 1 | I | 1021 | CME | 3 | 0 |
| 1 | I | 914 | CME | 1 | 0 |
| 1 | J | 1021 | CME | 3 | 0 |
| 1 | J | 914 | CME | 1 | 0 |
| 1 | K | 1021 | CME | 3 | 0 |
| 1 | K | 748 | CME | 1 | 0 |
| 1 | K | 914 | CME | 1 | 0 |
| 1 | L | 1021 | CME | 3 | 0 |
| 1 | L | 914 | CME | 1 | 0 |
| 1 | M | 1021 | CME | 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | N | 1021 | CME | 3 | 0 |
| 1 | N | 914 | CME | 1 | 0 |
| 1 | O | 1021 | CME | 3 | 0 |
| 1 | O | 914 | CME | 1 | 0 |
| 1 | P | 1021 | CME | 3 | 0 |
| 1 | P | 914 | CME | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|---------|
| 1 | A | 1018/1023 (99%) | -0.82 | 5 (0%) 91 92 | 3, 21, 66, 100 | 1 (0%) |
| 1 | B | 1018/1023 (99%) | -0.88 | 0 100 100 | 3, 21, 66, 100 | 1 (0%) |
| 1 | C | 1018/1023 (99%) | -0.76 | 1 (0%) 95 96 | 2, 19, 63, 98 | 1 (0%) |
| 1 | D | 1018/1023 (99%) | -0.79 | 0 100 100 | 5, 24, 67, 100 | 1 (0%) |
| 1 | E | 1018/1023 (99%) | -0.58 | 4 (0%) 93 93 | 15, 33, 74, 100 | 1 (0%) |
| 1 | F | 1018/1023 (99%) | -0.83 | 1 (0%) 95 96 | 3, 21, 66, 100 | 1 (0%) |
| 1 | G | 1018/1023 (99%) | -0.87 | 1 (0%) 95 96 | 7, 25, 68, 100 | 1 (0%) |
| 1 | H | 1018/1023 (99%) | -0.61 | 4 (0%) 93 93 | 14, 33, 73, 100 | 1 (0%) |
| 1 | I | 1018/1023 (99%) | -0.76 | 1 (0%) 95 96 | 10, 28, 70, 100 | 1 (0%) |
| 1 | J | 1018/1023 (99%) | -0.77 | 1 (0%) 95 96 | 8, 26, 69, 100 | 1 (0%) |
| 1 | K | 1018/1023 (99%) | -0.65 | 7 (0%) 89 90 | 17, 35, 76, 100 | 1 (0%) |
| 1 | L | 1018/1023 (99%) | -0.58 | 5 (0%) 91 92 | 16, 34, 75, 100 | 1 (0%) |
| 1 | M | 1018/1023 (99%) | -0.20 | 20 (1%) 68 72 | 22, 40, 79, 100 | 1 (0%) |
| 1 | N | 1018/1023 (99%) | -0.71 | 0 100 100 | 11, 29, 71, 100 | 1 (0%) |
| 1 | O | 1018/1023 (99%) | -0.78 | 2 (0%) 95 96 | 12, 30, 72, 100 | 1 (0%) |
| 1 | P | 1018/1023 (99%) | 0.32 | 78 (7%) 16 18 | 29, 47, 83, 100 | 1 (0%) |
| All | All | 16288/16368 (99%) | -0.64 | 130 (0%) 87 89 | 2, 30, 72, 100 | 16 (0%) |

All (130) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | K | 735 | HIS | 5.5 |
| 1 | P | 313 | VAL | 5.5 |
| 1 | P | 739 | HIS | 5.4 |
| 1 | P | 70 | PRO | 5.3 |
| 1 | O | 735 | HIS | 4.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | L | 735 | HIS | 4.7 |
| 1 | P | 143 | PHE | 4.6 |
| 1 | P | 732 | ALA | 4.4 |
| 1 | P | 115 | PRO | 4.3 |
| 1 | P | 133 | TRP | 4.2 |
| 1 | M | 575 | LEU | 4.1 |
| 1 | P | 731 | PRO | 4.1 |
| 1 | H | 735 | HIS | 4.0 |
| 1 | A | 580 | GLU | 4.0 |
| 1 | P | 55 | ASN | 3.9 |
| 1 | P | 158 | TRP | 3.9 |
| 1 | P | 129 | VAL | 3.9 |
| 1 | P | 149 | ALA | 3.7 |
| 1 | A | 582 | GLY | 3.7 |
| 1 | P | 203 | TRP | 3.7 |
| 1 | P | 364 | GLY | 3.6 |
| 1 | P | 97 | ALA | 3.6 |
| 1 | P | 141 | ILE | 3.6 |
| 1 | P | 204 | ARG | 3.5 |
| 1 | P | 73 | TRP | 3.5 |
| 1 | P | 34 | ALA | 3.5 |
| 1 | K | 734 | SER | 3.5 |
| 1 | P | 735 | HIS | 3.5 |
| 1 | L | 739 | HIS | 3.4 |
| 1 | P | 81 | ALA | 3.4 |
| 1 | P | 595 | THR | 3.3 |
| 1 | P | 68 | ALA | 3.3 |
| 1 | M | 66 | PRO | 3.2 |
| 1 | P | 799 | THR | 3.2 |
| 1 | P | 191 | TRP | 3.2 |
| 1 | M | 6 | SER | 3.2 |
| 1 | M | 162 | GLY | 3.1 |
| 1 | L | 687 | GLN | 3.1 |
| 1 | K | 730 | LEU | 3.0 |
| 1 | P | 733 | ALA | 3.0 |
| 1 | M | 177 | LEU | 3.0 |
| 1 | M | 73 | TRP | 3.0 |
| 1 | G | 735 | HIS | 3.0 |
| 1 | P | 180 | GLY | 2.9 |
| 1 | P | 684 | GLU | 2.9 |
| 1 | A | 735 | HIS | 2.9 |
| 1 | M | 69 | VAL | 2.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | P | 7 | LEU | 2.9 |
| 1 | P | 35 | SER | 2.9 |
| 1 | P | 9 | VAL | 2.8 |
| 1 | M | 149 | ALA | 2.8 |
| 1 | P | 209 | PHE | 2.8 |
| 1 | P | 317 | THR | 2.8 |
| 1 | M | 75 | GLU | 2.8 |
| 1 | P | 51 | LEU | 2.8 |
| 1 | P | 160 | GLY | 2.8 |
| 1 | C | 581 | ASN | 2.8 |
| 1 | P | 185 | ALA | 2.8 |
| 1 | P | 579 | ASP | 2.8 |
| 1 | P | 575 | LEU | 2.8 |
| 1 | A | 581 | ASN | 2.8 |
| 1 | E | 160 | GLY | 2.7 |
| 1 | P | 800 | ARG | 2.7 |
| 1 | P | 102 | ASN | 2.7 |
| 1 | P | 585 | TRP | 2.7 |
| 1 | P | 689 | GLU | 2.7 |
| 1 | M | 16 | TRP | 2.7 |
| 1 | K | 732 | ALA | 2.7 |
| 1 | P | 100 | TYR | 2.7 |
| 1 | E | 66 | PRO | 2.6 |
| 1 | M | 160 | GLY | 2.6 |
| 1 | P | 195 | SER | 2.6 |
| 1 | J | 581 | ASN | 2.6 |
| 1 | P | 85 | VAL | 2.6 |
| 1 | M | 735 | HIS | 2.6 |
| 1 | P | 174 | SER | 2.5 |
| 1 | M | 173 | LEU | 2.5 |
| 1 | P | 594 | ASP | 2.5 |
| 1 | P | 580 | GLU | 2.5 |
| 1 | P | 221 | GLN | 2.5 |
| 1 | P | 884 | LEU | 2.5 |
| 1 | K | 731 | PRO | 2.5 |
| 1 | E | 143 | PHE | 2.5 |
| 1 | P | 138 | GLN | 2.5 |
| 1 | F | 689 | GLU | 2.4 |
| 1 | P | 178 | ARG | 2.4 |
| 1 | P | 122 | CYS | 2.4 |
| 1 | M | 596 | PRO | 2.4 |
| 1 | P | 683 | PRO | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | M | 249 | GLU | 2.4 |
| 1 | P | 162 | GLY | 2.3 |
| 1 | K | 739 | HIS | 2.3 |
| 1 | P | 596 | PRO | 2.3 |
| 1 | P | 58 | TRP | 2.3 |
| 1 | H | 580 | GLU | 2.3 |
| 1 | I | 735 | HIS | 2.3 |
| 1 | P | 249 | GLU | 2.3 |
| 1 | M | 115 | PRO | 2.3 |
| 1 | P | 574 | SER | 2.3 |
| 1 | H | 4 | THR | 2.3 |
| 1 | H | 129 | VAL | 2.3 |
| 1 | M | 133 | TRP | 2.2 |
| 1 | P | 172 | ASP | 2.2 |
| 1 | P | 153 | TRP | 2.2 |
| 1 | P | 261 | TRP | 2.2 |
| 1 | M | 125 | LEU | 2.2 |
| 1 | P | 215 | LEU | 2.2 |
| 1 | P | 274 | PHE | 2.2 |
| 1 | A | 682 | LEU | 2.1 |
| 1 | P | 321 | THR | 2.1 |
| 1 | P | 65 | ALA | 2.1 |
| 1 | P | 86 | VAL | 2.1 |
| 1 | P | 131 | GLU | 2.1 |
| 1 | O | 733 | ALA | 2.1 |
| 1 | P | 202 | MET | 2.1 |
| 1 | P | 137 | GLY | 2.1 |
| 1 | L | 732 | ALA | 2.1 |
| 1 | M | 135 | GLN | 2.1 |
| 1 | M | 123 | TYR | 2.1 |
| 1 | P | 123 | TYR | 2.1 |
| 1 | P | 161 | TYR | 2.1 |
| 1 | E | 79 | PRO | 2.1 |
| 1 | P | 214 | LEU | 2.1 |
| 1 | P | 135 | GLN | 2.1 |
| 1 | P | 687 | GLN | 2.1 |
| 1 | K | 736 | ALA | 2.0 |
| 1 | P | 218 | PRO | 2.0 |
| 1 | P | 16 | TRP | 2.0 |
| 1 | P | 923 | SER | 2.0 |
| 1 | L | 578 | TYR | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 1 | CME | P | 748 | 10/11 | 0.92 | 0.12 | - | 44,54,100,100 | 0 |
| 1 | CME | P | 914 | 10/11 | 0.91 | 0.11 | - | 34,40,100,100 | 0 |
| 1 | CME | L | 914 | 10/11 | 0.96 | 0.09 | - | 21,27,100,100 | 0 |
| 1 | CME | G | 748 | 10/11 | 0.94 | 0.09 | - | 22,32,100,100 | 0 |
| 1 | CME | H | 914 | 10/11 | 0.96 | 0.11 | - | 19,25,100,100 | 0 |
| 1 | CME | G | 914 | 10/11 | 0.97 | 0.07 | - | 12,18,100,100 | 0 |
| 1 | CME | A | 1021 | 10/11 | 0.95 | 0.10 | - | 2,25,100,100 | 0 |
| 1 | CME | F | 914 | 10/11 | 0.97 | 0.12 | - | 8,14,100,100 | 0 |
| 1 | CME | C | 914 | 10/11 | 0.97 | 0.10 | - | 6,12,97,97 | 0 |
| 1 | CME | B | 914 | 10/11 | 0.97 | 0.08 | - | 8,14,99,99 | 0 |
| 1 | CME | C | 748 | 10/11 | 0.92 | 0.12 | - | 16,26,97,97 | 0 |
| 1 | CME | N | 1021 | 10/11 | 0.92 | 0.11 | - | 9,33,100,100 | 0 |
| 1 | CME | M | 748 | 10/11 | 0.96 | 0.10 | - | 37,47,100,100 | 0 |
| 1 | CME | O | 748 | 10/11 | 0.92 | 0.12 | - | 27,37,100,100 | 0 |
| 1 | CME | P | 1021 | 10/11 | 0.91 | 0.13 | - | 28,51,100,100 | 0 |
| 1 | CME | O | 914 | 10/11 | 0.96 | 0.08 | - | 17,23,100,100 | 0 |
| 1 | CME | E | 748 | 10/11 | 0.95 | 0.10 | - | 30,40,100,100 | 0 |
| 1 | CME | J | 914 | 10/11 | 0.97 | 0.10 | - | 13,19,100,100 | 0 |
| 1 | CME | L | 1021 | 10/11 | 0.95 | 0.09 | - | 15,38,100,100 | 0 |
| 1 | CME | D | 1021 | 10/11 | 0.94 | 0.13 | - | 4,27,100,100 | 0 |
| 1 | CME | E | 914 | 10/11 | 0.97 | 0.12 | - | 20,26,100,100 | 0 |
| 1 | CME | F | 748 | 10/11 | 0.95 | 0.09 | - | 18,28,100,100 | 0 |
| 1 | CME | N | 914 | 10/11 | 0.97 | 0.08 | - | 16,22,100,100 | 0 |
| 1 | CME | M | 1021 | 10/11 | 0.92 | 0.13 | - | 21,44,100,100 | 0 |
| 1 | CME | I | 914 | 10/11 | 0.97 | 0.11 | - | 15,21,100,100 | 0 |
| 1 | CME | I | 748 | 10/11 | 0.96 | 0.10 | - | 25,35,100,100 | 0 |
| 1 | CME | H | 748 | 10/11 | 0.93 | 0.13 | - | 29,39,100,100 | 0 |
| 1 | CME | K | 914 | 10/11 | 0.95 | 0.09 | - | 22,28,100,100 | 0 |
| 1 | CME | M | 914 | 10/11 | 0.95 | 0.13 | - | 27,33,100,100 | 0 |
| 1 | CME | B | 1021 | 10/11 | 0.95 | 0.08 | - | 2,25,99,99 | 0 |
| 1 | CME | J | 748 | 10/11 | 0.96 | 0.08 | - | 23,33,100,100 | 0 |
| 1 | CME | L | 748 | 10/11 | 0.90 | 0.17 | - | 31,41,100,100 | 0 |
| 1 | CME | N | 748 | 10/11 | 0.97 | 0.07 | - | 26,35,100,100 | 0 |
| 1 | CME | K | 1021 | 10/11 | 0.96 | 0.16 | - | 16,39,100,100 | 0 |
| 1 | CME | B | 748 | 10/11 | 0.93 | 0.08 | - | 18,28,99,99 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 1 | CME | K | 748 | 10/11 | 0.91 | 0.15 | - | 32,42,100,100 | 0 |
| 1 | CME | C | 1021 | 10/11 | 0.93 | 0.11 | - | 1,23,97,97 | 0 |
| 1 | CME | A | 914 | 10/11 | 0.97 | 0.10 | - | 8,14,100,100 | 0 |
| 1 | CME | D | 748 | 10/11 | 0.93 | 0.16 | - | 21,30,100,100 | 0 |
| 1 | CME | A | 748 | 10/11 | 0.96 | 0.09 | - | 18,28,100,100 | 0 |
| 1 | CME | F | 1021 | 10/11 | 0.93 | 0.11 | - | 2,25,100,100 | 0 |
| 1 | CME | D | 914 | 10/11 | 0.97 | 0.10 | - | 10,16,100,100 | 0 |
| 1 | CME | E | 1021 | 10/11 | 0.92 | 0.12 | - | 14,37,100,100 | 0 |
| 1 | CME | J | 1021 | 10/11 | 0.94 | 0.10 | - | 7,30,100,100 | 0 |
| 1 | CME | I | 1021 | 10/11 | 0.93 | 0.13 | - | 9,32,100,100 | 0 |
| 1 | CME | H | 1021 | 10/11 | 0.89 | 0.14 | - | 13,36,100,100 | 0 |
| 1 | CME | O | 1021 | 10/11 | 0.95 | 0.14 | - | 11,34,100,100 | 0 |
| 1 | CME | G | 1021 | 10/11 | 0.96 | 0.09 | - | 6,29,100,100 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2 | MG | A | 3002 | 1/1 | 0.97 | 0.12 | 1.25 | 18,18,18,18 | 0 |
| 2 | MG | J | 3002 | 1/1 | 0.95 | 0.12 | 1.11 | 23,23,23,23 | 0 |
| 2 | MG | C | 3002 | 1/1 | 0.94 | 0.11 | 0.31 | 16,16,16,16 | 0 |
| 2 | MG | D | 3002 | 1/1 | 0.96 | 0.10 | 0.31 | 21,21,21,21 | 0 |
| 2 | MG | N | 3002 | 1/1 | 0.94 | 0.13 | 0.27 | 26,26,26,26 | 0 |
| 2 | MG | F | 3001 | 1/1 | 0.88 | 0.10 | 0.25 | 18,18,18,18 | 0 |
| 2 | MG | O | 3002 | 1/1 | 0.96 | 0.12 | 0.03 | 27,27,27,27 | 0 |
| 2 | MG | M | 3002 | 1/1 | 0.90 | 0.19 | -0.07 | 37,37,37,37 | 0 |
| 2 | MG | A | 3001 | 1/1 | 0.91 | 0.09 | -0.09 | 18,18,18,18 | 0 |
| 2 | MG | H | 3002 | 1/1 | 0.98 | 0.12 | -0.36 | 30,30,30,30 | 0 |
| 2 | MG | I | 3002 | 1/1 | 0.84 | 0.10 | -0.48 | 25,25,25,25 | 0 |
| 2 | MG | F | 3002 | 1/1 | 0.95 | 0.08 | -0.73 | 19,19,19,19 | 0 |
| 2 | MG | L | 3002 | 1/1 | 0.97 | 0.09 | -0.88 | 31,31,31,31 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 2 | MG | E | 3002 | 1/1 | 0.88 | 0.10 | -1.00 | 30,30,30,30 | 0 |
| 2 | MG | M | 3001 | 1/1 | 0.91 | 0.10 | -1.08 | 37,37,37,37 | 0 |
| 2 | MG | P | 3001 | 1/1 | 0.85 | 0.10 | -1.24 | 44,44,44,44 | 0 |
| 2 | MG | K | 3001 | 1/1 | 0.96 | 0.08 | -1.52 | 32,32,32,32 | 0 |
| 2 | MG | K | 3002 | 1/1 | 0.93 | 0.08 | -1.73 | 32,32,32,32 | 0 |
| 2 | MG | I | 3001 | 1/1 | 0.95 | 0.05 | -1.96 | 25,25,25,25 | 0 |
| 2 | MG | B | 3001 | 1/1 | 0.97 | 0.08 | -2.00 | 18,18,18,18 | 0 |
| 2 | MG | J | 3001 | 1/1 | 0.93 | 0.04 | -2.25 | 23,23,23,23 | 0 |
| 2 | MG | L | 3001 | 1/1 | 0.84 | 0.06 | -2.28 | 31,31,31,31 | 0 |
| 2 | MG | P | 3002 | 1/1 | 0.83 | 0.10 | -2.96 | 44,44,44,44 | 0 |
| 2 | MG | D | 3001 | 1/1 | 0.93 | 0.04 | -3.46 | 20,20,20,20 | 0 |
| 2 | MG | G | 3001 | 1/1 | 0.95 | 0.04 | -3.57 | 22,22,22,22 | 0 |
| 2 | MG | B | 3002 | 1/1 | 0.97 | 0.06 | -3.66 | 18,18,18,18 | 0 |
| 2 | MG | H | 3001 | 1/1 | 0.94 | 0.04 | -3.97 | 29,29,29,29 | 0 |
| 2 | MG | E | 3001 | 1/1 | 0.97 | 0.03 | -4.24 | 30,30,30,30 | 0 |
| 2 | MG | G | 3002 | 1/1 | 0.96 | 0.05 | -4.39 | 22,22,22,22 | 0 |
| 2 | MG | O | 3001 | 1/1 | 0.98 | 0.05 | -5.18 | 27,27,27,27 | 0 |
| 2 | MG | C | 3001 | 1/1 | 0.97 | 0.04 | -5.54 | 16,16,16,16 | 0 |
| 2 | MG | N | 3001 | 1/1 | 0.92 | 0.04 | -9.20 | 26,26,26,26 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.