



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:13 AM GMT

PDB ID : 1QXP
Title : Crystal Structure of a mu-like calpain
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.
Deposited on : 2003-09-08
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

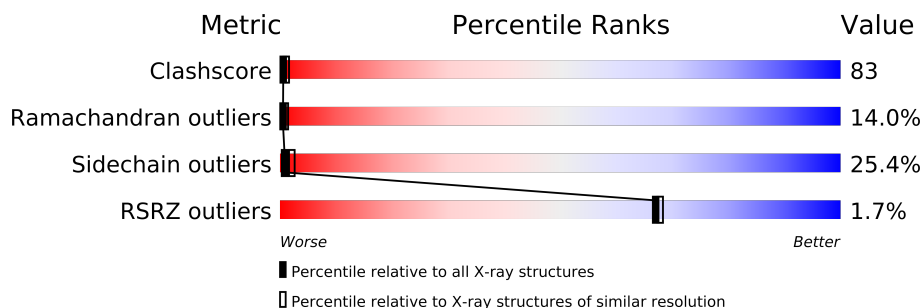
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 2295 (2.80-2.80) |
| Ramachandran outliers | 78287 | 2252 (2.80-2.80) |
| Sidechain outliers | 78261 | 2254 (2.80-2.80) |
| RSRZ outliers | 66119 | 1802 (2.80-2.80) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 900 |  |
| 1 | B | 900 |  |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12368 atoms, of which 0 are hydrogen and 0 are deuterium.

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 mu-like calpain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 783 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6053 | 3846 | 1037 | 1143 | 27 | | | |
| 1 | B | 788 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6003 | 3830 | 1015 | 1129 | 29 | | | |

There are 30 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 105 | SER | CYS | ENGINEERED | UNP P97571 |
| A | 702A | GLY | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702B | LYS | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702C | LEU | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702D | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702E | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702F | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702G | ILE | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702H | GLU | - | CLONING ARTIFACT | UNP Q07009 |
| A | 702I | HIS | - | EXPRESSION TAG | UNP Q07009 |
| A | 702J | HIS | - | EXPRESSION TAG | UNP Q07009 |
| A | 702K | HIS | - | EXPRESSION TAG | UNP Q07009 |
| A | 702L | HIS | - | EXPRESSION TAG | UNP Q07009 |
| A | 702M | HIS | - | EXPRESSION TAG | UNP Q07009 |
| A | 702N | HIS | - | EXPRESSION TAG | UNP Q07009 |
| B | 105 | SER | CYS | ENGINEERED | UNP P97571 |
| B | 702A | GLY | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702B | LYS | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702C | LEU | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702D | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702E | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702F | ALA | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702G | ILE | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702H | GLU | - | CLONING ARTIFACT | UNP Q07009 |
| B | 702I | HIS | - | EXPRESSION TAG | UNP Q07009 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 702J | HIS | - | EXPRESSION TAG | UNP Q07009 |
| B | 702K | HIS | - | EXPRESSION TAG | UNP Q07009 |
| B | 702L | HIS | - | EXPRESSION TAG | UNP Q07009 |
| B | 702M | HIS | - | EXPRESSION TAG | UNP Q07009 |
| B | 702N | HIS | - | EXPRESSION TAG | UNP Q07009 |

- Molecule 2 is water.

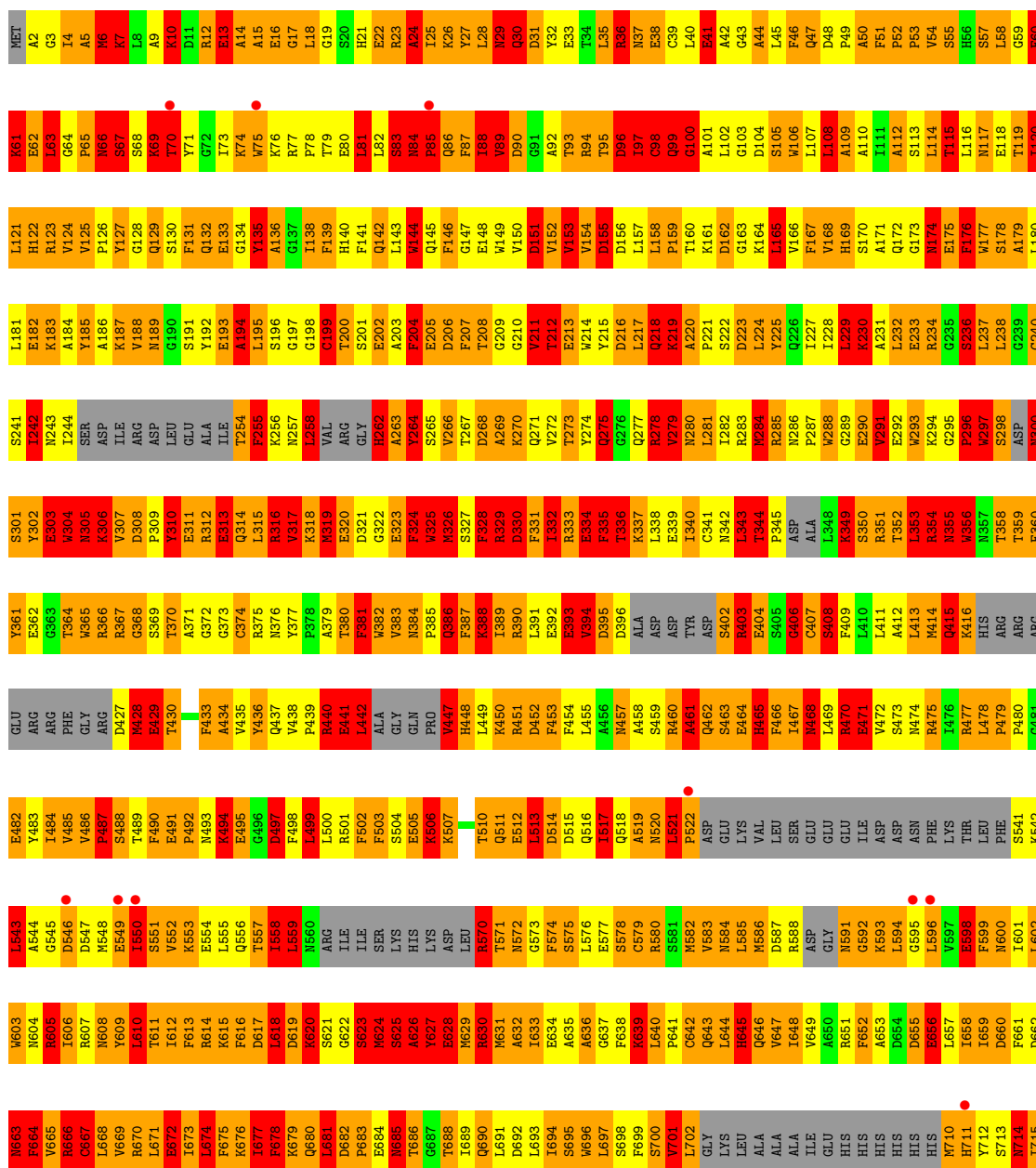
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2 | A | 172 | Total | O | 0 | 0 |
| | | | 172 | 172 | | |
| 2 | B | 140 | Total | O | 0 | 0 |
| | | | 140 | 140 | | |

3 Residue-property plots

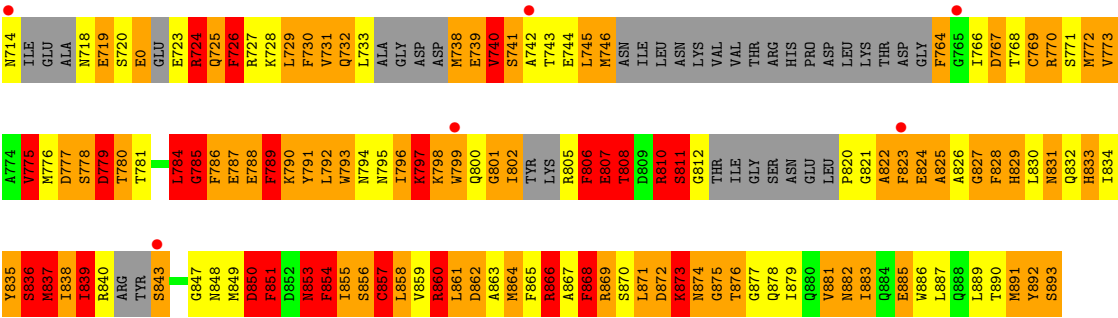
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: mu-like calpain

Chain A: 







4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00° | Depositor |
| Resolution (Å) | 91.29 – 2.80 49.81 – 2.69 | Depositor EDS |
| % Data completeness (in resolution range) | 91.6 (91.29-2.80) 87.3 (49.81-2.69) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.04 (at 2.69Å) | Xtriage |
| Refinement program | REFMAC 5.1.24 | Depositor |
| R, R_{free} | 0.229 , 0.311 0.241 , (Not available) | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 55.6 | Xtriage |
| Anisotropy | 0.074 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 75.5 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 0 of 55542 reflections | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 12368 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 | 3.70 | 964/6177 (15.6%) | 2.67 | 470/8354 (5.6%) |
| 1 | B | 3.71 | 932/6128 (15.2%) | 2.67 | 489/8288 (5.9%) |
| All | All | 3.70 | 1896/12305 (15.4%) | 2.67 | 959/16642 (5.8%) |

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 | 0 | 45 |
| 1 | B | 0 | 39 |
| All | All | 0 | 84 |

All (1896) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 67 | SER | CA-CB | 28.73 | 1.96 | 1.52 |
| 1 | A | 339 | GLU | CD-OE1 | 23.66 | 1.51 | 1.25 |
| 1 | A | 320 | GLU | CD-OE2 | 20.06 | 1.47 | 1.25 |
| 1 | B | 429 | GLU | CD-OE1 | 19.54 | 1.47 | 1.25 |
| 1 | A | 811 | SER | CA-CB | -18.37 | 1.25 | 1.52 |
| 1 | B | 185 | TYR | CD1-CE1 | -18.14 | 1.12 | 1.39 |
| 1 | B | 316 | ARG | CA-CB | 17.98 | 1.93 | 1.53 |
| 1 | B | 6 | MET | CG-SD | 17.54 | 2.26 | 1.81 |
| 1 | A | 680 | GLN | CA-CB | 17.33 | 1.92 | 1.53 |
| 1 | B | 869 | ARG | CA-CB | 17.27 | 1.92 | 1.53 |
| 1 | B | 806 | PHE | CB-CG | 16.50 | 1.79 | 1.51 |
| 1 | A | 428 | MET | CG-SD | 16.32 | 2.23 | 1.81 |
| 1 | A | 310 | TYR | CG-CD2 | 16.27 | 1.60 | 1.39 |
| 1 | A | 310 | TYR | CE2-CZ | 15.93 | 1.59 | 1.38 |
| 1 | A | 6 | MET | CG-SD | 15.67 | 2.21 | 1.81 |
| 1 | A | 671 | LEU | CA-CB | 15.34 | 1.89 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 436 | TYR | CD1-CE1 | 15.24 | 1.62 | 1.39 |
| 1 | B | 312 | ARG | CG-CD | 15.22 | 1.90 | 1.51 |
| 1 | B | 609 | TYR | CD1-CE1 | 15.16 | 1.62 | 1.39 |
| 1 | B | 291 | VAL | CA-CB | -15.02 | 1.23 | 1.54 |
| 1 | A | 75 | TRP | CB-CG | 15.01 | 1.77 | 1.50 |
| 1 | B | 332 | ILE | CB-CG2 | 14.84 | 1.98 | 1.52 |
| 1 | A | 452 | ASP | CB-CG | 14.82 | 1.82 | 1.51 |
| 1 | A | 193 | GLU | CD-OE2 | 14.79 | 1.42 | 1.25 |
| 1 | A | 460 | ARG | CZ-NH2 | 14.75 | 1.52 | 1.33 |
| 1 | A | 803 | TYR | CD1-CE1 | 14.67 | 1.61 | 1.39 |
| 1 | B | 824 | GLU | CA-CB | 14.57 | 1.86 | 1.53 |
| 1 | A | 337 | LYS | CE-NZ | 14.46 | 1.85 | 1.49 |
| 1 | B | 320 | GLU | CD-OE2 | 14.46 | 1.41 | 1.25 |
| 1 | A | 110 | ALA | CA-CB | -14.36 | 1.22 | 1.52 |
| 1 | B | 154 | VAL | CB-CG2 | -14.26 | 1.23 | 1.52 |
| 1 | B | 324 | PHE | CD1-CE1 | 14.19 | 1.67 | 1.39 |
| 1 | A | 331 | PHE | CE1-CZ | 14.07 | 1.64 | 1.37 |
| 1 | B | 233 | GLU | CD-OE1 | 13.99 | 1.41 | 1.25 |
| 1 | A | 317 | VAL | CA-CB | 13.98 | 1.84 | 1.54 |
| 1 | B | 440 | ARG | CG-CD | 13.94 | 1.86 | 1.51 |
| 1 | B | 726 | PHE | CE1-CZ | 13.87 | 1.63 | 1.37 |
| 1 | B | 328 | PHE | CD1-CE1 | -13.85 | 1.11 | 1.39 |
| 1 | B | 323 | GLU | CD-OE1 | 13.82 | 1.40 | 1.25 |
| 1 | A | 463 | SER | C-O | -13.50 | 0.97 | 1.23 |
| 1 | B | 176 | PHE | CE1-CZ | -13.37 | 1.11 | 1.37 |
| 1 | B | 669 | VAL | CA-CB | 13.31 | 1.82 | 1.54 |
| 1 | A | 429 | GLU | CD-OE1 | 13.31 | 1.40 | 1.25 |
| 1 | A | 360 | PHE | CE1-CZ | 13.30 | 1.62 | 1.37 |
| 1 | A | 225 | TYR | CD2-CE2 | 13.28 | 1.59 | 1.39 |
| 1 | B | 744 | GLU | CD-OE1 | 13.23 | 1.40 | 1.25 |
| 1 | A | 149 | TRP | CE3-CZ3 | -13.14 | 1.16 | 1.38 |
| 1 | A | 656 | GLU | CD-OE1 | 13.13 | 1.40 | 1.25 |
| 1 | A | 218 | GLN | CB-CG | 13.06 | 1.87 | 1.52 |
| 1 | B | 672 | GLU | CD-OE1 | 13.00 | 1.40 | 1.25 |
| 1 | A | 89 | VAL | CB-CG1 | 12.99 | 1.80 | 1.52 |
| 1 | A | 485 | VAL | CB-CG1 | -12.97 | 1.25 | 1.52 |
| 1 | A | 193 | GLU | CD-OE1 | 12.94 | 1.39 | 1.25 |
| 1 | B | 495 | GLU | CD-OE1 | 12.90 | 1.39 | 1.25 |
| 1 | A | 133 | GLU | CD-OE1 | 12.89 | 1.39 | 1.25 |
| 1 | A | 204 | PHE | CE2-CZ | 12.89 | 1.61 | 1.37 |
| 1 | B | 69 | LYS | CB-CG | 12.86 | 1.87 | 1.52 |
| 1 | A | 860 | ARG | CZ-NH2 | 12.81 | 1.49 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 616 | PHE | CE1-CZ | -12.78 | 1.13 | 1.37 |
| 1 | B | 361 | TYR | CD1-CE1 | 12.76 | 1.58 | 1.39 |
| 1 | B | 135 | TYR | CD1-CE1 | -12.75 | 1.20 | 1.39 |
| 1 | B | 297 | TRP | CZ3-CH2 | -12.64 | 1.19 | 1.40 |
| 1 | B | 226 | GLN | CG-CD | 12.60 | 1.80 | 1.51 |
| 1 | B | 441 | GLU | CA-CB | -12.58 | 1.26 | 1.53 |
| 1 | A | 329 | ARG | CZ-NH1 | 12.55 | 1.49 | 1.33 |
| 1 | A | 627 | TYR | CE2-CZ | -12.51 | 1.22 | 1.38 |
| 1 | A | 177 | TRP | CG-CD1 | -12.50 | 1.19 | 1.36 |
| 1 | B | 346 | ASP | CB-CG | 12.48 | 1.77 | 1.51 |
| 1 | A | 584 | ASN | CB-CG | -12.45 | 1.22 | 1.51 |
| 1 | B | 360 | PHE | CB-CG | -12.43 | 1.30 | 1.51 |
| 1 | B | 366 | ARG | NE-CZ | -12.41 | 1.17 | 1.33 |
| 1 | A | 41 | GLU | CG-CD | 12.39 | 1.70 | 1.51 |
| 1 | B | 328 | PHE | CE1-CZ | -12.34 | 1.13 | 1.37 |
| 1 | B | 90 | ASP | CB-CG | 12.34 | 1.77 | 1.51 |
| 1 | B | 678 | PHE | CD2-CE2 | -12.34 | 1.14 | 1.39 |
| 1 | B | 665 | VAL | CB-CG2 | -12.30 | 1.27 | 1.52 |
| 1 | B | 828 | PHE | CE2-CZ | 12.30 | 1.60 | 1.37 |
| 1 | B | 672 | GLU | CD-OE2 | 12.26 | 1.39 | 1.25 |
| 1 | B | 335 | PHE | CE2-CZ | 12.25 | 1.60 | 1.37 |
| 1 | B | 9 | ALA | CA-CB | -12.19 | 1.26 | 1.52 |
| 1 | B | 188 | VAL | CB-CG2 | -12.19 | 1.27 | 1.52 |
| 1 | B | 89 | VAL | CB-CG1 | 12.18 | 1.78 | 1.52 |
| 1 | B | 146 | PHE | CD2-CE2 | -12.18 | 1.14 | 1.39 |
| 1 | B | 362 | GLU | CG-CD | 12.11 | 1.70 | 1.51 |
| 1 | B | 643 | GLN | CG-CD | 12.10 | 1.78 | 1.51 |
| 1 | A | 392 | GLU | C-O | 12.10 | 1.46 | 1.23 |
| 1 | B | 313 | GLU | CB-CG | 12.09 | 1.75 | 1.52 |
| 1 | A | 174 | ASN | CB-CG | 12.06 | 1.78 | 1.51 |
| 1 | A | 434 | ALA | C-O | -12.04 | 1.00 | 1.23 |
| 1 | B | 369 | SER | CB-OG | -11.97 | 1.26 | 1.42 |
| 1 | A | 27 | TYR | CD1-CE1 | 11.86 | 1.57 | 1.39 |
| 1 | B | 690 | GLN | CB-CG | 11.81 | 1.84 | 1.52 |
| 1 | B | 142 | GLN | CB-CG | 11.77 | 1.84 | 1.52 |
| 1 | B | 341 | CYS | CB-SG | 11.73 | 2.02 | 1.82 |
| 1 | B | 87 | PHE | CE2-CZ | 11.72 | 1.59 | 1.37 |
| 1 | B | 464 | GLU | CG-CD | 11.71 | 1.69 | 1.51 |
| 1 | B | 176 | PHE | CE2-CZ | -11.71 | 1.15 | 1.37 |
| 1 | A | 303 | GLU | CD-OE2 | -11.70 | 1.12 | 1.25 |
| 1 | A | 826 | ALA | CA-CB | 11.66 | 1.76 | 1.52 |
| 1 | A | 773 | VAL | CB-CG1 | 11.64 | 1.77 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 394 | VAL | CB-CG2 | -11.63 | 1.28 | 1.52 |
| 1 | A | 124 | VAL | CB-CG2 | -11.57 | 1.28 | 1.52 |
| 1 | B | 883 | ILE | CA-CB | 11.57 | 1.81 | 1.54 |
| 1 | A | 665 | VAL | CB-CG2 | -11.54 | 1.28 | 1.52 |
| 1 | A | 616 | PHE | CG-CD2 | -11.52 | 1.21 | 1.38 |
| 1 | B | 225 | TYR | CE1-CZ | -11.50 | 1.23 | 1.38 |
| 1 | A | 379 | ALA | CA-CB | -11.49 | 1.28 | 1.52 |
| 1 | A | 652 | PHE | CD1-CE1 | 11.46 | 1.62 | 1.39 |
| 1 | B | 811 | SER | CA-CB | 11.42 | 1.70 | 1.52 |
| 1 | A | 387 | PHE | CE2-CZ | 11.42 | 1.59 | 1.37 |
| 1 | A | 669 | VAL | CB-CG1 | 11.40 | 1.76 | 1.52 |
| 1 | A | 631 | MET | SD-CE | 11.37 | 2.41 | 1.77 |
| 1 | B | 13 | GLU | CD-OE2 | 11.36 | 1.38 | 1.25 |
| 1 | B | 13 | GLU | CD-OE1 | 11.35 | 1.38 | 1.25 |
| 1 | A | 504 | SER | CB-OG | 11.32 | 1.56 | 1.42 |
| 1 | B | 68 | SER | C-O | -11.28 | 1.01 | 1.23 |
| 1 | B | 320 | GLU | CD-OE1 | 11.27 | 1.38 | 1.25 |
| 1 | A | 639 | LYS | CE-NZ | 11.26 | 1.77 | 1.49 |
| 1 | A | 280 | ASN | CG-OD1 | -11.23 | 0.99 | 1.24 |
| 1 | B | 199 | CYS | CB-SG | 11.18 | 2.01 | 1.82 |
| 1 | B | 198 | GLY | C-O | 11.17 | 1.41 | 1.23 |
| 1 | A | 613 | PHE | CB-CG | -11.09 | 1.32 | 1.51 |
| 1 | B | 881 | VAL | CB-CG2 | -11.08 | 1.29 | 1.52 |
| 1 | B | 740 | VAL | CB-CG1 | 11.02 | 1.76 | 1.52 |
| 1 | A | 41 | GLU | CD-OE1 | 11.00 | 1.37 | 1.25 |
| 1 | A | 831 | ASN | CG-OD1 | 10.99 | 1.48 | 1.24 |
| 1 | B | 579 | CYS | CA-CB | 10.99 | 1.78 | 1.53 |
| 1 | A | 503 | PHE | CE2-CZ | -10.97 | 1.16 | 1.37 |
| 1 | A | 99 | GLN | CA-CB | 10.96 | 1.78 | 1.53 |
| 1 | A | 274 | TYR | CE1-CZ | -10.96 | 1.24 | 1.38 |
| 1 | A | 215 | TYR | CE1-CZ | 10.96 | 1.52 | 1.38 |
| 1 | A | 505 | GLU | CG-CD | 10.96 | 1.68 | 1.51 |
| 1 | B | 335 | PHE | CD1-CE1 | 10.95 | 1.61 | 1.39 |
| 1 | A | 739 | GLU | CD-OE2 | 10.94 | 1.37 | 1.25 |
| 1 | B | 661 | PHE | CE2-CZ | 10.88 | 1.58 | 1.37 |
| 1 | B | 857 | CYS | CB-SG | 10.86 | 2.00 | 1.82 |
| 1 | A | 175 | GLU | CG-CD | 10.84 | 1.68 | 1.51 |
| 1 | A | 627 | TYR | CB-CG | 10.80 | 1.67 | 1.51 |
| 1 | A | 570 | ARG | CB-CG | 10.80 | 1.81 | 1.52 |
| 1 | A | 831 | ASN | CB-CG | 10.79 | 1.75 | 1.51 |
| 1 | A | 630 | ARG | CZ-NH2 | 10.78 | 1.47 | 1.33 |
| 1 | A | 166 | VAL | CB-CG2 | -10.75 | 1.30 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 7 | LYS | CD-CE | 10.73 | 1.78 | 1.51 |
| 1 | B | 638 | PHE | CG-CD1 | -10.73 | 1.22 | 1.38 |
| 1 | B | 328 | PHE | CG-CD2 | -10.73 | 1.22 | 1.38 |
| 1 | B | 135 | TYR | CD2-CE2 | -10.73 | 1.23 | 1.39 |
| 1 | A | 471 | GLU | C-O | -10.73 | 1.02 | 1.23 |
| 1 | B | 62 | GLU | CD-OE2 | 10.72 | 1.37 | 1.25 |
| 1 | B | 377 | TYR | CD1-CE1 | 10.72 | 1.55 | 1.39 |
| 1 | A | 115 | THR | CB-CG2 | 10.72 | 1.87 | 1.52 |
| 1 | B | 89 | VAL | CA-CB | 10.64 | 1.77 | 1.54 |
| 1 | B | 333 | ARG | CG-CD | 10.61 | 1.78 | 1.51 |
| 1 | B | 146 | PHE | CB-CG | 10.59 | 1.69 | 1.51 |
| 1 | B | 136 | ALA | N-CA | 10.56 | 1.67 | 1.46 |
| 1 | A | 112 | ALA | CA-CB | -10.56 | 1.30 | 1.52 |
| 1 | B | 577 | GLU | CD-OE1 | 10.54 | 1.37 | 1.25 |
| 1 | B | 778 | SER | CB-OG | 10.54 | 1.55 | 1.42 |
| 1 | A | 350 | SER | CB-OG | 10.53 | 1.55 | 1.42 |
| 1 | B | 699 | PHE | CE1-CZ | 10.53 | 1.57 | 1.37 |
| 1 | A | 362 | GLU | CG-CD | -10.53 | 1.36 | 1.51 |
| 1 | B | 123 | ARG | CZ-NH1 | 10.52 | 1.46 | 1.33 |
| 1 | B | 131 | PHE | CE1-CZ | 10.48 | 1.57 | 1.37 |
| 1 | A | 333 | ARG | CG-CD | 10.47 | 1.78 | 1.51 |
| 1 | B | 777 | ASP | CA-CB | 10.47 | 1.76 | 1.53 |
| 1 | A | 133 | GLU | CD-OE2 | 10.47 | 1.37 | 1.25 |
| 1 | B | 494 | LYS | CD-CE | 10.46 | 1.77 | 1.51 |
| 1 | B | 415 | GLN | CB-CG | -10.45 | 1.24 | 1.52 |
| 1 | B | 429 | GLU | CG-CD | 10.45 | 1.67 | 1.51 |
| 1 | B | 88 | ILE | CB-CG2 | -10.44 | 1.20 | 1.52 |
| 1 | B | 131 | PHE | CD1-CE1 | -10.42 | 1.18 | 1.39 |
| 1 | A | 453 | PHE | CE2-CZ | 10.41 | 1.57 | 1.37 |
| 1 | A | 483 | TYR | CD1-CE1 | -10.39 | 1.23 | 1.39 |
| 1 | A | 366 | ARG | CG-CD | 10.38 | 1.77 | 1.51 |
| 1 | B | 570 | ARG | N-CA | 10.37 | 1.67 | 1.46 |
| 1 | A | 868 | PHE | CG-CD1 | -10.35 | 1.23 | 1.38 |
| 1 | B | 193 | GLU | CG-CD | -10.35 | 1.36 | 1.51 |
| 1 | A | 615 | LYS | CE-NZ | 10.33 | 1.74 | 1.49 |
| 1 | A | 483 | TYR | CD2-CE2 | -10.32 | 1.23 | 1.39 |
| 1 | A | 512 | GLU | CG-CD | 10.32 | 1.67 | 1.51 |
| 1 | B | 141 | PHE | CE1-CZ | -10.32 | 1.17 | 1.37 |
| 1 | B | 338 | LEU | CA-CB | -10.31 | 1.30 | 1.53 |
| 1 | B | 208 | THR | C-O | 10.30 | 1.43 | 1.23 |
| 1 | B | 204 | PHE | CE2-CZ | 10.29 | 1.56 | 1.37 |
| 1 | A | 477 | ARG | CG-CD | 10.27 | 1.77 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | B | 310 | TYR | CD2-CE2 | -10.26 | 1.24 | 1.39 |
| 1 | A | 219 | LYS | CG-CD | 10.25 | 1.87 | 1.52 |
| 1 | A | 350 | SER | CA-CB | 10.24 | 1.68 | 1.52 |
| 1 | A | 436 | TYR | CE2-CZ | -10.23 | 1.25 | 1.38 |
| 1 | B | 553 | LYS | CA-CB | 10.22 | 1.76 | 1.53 |
| 1 | B | 775 | VAL | CB-CG2 | -10.21 | 1.31 | 1.52 |
| 1 | A | 207 | PHE | CD2-CE2 | 10.21 | 1.59 | 1.39 |
| 1 | B | 290 | GLU | CD-OE2 | 10.20 | 1.36 | 1.25 |
| 1 | B | 694 | ILE | CA-CB | 10.20 | 1.78 | 1.54 |
| 1 | B | 285 | ARG | CZ-NH1 | 10.19 | 1.46 | 1.33 |
| 1 | B | 740 | VAL | CB-CG2 | 10.18 | 1.74 | 1.52 |
| 1 | A | 608 | ASN | C-O | -10.18 | 1.04 | 1.23 |
| 1 | A | 462 | GLN | CA-CB | -10.18 | 1.31 | 1.53 |
| 1 | A | 167 | PHE | CG-CD2 | -10.16 | 1.23 | 1.38 |
| 1 | B | 48 | ASP | CB-CG | 10.16 | 1.73 | 1.51 |
| 1 | A | 339 | GLU | CD-OE2 | 10.13 | 1.36 | 1.25 |
| 1 | B | 230 | LYS | CD-CE | 10.10 | 1.76 | 1.51 |
| 1 | B | 34 | THR | N-CA | 10.09 | 1.66 | 1.46 |
| 1 | B | 799 | TRP | CB-CG | 10.09 | 1.68 | 1.50 |
| 1 | B | 690 | GLN | CG-CD | 10.08 | 1.74 | 1.51 |
| 1 | B | 243 | ASN | N-CA | 10.07 | 1.66 | 1.46 |
| 1 | A | 200 | THR | CA-CB | 10.06 | 1.79 | 1.53 |
| 1 | A | 609 | TYR | CZ-OH | 10.06 | 1.54 | 1.37 |
| 1 | B | 182 | GLU | CD-OE2 | 10.02 | 1.36 | 1.25 |
| 1 | A | 428 | MET | CB-CG | 10.02 | 1.83 | 1.51 |
| 1 | A | 390 | ARG | CZ-NH1 | 10.01 | 1.46 | 1.33 |
| 1 | A | 313 | GLU | CD-OE2 | 10.01 | 1.36 | 1.25 |
| 1 | A | 770 | ARG | C-O | -10.00 | 1.04 | 1.23 |
| 1 | A | 203 | ALA | CA-CB | -9.99 | 1.31 | 1.52 |
| 1 | B | 885 | GLU | C-O | -9.97 | 1.04 | 1.23 |
| 1 | B | 288 | TRP | CD2-CE2 | -9.96 | 1.29 | 1.41 |
| 1 | A | 301 | SER | CA-CB | 9.94 | 1.67 | 1.52 |
| 1 | B | 628 | GLU | CD-OE2 | 9.93 | 1.36 | 1.25 |
| 1 | B | 295 | GLY | N-CA | 9.93 | 1.60 | 1.46 |
| 1 | B | 828 | PHE | CE1-CZ | -9.92 | 1.18 | 1.37 |
| 1 | B | 435 | VAL | CB-CG2 | 9.92 | 1.73 | 1.52 |
| 1 | B | 621 | SER | CA-CB | 9.92 | 1.67 | 1.52 |
| 1 | B | 443 | ALA | CA-CB | 9.90 | 1.73 | 1.52 |
| 1 | A | 664 | PHE | CE1-CZ | 9.89 | 1.56 | 1.37 |
| 1 | B | 210 | GLY | C-O | -9.88 | 1.07 | 1.23 |
| 1 | B | 243 | ASN | C-O | 9.87 | 1.42 | 1.23 |
| 1 | A | 218 | GLN | CA-CB | 9.87 | 1.75 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 30 | GLN | C-O | -9.83 | 1.04 | 1.23 |
| 1 | B | 491 | GLU | CD-OE1 | 9.83 | 1.36 | 1.25 |
| 1 | B | 130 | SER | CB-OG | 9.81 | 1.55 | 1.42 |
| 1 | B | 149 | TRP | CG-CD1 | -9.81 | 1.23 | 1.36 |
| 1 | A | 215 | TYR | CE2-CZ | -9.81 | 1.25 | 1.38 |
| 1 | A | 166 | VAL | N-CA | 9.79 | 1.66 | 1.46 |
| 1 | A | 616 | PHE | CB-CG | 9.78 | 1.68 | 1.51 |
| 1 | B | 464 | GLU | CD-OE1 | 9.78 | 1.36 | 1.25 |
| 1 | B | 84 | ASN | CG-OD1 | 9.75 | 1.45 | 1.24 |
| 1 | A | 360 | PHE | CB-CG | -9.73 | 1.34 | 1.51 |
| 1 | B | 856 | SER | CA-CB | 9.72 | 1.67 | 1.52 |
| 1 | A | 265 | SER | CB-OG | 9.72 | 1.54 | 1.42 |
| 1 | A | 836 | SER | CA-CB | -9.70 | 1.38 | 1.52 |
| 1 | A | 370 | THR | C-O | -9.70 | 1.04 | 1.23 |
| 1 | A | 433 | PHE | CD1-CE1 | 9.70 | 1.58 | 1.39 |
| 1 | A | 870 | SER | CB-OG | 9.69 | 1.54 | 1.42 |
| 1 | B | 885 | GLU | CD-OE2 | 9.68 | 1.36 | 1.25 |
| 1 | A | 864 | MET | CA-CB | 9.68 | 1.75 | 1.53 |
| 1 | B | 598 | GLU | CD-OE2 | 9.68 | 1.36 | 1.25 |
| 1 | B | 772 | MET | SD-CE | 9.68 | 2.32 | 1.77 |
| 1 | B | 150 | VAL | CB-CG1 | -9.65 | 1.32 | 1.52 |
| 1 | B | 324 | PHE | N-CA | -9.64 | 1.27 | 1.46 |
| 1 | A | 488 | SER | CB-OG | 9.63 | 1.54 | 1.42 |
| 1 | A | 270 | LYS | CE-NZ | 9.63 | 1.73 | 1.49 |
| 1 | A | 757 | PRO | CG-CD | 9.62 | 1.82 | 1.50 |
| 1 | A | 176 | PHE | CE1-CZ | 9.62 | 1.55 | 1.37 |
| 1 | A | 318 | LYS | N-CA | 9.61 | 1.65 | 1.46 |
| 1 | B | 0 | GLU | CA-CB | 9.61 | 1.75 | 1.53 |
| 1 | A | 177 | TRP | CD2-CE2 | -9.61 | 1.29 | 1.41 |
| 1 | B | 291 | VAL | CB-CG2 | 9.61 | 1.73 | 1.52 |
| 1 | A | 26 | LYS | CE-NZ | 9.61 | 1.73 | 1.49 |
| 1 | A | 323 | GLU | CG-CD | 9.60 | 1.66 | 1.51 |
| 1 | A | 583 | VAL | CA-CB | 9.60 | 1.75 | 1.54 |
| 1 | B | 360 | PHE | CE2-CZ | 9.59 | 1.55 | 1.37 |
| 1 | B | 313 | GLU | CG-CD | 9.56 | 1.66 | 1.51 |
| 1 | B | 362 | GLU | C-O | 9.55 | 1.41 | 1.23 |
| 1 | B | 170 | SER | CB-OG | 9.54 | 1.54 | 1.42 |
| 1 | A | 202 | GLU | CD-OE2 | 9.54 | 1.36 | 1.25 |
| 1 | A | 744 | GLU | CD-OE1 | 9.47 | 1.36 | 1.25 |
| 1 | A | 591 | ASN | CB-CG | 9.45 | 1.72 | 1.51 |
| 1 | B | 203 | ALA | CA-CB | 9.45 | 1.72 | 1.52 |
| 1 | B | 387 | PHE | CB-CG | -9.44 | 1.35 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 572 | ASN | CA-C | 9.44 | 1.77 | 1.52 |
| 1 | A | 803 | TYR | CE2-CZ | 9.44 | 1.50 | 1.38 |
| 1 | A | 847 | GLY | C-O | 9.44 | 1.38 | 1.23 |
| 1 | B | 389 | ILE | C-O | 9.43 | 1.41 | 1.23 |
| 1 | A | 303 | GLU | CD-OE1 | 9.42 | 1.36 | 1.25 |
| 1 | A | 734 | ALA | CA-CB | 9.42 | 1.72 | 1.52 |
| 1 | A | 177 | TRP | CE3-CZ3 | -9.41 | 1.22 | 1.38 |
| 1 | A | 182 | GLU | CD-OE1 | 9.40 | 1.35 | 1.25 |
| 1 | A | 892 | TYR | CG-CD2 | -9.40 | 1.26 | 1.39 |
| 1 | A | 361 | TYR | CD1-CE1 | 9.40 | 1.53 | 1.39 |
| 1 | B | 26 | LYS | CB-CG | 9.39 | 1.77 | 1.52 |
| 1 | A | 135 | TYR | N-CA | -9.38 | 1.27 | 1.46 |
| 1 | A | 516 | GLN | CA-CB | -9.37 | 1.33 | 1.53 |
| 1 | A | 154 | VAL | CB-CG1 | 9.37 | 1.72 | 1.52 |
| 1 | B | 609 | TYR | CD2-CE2 | 9.36 | 1.53 | 1.39 |
| 1 | B | 477 | ARG | CB-CG | 9.36 | 1.77 | 1.52 |
| 1 | A | 471 | GLU | N-CA | 9.35 | 1.65 | 1.46 |
| 1 | B | 95 | THR | C-O | 9.35 | 1.41 | 1.23 |
| 1 | B | 786 | PHE | CA-CB | 9.35 | 1.74 | 1.53 |
| 1 | A | 382 | TRP | C-O | 9.35 | 1.41 | 1.23 |
| 1 | B | 175 | GLU | C-O | -9.34 | 1.05 | 1.23 |
| 1 | A | 320 | GLU | CA-CB | 9.32 | 1.74 | 1.53 |
| 1 | A | 453 | PHE | CD2-CE2 | -9.32 | 1.20 | 1.39 |
| 1 | B | 335 | PHE | CA-CB | 9.32 | 1.74 | 1.53 |
| 1 | A | 891 | MET | CA-CB | -9.31 | 1.33 | 1.53 |
| 1 | B | 811 | SER | CB-OG | 9.31 | 1.54 | 1.42 |
| 1 | B | 503 | PHE | CD2-CE2 | 9.31 | 1.57 | 1.39 |
| 1 | A | 630 | ARG | NE-CZ | 9.28 | 1.45 | 1.33 |
| 1 | A | 482 | GLU | CD-OE2 | 9.27 | 1.35 | 1.25 |
| 1 | B | 256 | LYS | CD-CE | 9.26 | 1.74 | 1.51 |
| 1 | A | 448 | HIS | N-CA | 9.26 | 1.64 | 1.46 |
| 1 | B | 83 | SER | C-O | 9.26 | 1.41 | 1.23 |
| 1 | B | 627 | TYR | CD1-CE1 | -9.26 | 1.25 | 1.39 |
| 1 | B | 13 | GLU | CG-CD | 9.25 | 1.65 | 1.51 |
| 1 | A | 377 | TYR | CD1-CE1 | -9.23 | 1.25 | 1.39 |
| 1 | A | 313 | GLU | CD-OE1 | 9.21 | 1.35 | 1.25 |
| 1 | A | 204 | PHE | CG-CD1 | 9.21 | 1.52 | 1.38 |
| 1 | B | 409 | PHE | CB-CG | -9.20 | 1.35 | 1.51 |
| 1 | A | 483 | TYR | CA-CB | -9.19 | 1.33 | 1.53 |
| 1 | B | 424 | PHE | C-O | 9.19 | 1.40 | 1.23 |
| 1 | B | 144 | TRP | CG-CD1 | -9.18 | 1.24 | 1.36 |
| 1 | B | 742 | ALA | N-CA | 9.18 | 1.64 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 234 | ARG | CG-CD | -9.16 | 1.29 | 1.51 |
| 1 | A | 877 | GLY | CA-C | 9.15 | 1.66 | 1.51 |
| 1 | A | 502 | PHE | CE2-CZ | -9.14 | 1.20 | 1.37 |
| 1 | A | 609 | TYR | CG-CD1 | -9.14 | 1.27 | 1.39 |
| 1 | A | 867 | ALA | CA-CB | 9.14 | 1.71 | 1.52 |
| 1 | A | 139 | PHE | CD2-CE2 | 9.13 | 1.57 | 1.39 |
| 1 | A | 188 | VAL | CB-CG2 | -9.13 | 1.33 | 1.52 |
| 1 | A | 122 | HIS | C-O | 9.12 | 1.40 | 1.23 |
| 1 | B | 487 | PRO | N-CD | -9.08 | 1.35 | 1.47 |
| 1 | B | 791 | TYR | CB-CG | 9.07 | 1.65 | 1.51 |
| 1 | B | 214 | TRP | CG-CD1 | -9.07 | 1.24 | 1.36 |
| 1 | B | 325 | TRP | CE3-CZ3 | 9.06 | 1.53 | 1.38 |
| 1 | A | 278 | ARG | C-O | -9.05 | 1.06 | 1.23 |
| 1 | A | 474 | ASN | CB-CG | 9.02 | 1.71 | 1.51 |
| 1 | B | 305 | ASN | CB-CG | 9.02 | 1.71 | 1.51 |
| 1 | B | 699 | PHE | CG-CD2 | 9.02 | 1.52 | 1.38 |
| 1 | A | 71 | TYR | CE2-CZ | -9.01 | 1.26 | 1.38 |
| 1 | A | 323 | GLU | CB-CG | 8.99 | 1.69 | 1.52 |
| 1 | A | 381 | PHE | CG-CD1 | 8.98 | 1.52 | 1.38 |
| 1 | A | 652 | PHE | CE2-CZ | 8.98 | 1.54 | 1.37 |
| 1 | B | 55 | SER | CA-CB | 8.96 | 1.66 | 1.52 |
| 1 | B | 627 | TYR | CG-CD1 | 8.96 | 1.50 | 1.39 |
| 1 | A | 678 | PHE | CD2-CE2 | -8.96 | 1.21 | 1.39 |
| 1 | A | 123 | ARG | CZ-NH1 | 8.95 | 1.44 | 1.33 |
| 1 | B | 133 | GLU | CG-CD | 8.95 | 1.65 | 1.51 |
| 1 | A | 113 | SER | CB-OG | 8.93 | 1.53 | 1.42 |
| 1 | B | 436 | TYR | CG-CD1 | 8.93 | 1.50 | 1.39 |
| 1 | B | 277 | GLN | CB-CG | 8.93 | 1.76 | 1.52 |
| 1 | A | 297 | TRP | CG-CD1 | 8.91 | 1.49 | 1.36 |
| 1 | B | 892 | TYR | CE2-CZ | 8.91 | 1.50 | 1.38 |
| 1 | A | 334 | GLU | CD-OE2 | 8.90 | 1.35 | 1.25 |
| 1 | B | 504 | SER | N-CA | 8.90 | 1.64 | 1.46 |
| 1 | A | 233 | GLU | CG-CD | 8.89 | 1.65 | 1.51 |
| 1 | B | 131 | PHE | CG-CD1 | -8.89 | 1.25 | 1.38 |
| 1 | A | 799 | TRP | C-O | -8.89 | 1.06 | 1.23 |
| 1 | A | 820 | PRO | CA-C | 8.88 | 1.70 | 1.52 |
| 1 | B | 113 | SER | C-O | 8.88 | 1.40 | 1.23 |
| 1 | B | 628 | GLU | CD-OE1 | 8.87 | 1.35 | 1.25 |
| 1 | A | 810 | ARG | NE-CZ | 8.87 | 1.44 | 1.33 |
| 1 | A | 858 | LEU | CA-CB | 8.85 | 1.74 | 1.53 |
| 1 | B | 348 | LEU | CA-CB | 8.84 | 1.74 | 1.53 |
| 1 | A | 502 | PHE | C-O | -8.83 | 1.06 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 75 | TRP | CG-CD1 | -8.83 | 1.24 | 1.36 |
| 1 | A | 168 | VAL | CB-CG1 | -8.81 | 1.34 | 1.52 |
| 1 | A | 406 | GLY | C-O | -8.80 | 1.09 | 1.23 |
| 1 | B | 71 | TYR | CE1-CZ | 8.80 | 1.50 | 1.38 |
| 1 | B | 482 | GLU | CD-OE1 | 8.80 | 1.35 | 1.25 |
| 1 | A | 233 | GLU | CD-OE2 | -8.79 | 1.16 | 1.25 |
| 1 | B | 382 | TRP | CE3-CZ3 | 8.79 | 1.53 | 1.38 |
| 1 | B | 647 | VAL | C-O | -8.78 | 1.06 | 1.23 |
| 1 | A | 570 | ARG | CG-CD | 8.78 | 1.73 | 1.51 |
| 1 | B | 166 | VAL | CB-CG2 | 8.78 | 1.71 | 1.52 |
| 1 | A | 550 | ILE | CA-CB | 8.76 | 1.75 | 1.54 |
| 1 | B | 624 | MET | SD-CE | -8.76 | 1.28 | 1.77 |
| 1 | B | 214 | TRP | CB-CG | -8.75 | 1.34 | 1.50 |
| 1 | A | 503 | PHE | CG-CD1 | -8.75 | 1.25 | 1.38 |
| 1 | A | 696 | TRP | C-O | -8.74 | 1.06 | 1.23 |
| 1 | B | 409 | PHE | CD2-CE2 | 8.73 | 1.56 | 1.39 |
| 1 | A | 498 | PHE | CB-CG | -8.73 | 1.36 | 1.51 |
| 1 | A | 393 | GLU | CD-OE2 | -8.73 | 1.16 | 1.25 |
| 1 | A | 453 | PHE | CB-CG | -8.72 | 1.36 | 1.51 |
| 1 | B | 463 | SER | CB-OG | 8.71 | 1.53 | 1.42 |
| 1 | A | 477 | ARG | NE-CZ | 8.71 | 1.44 | 1.33 |
| 1 | B | 502 | PHE | CD1-CE1 | 8.70 | 1.56 | 1.39 |
| 1 | A | 490 | PHE | CE2-CZ | -8.69 | 1.20 | 1.37 |
| 1 | A | 320 | GLU | CD-OE1 | 8.69 | 1.35 | 1.25 |
| 1 | A | 738 | MET | CA-CB | -8.68 | 1.34 | 1.53 |
| 1 | A | 498 | PHE | CE2-CZ | -8.67 | 1.20 | 1.37 |
| 1 | B | 394 | VAL | C-O | 8.67 | 1.39 | 1.23 |
| 1 | B | 52 | PRO | CA-C | -8.67 | 1.35 | 1.52 |
| 1 | A | 389 | ILE | CA-CB | -8.66 | 1.34 | 1.54 |
| 1 | B | 33 | GLU | CD-OE1 | 8.65 | 1.35 | 1.25 |
| 1 | A | 479 | PRO | CA-C | -8.65 | 1.35 | 1.52 |
| 1 | A | 468 | ASN | CB-CG | 8.64 | 1.71 | 1.51 |
| 1 | B | 677 | ILE | C-O | 8.64 | 1.39 | 1.23 |
| 1 | B | 791 | TYR | CD1-CE1 | 8.63 | 1.52 | 1.39 |
| 1 | A | 319 | MET | CG-SD | -8.62 | 1.58 | 1.81 |
| 1 | B | 19 | GLY | N-CA | -8.62 | 1.33 | 1.46 |
| 1 | B | 204 | PHE | CG-CD1 | 8.61 | 1.51 | 1.38 |
| 1 | A | 877 | GLY | N-CA | 8.61 | 1.58 | 1.46 |
| 1 | A | 155 | ASP | CB-CG | -8.61 | 1.33 | 1.51 |
| 1 | A | 463 | SER | CA-CB | -8.60 | 1.40 | 1.52 |
| 1 | A | 505 | GLU | CD-OE1 | 8.60 | 1.35 | 1.25 |
| 1 | B | 684 | GLU | CD-OE1 | 8.60 | 1.35 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 502 | PHE | CE2-CZ | -8.59 | 1.21 | 1.37 |
| 1 | B | 167 | PHE | CG-CD1 | -8.59 | 1.25 | 1.38 |
| 1 | B | 610 | LEU | CG-CD1 | 8.58 | 1.83 | 1.51 |
| 1 | A | 764 | PHE | CE1-CZ | -8.57 | 1.21 | 1.37 |
| 1 | B | 259 | VAL | CA-CB | 8.57 | 1.72 | 1.54 |
| 1 | A | 459 | SER | C-O | -8.56 | 1.07 | 1.23 |
| 1 | B | 94 | ARG | CA-CB | 8.56 | 1.72 | 1.53 |
| 1 | B | 656 | GLU | CD-OE1 | 8.55 | 1.35 | 1.25 |
| 1 | B | 772 | MET | C-O | 8.54 | 1.39 | 1.23 |
| 1 | A | 315 | LEU | C-O | -8.52 | 1.07 | 1.23 |
| 1 | A | 570 | ARG | NE-CZ | 8.52 | 1.44 | 1.33 |
| 1 | B | 385 | PRO | C-O | 8.51 | 1.40 | 1.23 |
| 1 | B | 143 | LEU | C-O | -8.50 | 1.07 | 1.23 |
| 1 | B | 508 | ALA | C-O | -8.50 | 1.07 | 1.23 |
| 1 | A | 799 | TRP | CE3-CZ3 | 8.49 | 1.52 | 1.38 |
| 1 | A | 656 | GLU | CD-OE2 | 8.49 | 1.34 | 1.25 |
| 1 | B | 465 | HIS | C-O | -8.49 | 1.07 | 1.23 |
| 1 | A | 436 | TYR | CD2-CE2 | 8.48 | 1.52 | 1.39 |
| 1 | B | 265 | SER | C-O | -8.48 | 1.07 | 1.23 |
| 1 | B | 54 | VAL | CB-CG2 | -8.47 | 1.35 | 1.52 |
| 1 | B | 39 | CYS | C-O | -8.46 | 1.07 | 1.23 |
| 1 | A | 186 | ALA | CA-CB | -8.46 | 1.34 | 1.52 |
| 1 | B | 360 | PHE | CD2-CE2 | 8.45 | 1.56 | 1.39 |
| 1 | B | 505 | GLU | CD-OE1 | 8.45 | 1.34 | 1.25 |
| 1 | A | 361 | TYR | CB-CG | 8.44 | 1.64 | 1.51 |
| 1 | A | 796 | ILE | CA-CB | 8.44 | 1.74 | 1.54 |
| 1 | A | 41 | GLU | CA-CB | 8.43 | 1.72 | 1.53 |
| 1 | B | 185 | TYR | CB-CG | 8.43 | 1.64 | 1.51 |
| 1 | A | 57 | SER | CB-OG | -8.43 | 1.31 | 1.42 |
| 1 | A | 353 | LEU | C-O | 8.41 | 1.39 | 1.23 |
| 1 | A | 310 | TYR | CE1-CZ | 8.40 | 1.49 | 1.38 |
| 1 | B | 418 | ARG | CZ-NH2 | 8.40 | 1.44 | 1.33 |
| 1 | A | 290 | GLU | C-O | 8.40 | 1.39 | 1.23 |
| 1 | A | 461 | ALA | N-CA | 8.39 | 1.63 | 1.46 |
| 1 | A | 868 | PHE | CD2-CE2 | -8.39 | 1.22 | 1.39 |
| 1 | B | 874 | ASN | N-CA | 8.39 | 1.63 | 1.46 |
| 1 | B | 166 | VAL | CB-CG1 | -8.38 | 1.35 | 1.52 |
| 1 | A | 618 | LEU | CG-CD2 | 8.38 | 1.82 | 1.51 |
| 1 | A | 454 | PHE | CE1-CZ | 8.38 | 1.53 | 1.37 |
| 1 | B | 780 | THR | CB-CG2 | 8.36 | 1.79 | 1.52 |
| 1 | A | 376 | ASN | N-CA | -8.36 | 1.29 | 1.46 |
| 1 | A | 502 | PHE | CB-CG | 8.35 | 1.65 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 546 | ASP | CA-CB | 8.35 | 1.72 | 1.53 |
| 1 | B | 211 | VAL | CB-CG1 | -8.35 | 1.35 | 1.52 |
| 1 | A | 631 | MET | CG-SD | 8.35 | 2.02 | 1.81 |
| 1 | A | 757 | PRO | CA-C | 8.35 | 1.69 | 1.52 |
| 1 | A | 772 | MET | CB-CG | 8.35 | 1.78 | 1.51 |
| 1 | A | 630 | ARG | CZ-NH1 | 8.31 | 1.43 | 1.33 |
| 1 | A | 800 | GLN | N-CA | -8.31 | 1.29 | 1.46 |
| 1 | A | 860 | ARG | CG-CD | 8.31 | 1.72 | 1.51 |
| 1 | B | 328 | PHE | CE2-CZ | -8.30 | 1.21 | 1.37 |
| 1 | B | 835 | TYR | CA-CB | 8.31 | 1.72 | 1.53 |
| 1 | B | 345 | PRO | CG-CD | 8.30 | 1.78 | 1.50 |
| 1 | B | 334 | GLU | N-CA | 8.30 | 1.62 | 1.46 |
| 1 | B | 865 | PHE | CB-CG | -8.30 | 1.37 | 1.51 |
| 1 | A | 670 | ARG | C-O | 8.29 | 1.39 | 1.23 |
| 1 | B | 366 | ARG | CZ-NH1 | 8.29 | 1.43 | 1.33 |
| 1 | A | 355 | ASN | CG-ND2 | 8.29 | 1.53 | 1.32 |
| 1 | B | 139 | PHE | N-CA | -8.29 | 1.29 | 1.46 |
| 1 | A | 776 | MET | CG-SD | -8.29 | 1.59 | 1.81 |
| 1 | B | 456 | ALA | CA-C | 8.28 | 1.74 | 1.52 |
| 1 | B | 839 | ILE | C-O | 8.28 | 1.39 | 1.23 |
| 1 | A | 447 | VAL | N-CA | 8.28 | 1.62 | 1.46 |
| 1 | B | 335 | PHE | CG-CD2 | 8.27 | 1.51 | 1.38 |
| 1 | A | 185 | TYR | CZ-OH | -8.27 | 1.23 | 1.37 |
| 1 | B | 642 | CYS | C-O | -8.27 | 1.07 | 1.23 |
| 1 | B | 118 | GLU | CD-OE1 | 8.27 | 1.34 | 1.25 |
| 1 | A | 175 | GLU | CD-OE2 | 8.26 | 1.34 | 1.25 |
| 1 | B | 680 | GLN | CA-CB | 8.26 | 1.72 | 1.53 |
| 1 | B | 854 | PHE | CE1-CZ | 8.26 | 1.53 | 1.37 |
| 1 | B | 32 | TYR | CE2-CZ | -8.26 | 1.27 | 1.38 |
| 1 | B | 256 | LYS | CB-CG | 8.26 | 1.74 | 1.52 |
| 1 | A | 739 | GLU | CD-OE1 | 8.25 | 1.34 | 1.25 |
| 1 | A | 862 | ASP | CB-CG | -8.25 | 1.34 | 1.51 |
| 1 | B | 851 | PHE | C-O | 8.24 | 1.39 | 1.23 |
| 1 | B | 192 | TYR | CG-CD1 | -8.24 | 1.28 | 1.39 |
| 1 | B | 34 | THR | CB-CG2 | -8.24 | 1.25 | 1.52 |
| 1 | B | 387 | PHE | CD1-CE1 | 8.24 | 1.55 | 1.39 |
| 1 | B | 324 | PHE | CB-CG | -8.23 | 1.37 | 1.51 |
| 1 | A | 739 | GLU | CB-CG | 8.22 | 1.67 | 1.52 |
| 1 | A | 775 | VAL | CA-CB | -8.21 | 1.37 | 1.54 |
| 1 | A | 279 | VAL | C-O | -8.21 | 1.07 | 1.23 |
| 1 | A | 502 | PHE | CD1-CE1 | -8.21 | 1.22 | 1.39 |
| 1 | B | 164 | LYS | CG-CD | 8.21 | 1.80 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 123 | ARG | NE-CZ | 8.20 | 1.43 | 1.33 |
| 1 | B | 182 | GLU | CA-CB | -8.20 | 1.35 | 1.53 |
| 1 | A | 580 | ARG | N-CA | -8.19 | 1.29 | 1.46 |
| 1 | A | 891 | MET | C-O | -8.19 | 1.07 | 1.23 |
| 1 | A | 106 | TRP | C-O | -8.19 | 1.07 | 1.23 |
| 1 | B | 470 | ARG | CB-CG | 8.19 | 1.74 | 1.52 |
| 1 | A | 392 | GLU | CD-OE2 | 8.19 | 1.34 | 1.25 |
| 1 | A | 10 | LYS | N-CA | 8.19 | 1.62 | 1.46 |
| 1 | A | 492 | PRO | C-O | -8.19 | 1.06 | 1.23 |
| 1 | B | 201 | SER | C-O | -8.18 | 1.07 | 1.23 |
| 1 | A | 331 | PHE | CB-CG | -8.18 | 1.37 | 1.51 |
| 1 | B | 396 | ASP | C-O | 8.18 | 1.38 | 1.23 |
| 1 | A | 382 | TRP | CE3-CZ3 | 8.17 | 1.52 | 1.38 |
| 1 | B | 403 | ARG | N-CA | 8.17 | 1.62 | 1.46 |
| 1 | B | 118 | GLU | CD-OE2 | -8.17 | 1.16 | 1.25 |
| 1 | A | 833 | HIS | CA-C | 8.16 | 1.74 | 1.52 |
| 1 | A | 329 | ARG | N-CA | 8.15 | 1.62 | 1.46 |
| 1 | B | 74 | LYS | C-O | 8.15 | 1.38 | 1.23 |
| 1 | A | 478 | LEU | CG-CD1 | 8.14 | 1.81 | 1.51 |
| 1 | B | 69 | LYS | C-O | 8.14 | 1.38 | 1.23 |
| 1 | A | 144 | TRP | CB-CG | -8.13 | 1.35 | 1.50 |
| 1 | A | 361 | TYR | CE1-CZ | -8.12 | 1.27 | 1.38 |
| 1 | B | 345 | PRO | CA-CB | 8.12 | 1.69 | 1.53 |
| 1 | A | 415 | GLN | N-CA | 8.11 | 1.62 | 1.46 |
| 1 | B | 417 | HIS | CA-CB | 8.11 | 1.71 | 1.53 |
| 1 | A | 367 | ARG | C-O | -8.10 | 1.07 | 1.23 |
| 1 | B | 363 | GLY | N-CA | 8.10 | 1.58 | 1.46 |
| 1 | B | 399 | ASP | C-O | 8.10 | 1.38 | 1.23 |
| 1 | A | 436 | TYR | C-O | 8.10 | 1.38 | 1.23 |
| 1 | B | 264 | TYR | CD2-CE2 | -8.09 | 1.27 | 1.39 |
| 1 | B | 583 | VAL | CA-CB | 8.09 | 1.71 | 1.54 |
| 1 | B | 409 | PHE | CG-CD2 | -8.09 | 1.26 | 1.38 |
| 1 | B | 237 | LEU | C-O | -8.09 | 1.07 | 1.23 |
| 1 | B | 88 | ILE | CA-C | -8.08 | 1.31 | 1.52 |
| 1 | A | 328 | PHE | C-O | -8.08 | 1.07 | 1.23 |
| 1 | A | 133 | GLU | CA-C | 8.08 | 1.74 | 1.52 |
| 1 | B | 61 | LYS | CA-CB | 8.07 | 1.71 | 1.53 |
| 1 | B | 6 | MET | SD-CE | 8.07 | 2.23 | 1.77 |
| 1 | B | 349 | LYS | CA-C | -8.06 | 1.31 | 1.52 |
| 1 | B | 380 | THR | C-O | 8.06 | 1.38 | 1.23 |
| 1 | A | 436 | TYR | CG-CD1 | 8.06 | 1.49 | 1.39 |
| 1 | A | 760 | LYS | CA-C | 8.05 | 1.73 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 54 | VAL | CA-CB | -8.05 | 1.37 | 1.54 |
| 1 | A | 354 | ARG | NE-CZ | 8.04 | 1.43 | 1.33 |
| 1 | A | 19 | GLY | N-CA | 8.04 | 1.58 | 1.46 |
| 1 | A | 387 | PHE | CD1-CE1 | 8.04 | 1.55 | 1.39 |
| 1 | B | 38 | GLU | CD-OE2 | 8.03 | 1.34 | 1.25 |
| 1 | A | 803 | TYR | CE1-CZ | -8.03 | 1.28 | 1.38 |
| 1 | A | 301 | SER | CB-OG | 8.03 | 1.52 | 1.42 |
| 1 | B | 400 | TYR | CD2-CE2 | 8.01 | 1.51 | 1.39 |
| 1 | A | 688 | THR | CB-CG2 | 8.00 | 1.78 | 1.52 |
| 1 | B | 418 | ARG | N-CA | 8.00 | 1.62 | 1.46 |
| 1 | A | 264 | TYR | CD1-CE1 | 8.00 | 1.51 | 1.39 |
| 1 | B | 120 | ILE | C-O | -7.99 | 1.08 | 1.23 |
| 1 | A | 740 | VAL | CB-CG1 | -7.99 | 1.36 | 1.52 |
| 1 | A | 213 | GLU | CB-CG | -7.99 | 1.36 | 1.52 |
| 1 | B | 277 | GLN | CG-CD | 7.98 | 1.69 | 1.51 |
| 1 | A | 433 | PHE | CG-CD1 | -7.97 | 1.26 | 1.38 |
| 1 | A | 623 | SER | C-O | -7.97 | 1.08 | 1.23 |
| 1 | B | 200 | THR | N-CA | 7.96 | 1.62 | 1.46 |
| 1 | A | 130 | SER | CB-OG | 7.96 | 1.52 | 1.42 |
| 1 | A | 144 | TRP | N-CA | 7.94 | 1.62 | 1.46 |
| 1 | B | 788 | GLU | CA-CB | 7.94 | 1.71 | 1.53 |
| 1 | A | 483 | TYR | CB-CG | 7.94 | 1.63 | 1.51 |
| 1 | B | 416 | LYS | CD-CE | 7.94 | 1.71 | 1.51 |
| 1 | A | 324 | PHE | CD2-CE2 | -7.94 | 1.23 | 1.39 |
| 1 | B | 656 | GLU | C-O | 7.94 | 1.38 | 1.23 |
| 1 | B | 183 | LYS | CD-CE | 7.93 | 1.71 | 1.51 |
| 1 | A | 386 | GLN | C-O | -7.93 | 1.08 | 1.23 |
| 1 | A | 740 | VAL | CB-CG2 | -7.93 | 1.36 | 1.52 |
| 1 | A | 873 | LYS | C-O | 7.92 | 1.38 | 1.23 |
| 1 | A | 350 | SER | CA-C | -7.91 | 1.32 | 1.52 |
| 1 | B | 398 | ASP | C-N | 7.90 | 1.52 | 1.34 |
| 1 | A | 655 | ASP | CB-CG | 7.88 | 1.68 | 1.51 |
| 1 | A | 790 | LYS | CA-CB | 7.86 | 1.71 | 1.53 |
| 1 | B | 290 | GLU | CD-OE1 | 7.86 | 1.34 | 1.25 |
| 1 | B | 729 | LEU | C-O | 7.86 | 1.38 | 1.23 |
| 1 | B | 613 | PHE | CE2-CZ | 7.85 | 1.52 | 1.37 |
| 1 | A | 214 | TRP | CG-CD1 | -7.84 | 1.25 | 1.36 |
| 1 | A | 731 | VAL | CB-CG1 | 7.84 | 1.69 | 1.52 |
| 1 | A | 882 | ASN | C-O | 7.84 | 1.38 | 1.23 |
| 1 | B | 843 | SER | CA-CB | 7.84 | 1.64 | 1.52 |
| 1 | A | 225 | TYR | CD1-CE1 | 7.83 | 1.51 | 1.39 |
| 1 | A | 821 | GLY | C-O | 7.82 | 1.36 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 89 | VAL | CB-CG2 | 7.82 | 1.69 | 1.52 |
| 1 | B | 331 | PHE | CD1-CE1 | -7.82 | 1.23 | 1.39 |
| 1 | A | 385 | PRO | CA-C | -7.82 | 1.37 | 1.52 |
| 1 | B | 613 | PHE | CB-CG | -7.82 | 1.38 | 1.51 |
| 1 | A | 377 | TYR | C-O | -7.81 | 1.08 | 1.23 |
| 1 | A | 789 | PHE | CA-C | -7.80 | 1.32 | 1.52 |
| 1 | A | 241 | SER | CA-CB | 7.80 | 1.64 | 1.52 |
| 1 | A | 649 | VAL | CA-CB | 7.79 | 1.71 | 1.54 |
| 1 | B | 331 | PHE | CD2-CE2 | -7.79 | 1.23 | 1.39 |
| 1 | A | 167 | PHE | C-O | 7.79 | 1.38 | 1.23 |
| 1 | A | 468 | ASN | CG-ND2 | 7.79 | 1.52 | 1.32 |
| 1 | B | 125 | VAL | C-O | 7.78 | 1.38 | 1.23 |
| 1 | B | 647 | VAL | CB-CG2 | -7.78 | 1.36 | 1.52 |
| 1 | A | 662 | ASP | CB-CG | -7.78 | 1.35 | 1.51 |
| 1 | B | 17 | GLY | CA-C | 7.78 | 1.64 | 1.51 |
| 1 | A | 833 | HIS | C-O | 7.77 | 1.38 | 1.23 |
| 1 | A | 332 | ILE | CB-CG1 | 7.77 | 1.75 | 1.54 |
| 1 | A | 413 | LEU | C-O | -7.77 | 1.08 | 1.23 |
| 1 | A | 616 | PHE | CE2-CZ | -7.77 | 1.22 | 1.37 |
| 1 | A | 19 | GLY | CA-C | 7.76 | 1.64 | 1.51 |
| 1 | A | 119 | THR | N-CA | -7.76 | 1.30 | 1.46 |
| 1 | B | 495 | GLU | CD-OE2 | 7.76 | 1.34 | 1.25 |
| 1 | A | 440 | ARG | C-O | 7.76 | 1.38 | 1.23 |
| 1 | A | 450 | LYS | CD-CE | 7.76 | 1.70 | 1.51 |
| 1 | A | 213 | GLU | CD-OE2 | -7.75 | 1.17 | 1.25 |
| 1 | A | 89 | VAL | CA-CB | 7.75 | 1.71 | 1.54 |
| 1 | A | 148 | GLU | CD-OE1 | 7.75 | 1.34 | 1.25 |
| 1 | A | 314 | GLN | CG-CD | 7.75 | 1.68 | 1.51 |
| 1 | A | 27 | TYR | CZ-OH | -7.74 | 1.24 | 1.37 |
| 1 | A | 278 | ARG | CA-C | -7.73 | 1.32 | 1.52 |
| 1 | B | 259 | VAL | CA-C | 7.73 | 1.73 | 1.52 |
| 1 | A | 311 | GLU | CD-OE1 | -7.72 | 1.17 | 1.25 |
| 1 | A | 382 | TRP | CD2-CE2 | -7.72 | 1.32 | 1.41 |
| 1 | B | 73 | ILE | C-O | -7.72 | 1.08 | 1.23 |
| 1 | A | 242 | ILE | C-O | -7.72 | 1.08 | 1.23 |
| 1 | A | 613 | PHE | CG-CD2 | -7.72 | 1.27 | 1.38 |
| 1 | B | 38 | GLU | C-O | -7.71 | 1.08 | 1.23 |
| 1 | A | 177 | TRP | CB-CG | -7.71 | 1.36 | 1.50 |
| 1 | A | 404 | GLU | CD-OE1 | 7.71 | 1.34 | 1.25 |
| 1 | A | 429 | GLU | N-CA | -7.70 | 1.30 | 1.46 |
| 1 | B | 159 | PRO | C-O | -7.70 | 1.07 | 1.23 |
| 1 | A | 26 | LYS | CD-CE | 7.70 | 1.70 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 366 | ARG | N-CA | 7.70 | 1.61 | 1.46 |
| 1 | B | 454 | PHE | CB-CG | 7.70 | 1.64 | 1.51 |
| 1 | A | 635 | ALA | N-CA | 7.69 | 1.61 | 1.46 |
| 1 | B | 349 | LYS | CE-NZ | 7.69 | 1.68 | 1.49 |
| 1 | A | 217 | LEU | CA-C | -7.68 | 1.32 | 1.52 |
| 1 | A | 764 | PHE | N-CA | 7.68 | 1.61 | 1.46 |
| 1 | B | 416 | LYS | CB-CG | 7.68 | 1.73 | 1.52 |
| 1 | A | 30 | GLN | CD-NE2 | 7.68 | 1.52 | 1.32 |
| 1 | A | 507 | LYS | CD-CE | 7.68 | 1.70 | 1.51 |
| 1 | A | 553 | LYS | CA-CB | 7.66 | 1.70 | 1.53 |
| 1 | B | 284 | MET | CB-CG | 7.66 | 1.75 | 1.51 |
| 1 | A | 666 | ARG | CZ-NH1 | 7.66 | 1.43 | 1.33 |
| 1 | A | 778 | SER | C-O | 7.66 | 1.38 | 1.23 |
| 1 | B | 470 | ARG | CZ-NH1 | -7.66 | 1.23 | 1.33 |
| 1 | B | 508 | ALA | CA-CB | 7.66 | 1.68 | 1.52 |
| 1 | A | 637 | GLY | C-O | 7.66 | 1.35 | 1.23 |
| 1 | A | 494 | LYS | CE-NZ | 7.65 | 1.68 | 1.49 |
| 1 | A | 69 | LYS | CE-NZ | -7.65 | 1.29 | 1.49 |
| 1 | A | 141 | PHE | CG-CD2 | 7.65 | 1.50 | 1.38 |
| 1 | A | 647 | VAL | CB-CG1 | 7.65 | 1.69 | 1.52 |
| 1 | A | 355 | ASN | CG-OD1 | 7.64 | 1.40 | 1.24 |
| 1 | A | 787 | GLU | CD-OE2 | 7.64 | 1.34 | 1.25 |
| 1 | A | 803 | TYR | CG-CD1 | -7.64 | 1.29 | 1.39 |
| 1 | A | 800 | GLN | CB-CG | -7.63 | 1.31 | 1.52 |
| 1 | B | 297 | TRP | CD2-CE2 | -7.63 | 1.32 | 1.41 |
| 1 | B | 346 | ASP | CG-OD1 | 7.63 | 1.43 | 1.25 |
| 1 | A | 881 | VAL | CB-CG1 | -7.63 | 1.36 | 1.52 |
| 1 | A | 45 | LEU | C-O | 7.63 | 1.37 | 1.23 |
| 1 | A | 763 | GLY | C-O | 7.63 | 1.35 | 1.23 |
| 1 | B | 412 | ALA | C-O | 7.62 | 1.37 | 1.23 |
| 1 | B | 655 | ASP | CB-CG | 7.62 | 1.67 | 1.51 |
| 1 | A | 61 | LYS | CA-CB | 7.62 | 1.70 | 1.53 |
| 1 | A | 602 | LEU | CG-CD1 | 7.62 | 1.80 | 1.51 |
| 1 | B | 451 | ARG | CG-CD | 7.61 | 1.71 | 1.51 |
| 1 | B | 472 | VAL | C-O | 7.61 | 1.37 | 1.23 |
| 1 | A | 388 | LYS | CE-NZ | 7.61 | 1.68 | 1.49 |
| 1 | B | 181 | LEU | CG-CD1 | -7.61 | 1.23 | 1.51 |
| 1 | A | 313 | GLU | CG-CD | 7.60 | 1.63 | 1.51 |
| 1 | B | 377 | TYR | CD2-CE2 | 7.60 | 1.50 | 1.39 |
| 1 | A | 340 | ILE | CB-CG2 | 7.59 | 1.76 | 1.52 |
| 1 | A | 356 | TRP | CB-CG | -7.59 | 1.36 | 1.50 |
| 1 | B | 152 | VAL | C-O | -7.59 | 1.08 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 215 | TYR | CG-CD2 | -7.59 | 1.29 | 1.39 |
| 1 | B | 278 | ARG | CG-CD | 7.59 | 1.71 | 1.51 |
| 1 | A | 543 | LEU | C-O | 7.58 | 1.37 | 1.23 |
| 1 | B | 41 | GLU | CD-OE1 | 7.58 | 1.33 | 1.25 |
| 1 | B | 550 | ILE | CA-CB | -7.58 | 1.37 | 1.54 |
| 1 | B | 331 | PHE | CB-CG | -7.57 | 1.38 | 1.51 |
| 1 | A | 878 | GLN | CD-OE1 | 7.57 | 1.40 | 1.24 |
| 1 | A | 127 | TYR | CE2-CZ | 7.57 | 1.48 | 1.38 |
| 1 | A | 797 | LYS | CB-CG | 7.56 | 1.73 | 1.52 |
| 1 | A | 800 | GLN | C-O | 7.56 | 1.37 | 1.23 |
| 1 | A | 106 | TRP | CB-CG | -7.55 | 1.36 | 1.50 |
| 1 | B | 182 | GLU | N-CA | 7.55 | 1.61 | 1.46 |
| 1 | A | 129 | GLN | CD-NE2 | 7.55 | 1.51 | 1.32 |
| 1 | A | 275 | GLN | N-CA | -7.55 | 1.31 | 1.46 |
| 1 | A | 882 | ASN | CB-CG | 7.55 | 1.68 | 1.51 |
| 1 | A | 490 | PHE | CG-CD2 | -7.54 | 1.27 | 1.38 |
| 1 | A | 656 | GLU | CG-CD | 7.54 | 1.63 | 1.51 |
| 1 | A | 109 | ALA | CA-CB | 7.54 | 1.68 | 1.52 |
| 1 | B | 837 | MET | CA-C | 7.54 | 1.72 | 1.52 |
| 1 | A | 845 | GLU | CA-C | 7.54 | 1.72 | 1.52 |
| 1 | B | 471 | GLU | CG-CD | 7.54 | 1.63 | 1.51 |
| 1 | B | 648 | ILE | CB-CG2 | -7.53 | 1.29 | 1.52 |
| 1 | A | 579 | CYS | CB-SG | 7.52 | 1.95 | 1.82 |
| 1 | A | 628 | GLU | CD-OE1 | 7.51 | 1.33 | 1.25 |
| 1 | B | 503 | PHE | C-O | -7.51 | 1.09 | 1.23 |
| 1 | A | 225 | TYR | CG-CD1 | 7.51 | 1.49 | 1.39 |
| 1 | A | 306 | LYS | C-O | -7.50 | 1.09 | 1.23 |
| 1 | A | 385 | PRO | C-O | -7.50 | 1.08 | 1.23 |
| 1 | B | 303 | GLU | CD-OE2 | 7.50 | 1.33 | 1.25 |
| 1 | B | 192 | TYR | CZ-OH | 7.50 | 1.50 | 1.37 |
| 1 | B | 471 | GLU | CD-OE1 | 7.50 | 1.33 | 1.25 |
| 1 | A | 450 | LYS | CE-NZ | 7.49 | 1.67 | 1.49 |
| 1 | B | 649 | VAL | CB-CG2 | -7.49 | 1.37 | 1.52 |
| 1 | A | 466 | PHE | CD2-CE2 | 7.49 | 1.54 | 1.39 |
| 1 | B | 303 | GLU | CD-OE1 | 7.49 | 1.33 | 1.25 |
| 1 | A | 883 | ILE | CB-CG2 | 7.48 | 1.76 | 1.52 |
| 1 | A | 316 | ARG | CA-CB | 7.48 | 1.70 | 1.53 |
| 1 | A | 383 | VAL | C-O | -7.47 | 1.09 | 1.23 |
| 1 | A | 65 | PRO | CB-CG | 7.47 | 1.87 | 1.50 |
| 1 | B | 50 | ALA | C-O | 7.46 | 1.37 | 1.23 |
| 1 | B | 403 | ARG | CA-C | 7.46 | 1.72 | 1.52 |
| 1 | A | 769 | CYS | CB-SG | 7.46 | 1.95 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 444 | GLY | C-O | 7.46 | 1.35 | 1.23 |
| 1 | B | 344 | THR | N-CA | 7.46 | 1.61 | 1.46 |
| 1 | A | 436 | TYR | CG-CD2 | -7.46 | 1.29 | 1.39 |
| 1 | B | 436 | TYR | CZ-OH | 7.46 | 1.50 | 1.37 |
| 1 | A | 324 | PHE | CB-CG | -7.45 | 1.38 | 1.51 |
| 1 | A | 382 | TRP | CB-CG | 7.45 | 1.63 | 1.50 |
| 1 | B | 79 | THR | CB-CG2 | -7.45 | 1.27 | 1.52 |
| 1 | B | 560 | ASN | CA-CB | 7.45 | 1.72 | 1.53 |
| 1 | A | 808 | THR | CB-CG2 | 7.44 | 1.76 | 1.52 |
| 1 | B | 101 | ALA | CA-CB | 7.44 | 1.68 | 1.52 |
| 1 | A | 636 | ALA | CA-CB | -7.43 | 1.36 | 1.52 |
| 1 | B | 42 | ALA | CA-CB | -7.43 | 1.36 | 1.52 |
| 1 | A | 854 | PHE | CE1-CZ | 7.42 | 1.51 | 1.37 |
| 1 | A | 777 | ASP | C-O | -7.41 | 1.09 | 1.23 |
| 1 | A | 117 | ASN | CG-ND2 | 7.41 | 1.51 | 1.32 |
| 1 | B | 634 | GLU | CD-OE2 | 7.41 | 1.33 | 1.25 |
| 1 | B | 464 | GLU | CD-OE2 | 7.40 | 1.33 | 1.25 |
| 1 | A | 600 | ASN | CA-CB | 7.39 | 1.72 | 1.53 |
| 1 | B | 767 | ASP | CA-CB | 7.39 | 1.70 | 1.53 |
| 1 | A | 44 | ALA | N-CA | 7.39 | 1.61 | 1.46 |
| 1 | B | 140 | HIS | CA-CB | -7.39 | 1.37 | 1.53 |
| 1 | B | 335 | PHE | CD2-CE2 | 7.38 | 1.54 | 1.39 |
| 1 | A | 131 | PHE | CB-CG | -7.38 | 1.38 | 1.51 |
| 1 | A | 413 | LEU | CG-CD1 | 7.38 | 1.79 | 1.51 |
| 1 | B | 74 | LYS | CA-C | 7.38 | 1.72 | 1.52 |
| 1 | B | 572 | ASN | C-O | 7.38 | 1.37 | 1.23 |
| 1 | A | 25 | ILE | CB-CG2 | -7.37 | 1.29 | 1.52 |
| 1 | A | 285 | ARG | CB-CG | 7.37 | 1.72 | 1.52 |
| 1 | B | 312 | ARG | C-O | -7.37 | 1.09 | 1.23 |
| 1 | B | 312 | ARG | CB-CG | 7.37 | 1.72 | 1.52 |
| 1 | A | 297 | TRP | CD2-CE2 | 7.36 | 1.50 | 1.41 |
| 1 | B | 643 | GLN | CD-OE1 | 7.36 | 1.40 | 1.24 |
| 1 | B | 369 | SER | C-O | -7.35 | 1.09 | 1.23 |
| 1 | A | 71 | TYR | CB-CG | 7.35 | 1.62 | 1.51 |
| 1 | A | 874 | ASN | CB-CG | 7.35 | 1.68 | 1.51 |
| 1 | B | 185 | TYR | CD2-CE2 | -7.34 | 1.28 | 1.39 |
| 1 | B | 351 | ARG | CA-CB | 7.33 | 1.70 | 1.53 |
| 1 | B | 429 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | A | 255 | PHE | N-CA | 7.32 | 1.60 | 1.46 |
| 1 | B | 288 | TRP | CZ3-CH2 | -7.32 | 1.28 | 1.40 |
| 1 | A | 174 | ASN | CA-C | 7.31 | 1.72 | 1.52 |
| 1 | A | 427 | ASP | N-CA | 7.30 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 399 | ASP | CG-OD2 | 7.30 | 1.42 | 1.25 |
| 1 | A | 659 | ILE | CA-CB | -7.30 | 1.38 | 1.54 |
| 1 | A | 329 | ARG | CB-CG | 7.30 | 1.72 | 1.52 |
| 1 | B | 512 | GLU | CD-OE2 | -7.29 | 1.17 | 1.25 |
| 1 | A | 504 | SER | CA-CB | 7.29 | 1.63 | 1.52 |
| 1 | A | 778 | SER | CB-OG | 7.29 | 1.51 | 1.42 |
| 1 | B | 793 | TRP | CB-CG | 7.28 | 1.63 | 1.50 |
| 1 | A | 437 | GLN | C-O | 7.28 | 1.37 | 1.23 |
| 1 | A | 375 | ARG | C-O | -7.27 | 1.09 | 1.23 |
| 1 | A | 381 | PHE | CD2-CE2 | 7.27 | 1.53 | 1.39 |
| 1 | A | 176 | PHE | CG-CD2 | 7.27 | 1.49 | 1.38 |
| 1 | A | 10 | LYS | CE-NZ | 7.27 | 1.67 | 1.49 |
| 1 | A | 320 | GLU | CB-CG | 7.27 | 1.66 | 1.52 |
| 1 | A | 380 | THR | N-CA | -7.26 | 1.31 | 1.46 |
| 1 | A | 658 | ILE | CB-CG2 | -7.26 | 1.30 | 1.52 |
| 1 | A | 120 | ILE | C-O | -7.26 | 1.09 | 1.23 |
| 1 | A | 712 | TYR | CA-CB | 7.26 | 1.70 | 1.53 |
| 1 | A | 199 | CYS | CB-SG | -7.25 | 1.70 | 1.82 |
| 1 | A | 593 | LYS | CA-CB | 7.25 | 1.69 | 1.53 |
| 1 | B | 96 | ASP | C-O | -7.25 | 1.09 | 1.23 |
| 1 | A | 674 | LEU | CA-CB | -7.25 | 1.37 | 1.53 |
| 1 | B | 479 | PRO | CA-CB | -7.25 | 1.39 | 1.53 |
| 1 | B | 354 | ARG | N-CA | 7.25 | 1.60 | 1.46 |
| 1 | A | 119 | THR | CA-CB | -7.24 | 1.34 | 1.53 |
| 1 | B | 791 | TYR | CD2-CE2 | 7.24 | 1.50 | 1.39 |
| 1 | A | 185 | TYR | CE1-CZ | -7.24 | 1.29 | 1.38 |
| 1 | B | 599 | PHE | CE1-CZ | 7.24 | 1.51 | 1.37 |
| 1 | A | 734 | ALA | C-O | 7.23 | 1.37 | 1.23 |
| 1 | A | 802 | ILE | CA-CB | -7.22 | 1.38 | 1.54 |
| 1 | B | 129 | GLN | C-O | -7.22 | 1.09 | 1.23 |
| 1 | B | 647 | VAL | CB-CG1 | -7.22 | 1.37 | 1.52 |
| 1 | B | 237 | LEU | N-CA | 7.21 | 1.60 | 1.46 |
| 1 | B | 399 | ASP | CB-CG | 7.21 | 1.66 | 1.51 |
| 1 | B | 322 | GLY | CA-C | 7.21 | 1.63 | 1.51 |
| 1 | B | 59 | GLY | N-CA | 7.21 | 1.56 | 1.46 |
| 1 | A | 812 | GLY | N-CA | 7.20 | 1.56 | 1.46 |
| 1 | B | 480 | PRO | N-CD | -7.20 | 1.37 | 1.47 |
| 1 | B | 160 | THR | N-CA | -7.20 | 1.31 | 1.46 |
| 1 | A | 611 | THR | CA-CB | -7.20 | 1.34 | 1.53 |
| 1 | A | 666 | ARG | CZ-NH2 | 7.19 | 1.42 | 1.33 |
| 1 | A | 369 | SER | CB-OG | 7.18 | 1.51 | 1.42 |
| 1 | B | 24 | ALA | CA-CB | -7.18 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 342 | ASN | C-O | -7.18 | 1.09 | 1.23 |
| 1 | B | 378 | PRO | CA-C | -7.18 | 1.38 | 1.52 |
| 1 | B | 228 | ILE | CB-CG2 | 7.18 | 1.75 | 1.52 |
| 1 | B | 826 | ALA | CA-CB | 7.18 | 1.67 | 1.52 |
| 1 | B | 378 | PRO | CG-CD | 7.17 | 1.74 | 1.50 |
| 1 | A | 16 | GLU | CD-OE2 | 7.17 | 1.33 | 1.25 |
| 1 | A | 341 | CYS | CA-C | 7.17 | 1.71 | 1.52 |
| 1 | A | 860 | ARG | CZ-NH1 | 7.17 | 1.42 | 1.33 |
| 1 | A | 516 | GLN | N-CA | 7.17 | 1.60 | 1.46 |
| 1 | B | 329 | ARG | NE-CZ | 7.17 | 1.42 | 1.33 |
| 1 | B | 90 | ASP | CA-CB | 7.16 | 1.69 | 1.53 |
| 1 | B | 764 | PHE | CD2-CE2 | 7.16 | 1.53 | 1.39 |
| 1 | B | 349 | LYS | CD-CE | 7.15 | 1.69 | 1.51 |
| 1 | A | 194 | ALA | CA-CB | -7.15 | 1.37 | 1.52 |
| 1 | A | 437 | GLN | CD-NE2 | 7.15 | 1.50 | 1.32 |
| 1 | B | 278 | ARG | CB-CG | 7.15 | 1.71 | 1.52 |
| 1 | B | 167 | PHE | C-O | 7.14 | 1.36 | 1.23 |
| 1 | A | 99 | GLN | N-CA | 7.14 | 1.60 | 1.46 |
| 1 | B | 120 | ILE | CB-CG2 | 7.14 | 1.75 | 1.52 |
| 1 | B | 256 | LYS | N-CA | 7.13 | 1.60 | 1.46 |
| 1 | B | 473 | SER | C-O | -7.13 | 1.09 | 1.23 |
| 1 | B | 854 | PHE | CG-CD2 | 7.13 | 1.49 | 1.38 |
| 1 | B | 281 | LEU | C-O | 7.12 | 1.36 | 1.23 |
| 1 | B | 719 | GLU | CD-OE2 | 7.12 | 1.33 | 1.25 |
| 1 | B | 726 | PHE | CD1-CE1 | 7.12 | 1.53 | 1.39 |
| 1 | B | 389 | ILE | CB-CG1 | -7.12 | 1.34 | 1.54 |
| 1 | B | 687 | GLY | CA-C | 7.12 | 1.63 | 1.51 |
| 1 | A | 385 | PRO | N-CA | -7.11 | 1.35 | 1.47 |
| 1 | B | 296 | PRO | CB-CG | -7.11 | 1.14 | 1.50 |
| 1 | A | 51 | PHE | CG-CD1 | 7.11 | 1.49 | 1.38 |
| 1 | A | 448 | HIS | C-O | -7.11 | 1.09 | 1.23 |
| 1 | A | 7 | LYS | CE-NZ | 7.11 | 1.66 | 1.49 |
| 1 | A | 434 | ALA | CA-CB | -7.11 | 1.37 | 1.52 |
| 1 | A | 439 | PRO | C-O | 7.10 | 1.37 | 1.23 |
| 1 | A | 822 | ALA | N-CA | 7.10 | 1.60 | 1.46 |
| 1 | B | 892 | TYR | CE1-CZ | 7.10 | 1.47 | 1.38 |
| 1 | A | 92 | ALA | C-O | 7.09 | 1.36 | 1.23 |
| 1 | A | 288 | TRP | CB-CG | -7.09 | 1.37 | 1.50 |
| 1 | B | 215 | TYR | CE2-CZ | -7.09 | 1.29 | 1.38 |
| 1 | B | 296 | PRO | CA-C | 7.09 | 1.67 | 1.52 |
| 1 | B | 192 | TYR | CG-CD2 | -7.08 | 1.29 | 1.39 |
| 1 | A | 262 | HIS | N-CA | 7.08 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 586 | MET | CG-SD | 7.08 | 1.99 | 1.81 |
| 1 | B | 872 | ASP | CB-CG | -7.08 | 1.36 | 1.51 |
| 1 | B | 539 | LEU | CA-C | 7.08 | 1.71 | 1.52 |
| 1 | A | 41 | GLU | CB-CG | 7.07 | 1.65 | 1.52 |
| 1 | A | 892 | TYR | CZ-OH | -7.07 | 1.25 | 1.37 |
| 1 | A | 696 | TRP | CB-CG | -7.07 | 1.37 | 1.50 |
| 1 | B | 20 | SER | CB-OG | 7.07 | 1.51 | 1.42 |
| 1 | A | 884 | GLN | CD-NE2 | 7.06 | 1.50 | 1.32 |
| 1 | B | 503 | PHE | CB-CG | -7.06 | 1.39 | 1.51 |
| 1 | A | 673 | ILE | CA-CB | 7.05 | 1.71 | 1.54 |
| 1 | A | 833 | HIS | N-CA | 7.05 | 1.60 | 1.46 |
| 1 | B | 382 | TRP | C-O | 7.05 | 1.36 | 1.23 |
| 1 | A | 41 | GLU | CD-OE2 | 7.05 | 1.33 | 1.25 |
| 1 | A | 387 | PHE | CG-CD2 | 7.05 | 1.49 | 1.38 |
| 1 | B | 438 | VAL | CB-CG2 | 7.05 | 1.67 | 1.52 |
| 1 | A | 51 | PHE | CD2-CE2 | -7.04 | 1.25 | 1.39 |
| 1 | A | 192 | TYR | CE1-CZ | -7.04 | 1.29 | 1.38 |
| 1 | A | 598 | GLU | C-O | -7.04 | 1.09 | 1.23 |
| 1 | B | 409 | PHE | CD1-CE1 | 7.04 | 1.53 | 1.39 |
| 1 | B | 498 | PHE | C-O | 7.04 | 1.36 | 1.23 |
| 1 | A | 204 | PHE | CD2-CE2 | -7.04 | 1.25 | 1.39 |
| 1 | A | 241 | SER | CB-OG | 7.03 | 1.51 | 1.42 |
| 1 | A | 152 | VAL | CB-CG2 | -7.03 | 1.38 | 1.52 |
| 1 | A | 110 | ALA | N-CA | 7.03 | 1.60 | 1.46 |
| 1 | A | 789 | PHE | CD2-CE2 | -7.03 | 1.25 | 1.39 |
| 1 | A | 76 | LYS | CB-CG | 7.03 | 1.71 | 1.52 |
| 1 | B | 131 | PHE | C-O | -7.02 | 1.10 | 1.23 |
| 1 | B | 271 | GLN | CG-CD | 7.02 | 1.67 | 1.51 |
| 1 | B | 664 | PHE | CD2-CE2 | 7.02 | 1.53 | 1.39 |
| 1 | B | 499 | LEU | C-O | 7.01 | 1.36 | 1.23 |
| 1 | A | 236 | SER | CA-CB | -7.01 | 1.42 | 1.52 |
| 1 | B | 450 | LYS | CB-CG | 7.00 | 1.71 | 1.52 |
| 1 | B | 236 | SER | CB-OG | 7.00 | 1.51 | 1.42 |
| 1 | B | 22 | GLU | CD-OE1 | 7.00 | 1.33 | 1.25 |
| 1 | A | 485 | VAL | C-O | -6.99 | 1.10 | 1.23 |
| 1 | A | 183 | LYS | N-CA | 6.99 | 1.60 | 1.46 |
| 1 | A | 96 | ASP | CA-C | -6.99 | 1.34 | 1.52 |
| 1 | B | 854 | PHE | CE2-CZ | 6.99 | 1.50 | 1.37 |
| 1 | B | 811 | SER | CA-C | 6.98 | 1.71 | 1.52 |
| 1 | A | 12 | ARG | CA-C | 6.98 | 1.71 | 1.52 |
| 1 | B | 230 | LYS | CB-CG | -6.98 | 1.33 | 1.52 |
| 1 | B | 670 | ARG | CZ-NH2 | -6.98 | 1.24 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 211 | VAL | CA-C | -6.96 | 1.34 | 1.52 |
| 1 | B | 23 | ARG | CB-CG | 6.96 | 1.71 | 1.52 |
| 1 | B | 382 | TRP | CB-CG | -6.96 | 1.37 | 1.50 |
| 1 | A | 381 | PHE | CB-CG | -6.95 | 1.39 | 1.51 |
| 1 | A | 384 | ASN | CG-ND2 | 6.95 | 1.50 | 1.32 |
| 1 | A | 452 | ASP | C-O | 6.95 | 1.36 | 1.23 |
| 1 | A | 638 | PHE | CE2-CZ | 6.95 | 1.50 | 1.37 |
| 1 | A | 334 | GLU | CB-CG | -6.95 | 1.39 | 1.52 |
| 1 | B | 135 | TYR | CG-CD2 | -6.94 | 1.30 | 1.39 |
| 1 | A | 412 | ALA | CA-C | -6.94 | 1.34 | 1.52 |
| 1 | A | 736 | ASP | CB-CG | 6.94 | 1.66 | 1.51 |
| 1 | B | 504 | SER | CA-CB | 6.94 | 1.63 | 1.52 |
| 1 | B | 96 | ASP | CA-C | -6.93 | 1.34 | 1.52 |
| 1 | B | 366 | ARG | CG-CD | 6.93 | 1.69 | 1.51 |
| 1 | A | 164 | LYS | C-O | 6.92 | 1.36 | 1.23 |
| 1 | A | 217 | LEU | CG-CD2 | -6.92 | 1.26 | 1.51 |
| 1 | B | 636 | ALA | C-O | 6.92 | 1.36 | 1.23 |
| 1 | A | 550 | ILE | CA-C | 6.92 | 1.71 | 1.52 |
| 1 | B | 192 | TYR | CD2-CE2 | -6.91 | 1.28 | 1.39 |
| 1 | B | 631 | MET | SD-CE | 6.90 | 2.16 | 1.77 |
| 1 | B | 764 | PHE | CE1-CZ | 6.90 | 1.50 | 1.37 |
| 1 | B | 636 | ALA | CA-CB | -6.90 | 1.38 | 1.52 |
| 1 | B | 341 | CYS | C-O | -6.89 | 1.10 | 1.23 |
| 1 | B | 777 | ASP | N-CA | 6.89 | 1.60 | 1.46 |
| 1 | A | 244 | ILE | CA-CB | 6.89 | 1.70 | 1.54 |
| 1 | A | 306 | LYS | CE-NZ | 6.89 | 1.66 | 1.49 |
| 1 | A | 623 | SER | CB-OG | 6.89 | 1.51 | 1.42 |
| 1 | B | 491 | GLU | CG-CD | 6.88 | 1.62 | 1.51 |
| 1 | A | 214 | TRP | CD2-CE2 | -6.88 | 1.33 | 1.41 |
| 1 | A | 257 | ASN | C-O | 6.88 | 1.36 | 1.23 |
| 1 | A | 610 | LEU | CG-CD2 | 6.88 | 1.77 | 1.51 |
| 1 | A | 266 | VAL | C-O | 6.87 | 1.36 | 1.23 |
| 1 | A | 151 | ASP | CG-OD1 | 6.87 | 1.41 | 1.25 |
| 1 | A | 139 | PHE | CE1-CZ | 6.87 | 1.50 | 1.37 |
| 1 | B | 360 | PHE | CD1-CE1 | 6.87 | 1.52 | 1.39 |
| 1 | A | 281 | LEU | CA-C | -6.86 | 1.35 | 1.52 |
| 1 | B | 398 | ASP | CG-OD1 | 6.86 | 1.41 | 1.25 |
| 1 | B | 699 | PHE | CD2-CE2 | 6.86 | 1.52 | 1.39 |
| 1 | B | 343 | LEU | CG-CD2 | 6.86 | 1.77 | 1.51 |
| 1 | A | 178 | SER | C-O | 6.86 | 1.36 | 1.23 |
| 1 | A | 756 | HIS | N-CA | 6.86 | 1.60 | 1.46 |
| 1 | A | 67 | SER | CA-CB | 6.85 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 871 | LEU | C-O | -6.85 | 1.10 | 1.23 |
| 1 | B | 2 | ALA | N-CA | 6.85 | 1.60 | 1.46 |
| 1 | A | 820 | PRO | N-CA | 6.85 | 1.58 | 1.47 |
| 1 | A | 466 | PHE | CE2-CZ | 6.85 | 1.50 | 1.37 |
| 1 | B | 164 | LYS | CB-CG | 6.85 | 1.71 | 1.52 |
| 1 | B | 11 | ASP | CA-C | 6.84 | 1.70 | 1.52 |
| 1 | A | 380 | THR | CA-CB | -6.84 | 1.35 | 1.53 |
| 1 | A | 656 | GLU | CB-CG | 6.84 | 1.65 | 1.52 |
| 1 | B | 851 | PHE | CD1-CE1 | 6.83 | 1.52 | 1.39 |
| 1 | B | 329 | ARG | CZ-NH2 | 6.83 | 1.42 | 1.33 |
| 1 | B | 451 | ARG | NE-CZ | 6.83 | 1.42 | 1.33 |
| 1 | A | 222 | SER | C-O | 6.83 | 1.36 | 1.23 |
| 1 | A | 200 | THR | CB-CG2 | 6.82 | 1.74 | 1.52 |
| 1 | B | 699 | PHE | CD1-CE1 | 6.82 | 1.52 | 1.39 |
| 1 | B | 738 | MET | CG-SD | 6.82 | 1.98 | 1.81 |
| 1 | B | 780 | THR | C-O | -6.82 | 1.10 | 1.23 |
| 1 | A | 312 | ARG | CZ-NH2 | 6.82 | 1.42 | 1.33 |
| 1 | B | 616 | PHE | CB-CG | -6.81 | 1.39 | 1.51 |
| 1 | B | 627 | TYR | CE2-CZ | 6.81 | 1.47 | 1.38 |
| 1 | A | 155 | ASP | CG-OD1 | 6.80 | 1.41 | 1.25 |
| 1 | A | 436 | TYR | CZ-OH | -6.80 | 1.26 | 1.37 |
| 1 | A | 374 | CYS | C-O | -6.80 | 1.10 | 1.23 |
| 1 | B | 267 | THR | N-CA | -6.80 | 1.32 | 1.46 |
| 1 | B | 319 | MET | CG-SD | 6.79 | 1.98 | 1.81 |
| 1 | B | 329 | ARG | CA-C | 6.79 | 1.70 | 1.52 |
| 1 | B | 452 | ASP | CB-CG | 6.79 | 1.66 | 1.51 |
| 1 | B | 843 | SER | N-CA | 6.79 | 1.59 | 1.46 |
| 1 | B | 22 | GLU | CG-CD | 6.79 | 1.62 | 1.51 |
| 1 | B | 481 | GLY | C-O | 6.78 | 1.34 | 1.23 |
| 1 | A | 678 | PHE | CE2-CZ | 6.78 | 1.50 | 1.37 |
| 1 | B | 681 | LEU | C-O | 6.78 | 1.36 | 1.23 |
| 1 | A | 803 | TYR | CB-CG | -6.77 | 1.41 | 1.51 |
| 1 | B | 294 | LYS | CG-CD | 6.77 | 1.75 | 1.52 |
| 1 | B | 678 | PHE | CD1-CE1 | -6.77 | 1.25 | 1.39 |
| 1 | B | 885 | GLU | CB-CG | 6.76 | 1.65 | 1.52 |
| 1 | A | 871 | LEU | CA-C | -6.76 | 1.35 | 1.52 |
| 1 | B | 505 | GLU | CB-CG | 6.76 | 1.65 | 1.52 |
| 1 | B | 231 | ALA | N-CA | 6.75 | 1.59 | 1.46 |
| 1 | A | 663 | ASN | CB-CG | 6.75 | 1.66 | 1.51 |
| 1 | B | 666 | ARG | C-O | -6.75 | 1.10 | 1.23 |
| 1 | A | 783 | LYS | C-O | 6.74 | 1.36 | 1.23 |
| 1 | A | 863 | ALA | CA-CB | -6.74 | 1.38 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 87 | PHE | CD1-CE1 | 6.74 | 1.52 | 1.39 |
| 1 | B | 335 | PHE | CB-CG | 6.74 | 1.62 | 1.51 |
| 1 | B | 361 | TYR | CG-CD1 | 6.74 | 1.48 | 1.39 |
| 1 | B | 587 | ASP | CB-CG | 6.74 | 1.66 | 1.51 |
| 1 | B | 433 | PHE | CE2-CZ | -6.74 | 1.24 | 1.37 |
| 1 | B | 607 | ARG | CB-CG | 6.73 | 1.70 | 1.52 |
| 1 | A | 652 | PHE | CE1-CZ | -6.73 | 1.24 | 1.37 |
| 1 | B | 491 | GLU | CD-OE2 | 6.73 | 1.33 | 1.25 |
| 1 | B | 175 | GLU | CB-CG | 6.71 | 1.65 | 1.52 |
| 1 | B | 727 | ARG | C-O | 6.71 | 1.36 | 1.23 |
| 1 | B | 340 | ILE | CB-CG2 | -6.71 | 1.32 | 1.52 |
| 1 | B | 616 | PHE | CD2-CE2 | -6.70 | 1.25 | 1.39 |
| 1 | A | 167 | PHE | CA-CB | -6.70 | 1.39 | 1.53 |
| 1 | A | 149 | TRP | CE2-CZ2 | -6.69 | 1.28 | 1.39 |
| 1 | A | 616 | PHE | C-O | 6.69 | 1.36 | 1.23 |
| 1 | A | 767 | ASP | CG-OD1 | 6.69 | 1.40 | 1.25 |
| 1 | B | 177 | TRP | CB-CG | -6.69 | 1.38 | 1.50 |
| 1 | A | 349 | LYS | C-O | 6.68 | 1.36 | 1.23 |
| 1 | A | 514 | ASP | CG-OD2 | 6.68 | 1.40 | 1.25 |
| 1 | B | 424 | PHE | C-N | 6.68 | 1.45 | 1.33 |
| 1 | A | 58 | LEU | C-O | 6.68 | 1.36 | 1.23 |
| 1 | A | 780 | THR | CA-CB | -6.67 | 1.35 | 1.53 |
| 1 | A | 273 | THR | CB-CG2 | 6.67 | 1.74 | 1.52 |
| 1 | A | 214 | TRP | CZ3-CH2 | -6.67 | 1.29 | 1.40 |
| 1 | B | 483 | TYR | CG-CD2 | -6.67 | 1.30 | 1.39 |
| 1 | A | 243 | ASN | N-CA | 6.66 | 1.59 | 1.46 |
| 1 | B | 518 | GLN | N-CA | 6.66 | 1.59 | 1.46 |
| 1 | A | 278 | ARG | CZ-NH2 | 6.65 | 1.41 | 1.33 |
| 1 | A | 393 | GLU | C-O | 6.65 | 1.35 | 1.23 |
| 1 | B | 113 | SER | CB-OG | 6.65 | 1.50 | 1.42 |
| 1 | A | 133 | GLU | CG-CD | 6.65 | 1.61 | 1.51 |
| 1 | A | 859 | VAL | CA-CB | -6.64 | 1.40 | 1.54 |
| 1 | A | 702 | LEU | N-CA | 6.64 | 1.59 | 1.46 |
| 1 | A | 105 | SER | CB-OG | 6.64 | 1.50 | 1.42 |
| 1 | A | 764 | PHE | CE2-CZ | -6.64 | 1.24 | 1.37 |
| 1 | B | 512 | GLU | CG-CD | 6.64 | 1.61 | 1.51 |
| 1 | B | 176 | PHE | CG-CD1 | -6.63 | 1.28 | 1.38 |
| 1 | B | 519 | ALA | C-O | -6.63 | 1.10 | 1.23 |
| 1 | A | 331 | PHE | CA-CB | -6.63 | 1.39 | 1.53 |
| 1 | A | 686 | THR | N-CA | 6.63 | 1.59 | 1.46 |
| 1 | B | 324 | PHE | CA-C | -6.63 | 1.35 | 1.52 |
| 1 | B | 308 | ASP | C-O | 6.62 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 474 | ASN | N-CA | -6.62 | 1.33 | 1.46 |
| 1 | B | 843 | SER | CA-C | 6.62 | 1.70 | 1.52 |
| 1 | A | 335 | PHE | CG-CD1 | 6.61 | 1.48 | 1.38 |
| 1 | B | 639 | LYS | CA-CB | 6.61 | 1.68 | 1.53 |
| 1 | A | 408 | SER | CB-OG | -6.61 | 1.33 | 1.42 |
| 1 | A | 148 | GLU | CG-CD | 6.61 | 1.61 | 1.51 |
| 1 | B | 344 | THR | C-O | -6.61 | 1.10 | 1.23 |
| 1 | A | 332 | ILE | CA-CB | 6.61 | 1.70 | 1.54 |
| 1 | B | 153 | VAL | CA-CB | -6.60 | 1.40 | 1.54 |
| 1 | B | 48 | ASP | N-CA | -6.60 | 1.33 | 1.46 |
| 1 | B | 483 | TYR | CE2-CZ | 6.59 | 1.47 | 1.38 |
| 1 | A | 795 | ASN | C-O | -6.59 | 1.10 | 1.23 |
| 1 | A | 760 | LYS | C-O | 6.59 | 1.35 | 1.23 |
| 1 | A | 694 | ILE | CA-CB | 6.59 | 1.70 | 1.54 |
| 1 | B | 400 | TYR | CG-CD1 | 6.58 | 1.47 | 1.39 |
| 1 | A | 288 | TRP | CE2-CZ2 | -6.58 | 1.28 | 1.39 |
| 1 | A | 730 | PHE | CD2-CE2 | 6.58 | 1.52 | 1.39 |
| 1 | A | 633 | ILE | CB-CG2 | -6.58 | 1.32 | 1.52 |
| 1 | A | 22 | GLU | CG-CD | 6.58 | 1.61 | 1.51 |
| 1 | B | 284 | MET | CG-SD | -6.58 | 1.64 | 1.81 |
| 1 | B | 640 | LEU | N-CA | 6.58 | 1.59 | 1.46 |
| 1 | B | 502 | PHE | CA-C | -6.57 | 1.35 | 1.52 |
| 1 | B | 806 | PHE | CD1-CE1 | 6.57 | 1.52 | 1.39 |
| 1 | B | 135 | TYR | CB-CG | 6.57 | 1.61 | 1.51 |
| 1 | A | 355 | ASN | CB-CG | 6.56 | 1.66 | 1.51 |
| 1 | B | 726 | PHE | CD2-CE2 | 6.56 | 1.52 | 1.39 |
| 1 | B | 373 | GLY | C-O | -6.55 | 1.13 | 1.23 |
| 1 | B | 477 | ARG | CD-NE | -6.55 | 1.35 | 1.46 |
| 1 | A | 40 | LEU | C-O | -6.55 | 1.10 | 1.23 |
| 1 | B | 227 | ILE | CA-CB | -6.55 | 1.39 | 1.54 |
| 1 | B | 505 | GLU | C-O | -6.55 | 1.10 | 1.23 |
| 1 | B | 61 | LYS | N-CA | 6.55 | 1.59 | 1.46 |
| 1 | A | 661 | PHE | CG-CD2 | -6.55 | 1.28 | 1.38 |
| 1 | A | 663 | ASN | CA-CB | -6.55 | 1.36 | 1.53 |
| 1 | B | 675 | PHE | CD1-CE1 | -6.54 | 1.26 | 1.39 |
| 1 | B | 8 | LEU | CG-CD2 | 6.54 | 1.76 | 1.51 |
| 1 | B | 213 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | B | 483 | TYR | CZ-OH | 6.53 | 1.49 | 1.37 |
| 1 | B | 162 | ASP | CA-C | 6.53 | 1.70 | 1.52 |
| 1 | B | 277 | GLN | CD-OE1 | 6.53 | 1.38 | 1.24 |
| 1 | A | 354 | ARG | CG-CD | -6.53 | 1.35 | 1.51 |
| 1 | A | 500 | LEU | C-O | 6.53 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 746 | MET | CG-SD | -6.53 | 1.64 | 1.81 |
| 1 | B | 390 | ARG | CD-NE | -6.53 | 1.35 | 1.46 |
| 1 | A | 667 | CYS | CB-SG | 6.52 | 1.93 | 1.82 |
| 1 | B | 384 | ASN | CA-CB | -6.52 | 1.36 | 1.53 |
| 1 | B | 92 | ALA | CA-CB | 6.52 | 1.66 | 1.52 |
| 1 | A | 100 | GLY | CA-C | 6.51 | 1.62 | 1.51 |
| 1 | B | 123 | ARG | CB-CG | 6.50 | 1.70 | 1.52 |
| 1 | B | 137 | GLY | C-O | -6.50 | 1.13 | 1.23 |
| 1 | B | 185 | TYR | CE2-CZ | 6.50 | 1.47 | 1.38 |
| 1 | B | 524 | GLU | CD-OE1 | 6.50 | 1.32 | 1.25 |
| 1 | B | 354 | ARG | C-O | -6.50 | 1.10 | 1.23 |
| 1 | A | 629 | MET | CA-CB | 6.50 | 1.68 | 1.53 |
| 1 | B | 892 | TYR | CZ-OH | 6.50 | 1.48 | 1.37 |
| 1 | B | 613 | PHE | CG-CD2 | -6.50 | 1.29 | 1.38 |
| 1 | B | 274 | TYR | CE2-CZ | -6.49 | 1.30 | 1.38 |
| 1 | B | 537 | LYS | CG-CD | 6.49 | 1.74 | 1.52 |
| 1 | B | 499 | LEU | N-CA | -6.49 | 1.33 | 1.46 |
| 1 | B | 41 | GLU | N-CA | -6.49 | 1.33 | 1.46 |
| 1 | B | 304 | TRP | C-O | -6.49 | 1.11 | 1.23 |
| 1 | A | 615 | LYS | CB-CG | 6.48 | 1.70 | 1.52 |
| 1 | A | 33 | GLU | CD-OE1 | 6.47 | 1.32 | 1.25 |
| 1 | B | 46 | PHE | CE1-CZ | -6.47 | 1.25 | 1.37 |
| 1 | B | 331 | PHE | CG-CD1 | -6.46 | 1.29 | 1.38 |
| 1 | B | 787 | GLU | CD-OE1 | -6.46 | 1.18 | 1.25 |
| 1 | A | 291 | VAL | C-O | 6.46 | 1.35 | 1.23 |
| 1 | B | 377 | TYR | CG-CD2 | -6.46 | 1.30 | 1.39 |
| 1 | A | 465 | HIS | N-CA | 6.45 | 1.59 | 1.46 |
| 1 | B | 645 | HIS | CA-C | -6.45 | 1.36 | 1.52 |
| 1 | B | 599 | PHE | CB-CG | -6.45 | 1.40 | 1.51 |
| 1 | B | 294 | LYS | CE-NZ | 6.44 | 1.65 | 1.49 |
| 1 | A | 513 | LEU | C-O | 6.44 | 1.35 | 1.23 |
| 1 | B | 123 | ARG | NE-CZ | 6.44 | 1.41 | 1.33 |
| 1 | B | 177 | TRP | CE3-CZ3 | 6.44 | 1.49 | 1.38 |
| 1 | B | 808 | THR | CA-C | 6.43 | 1.69 | 1.52 |
| 1 | A | 845 | GLU | CA-CB | 6.43 | 1.68 | 1.53 |
| 1 | B | 225 | TYR | CG-CD1 | -6.43 | 1.30 | 1.39 |
| 1 | B | 436 | TYR | CA-CB | -6.43 | 1.39 | 1.53 |
| 1 | A | 133 | GLU | C-O | 6.43 | 1.35 | 1.23 |
| 1 | B | 335 | PHE | CG-CD1 | 6.43 | 1.48 | 1.38 |
| 1 | A | 859 | VAL | CB-CG2 | 6.42 | 1.66 | 1.52 |
| 1 | B | 398 | ASP | CG-OD2 | 6.42 | 1.40 | 1.25 |
| 1 | B | 847 | GLY | C-O | 6.41 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 492 | PRO | CA-CB | -6.41 | 1.40 | 1.53 |
| 1 | B | 60 | PHE | CA-CB | -6.40 | 1.39 | 1.53 |
| 1 | B | 8 | LEU | N-CA | -6.40 | 1.33 | 1.46 |
| 1 | B | 242 | ILE | CB-CG2 | -6.40 | 1.33 | 1.52 |
| 1 | A | 30 | GLN | CG-CD | -6.40 | 1.36 | 1.51 |
| 1 | A | 388 | LYS | CG-CD | 6.40 | 1.74 | 1.52 |
| 1 | A | 797 | LYS | CG-CD | 6.40 | 1.74 | 1.52 |
| 1 | A | 38 | GLU | CD-OE1 | 6.39 | 1.32 | 1.25 |
| 1 | A | 62 | GLU | CA-C | -6.39 | 1.36 | 1.52 |
| 1 | A | 385 | PRO | CG-CD | -6.39 | 1.29 | 1.50 |
| 1 | B | 264 | TYR | CZ-OH | -6.39 | 1.26 | 1.37 |
| 1 | A | 506 | LYS | CD-CE | 6.39 | 1.67 | 1.51 |
| 1 | B | 718 | ASN | CA-CB | 6.38 | 1.69 | 1.53 |
| 1 | B | 789 | PHE | C-O | 6.38 | 1.35 | 1.23 |
| 1 | A | 368 | GLY | CA-C | -6.38 | 1.41 | 1.51 |
| 1 | B | 603 | TRP | CE3-CZ3 | 6.38 | 1.49 | 1.38 |
| 1 | A | 390 | ARG | CB-CG | 6.37 | 1.69 | 1.52 |
| 1 | A | 520 | ASN | CA-CB | -6.37 | 1.36 | 1.53 |
| 1 | B | 348 | LEU | CG-CD1 | 6.36 | 1.75 | 1.51 |
| 1 | B | 871 | LEU | CA-CB | -6.36 | 1.39 | 1.53 |
| 1 | A | 95 | THR | CA-CB | -6.36 | 1.36 | 1.53 |
| 1 | A | 459 | SER | CA-C | -6.36 | 1.36 | 1.52 |
| 1 | A | 519 | ALA | C-O | 6.36 | 1.35 | 1.23 |
| 1 | A | 740 | VAL | CA-CB | -6.35 | 1.41 | 1.54 |
| 1 | A | 831 | ASN | CG-ND2 | 6.35 | 1.48 | 1.32 |
| 1 | A | 520 | ASN | CB-CG | -6.35 | 1.36 | 1.51 |
| 1 | A | 304 | TRP | CZ3-CH2 | 6.34 | 1.50 | 1.40 |
| 1 | A | 450 | LYS | CA-C | -6.34 | 1.36 | 1.52 |
| 1 | B | 851 | PHE | CB-CG | -6.34 | 1.40 | 1.51 |
| 1 | B | 881 | VAL | CB-CG1 | 6.34 | 1.66 | 1.52 |
| 1 | A | 238 | LEU | N-CA | -6.33 | 1.33 | 1.46 |
| 1 | A | 367 | ARG | N-CA | -6.33 | 1.33 | 1.46 |
| 1 | B | 266 | VAL | CA-CB | 6.33 | 1.68 | 1.54 |
| 1 | B | 777 | ASP | C-O | 6.33 | 1.35 | 1.23 |
| 1 | B | 182 | GLU | CG-CD | 6.33 | 1.61 | 1.51 |
| 1 | A | 331 | PHE | C-O | 6.33 | 1.35 | 1.23 |
| 1 | B | 685 | ASN | CB-CG | 6.33 | 1.65 | 1.51 |
| 1 | B | 402 | SER | C-N | 6.31 | 1.48 | 1.34 |
| 1 | A | 628 | GLU | N-CA | -6.31 | 1.33 | 1.46 |
| 1 | A | 793 | TRP | CG-CD2 | -6.31 | 1.32 | 1.43 |
| 1 | B | 172 | GLN | CB-CG | 6.30 | 1.69 | 1.52 |
| 1 | A | 517 | ILE | CA-C | 6.30 | 1.69 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 87 | PHE | CB-CG | -6.29 | 1.40 | 1.51 |
| 1 | B | 20 | SER | N-CA | 6.29 | 1.58 | 1.46 |
| 1 | A | 511 | GLN | C-O | -6.29 | 1.11 | 1.23 |
| 1 | A | 750 | ASN | CA-CB | 6.29 | 1.69 | 1.53 |
| 1 | B | 806 | PHE | CG-CD2 | 6.28 | 1.48 | 1.38 |
| 1 | A | 282 | ILE | C-O | 6.28 | 1.35 | 1.23 |
| 1 | A | 464 | GLU | CB-CG | 6.28 | 1.64 | 1.52 |
| 1 | B | 375 | ARG | CZ-NH1 | 6.28 | 1.41 | 1.33 |
| 1 | B | 729 | LEU | CG-CD2 | 6.28 | 1.75 | 1.51 |
| 1 | B | 828 | PHE | CG-CD1 | 6.28 | 1.48 | 1.38 |
| 1 | B | 80 | GLU | CD-OE2 | 6.27 | 1.32 | 1.25 |
| 1 | B | 330 | ASP | CB-CG | 6.27 | 1.65 | 1.51 |
| 1 | B | 351 | ARG | C-O | 6.27 | 1.35 | 1.23 |
| 1 | B | 426 | ARG | CG-CD | 6.27 | 1.67 | 1.51 |
| 1 | A | 652 | PHE | CA-CB | -6.27 | 1.40 | 1.53 |
| 1 | B | 310 | TYR | CE1-CZ | 6.25 | 1.46 | 1.38 |
| 1 | A | 628 | GLU | C-O | 6.25 | 1.35 | 1.23 |
| 1 | B | 264 | TYR | CE1-CZ | -6.25 | 1.30 | 1.38 |
| 1 | B | 154 | VAL | CA-CB | -6.24 | 1.41 | 1.54 |
| 1 | A | 17 | GLY | C-O | -6.24 | 1.13 | 1.23 |
| 1 | B | 308 | ASP | CG-OD2 | 6.24 | 1.39 | 1.25 |
| 1 | A | 713 | SER | C-O | 6.24 | 1.35 | 1.23 |
| 1 | B | 823 | PHE | CB-CG | 6.24 | 1.61 | 1.51 |
| 1 | A | 888 | GLN | CB-CG | 6.23 | 1.69 | 1.52 |
| 1 | B | 272 | VAL | CB-CG2 | 6.23 | 1.66 | 1.52 |
| 1 | B | 374 | CYS | CB-SG | -6.22 | 1.71 | 1.82 |
| 1 | B | 390 | ARG | CG-CD | -6.22 | 1.36 | 1.51 |
| 1 | A | 212 | THR | C-O | 6.21 | 1.35 | 1.23 |
| 1 | A | 370 | THR | CA-CB | -6.21 | 1.37 | 1.53 |
| 1 | B | 14 | ALA | CA-CB | -6.21 | 1.39 | 1.52 |
| 1 | A | 557 | THR | C-O | 6.21 | 1.35 | 1.23 |
| 1 | B | 738 | MET | CB-CG | 6.21 | 1.71 | 1.51 |
| 1 | B | 510 | THR | CB-CG2 | 6.20 | 1.72 | 1.52 |
| 1 | B | 402 | SER | C-O | 6.20 | 1.35 | 1.23 |
| 1 | A | 466 | PHE | CE1-CZ | -6.20 | 1.25 | 1.37 |
| 1 | A | 609 | TYR | CE1-CZ | 6.20 | 1.46 | 1.38 |
| 1 | B | 638 | PHE | CE1-CZ | -6.20 | 1.25 | 1.37 |
| 1 | B | 665 | VAL | C-O | 6.19 | 1.35 | 1.23 |
| 1 | B | 189 | ASN | N-CA | -6.18 | 1.33 | 1.46 |
| 1 | B | 46 | PHE | CG-CD2 | -6.18 | 1.29 | 1.38 |
| 1 | B | 680 | GLN | C-O | -6.18 | 1.11 | 1.23 |
| 1 | B | 61 | LYS | CE-NZ | 6.18 | 1.64 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 728 | LYS | CA-CB | 6.18 | 1.67 | 1.53 |
| 1 | A | 696 | TRP | CA-C | -6.18 | 1.36 | 1.52 |
| 1 | A | 205 | GLU | CG-CD | 6.17 | 1.61 | 1.51 |
| 1 | B | 304 | TRP | N-CA | 6.17 | 1.58 | 1.46 |
| 1 | A | 492 | PRO | CA-C | -6.17 | 1.40 | 1.52 |
| 1 | A | 856 | SER | C-O | -6.17 | 1.11 | 1.23 |
| 1 | A | 511 | GLN | CG-CD | 6.16 | 1.65 | 1.51 |
| 1 | B | 46 | PHE | CD1-CE1 | 6.16 | 1.51 | 1.39 |
| 1 | B | 323 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 1 | A | 797 | LYS | C-O | -6.16 | 1.11 | 1.23 |
| 1 | A | 81 | LEU | C-O | -6.16 | 1.11 | 1.23 |
| 1 | A | 495 | GLU | CD-OE1 | 6.16 | 1.32 | 1.25 |
| 1 | B | 631 | MET | CG-SD | 6.15 | 1.97 | 1.81 |
| 1 | A | 125 | VAL | N-CA | 6.15 | 1.58 | 1.46 |
| 1 | A | 361 | TYR | C-O | 6.15 | 1.35 | 1.23 |
| 1 | A | 367 | ARG | NE-CZ | 6.15 | 1.41 | 1.33 |
| 1 | B | 397 | ALA | CA-C | 6.14 | 1.69 | 1.52 |
| 1 | B | 682 | ASP | CB-CG | -6.14 | 1.38 | 1.51 |
| 1 | A | 870 | SER | CA-CB | 6.14 | 1.62 | 1.52 |
| 1 | B | 130 | SER | CA-CB | -6.14 | 1.43 | 1.52 |
| 1 | B | 293 | TRP | CZ3-CH2 | 6.14 | 1.49 | 1.40 |
| 1 | A | 47 | GLN | CA-CB | -6.14 | 1.40 | 1.53 |
| 1 | A | 65 | PRO | CA-C | 6.14 | 1.65 | 1.52 |
| 1 | A | 359 | THR | N-CA | -6.14 | 1.34 | 1.46 |
| 1 | A | 264 | TYR | CZ-OH | 6.13 | 1.48 | 1.37 |
| 1 | A | 609 | TYR | CD1-CE1 | 6.13 | 1.48 | 1.39 |
| 1 | B | 730 | PHE | C-O | 6.13 | 1.35 | 1.23 |
| 1 | B | 480 | PRO | CB-CG | 6.13 | 1.80 | 1.50 |
| 1 | B | 16 | GLU | CD-OE2 | -6.13 | 1.19 | 1.25 |
| 1 | B | 450 | LYS | C-O | 6.13 | 1.34 | 1.23 |
| 1 | A | 823 | PHE | CB-CG | 6.12 | 1.61 | 1.51 |
| 1 | A | 634 | GLU | CG-CD | 6.12 | 1.61 | 1.51 |
| 1 | B | 668 | LEU | CG-CD2 | 6.12 | 1.74 | 1.51 |
| 1 | B | 796 | ILE | CA-C | 6.12 | 1.68 | 1.52 |
| 1 | A | 492 | PRO | N-CA | -6.12 | 1.36 | 1.47 |
| 1 | A | 117 | ASN | CB-CG | 6.11 | 1.65 | 1.51 |
| 1 | B | 231 | ALA | C-O | -6.11 | 1.11 | 1.23 |
| 1 | A | 511 | GLN | CB-CG | 6.11 | 1.69 | 1.52 |
| 1 | A | 518 | GLN | CA-C | 6.11 | 1.68 | 1.52 |
| 1 | B | 27 | TYR | CD1-CE1 | 6.10 | 1.48 | 1.39 |
| 1 | B | 507 | LYS | CB-CG | 6.10 | 1.69 | 1.52 |
| 1 | B | 56 | HIS | CA-C | 6.10 | 1.68 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 182 | GLU | CD-OE1 | -6.10 | 1.19 | 1.25 |
| 1 | A | 780 | THR | CB-CG2 | -6.09 | 1.32 | 1.52 |
| 1 | B | 806 | PHE | CE2-CZ | 6.09 | 1.49 | 1.37 |
| 1 | A | 89 | VAL | C-O | -6.09 | 1.11 | 1.23 |
| 1 | B | 168 | VAL | CB-CG1 | 6.09 | 1.65 | 1.52 |
| 1 | B | 52 | PRO | C-O | -6.09 | 1.11 | 1.23 |
| 1 | B | 138 | ILE | CB-CG2 | -6.08 | 1.33 | 1.52 |
| 1 | B | 192 | TYR | CE2-CZ | -6.08 | 1.30 | 1.38 |
| 1 | B | 632 | ALA | C-O | 6.08 | 1.34 | 1.23 |
| 1 | B | 428 | MET | CG-SD | -6.08 | 1.65 | 1.81 |
| 1 | B | 475 | ARG | CB-CG | 6.08 | 1.69 | 1.52 |
| 1 | A | 99 | GLN | CA-C | -6.08 | 1.37 | 1.52 |
| 1 | A | 888 | GLN | C-O | 6.08 | 1.34 | 1.23 |
| 1 | B | 725 | GLN | CA-CB | 6.08 | 1.67 | 1.53 |
| 1 | A | 74 | LYS | CG-CD | 6.07 | 1.73 | 1.52 |
| 1 | B | 150 | VAL | CA-C | 6.07 | 1.68 | 1.52 |
| 1 | B | 153 | VAL | C-O | 6.07 | 1.34 | 1.23 |
| 1 | A | 298 | SER | CA-CB | -6.06 | 1.43 | 1.52 |
| 1 | A | 304 | TRP | CB-CG | 6.06 | 1.61 | 1.50 |
| 1 | A | 772 | MET | N-CA | -6.06 | 1.34 | 1.46 |
| 1 | B | 143 | LEU | CA-CB | 6.06 | 1.67 | 1.53 |
| 1 | B | 585 | LEU | CG-CD1 | 6.06 | 1.74 | 1.51 |
| 1 | B | 859 | VAL | C-O | -6.06 | 1.11 | 1.23 |
| 1 | A | 31 | ASP | CG-OD1 | 6.06 | 1.39 | 1.25 |
| 1 | A | 394 | VAL | C-O | -6.05 | 1.11 | 1.23 |
| 1 | B | 167 | PHE | CG-CD2 | -6.05 | 1.29 | 1.38 |
| 1 | A | 756 | HIS | CG-CD2 | 6.05 | 1.46 | 1.35 |
| 1 | B | 187 | LYS | CD-CE | 6.05 | 1.66 | 1.51 |
| 1 | A | 585 | LEU | CG-CD2 | 6.05 | 1.74 | 1.51 |
| 1 | A | 5 | ALA | C-O | -6.04 | 1.11 | 1.23 |
| 1 | A | 125 | VAL | CB-CG1 | -6.04 | 1.40 | 1.52 |
| 1 | A | 558 | ILE | CA-CB | -6.04 | 1.41 | 1.54 |
| 1 | A | 794 | ASN | N-CA | -6.04 | 1.34 | 1.46 |
| 1 | A | 133 | GLU | CB-CG | 6.04 | 1.63 | 1.52 |
| 1 | B | 164 | LYS | C-O | 6.03 | 1.34 | 1.23 |
| 1 | B | 885 | GLU | CG-CD | 6.03 | 1.60 | 1.51 |
| 1 | A | 266 | VAL | CB-CG1 | -6.03 | 1.40 | 1.52 |
| 1 | B | 54 | VAL | C-O | -6.03 | 1.11 | 1.23 |
| 1 | A | 178 | SER | CB-OG | 6.02 | 1.50 | 1.42 |
| 1 | B | 322 | GLY | C-O | 6.01 | 1.33 | 1.23 |
| 1 | B | 325 | TRP | CG-CD1 | -6.01 | 1.28 | 1.36 |
| 1 | A | 129 | GLN | C-O | -6.01 | 1.11 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 483 | TYR | CD2-CE2 | 6.01 | 1.48 | 1.39 |
| 1 | A | 440 | ARG | C-N | 6.00 | 1.47 | 1.34 |
| 1 | A | 885 | GLU | CD-OE1 | 6.00 | 1.32 | 1.25 |
| 1 | B | 49 | PRO | N-CD | -6.00 | 1.39 | 1.47 |
| 1 | B | 57 | SER | CB-OG | 6.00 | 1.50 | 1.42 |
| 1 | B | 502 | PHE | CA-CB | 6.00 | 1.67 | 1.53 |
| 1 | A | 613 | PHE | CD2-CE2 | 5.99 | 1.51 | 1.39 |
| 1 | B | 490 | PHE | C-O | -5.99 | 1.11 | 1.23 |
| 1 | B | 62 | GLU | C-O | 5.99 | 1.34 | 1.23 |
| 1 | B | 472 | VAL | CB-CG1 | -5.99 | 1.40 | 1.52 |
| 1 | B | 518 | GLN | CG-CD | 5.99 | 1.64 | 1.51 |
| 1 | A | 142 | GLN | CB-CG | -5.98 | 1.36 | 1.52 |
| 1 | B | 443 | ALA | N-CA | 5.98 | 1.58 | 1.46 |
| 1 | A | 487 | PRO | N-CA | -5.98 | 1.37 | 1.47 |
| 1 | A | 788 | GLU | C-O | -5.98 | 1.11 | 1.23 |
| 1 | B | 387 | PHE | CE2-CZ | 5.98 | 1.48 | 1.37 |
| 1 | A | 215 | TYR | CA-CB | -5.97 | 1.40 | 1.53 |
| 1 | B | 418 | ARG | CZ-NH1 | 5.97 | 1.40 | 1.33 |
| 1 | A | 451 | ARG | CZ-NH1 | 5.97 | 1.40 | 1.33 |
| 1 | A | 545 | GLY | CA-C | 5.97 | 1.61 | 1.51 |
| 1 | A | 596 | LEU | N-CA | 5.96 | 1.58 | 1.46 |
| 1 | B | 646 | GLN | CG-CD | 5.96 | 1.64 | 1.51 |
| 1 | A | 206 | ASP | CB-CG | 5.96 | 1.64 | 1.51 |
| 1 | A | 392 | GLU | CA-CB | -5.96 | 1.40 | 1.53 |
| 1 | B | 26 | LYS | CG-CD | 5.96 | 1.72 | 1.52 |
| 1 | B | 225 | TYR | CG-CD2 | -5.96 | 1.31 | 1.39 |
| 1 | B | 176 | PHE | CB-CG | -5.96 | 1.41 | 1.51 |
| 1 | A | 368 | GLY | C-O | 5.95 | 1.33 | 1.23 |
| 1 | B | 651 | ARG | NE-CZ | 5.95 | 1.40 | 1.33 |
| 1 | B | 342 | ASN | CA-CB | -5.95 | 1.37 | 1.53 |
| 1 | B | 435 | VAL | CB-CG1 | 5.95 | 1.65 | 1.52 |
| 1 | A | 570 | ARG | CA-CB | 5.95 | 1.67 | 1.53 |
| 1 | B | 27 | TYR | CG-CD2 | -5.94 | 1.31 | 1.39 |
| 1 | A | 713 | SER | N-CA | 5.94 | 1.58 | 1.46 |
| 1 | B | 451 | ARG | CD-NE | 5.94 | 1.56 | 1.46 |
| 1 | B | 49 | PRO | N-CA | -5.94 | 1.37 | 1.47 |
| 1 | B | 125 | VAL | CB-CG2 | -5.93 | 1.40 | 1.52 |
| 1 | A | 114 | LEU | N-CA | 5.93 | 1.58 | 1.46 |
| 1 | A | 889 | LEU | C-O | -5.93 | 1.12 | 1.23 |
| 1 | B | 643 | GLN | CA-CB | 5.93 | 1.67 | 1.53 |
| 1 | B | 9 | ALA | C-O | 5.93 | 1.34 | 1.23 |
| 1 | A | 124 | VAL | CA-C | -5.92 | 1.37 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 409 | PHE | CD1-CE1 | 5.92 | 1.51 | 1.39 |
| 1 | A | 542 | LYS | N-CA | 5.91 | 1.58 | 1.46 |
| 1 | A | 700 | SER | CB-OG | -5.91 | 1.34 | 1.42 |
| 1 | A | 65 | PRO | C-O | 5.91 | 1.35 | 1.23 |
| 1 | B | 597 | VAL | CA-C | 5.91 | 1.68 | 1.52 |
| 1 | A | 167 | PHE | N-CA | -5.91 | 1.34 | 1.46 |
| 1 | B | 673 | ILE | CA-C | 5.91 | 1.68 | 1.52 |
| 1 | B | 194 | ALA | CA-CB | -5.91 | 1.40 | 1.52 |
| 1 | A | 503 | PHE | CB-CG | -5.91 | 1.41 | 1.51 |
| 1 | A | 865 | PHE | CE2-CZ | 5.90 | 1.48 | 1.37 |
| 1 | B | 746 | MET | CG-SD | 5.90 | 1.96 | 1.81 |
| 1 | B | 21 | HIS | C-O | -5.90 | 1.12 | 1.23 |
| 1 | B | 348 | LEU | CB-CG | 5.90 | 1.69 | 1.52 |
| 1 | A | 392 | GLU | CD-OE1 | 5.90 | 1.32 | 1.25 |
| 1 | A | 795 | ASN | CB-CG | -5.90 | 1.37 | 1.51 |
| 1 | A | 27 | TYR | CD2-CE2 | -5.89 | 1.30 | 1.39 |
| 1 | A | 274 | TYR | CE2-CZ | -5.89 | 1.30 | 1.38 |
| 1 | A | 743 | THR | C-O | 5.89 | 1.34 | 1.23 |
| 1 | A | 312 | ARG | CZ-NH1 | 5.88 | 1.40 | 1.33 |
| 1 | A | 789 | PHE | CE2-CZ | 5.88 | 1.48 | 1.37 |
| 1 | B | 641 | PRO | CG-CD | 5.88 | 1.70 | 1.50 |
| 1 | A | 57 | SER | CA-CB | -5.88 | 1.44 | 1.52 |
| 1 | B | 294 | LYS | CD-CE | 5.88 | 1.66 | 1.51 |
| 1 | B | 601 | ILE | CA-CB | 5.88 | 1.68 | 1.54 |
| 1 | B | 172 | GLN | CG-CD | -5.88 | 1.37 | 1.51 |
| 1 | A | 676 | LYS | CA-CB | 5.88 | 1.66 | 1.53 |
| 1 | A | 331 | PHE | CE2-CZ | -5.88 | 1.26 | 1.37 |
| 1 | A | 192 | TYR | CE2-CZ | 5.87 | 1.46 | 1.38 |
| 1 | B | 372 | GLY | C-O | 5.87 | 1.33 | 1.23 |
| 1 | A | 134 | GLY | CA-C | 5.87 | 1.61 | 1.51 |
| 1 | B | 453 | PHE | CE1-CZ | 5.87 | 1.48 | 1.37 |
| 1 | B | 447 | VAL | C-O | -5.86 | 1.12 | 1.23 |
| 1 | A | 643 | GLN | CG-CD | -5.86 | 1.37 | 1.51 |
| 1 | A | 713 | SER | CA-C | 5.86 | 1.68 | 1.52 |
| 1 | A | 124 | VAL | CA-CB | 5.86 | 1.67 | 1.54 |
| 1 | B | 232 | LEU | CG-CD1 | -5.86 | 1.30 | 1.51 |
| 1 | A | 325 | TRP | CG-CD1 | -5.85 | 1.28 | 1.36 |
| 1 | B | 360 | PHE | CG-CD2 | -5.85 | 1.29 | 1.38 |
| 1 | B | 789 | PHE | CG-CD2 | 5.85 | 1.47 | 1.38 |
| 1 | B | 876 | THR | CA-C | -5.85 | 1.37 | 1.52 |
| 1 | A | 451 | ARG | C-O | 5.84 | 1.34 | 1.23 |
| 1 | B | 351 | ARG | CA-C | 5.84 | 1.68 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 241 | SER | CB-OG | 5.84 | 1.49 | 1.42 |
| 1 | A | 109 | ALA | CA-C | 5.84 | 1.68 | 1.52 |
| 1 | B | 487 | PRO | C-O | 5.84 | 1.34 | 1.23 |
| 1 | B | 383 | VAL | CB-CG2 | -5.83 | 1.40 | 1.52 |
| 1 | A | 586 | MET | C-O | 5.83 | 1.34 | 1.23 |
| 1 | A | 149 | TRP | CB-CG | -5.83 | 1.39 | 1.50 |
| 1 | B | 57 | SER | N-CA | -5.83 | 1.34 | 1.46 |
| 1 | B | 404 | GLU | CD-OE1 | 5.83 | 1.32 | 1.25 |
| 1 | B | 33 | GLU | CB-CG | 5.83 | 1.63 | 1.52 |
| 1 | A | 273 | THR | CA-CB | -5.82 | 1.38 | 1.53 |
| 1 | B | 99 | GLN | C-O | -5.82 | 1.12 | 1.23 |
| 1 | B | 342 | ASN | CG-OD1 | 5.82 | 1.36 | 1.24 |
| 1 | B | 582 | MET | SD-CE | 5.82 | 2.10 | 1.77 |
| 1 | A | 594 | LEU | CA-C | -5.82 | 1.37 | 1.52 |
| 1 | B | 105 | SER | N-CA | -5.82 | 1.34 | 1.46 |
| 1 | B | 835 | TYR | C-O | 5.82 | 1.34 | 1.23 |
| 1 | A | 62 | GLU | CG-CD | 5.81 | 1.60 | 1.51 |
| 1 | B | 163 | GLY | C-O | -5.81 | 1.14 | 1.23 |
| 1 | A | 556 | GLN | C-O | 5.80 | 1.34 | 1.23 |
| 1 | B | 607 | ARG | NE-CZ | 5.80 | 1.40 | 1.33 |
| 1 | A | 365 | TRP | CG-CD1 | -5.80 | 1.28 | 1.36 |
| 1 | A | 294 | LYS | C-O | 5.80 | 1.34 | 1.23 |
| 1 | A | 642 | CYS | N-CA | 5.80 | 1.57 | 1.46 |
| 1 | A | 800 | GLN | CA-CB | -5.80 | 1.41 | 1.53 |
| 1 | B | 882 | ASN | CB-CG | 5.80 | 1.64 | 1.51 |
| 1 | B | 148 | GLU | CD-OE1 | -5.79 | 1.19 | 1.25 |
| 1 | A | 71 | TYR | CD2-CE2 | -5.79 | 1.30 | 1.39 |
| 1 | B | 259 | VAL | C-O | 5.79 | 1.34 | 1.23 |
| 1 | B | 647 | VAL | CA-CB | 5.79 | 1.67 | 1.54 |
| 1 | A | 176 | PHE | CA-CB | -5.79 | 1.41 | 1.53 |
| 1 | A | 767 | ASP | CG-OD2 | 5.79 | 1.38 | 1.25 |
| 1 | B | 76 | LYS | CD-CE | 5.79 | 1.65 | 1.51 |
| 1 | A | 175 | GLU | C-O | 5.79 | 1.34 | 1.23 |
| 1 | A | 97 | ILE | C-O | -5.79 | 1.12 | 1.23 |
| 1 | A | 165 | LEU | CA-CB | 5.79 | 1.67 | 1.53 |
| 1 | B | 15 | ALA | CA-CB | 5.79 | 1.64 | 1.52 |
| 1 | B | 193 | GLU | CA-C | -5.79 | 1.38 | 1.52 |
| 1 | A | 454 | PHE | CD1-CE1 | -5.78 | 1.27 | 1.39 |
| 1 | A | 862 | ASP | CG-OD2 | -5.78 | 1.12 | 1.25 |
| 1 | B | 207 | PHE | CD2-CE2 | 5.78 | 1.50 | 1.39 |
| 1 | B | 229 | LEU | CG-CD1 | -5.78 | 1.30 | 1.51 |
| 1 | B | 386 | GLN | CA-CB | -5.78 | 1.41 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 98 | CYS | C-O | -5.77 | 1.12 | 1.23 |
| 1 | B | 46 | PHE | C-O | -5.77 | 1.12 | 1.23 |
| 1 | B | 887 | LEU | CG-CD2 | -5.77 | 1.30 | 1.51 |
| 1 | A | 634 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | B | 178 | SER | N-CA | 5.77 | 1.57 | 1.46 |
| 1 | B | 216 | ASP | CB-CG | -5.76 | 1.39 | 1.51 |
| 1 | A | 437 | GLN | N-CA | -5.76 | 1.34 | 1.46 |
| 1 | A | 647 | VAL | CB-CG2 | 5.76 | 1.65 | 1.52 |
| 1 | B | 415 | GLN | CD-NE2 | 5.75 | 1.47 | 1.32 |
| 1 | B | 311 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 1 | B | 277 | GLN | CA-C | -5.75 | 1.38 | 1.52 |
| 1 | B | 269 | ALA | N-CA | 5.75 | 1.57 | 1.46 |
| 1 | B | 663 | ASN | CA-C | -5.75 | 1.38 | 1.52 |
| 1 | B | 329 | ARG | C-N | 5.74 | 1.47 | 1.34 |
| 1 | A | 751 | LYS | N-CA | 5.74 | 1.57 | 1.46 |
| 1 | A | 134 | GLY | C-O | 5.74 | 1.32 | 1.23 |
| 1 | A | 80 | GLU | CD-OE1 | 5.74 | 1.31 | 1.25 |
| 1 | A | 511 | GLN | CD-OE1 | 5.74 | 1.36 | 1.24 |
| 1 | B | 185 | TYR | CE1-CZ | -5.74 | 1.31 | 1.38 |
| 1 | A | 175 | GLU | N-CA | 5.73 | 1.57 | 1.46 |
| 1 | A | 778 | SER | CA-CB | 5.73 | 1.61 | 1.52 |
| 1 | A | 744 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 1 | A | 696 | TRP | CG-CD1 | -5.73 | 1.28 | 1.36 |
| 1 | A | 33 | GLU | CD-OE2 | 5.73 | 1.31 | 1.25 |
| 1 | A | 86 | GLN | CD-OE1 | 5.72 | 1.36 | 1.24 |
| 1 | B | 384 | ASN | C-O | 5.72 | 1.34 | 1.23 |
| 1 | A | 671 | LEU | C-O | -5.72 | 1.12 | 1.23 |
| 1 | B | 72 | GLY | C-O | 5.72 | 1.32 | 1.23 |
| 1 | B | 456 | ALA | N-CA | 5.72 | 1.57 | 1.46 |
| 1 | A | 289 | GLY | N-CA | -5.72 | 1.37 | 1.46 |
| 1 | B | 807 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | A | 831 | ASN | CA-C | -5.71 | 1.38 | 1.52 |
| 1 | A | 127 | TYR | CD2-CE2 | -5.71 | 1.30 | 1.39 |
| 1 | A | 387 | PHE | CG-CD1 | 5.71 | 1.47 | 1.38 |
| 1 | B | 425 | GLY | N-CA | 5.71 | 1.54 | 1.46 |
| 1 | B | 873 | LYS | CA-CB | 5.71 | 1.66 | 1.53 |
| 1 | B | 436 | TYR | CG-CD2 | -5.71 | 1.31 | 1.39 |
| 1 | B | 223 | ASP | CA-C | -5.70 | 1.38 | 1.52 |
| 1 | B | 292 | GLU | CA-CB | 5.70 | 1.66 | 1.53 |
| 1 | B | 638 | PHE | CB-CG | -5.70 | 1.41 | 1.51 |
| 1 | B | 714 | ASN | C-O | 5.70 | 1.34 | 1.23 |
| 1 | A | 627 | TYR | CG-CD1 | -5.70 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 664 | PHE | CE2-CZ | -5.70 | 1.26 | 1.37 |
| 1 | A | 601 | ILE | C-O | 5.70 | 1.34 | 1.23 |
| 1 | A | 871 | LEU | CG-CD1 | 5.70 | 1.73 | 1.51 |
| 1 | A | 179 | ALA | C-O | -5.70 | 1.12 | 1.23 |
| 1 | B | 883 | ILE | CB-CG2 | 5.70 | 1.70 | 1.52 |
| 1 | B | 225 | TYR | CA-C | -5.70 | 1.38 | 1.52 |
| 1 | B | 321 | ASP | C-O | 5.69 | 1.34 | 1.23 |
| 1 | B | 713 | SER | CA-C | 5.69 | 1.67 | 1.52 |
| 1 | A | 768 | THR | CA-CB | -5.69 | 1.38 | 1.53 |
| 1 | A | 791 | TYR | CG-CD2 | 5.69 | 1.46 | 1.39 |
| 1 | B | 278 | ARG | CD-NE | 5.69 | 1.56 | 1.46 |
| 1 | A | 541 | SER | N-CA | 5.68 | 1.57 | 1.46 |
| 1 | A | 362 | GLU | N-CA | 5.68 | 1.57 | 1.46 |
| 1 | B | 217 | LEU | N-CA | 5.68 | 1.57 | 1.46 |
| 1 | A | 333 | ARG | CB-CG | 5.68 | 1.67 | 1.52 |
| 1 | A | 407 | CYS | CA-CB | -5.68 | 1.41 | 1.53 |
| 1 | A | 603 | TRP | CE2-CZ2 | -5.68 | 1.30 | 1.39 |
| 1 | A | 737 | ASP | C-O | 5.68 | 1.34 | 1.23 |
| 1 | B | 288 | TRP | CG-CD1 | -5.68 | 1.28 | 1.36 |
| 1 | A | 867 | ALA | C-N | -5.67 | 1.21 | 1.34 |
| 1 | A | 831 | ASN | N-CA | -5.67 | 1.35 | 1.46 |
| 1 | A | 646 | GLN | CB-CG | 5.67 | 1.67 | 1.52 |
| 1 | A | 510 | THR | C-O | -5.67 | 1.12 | 1.23 |
| 1 | A | 739 | GLU | CG-CD | -5.67 | 1.43 | 1.51 |
| 1 | B | 51 | PHE | CB-CG | -5.67 | 1.41 | 1.51 |
| 1 | B | 473 | SER | N-CA | -5.67 | 1.35 | 1.46 |
| 1 | A | 390 | ARG | CA-C | 5.66 | 1.67 | 1.52 |
| 1 | B | 501 | ARG | CB-CG | 5.66 | 1.67 | 1.52 |
| 1 | A | 886 | TRP | CD2-CE2 | -5.66 | 1.34 | 1.41 |
| 1 | B | 368 | GLY | CA-C | 5.66 | 1.60 | 1.51 |
| 1 | A | 186 | ALA | C-O | 5.66 | 1.34 | 1.23 |
| 1 | A | 891 | MET | SD-CE | 5.66 | 2.09 | 1.77 |
| 1 | A | 660 | ASP | CA-CB | -5.65 | 1.41 | 1.53 |
| 1 | B | 75 | TRP | CZ3-CH2 | -5.65 | 1.31 | 1.40 |
| 1 | B | 478 | LEU | CG-CD2 | -5.65 | 1.30 | 1.51 |
| 1 | B | 855 | ILE | N-CA | 5.65 | 1.57 | 1.46 |
| 1 | B | 53 | PRO | CA-C | -5.64 | 1.41 | 1.52 |
| 1 | A | 402 | SER | CA-CB | 5.64 | 1.61 | 1.52 |
| 1 | B | 478 | LEU | CB-CG | 5.64 | 1.69 | 1.52 |
| 1 | A | 790 | LYS | CA-C | 5.64 | 1.67 | 1.52 |
| 1 | A | 70 | THR | CA-CB | 5.64 | 1.68 | 1.53 |
| 1 | A | 603 | TRP | CG-CD1 | 5.64 | 1.44 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 619 | ASP | N-CA | -5.64 | 1.35 | 1.46 |
| 1 | B | 8 | LEU | C-O | 5.64 | 1.34 | 1.23 |
| 1 | A | 477 | ARG | CD-NE | 5.64 | 1.56 | 1.46 |
| 1 | A | 572 | ASN | CG-OD1 | 5.64 | 1.36 | 1.24 |
| 1 | A | 120 | ILE | CG1-CD1 | 5.63 | 1.89 | 1.50 |
| 1 | A | 404 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | A | 695 | SER | N-CA | 5.63 | 1.57 | 1.46 |
| 1 | B | 624 | MET | CA-C | 5.63 | 1.67 | 1.52 |
| 1 | A | 185 | TYR | CD1-CE1 | 5.63 | 1.47 | 1.39 |
| 1 | A | 479 | PRO | C-O | -5.63 | 1.11 | 1.23 |
| 1 | A | 854 | PHE | C-O | 5.63 | 1.34 | 1.23 |
| 1 | A | 438 | VAL | CB-CG2 | -5.63 | 1.41 | 1.52 |
| 1 | A | 850 | ASP | C-O | -5.63 | 1.12 | 1.23 |
| 1 | A | 43 | GLY | C-O | -5.62 | 1.14 | 1.23 |
| 1 | A | 141 | PHE | CA-CB | -5.62 | 1.41 | 1.53 |
| 1 | A | 578 | SER | N-CA | 5.62 | 1.57 | 1.46 |
| 1 | A | 854 | PHE | CA-CB | -5.62 | 1.41 | 1.53 |
| 1 | A | 189 | ASN | C-O | 5.62 | 1.34 | 1.23 |
| 1 | B | 683 | PRO | CG-CD | 5.62 | 1.69 | 1.50 |
| 1 | B | 157 | LEU | CA-CB | 5.62 | 1.66 | 1.53 |
| 1 | A | 238 | LEU | CG-CD1 | 5.62 | 1.72 | 1.51 |
| 1 | A | 145 | GLN | CA-CB | -5.62 | 1.41 | 1.53 |
| 1 | A | 608 | ASN | C-N | -5.62 | 1.21 | 1.34 |
| 1 | A | 685 | ASN | CA-C | 5.61 | 1.67 | 1.52 |
| 1 | B | 138 | ILE | N-CA | 5.61 | 1.57 | 1.46 |
| 1 | A | 415 | GLN | CB-CG | -5.61 | 1.37 | 1.52 |
| 1 | B | 126 | PRO | C-O | -5.60 | 1.12 | 1.23 |
| 1 | A | 122 | HIS | CB-CG | -5.60 | 1.40 | 1.50 |
| 1 | B | 575 | SER | CA-CB | -5.60 | 1.44 | 1.52 |
| 1 | A | 13 | GLU | N-CA | -5.60 | 1.35 | 1.46 |
| 1 | A | 607 | ARG | CG-CD | -5.60 | 1.38 | 1.51 |
| 1 | B | 280 | ASN | CB-CG | 5.60 | 1.64 | 1.51 |
| 1 | B | 11 | ASP | CG-OD2 | 5.60 | 1.38 | 1.25 |
| 1 | B | 789 | PHE | CE1-CZ | 5.60 | 1.48 | 1.37 |
| 1 | A | 869 | ARG | CZ-NH1 | 5.59 | 1.40 | 1.33 |
| 1 | A | 153 | VAL | CB-CG2 | 5.59 | 1.64 | 1.52 |
| 1 | A | 388 | LYS | C-O | 5.59 | 1.33 | 1.23 |
| 1 | A | 233 | GLU | CB-CG | -5.59 | 1.41 | 1.52 |
| 1 | B | 134 | GLY | C-O | -5.58 | 1.14 | 1.23 |
| 1 | A | 674 | LEU | CG-CD1 | -5.58 | 1.31 | 1.51 |
| 1 | A | 866 | ARG | C-O | 5.58 | 1.33 | 1.23 |
| 1 | B | 274 | TYR | CG-CD1 | -5.58 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 26 | LYS | C-O | -5.57 | 1.12 | 1.23 |
| 1 | B | 452 | ASP | CG-OD1 | 5.57 | 1.38 | 1.25 |
| 1 | A | 114 | LEU | CG-CD1 | 5.57 | 1.72 | 1.51 |
| 1 | A | 265 | SER | C-O | -5.57 | 1.12 | 1.23 |
| 1 | B | 580 | ARG | CG-CD | 5.57 | 1.65 | 1.51 |
| 1 | A | 174 | ASN | CG-OD1 | 5.57 | 1.36 | 1.24 |
| 1 | A | 491 | GLU | CD-OE1 | 5.57 | 1.31 | 1.25 |
| 1 | A | 324 | PHE | CG-CD2 | -5.57 | 1.30 | 1.38 |
| 1 | A | 631 | MET | C-O | 5.57 | 1.33 | 1.23 |
| 1 | B | 310 | TYR | CA-C | -5.57 | 1.38 | 1.52 |
| 1 | B | 643 | GLN | C-O | -5.57 | 1.12 | 1.23 |
| 1 | B | 467 | ILE | CB-CG2 | 5.56 | 1.70 | 1.52 |
| 1 | A | 229 | LEU | N-CA | -5.56 | 1.35 | 1.46 |
| 1 | B | 854 | PHE | CG-CD1 | 5.56 | 1.47 | 1.38 |
| 1 | A | 498 | PHE | CG-CD2 | -5.56 | 1.30 | 1.38 |
| 1 | A | 632 | ALA | CA-CB | -5.56 | 1.40 | 1.52 |
| 1 | A | 94 | ARG | C-O | -5.55 | 1.12 | 1.23 |
| 1 | A | 120 | ILE | CA-CB | 5.55 | 1.67 | 1.54 |
| 1 | A | 617 | ASP | CG-OD1 | 5.55 | 1.38 | 1.25 |
| 1 | B | 656 | GLU | CG-CD | 5.55 | 1.60 | 1.51 |
| 1 | B | 439 | PRO | CA-CB | -5.55 | 1.42 | 1.53 |
| 1 | B | 868 | PHE | N-CA | -5.55 | 1.35 | 1.46 |
| 1 | A | 146 | PHE | CD1-CE1 | 5.55 | 1.50 | 1.39 |
| 1 | A | 475 | ARG | CG-CD | 5.54 | 1.65 | 1.51 |
| 1 | A | 714 | ASN | C-O | 5.54 | 1.33 | 1.23 |
| 1 | A | 334 | GLU | CD-OE1 | 5.54 | 1.31 | 1.25 |
| 1 | B | 206 | ASP | CB-CG | -5.54 | 1.40 | 1.51 |
| 1 | B | 488 | SER | C-O | 5.54 | 1.33 | 1.23 |
| 1 | B | 640 | LEU | C-O | -5.54 | 1.12 | 1.23 |
| 1 | B | 710 | MET | CA-CB | 5.54 | 1.66 | 1.53 |
| 1 | A | 320 | GLU | CG-CD | -5.53 | 1.43 | 1.51 |
| 1 | A | 388 | LYS | CD-CE | 5.53 | 1.65 | 1.51 |
| 1 | B | 90 | ASP | CG-OD2 | 5.53 | 1.38 | 1.25 |
| 1 | B | 583 | VAL | CB-CG1 | -5.53 | 1.41 | 1.52 |
| 1 | A | 454 | PHE | CB-CG | -5.53 | 1.42 | 1.51 |
| 1 | A | 204 | PHE | CB-CG | -5.53 | 1.42 | 1.51 |
| 1 | B | 615 | LYS | CB-CG | 5.53 | 1.67 | 1.52 |
| 1 | B | 264 | TYR | CB-CG | -5.53 | 1.43 | 1.51 |
| 1 | B | 89 | VAL | CA-C | -5.53 | 1.38 | 1.52 |
| 1 | B | 381 | PHE | CB-CG | -5.52 | 1.42 | 1.51 |
| 1 | B | 460 | ARG | CG-CD | 5.52 | 1.65 | 1.51 |
| 1 | B | 524 | GLU | CA-C | 5.52 | 1.67 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 36 | ARG | NE-CZ | 5.52 | 1.40 | 1.33 |
| 1 | A | 678 | PHE | CD1-CE1 | 5.52 | 1.50 | 1.39 |
| 1 | A | 12 | ARG | NE-CZ | 5.52 | 1.40 | 1.33 |
| 1 | A | 616 | PHE | CG-CD1 | -5.52 | 1.30 | 1.38 |
| 1 | A | 9 | ALA | CA-CB | 5.52 | 1.64 | 1.52 |
| 1 | B | 196 | SER | CB-OG | -5.52 | 1.35 | 1.42 |
| 1 | B | 157 | LEU | CG-CD1 | -5.51 | 1.31 | 1.51 |
| 1 | B | 454 | PHE | CE1-CZ | 5.51 | 1.47 | 1.37 |
| 1 | A | 665 | VAL | N-CA | 5.51 | 1.57 | 1.46 |
| 1 | A | 663 | ASN | N-CA | 5.51 | 1.57 | 1.46 |
| 1 | A | 468 | ASN | C-O | 5.50 | 1.33 | 1.23 |
| 1 | A | 214 | TRP | CZ2-CH2 | -5.50 | 1.26 | 1.37 |
| 1 | A | 571 | THR | CA-CB | 5.50 | 1.67 | 1.53 |
| 1 | B | 491 | GLU | CB-CG | 5.50 | 1.62 | 1.52 |
| 1 | A | 884 | GLN | N-CA | -5.50 | 1.35 | 1.46 |
| 1 | A | 344 | THR | N-CA | -5.49 | 1.35 | 1.46 |
| 1 | A | 83 | SER | C-O | -5.49 | 1.12 | 1.23 |
| 1 | A | 830 | LEU | N-CA | 5.49 | 1.57 | 1.46 |
| 1 | B | 377 | TYR | C-O | 5.48 | 1.33 | 1.23 |
| 1 | B | 684 | GLU | CD-OE2 | 5.48 | 1.31 | 1.25 |
| 1 | A | 503 | PHE | CD2-CE2 | -5.48 | 1.28 | 1.39 |
| 1 | B | 183 | LYS | CE-NZ | 5.48 | 1.62 | 1.49 |
| 1 | B | 521 | LEU | C-O | 5.48 | 1.33 | 1.23 |
| 1 | B | 661 | PHE | CB-CG | 5.48 | 1.60 | 1.51 |
| 1 | B | 837 | MET | C-O | 5.48 | 1.33 | 1.23 |
| 1 | B | 475 | ARG | N-CA | -5.47 | 1.35 | 1.46 |
| 1 | A | 138 | ILE | CB-CG2 | 5.47 | 1.69 | 1.52 |
| 1 | B | 634 | GLU | CB-CG | 5.47 | 1.62 | 1.52 |
| 1 | A | 459 | SER | CB-OG | -5.47 | 1.35 | 1.42 |
| 1 | A | 460 | ARG | CA-C | -5.47 | 1.38 | 1.52 |
| 1 | B | 325 | TRP | CZ2-CH2 | 5.47 | 1.47 | 1.37 |
| 1 | B | 31 | ASP | CG-OD1 | 5.47 | 1.38 | 1.25 |
| 1 | A | 497 | ASP | CB-CG | 5.47 | 1.63 | 1.51 |
| 1 | B | 349 | LYS | CB-CG | -5.47 | 1.37 | 1.52 |
| 1 | B | 27 | TYR | CA-CB | -5.46 | 1.42 | 1.53 |
| 1 | A | 209 | GLY | C-O | -5.46 | 1.15 | 1.23 |
| 1 | B | 87 | PHE | CD2-CE2 | 5.46 | 1.50 | 1.39 |
| 1 | B | 697 | LEU | CA-CB | 5.46 | 1.66 | 1.53 |
| 1 | A | 661 | PHE | CA-C | 5.46 | 1.67 | 1.52 |
| 1 | B | 223 | ASP | CB-CG | -5.46 | 1.40 | 1.51 |
| 1 | A | 860 | ARG | NE-CZ | 5.46 | 1.40 | 1.33 |
| 1 | B | 28 | LEU | C-O | 5.46 | 1.33 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 377 | TYR | N-CA | -5.46 | 1.35 | 1.46 |
| 1 | A | 51 | PHE | CE2-CZ | 5.45 | 1.47 | 1.37 |
| 1 | A | 129 | GLN | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | A | 311 | GLU | C-O | 5.45 | 1.33 | 1.23 |
| 1 | A | 271 | GLN | CA-C | 5.45 | 1.67 | 1.52 |
| 1 | A | 495 | GLU | CA-CB | -5.45 | 1.42 | 1.53 |
| 1 | A | 118 | GLU | CB-CG | 5.45 | 1.62 | 1.52 |
| 1 | A | 243 | ASN | CA-C | 5.45 | 1.67 | 1.52 |
| 1 | B | 60 | PHE | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | B | 61 | LYS | CD-CE | 5.45 | 1.64 | 1.51 |
| 1 | A | 364 | THR | CA-C | 5.44 | 1.67 | 1.52 |
| 1 | A | 23 | ARG | CA-C | 5.44 | 1.67 | 1.52 |
| 1 | B | 660 | ASP | C-O | 5.44 | 1.33 | 1.23 |
| 1 | B | 742 | ALA | CA-CB | 5.44 | 1.63 | 1.52 |
| 1 | B | 824 | GLU | CA-C | 5.43 | 1.67 | 1.52 |
| 1 | A | 84 | ASN | C-N | 5.43 | 1.44 | 1.34 |
| 1 | B | 400 | TYR | N-CA | 5.43 | 1.57 | 1.46 |
| 1 | A | 652 | PHE | C-O | 5.43 | 1.33 | 1.23 |
| 1 | A | 127 | TYR | CE1-CZ | -5.43 | 1.31 | 1.38 |
| 1 | B | 31 | ASP | CB-CG | 5.43 | 1.63 | 1.51 |
| 1 | B | 608 | ASN | CA-C | 5.43 | 1.67 | 1.52 |
| 1 | B | 797 | LYS | CB-CG | 5.42 | 1.67 | 1.52 |
| 1 | A | 518 | GLN | CA-CB | -5.42 | 1.42 | 1.53 |
| 1 | B | 392 | GLU | CD-OE2 | 5.42 | 1.31 | 1.25 |
| 1 | A | 861 | LEU | CG-CD2 | 5.42 | 1.71 | 1.51 |
| 1 | B | 267 | THR | CA-CB | 5.42 | 1.67 | 1.53 |
| 1 | A | 177 | TRP | CG-CD2 | 5.42 | 1.52 | 1.43 |
| 1 | B | 77 | ARG | CG-CD | -5.41 | 1.38 | 1.51 |
| 1 | A | 749 | LEU | CG-CD2 | 5.41 | 1.71 | 1.51 |
| 1 | A | 892 | TYR | CA-CB | 5.41 | 1.65 | 1.53 |
| 1 | A | 648 | ILE | CA-CB | -5.40 | 1.42 | 1.54 |
| 1 | B | 149 | TRP | CZ3-CH2 | -5.40 | 1.31 | 1.40 |
| 1 | B | 197 | GLY | CA-C | 5.40 | 1.60 | 1.51 |
| 1 | B | 206 | ASP | C-O | -5.40 | 1.13 | 1.23 |
| 1 | B | 219 | LYS | CA-C | 5.40 | 1.67 | 1.52 |
| 1 | A | 277 | GLN | C-O | 5.40 | 1.33 | 1.23 |
| 1 | B | 7 | LYS | CE-NZ | 5.40 | 1.62 | 1.49 |
| 1 | B | 400 | TYR | CA-C | 5.40 | 1.67 | 1.52 |
| 1 | B | 129 | GLN | CA-CB | -5.39 | 1.42 | 1.53 |
| 1 | B | 319 | MET | C-O | 5.39 | 1.33 | 1.23 |
| 1 | A | 240 | CYS | N-CA | -5.39 | 1.35 | 1.46 |
| 1 | A | 409 | PHE | CG-CD1 | 5.39 | 1.46 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 283 | ARG | CA-C | -5.39 | 1.39 | 1.52 |
| 1 | A | 168 | VAL | CA-CB | -5.39 | 1.43 | 1.54 |
| 1 | B | 555 | LEU | N-CA | 5.39 | 1.57 | 1.46 |
| 1 | B | 467 | ILE | CB-CG1 | 5.38 | 1.69 | 1.54 |
| 1 | A | 202 | GLU | CD-OE1 | 5.38 | 1.31 | 1.25 |
| 1 | A | 288 | TRP | CE3-CZ3 | -5.38 | 1.29 | 1.38 |
| 1 | A | 225 | TYR | CB-CG | -5.38 | 1.43 | 1.51 |
| 1 | B | 169 | HIS | N-CA | -5.38 | 1.35 | 1.46 |
| 1 | B | 382 | TRP | CG-CD1 | -5.37 | 1.29 | 1.36 |
| 1 | B | 557 | THR | CB-CG2 | 5.37 | 1.70 | 1.52 |
| 1 | B | 304 | TRP | CA-CB | 5.37 | 1.65 | 1.53 |
| 1 | A | 884 | GLN | CG-CD | 5.36 | 1.63 | 1.51 |
| 1 | B | 15 | ALA | N-CA | 5.36 | 1.57 | 1.46 |
| 1 | B | 152 | VAL | CA-CB | -5.36 | 1.43 | 1.54 |
| 1 | B | 700 | SER | CB-OG | -5.36 | 1.35 | 1.42 |
| 1 | B | 615 | LYS | CD-CE | 5.36 | 1.64 | 1.51 |
| 1 | B | 214 | TRP | CZ3-CH2 | 5.36 | 1.48 | 1.40 |
| 1 | A | 298 | SER | N-CA | 5.35 | 1.57 | 1.46 |
| 1 | A | 311 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | A | 770 | ARG | C-N | -5.35 | 1.21 | 1.34 |
| 1 | B | 577 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 |
| 1 | B | 609 | TYR | CA-CB | 5.35 | 1.65 | 1.53 |
| 1 | A | 831 | ASN | CA-CB | 5.35 | 1.67 | 1.53 |
| 1 | B | 607 | ARG | CZ-NH1 | 5.35 | 1.40 | 1.33 |
| 1 | B | 584 | ASN | CA-C | 5.35 | 1.66 | 1.52 |
| 1 | A | 873 | LYS | CA-C | 5.35 | 1.66 | 1.52 |
| 1 | A | 359 | THR | CB-CG2 | -5.34 | 1.34 | 1.52 |
| 1 | B | 784 | LEU | C-O | -5.34 | 1.13 | 1.23 |
| 1 | A | 623 | SER | N-CA | -5.34 | 1.35 | 1.46 |
| 1 | B | 23 | ARG | C-N | -5.34 | 1.21 | 1.34 |
| 1 | B | 225 | TYR | CZ-OH | 5.34 | 1.47 | 1.37 |
| 1 | A | 668 | LEU | C-O | 5.34 | 1.33 | 1.23 |
| 1 | B | 521 | LEU | N-CA | 5.34 | 1.57 | 1.46 |
| 1 | A | 338 | LEU | CG-CD2 | -5.34 | 1.32 | 1.51 |
| 1 | B | 596 | LEU | C-O | 5.33 | 1.33 | 1.23 |
| 1 | A | 107 | LEU | CG-CD2 | -5.33 | 1.32 | 1.51 |
| 1 | A | 166 | VAL | CA-CB | -5.33 | 1.43 | 1.54 |
| 1 | A | 458 | ALA | CA-CB | -5.33 | 1.41 | 1.52 |
| 1 | B | 261 | GLY | CA-C | 5.33 | 1.60 | 1.51 |
| 1 | B | 283 | ARG | NE-CZ | 5.33 | 1.40 | 1.33 |
| 1 | A | 313 | GLU | CB-CG | -5.33 | 1.42 | 1.52 |
| 1 | A | 645 | HIS | C-N | -5.33 | 1.21 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 660 | ASP | N-CA | -5.33 | 1.35 | 1.46 |
| 1 | A | 777 | ASP | CA-CB | 5.33 | 1.65 | 1.53 |
| 1 | B | 664 | PHE | CD1-CE1 | 5.33 | 1.50 | 1.39 |
| 1 | A | 271 | GLN | CD-OE1 | 5.33 | 1.35 | 1.24 |
| 1 | B | 851 | PHE | CG-CD1 | -5.33 | 1.30 | 1.38 |
| 1 | A | 730 | PHE | N-CA | 5.33 | 1.56 | 1.46 |
| 1 | A | 87 | PHE | CG-CD2 | -5.32 | 1.30 | 1.38 |
| 1 | A | 313 | GLU | CA-CB | -5.32 | 1.42 | 1.53 |
| 1 | A | 60 | PHE | CG-CD2 | 5.32 | 1.46 | 1.38 |
| 1 | A | 809 | ASP | CA-C | 5.32 | 1.66 | 1.52 |
| 1 | B | 33 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | B | 326 | MET | N-CA | -5.32 | 1.35 | 1.46 |
| 1 | B | 188 | VAL | N-CA | 5.31 | 1.56 | 1.46 |
| 1 | B | 502 | PHE | CG-CD1 | -5.31 | 1.30 | 1.38 |
| 1 | A | 470 | ARG | CZ-NH2 | -5.31 | 1.26 | 1.33 |
| 1 | A | 503 | PHE | CE1-CZ | -5.31 | 1.27 | 1.37 |
| 1 | A | 213 | GLU | C-O | -5.31 | 1.13 | 1.23 |
| 1 | B | 356 | TRP | CA-CB | -5.30 | 1.42 | 1.53 |
| 1 | B | 95 | THR | N-CA | 5.30 | 1.56 | 1.46 |
| 1 | A | 123 | ARG | CB-CG | -5.30 | 1.38 | 1.52 |
| 1 | A | 544 | ALA | CA-CB | 5.30 | 1.63 | 1.52 |
| 1 | A | 670 | ARG | CZ-NH1 | 5.30 | 1.40 | 1.33 |
| 1 | B | 634 | GLU | CG-CD | 5.30 | 1.59 | 1.51 |
| 1 | B | 181 | LEU | CA-C | -5.29 | 1.39 | 1.52 |
| 1 | A | 230 | LYS | CE-NZ | 5.29 | 1.62 | 1.49 |
| 1 | A | 66 | ASN | C-O | -5.29 | 1.13 | 1.23 |
| 1 | B | 720 | SER | CA-CB | 5.29 | 1.60 | 1.52 |
| 1 | A | 335 | PHE | CB-CG | 5.29 | 1.60 | 1.51 |
| 1 | A | 498 | PHE | CG-CD1 | -5.29 | 1.30 | 1.38 |
| 1 | B | 892 | TYR | C-O | 5.28 | 1.33 | 1.23 |
| 1 | A | 464 | GLU | CG-CD | 5.28 | 1.59 | 1.51 |
| 1 | A | 626 | ALA | N-CA | -5.28 | 1.35 | 1.46 |
| 1 | B | 18 | LEU | N-CA | -5.28 | 1.35 | 1.46 |
| 1 | A | 784 | LEU | C-O | 5.28 | 1.33 | 1.23 |
| 1 | B | 133 | GLU | N-CA | 5.28 | 1.56 | 1.46 |
| 1 | B | 391 | LEU | CA-CB | 5.28 | 1.65 | 1.53 |
| 1 | B | 456 | ALA | CA-CB | 5.28 | 1.63 | 1.52 |
| 1 | A | 669 | VAL | C-N | -5.27 | 1.22 | 1.34 |
| 1 | A | 789 | PHE | C-O | -5.27 | 1.13 | 1.23 |
| 1 | B | 388 | LYS | CA-C | -5.27 | 1.39 | 1.52 |
| 1 | B | 540 | PHE | CB-CG | 5.27 | 1.60 | 1.51 |
| 1 | B | 655 | ASP | CA-CB | 5.27 | 1.65 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 185 | TYR | CD2-CE2 | -5.27 | 1.31 | 1.39 |
| 1 | B | 415 | GLN | N-CA | 5.27 | 1.56 | 1.46 |
| 1 | B | 2 | ALA | C-O | 5.27 | 1.33 | 1.23 |
| 1 | B | 315 | LEU | CA-C | -5.26 | 1.39 | 1.52 |
| 1 | B | 318 | LYS | C-O | 5.26 | 1.33 | 1.23 |
| 1 | A | 511 | GLN | CD-NE2 | 5.26 | 1.46 | 1.32 |
| 1 | B | 392 | GLU | C-O | 5.26 | 1.33 | 1.23 |
| 1 | A | 434 | ALA | CA-C | -5.26 | 1.39 | 1.52 |
| 1 | A | 475 | ARG | CZ-NH1 | 5.26 | 1.39 | 1.33 |
| 1 | A | 691 | LEU | C-O | -5.26 | 1.13 | 1.23 |
| 1 | B | 509 | GLY | CA-C | -5.25 | 1.43 | 1.51 |
| 1 | B | 325 | TRP | CB-CG | 5.25 | 1.59 | 1.50 |
| 1 | B | 396 | ASP | C-N | 5.25 | 1.46 | 1.34 |
| 1 | A | 675 | PHE | CE2-CZ | -5.25 | 1.27 | 1.37 |
| 1 | B | 726 | PHE | CB-CG | -5.25 | 1.42 | 1.51 |
| 1 | B | 769 | CYS | CA-C | -5.25 | 1.39 | 1.52 |
| 1 | A | 308 | ASP | CG-OD1 | 5.25 | 1.37 | 1.25 |
| 1 | A | 275 | GLN | CD-NE2 | -5.24 | 1.19 | 1.32 |
| 1 | A | 520 | ASN | C-O | 5.24 | 1.33 | 1.23 |
| 1 | B | 156 | ASP | C-O | 5.24 | 1.33 | 1.23 |
| 1 | B | 583 | VAL | N-CA | -5.24 | 1.35 | 1.46 |
| 1 | A | 28 | LEU | N-CA | 5.24 | 1.56 | 1.46 |
| 1 | A | 218 | GLN | C-O | -5.24 | 1.13 | 1.23 |
| 1 | A | 218 | GLN | CD-OE1 | 5.23 | 1.35 | 1.24 |
| 1 | A | 254 | THR | C-O | 5.23 | 1.33 | 1.23 |
| 1 | A | 315 | LEU | CA-CB | 5.23 | 1.65 | 1.53 |
| 1 | B | 241 | SER | CA-C | -5.23 | 1.39 | 1.52 |
| 1 | B | 376 | ASN | CG-ND2 | 5.23 | 1.46 | 1.32 |
| 1 | A | 38 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | B | 456 | ALA | C-O | 5.22 | 1.33 | 1.23 |
| 1 | A | 670 | ARG | NE-CZ | -5.22 | 1.26 | 1.33 |
| 1 | A | 672 | GLU | CD-OE1 | 5.22 | 1.31 | 1.25 |
| 1 | A | 892 | TYR | CD2-CE2 | 5.22 | 1.47 | 1.39 |
| 1 | A | 50 | ALA | C-O | 5.21 | 1.33 | 1.23 |
| 1 | B | 36 | ARG | NE-CZ | 5.21 | 1.39 | 1.33 |
| 1 | B | 155 | ASP | CA-CB | -5.21 | 1.42 | 1.53 |
| 1 | B | 426 | ARG | C-O | 5.21 | 1.33 | 1.23 |
| 1 | B | 514 | ASP | C-O | 5.21 | 1.33 | 1.23 |
| 1 | A | 187 | LYS | CD-CE | 5.21 | 1.64 | 1.51 |
| 1 | B | 263 | ALA | N-CA | 5.21 | 1.56 | 1.46 |
| 1 | B | 297 | TRP | CA-CB | -5.21 | 1.42 | 1.53 |
| 1 | A | 503 | PHE | CG-CD2 | -5.21 | 1.30 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 203 | ALA | C-O | 5.20 | 1.33 | 1.23 |
| 1 | A | 614 | ARG | CZ-NH1 | 5.20 | 1.39 | 1.33 |
| 1 | B | 519 | ALA | C-N | -5.20 | 1.22 | 1.34 |
| 1 | A | 23 | ARG | CG-CD | 5.20 | 1.65 | 1.51 |
| 1 | A | 558 | ILE | CB-CG2 | 5.20 | 1.69 | 1.52 |
| 1 | A | 275 | GLN | C-N | -5.20 | 1.23 | 1.33 |
| 1 | B | 305 | ASN | CG-ND2 | 5.20 | 1.45 | 1.32 |
| 1 | A | 414 | MET | SD-CE | 5.20 | 2.06 | 1.77 |
| 1 | A | 774 | ALA | C-O | -5.19 | 1.13 | 1.23 |
| 1 | B | 81 | LEU | CG-CD2 | 5.19 | 1.71 | 1.51 |
| 1 | B | 226 | GLN | CA-C | 5.19 | 1.66 | 1.52 |
| 1 | B | 345 | PRO | C-O | -5.19 | 1.12 | 1.23 |
| 1 | A | 220 | ALA | C-N | -5.19 | 1.24 | 1.34 |
| 1 | A | 238 | LEU | CA-CB | -5.19 | 1.41 | 1.53 |
| 1 | B | 284 | MET | C-O | 5.19 | 1.33 | 1.23 |
| 1 | B | 475 | ARG | CZ-NH2 | -5.19 | 1.26 | 1.33 |
| 1 | B | 454 | PHE | CD1-CE1 | -5.19 | 1.28 | 1.39 |
| 1 | A | 374 | CYS | CB-SG | 5.19 | 1.91 | 1.82 |
| 1 | A | 639 | LYS | CD-CE | 5.19 | 1.64 | 1.51 |
| 1 | B | 341 | CYS | CA-C | -5.18 | 1.39 | 1.52 |
| 1 | A | 358 | THR | CA-C | 5.18 | 1.66 | 1.52 |
| 1 | B | 494 | LYS | CG-CD | 5.18 | 1.70 | 1.52 |
| 1 | B | 36 | ARG | CG-CD | -5.18 | 1.39 | 1.51 |
| 1 | B | 174 | ASN | CA-CB | 5.18 | 1.66 | 1.53 |
| 1 | A | 490 | PHE | CG-CD1 | -5.17 | 1.30 | 1.38 |
| 1 | B | 311 | GLU | N-CA | 5.17 | 1.56 | 1.46 |
| 1 | B | 854 | PHE | N-CA | -5.17 | 1.36 | 1.46 |
| 1 | A | 677 | ILE | N-CA | -5.17 | 1.36 | 1.46 |
| 1 | B | 771 | SER | CA-CB | -5.17 | 1.45 | 1.52 |
| 1 | B | 78 | PRO | CA-CB | -5.17 | 1.43 | 1.53 |
| 1 | B | 313 | GLU | CD-OE1 | 5.17 | 1.31 | 1.25 |
| 1 | B | 806 | PHE | CA-CB | 5.17 | 1.65 | 1.53 |
| 1 | A | 237 | LEU | N-CA | 5.17 | 1.56 | 1.46 |
| 1 | A | 323 | GLU | C-O | 5.17 | 1.33 | 1.23 |
| 1 | B | 288 | TRP | CE3-CZ3 | -5.16 | 1.29 | 1.38 |
| 1 | B | 313 | GLU | CD-OE2 | -5.16 | 1.20 | 1.25 |
| 1 | B | 617 | ASP | CB-CG | -5.16 | 1.41 | 1.51 |
| 1 | A | 823 | PHE | CD2-CE2 | -5.16 | 1.28 | 1.39 |
| 1 | B | 618 | LEU | CA-C | 5.16 | 1.66 | 1.52 |
| 1 | A | 702 | LEU | CA-CB | 5.16 | 1.65 | 1.53 |
| 1 | A | 337 | LYS | CG-CD | -5.15 | 1.34 | 1.52 |
| 1 | A | 593 | LYS | N-CA | -5.15 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 144 | TRP | CZ3-CH2 | -5.15 | 1.31 | 1.40 |
| 1 | A | 874 | ASN | CG-ND2 | 5.15 | 1.45 | 1.32 |
| 1 | B | 891 | MET | C-O | 5.15 | 1.33 | 1.23 |
| 1 | A | 681 | LEU | C-O | -5.15 | 1.13 | 1.23 |
| 1 | A | 94 | ARG | NE-CZ | 5.14 | 1.39 | 1.33 |
| 1 | A | 601 | ILE | N-CA | 5.14 | 1.56 | 1.46 |
| 1 | B | 839 | ILE | CA-C | 5.14 | 1.66 | 1.52 |
| 1 | A | 582 | MET | CA-CB | -5.14 | 1.42 | 1.53 |
| 1 | B | 829 | HIS | C-O | -5.14 | 1.13 | 1.23 |
| 1 | B | 30 | GLN | CG-CD | -5.14 | 1.39 | 1.51 |
| 1 | B | 47 | GLN | CB-CG | 5.14 | 1.66 | 1.52 |
| 1 | B | 207 | PHE | CD1-CE1 | 5.14 | 1.49 | 1.39 |
| 1 | B | 581 | SER | CA-CB | 5.14 | 1.60 | 1.52 |
| 1 | A | 286 | ASN | CA-CB | -5.13 | 1.39 | 1.53 |
| 1 | A | 88 | ILE | C-O | 5.13 | 1.33 | 1.23 |
| 1 | A | 124 | VAL | C-O | -5.13 | 1.13 | 1.23 |
| 1 | B | 426 | ARG | CZ-NH2 | 5.13 | 1.39 | 1.33 |
| 1 | B | 467 | ILE | N-CA | 5.13 | 1.56 | 1.46 |
| 1 | A | 491 | GLU | CA-CB | -5.13 | 1.42 | 1.53 |
| 1 | B | 375 | ARG | C-O | 5.13 | 1.33 | 1.23 |
| 1 | A | 356 | TRP | CD2-CE2 | 5.12 | 1.47 | 1.41 |
| 1 | A | 603 | TRP | CZ3-CH2 | -5.12 | 1.31 | 1.40 |
| 1 | B | 17 | GLY | N-CA | 5.12 | 1.53 | 1.46 |
| 1 | A | 470 | ARG | CG-CD | -5.12 | 1.39 | 1.51 |
| 1 | B | 311 | GLU | C-O | -5.12 | 1.13 | 1.23 |
| 1 | B | 48 | ASP | CG-OD2 | 5.12 | 1.37 | 1.25 |
| 1 | B | 133 | GLU | CD-OE1 | 5.12 | 1.31 | 1.25 |
| 1 | A | 741 | SER | CA-CB | 5.12 | 1.60 | 1.52 |
| 1 | B | 678 | PHE | C-O | 5.12 | 1.33 | 1.23 |
| 1 | A | 383 | VAL | CA-CB | -5.11 | 1.44 | 1.54 |
| 1 | B | 57 | SER | CA-C | -5.11 | 1.39 | 1.52 |
| 1 | B | 94 | ARG | C-O | -5.11 | 1.13 | 1.23 |
| 1 | B | 468 | ASN | CB-CG | 5.11 | 1.62 | 1.51 |
| 1 | A | 679 | LYS | CA-CB | -5.11 | 1.42 | 1.53 |
| 1 | A | 648 | ILE | CB-CG2 | -5.11 | 1.37 | 1.52 |
| 1 | B | 47 | GLN | C-O | -5.11 | 1.13 | 1.23 |
| 1 | A | 131 | PHE | CG-CD2 | -5.11 | 1.31 | 1.38 |
| 1 | A | 317 | VAL | CB-CG2 | -5.11 | 1.42 | 1.52 |
| 1 | B | 192 | TYR | CE1-CZ | -5.11 | 1.31 | 1.38 |
| 1 | A | 27 | TYR | CE1-CZ | -5.10 | 1.31 | 1.38 |
| 1 | B | 580 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.33 |
| 1 | B | 427 | ASP | CA-C | 5.10 | 1.66 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 638 | PHE | CD2-CE2 | -5.09 | 1.29 | 1.39 |
| 1 | B | 690 | GLN | C-O | -5.09 | 1.13 | 1.23 |
| 1 | B | 827 | GLY | C-O | -5.09 | 1.15 | 1.23 |
| 1 | A | 135 | TYR | CB-CG | 5.09 | 1.59 | 1.51 |
| 1 | A | 356 | TRP | CZ3-CH2 | 5.09 | 1.48 | 1.40 |
| 1 | A | 385 | PRO | CA-CB | -5.09 | 1.43 | 1.53 |
| 1 | A | 644 | LEU | CG-CD1 | -5.09 | 1.33 | 1.51 |
| 1 | B | 572 | ASN | C-N | 5.09 | 1.42 | 1.33 |
| 1 | A | 415 | GLN | C-O | -5.09 | 1.13 | 1.23 |
| 1 | B | 447 | VAL | C-N | -5.09 | 1.22 | 1.34 |
| 1 | B | 349 | LYS | N-CA | 5.08 | 1.56 | 1.46 |
| 1 | B | 674 | LEU | C-O | 5.08 | 1.33 | 1.23 |
| 1 | A | 208 | THR | C-O | 5.08 | 1.32 | 1.23 |
| 1 | B | 161 | LYS | CG-CD | 5.08 | 1.69 | 1.52 |
| 1 | B | 627 | TYR | CD2-CE2 | 5.08 | 1.47 | 1.39 |
| 1 | B | 356 | TRP | CZ3-CH2 | 5.07 | 1.48 | 1.40 |
| 1 | B | 6 | MET | CA-C | -5.07 | 1.39 | 1.52 |
| 1 | A | 625 | SER | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | B | 112 | ALA | CA-C | 5.07 | 1.66 | 1.52 |
| 1 | B | 220 | ALA | C-N | -5.07 | 1.24 | 1.34 |
| 1 | B | 773 | VAL | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | B | 810 | ARG | C-O | 5.07 | 1.32 | 1.23 |
| 1 | A | 18 | LEU | CA-C | -5.07 | 1.39 | 1.52 |
| 1 | A | 763 | GLY | N-CA | 5.07 | 1.53 | 1.46 |
| 1 | B | 881 | VAL | C-O | 5.07 | 1.32 | 1.23 |
| 1 | A | 876 | THR | CB-OG1 | 5.07 | 1.53 | 1.43 |
| 1 | B | 213 | GLU | CA-CB | 5.06 | 1.65 | 1.53 |
| 1 | A | 199 | CYS | N-CA | -5.06 | 1.36 | 1.46 |
| 1 | A | 293 | TRP | CA-C | -5.06 | 1.39 | 1.52 |
| 1 | B | 482 | GLU | CG-CD | 5.06 | 1.59 | 1.51 |
| 1 | A | 886 | TRP | CB-CG | 5.06 | 1.59 | 1.50 |
| 1 | A | 482 | GLU | CG-CD | 5.06 | 1.59 | 1.51 |
| 1 | A | 336 | THR | CA-C | -5.05 | 1.39 | 1.52 |
| 1 | A | 751 | LYS | CD-CE | 5.05 | 1.63 | 1.51 |
| 1 | B | 376 | ASN | C-O | -5.05 | 1.13 | 1.23 |
| 1 | B | 638 | PHE | CG-CD2 | -5.05 | 1.31 | 1.38 |
| 1 | B | 384 | ASN | CB-CG | -5.05 | 1.39 | 1.51 |
| 1 | A | 381 | PHE | CE1-CZ | 5.05 | 1.47 | 1.37 |
| 1 | A | 614 | ARG | CB-CG | 5.05 | 1.66 | 1.52 |
| 1 | A | 734 | ALA | N-CA | 5.05 | 1.56 | 1.46 |
| 1 | B | 222 | SER | CA-CB | -5.05 | 1.45 | 1.52 |
| 1 | B | 370 | THR | C-O | 5.05 | 1.32 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 361 | TYR | CA-C | -5.04 | 1.39 | 1.52 |
| 1 | B | 329 | ARG | CB-CG | 5.04 | 1.66 | 1.52 |
| 1 | A | 856 | SER | CA-C | -5.04 | 1.39 | 1.52 |
| 1 | B | 701 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |
| 1 | B | 621 | SER | C-O | 5.03 | 1.32 | 1.23 |
| 1 | B | 673 | ILE | CG1-CD1 | -5.03 | 1.15 | 1.50 |
| 1 | A | 351 | ARG | CB-CG | 5.03 | 1.66 | 1.52 |
| 1 | B | 295 | GLY | CA-C | 5.03 | 1.59 | 1.51 |
| 1 | A | 46 | PHE | CE1-CZ | 5.03 | 1.47 | 1.37 |
| 1 | A | 323 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 |
| 1 | A | 416 | LYS | CB-CG | 5.03 | 1.66 | 1.52 |
| 1 | A | 146 | PHE | C-O | -5.03 | 1.13 | 1.23 |
| 1 | A | 868 | PHE | CE1-CZ | -5.03 | 1.27 | 1.37 |
| 1 | B | 205 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 |
| 1 | B | 95 | THR | CB-CG2 | 5.02 | 1.69 | 1.52 |
| 1 | A | 457 | ASN | CG-OD1 | 5.02 | 1.34 | 1.24 |
| 1 | B | 117 | ASN | C-O | 5.02 | 1.32 | 1.23 |
| 1 | B | 435 | VAL | C-O | -5.02 | 1.13 | 1.23 |
| 1 | A | 351 | ARG | NE-CZ | 5.02 | 1.39 | 1.33 |
| 1 | B | 225 | TYR | CD1-CE1 | -5.02 | 1.31 | 1.39 |
| 1 | A | 875 | GLY | N-CA | -5.01 | 1.38 | 1.46 |
| 1 | B | 365 | TRP | C-O | -5.01 | 1.13 | 1.23 |
| 1 | A | 200 | THR | CB-OG1 | 5.01 | 1.53 | 1.43 |
| 1 | B | 343 | LEU | CB-CG | -5.01 | 1.38 | 1.52 |
| 1 | B | 853 | ASN | CB-CG | 5.01 | 1.62 | 1.51 |
| 1 | B | 836 | SER | CA-CB | 5.00 | 1.60 | 1.52 |
| 1 | A | 547 | ASP | N-CA | 5.00 | 1.56 | 1.46 |
| 1 | B | 27 | TYR | CB-CG | -5.00 | 1.44 | 1.51 |
| 1 | A | 105 | SER | CA-C | 5.00 | 1.66 | 1.52 |
| 1 | A | 375 | ARG | C-N | -5.00 | 1.22 | 1.34 |
| 1 | A | 579 | CYS | C-O | 5.00 | 1.32 | 1.23 |
| 1 | B | 700 | SER | C-O | 5.00 | 1.32 | 1.23 |

All (959) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 460 | ARG | NE-CZ-NH1 | -29.77 | 105.41 | 120.30 |
| 1 | A | 329 | ARG | NE-CZ-NH1 | 26.14 | 133.37 | 120.30 |
| 1 | A | 329 | ARG | NE-CZ-NH2 | -24.17 | 108.22 | 120.30 |
| 1 | B | 514 | ASP | CB-CG-OD2 | -18.56 | 101.59 | 118.30 |
| 1 | A | 285 | ARG | NE-CZ-NH2 | -15.96 | 112.32 | 120.30 |
| 1 | B | 285 | ARG | NE-CZ-NH1 | 15.90 | 128.25 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 614 | ARG | NE-CZ-NH2 | -15.75 | 112.43 | 120.30 |
| 1 | A | 278 | ARG | NE-CZ-NH1 | -15.65 | 112.48 | 120.30 |
| 1 | B | 501 | ARG | NE-CZ-NH2 | -15.59 | 112.50 | 120.30 |
| 1 | B | 315 | LEU | CA-CB-CG | 15.47 | 150.88 | 115.30 |
| 1 | B | 514 | ASP | CB-CG-OD1 | 15.47 | 132.22 | 118.30 |
| 1 | B | 501 | ARG | NE-CZ-NH1 | 15.35 | 127.97 | 120.30 |
| 1 | B | 375 | ARG | NE-CZ-NH1 | 15.28 | 127.94 | 120.30 |
| 1 | A | 477 | ARG | NE-CZ-NH2 | 15.27 | 127.93 | 120.30 |
| 1 | A | 460 | ARG | NE-CZ-NH2 | 15.14 | 127.87 | 120.30 |
| 1 | B | 285 | ARG | NE-CZ-NH2 | -15.11 | 112.74 | 120.30 |
| 1 | B | 779 | ASP | CB-CG-OD2 | 14.97 | 131.78 | 118.30 |
| 1 | A | 31 | ASP | CB-CG-OD2 | -14.81 | 104.97 | 118.30 |
| 1 | A | 396 | ASP | CB-CG-OD1 | 14.80 | 131.62 | 118.30 |
| 1 | B | 330 | ASP | CB-CG-OD2 | 14.77 | 131.59 | 118.30 |
| 1 | B | 308 | ASP | CB-CG-OD1 | -14.67 | 105.09 | 118.30 |
| 1 | B | 366 | ARG | NE-CZ-NH1 | -14.67 | 112.96 | 120.30 |
| 1 | B | 470 | ARG | NE-CZ-NH2 | 14.62 | 127.61 | 120.30 |
| 1 | A | 497 | ASP | CB-CG-OD1 | -14.24 | 105.48 | 118.30 |
| 1 | B | 375 | ARG | NE-CZ-NH2 | -14.23 | 113.19 | 120.30 |
| 1 | A | 756 | HIS | C-N-CD | -13.92 | 89.97 | 120.60 |
| 1 | A | 354 | ARG | NE-CZ-NH2 | 13.84 | 127.22 | 120.30 |
| 1 | A | 860 | ARG | NE-CZ-NH1 | -13.83 | 113.39 | 120.30 |
| 1 | A | 175 | GLU | OE1-CD-OE2 | -13.59 | 107.00 | 123.30 |
| 1 | B | 398 | ASP | CA-C-N | 13.51 | 146.92 | 117.20 |
| 1 | B | 670 | ARG | NE-CZ-NH1 | 13.11 | 126.86 | 120.30 |
| 1 | A | 662 | ASP | CB-CG-OD1 | -13.09 | 106.52 | 118.30 |
| 1 | B | 470 | ARG | NE-CZ-NH1 | -12.92 | 113.84 | 120.30 |
| 1 | B | 36 | ARG | NE-CZ-NH1 | 12.89 | 126.74 | 120.30 |
| 1 | A | 614 | ARG | NE-CZ-NH1 | 12.84 | 126.72 | 120.30 |
| 1 | B | 512 | GLU | OE1-CD-OE2 | -12.72 | 108.03 | 123.30 |
| 1 | B | 497 | ASP | CB-CG-OD1 | 12.69 | 129.72 | 118.30 |
| 1 | A | 390 | ARG | NE-CZ-NH2 | -12.41 | 114.10 | 120.30 |
| 1 | A | 810 | ARG | NE-CZ-NH2 | 12.39 | 126.50 | 120.30 |
| 1 | A | 94 | ARG | NE-CZ-NH1 | 12.34 | 126.47 | 120.30 |
| 1 | B | 216 | ASP | CB-CG-OD1 | -12.28 | 107.25 | 118.30 |
| 1 | B | 346 | ASP | CB-CG-OD1 | 12.20 | 129.28 | 118.30 |
| 1 | A | 395 | ASP | CB-CG-OD1 | -12.12 | 107.39 | 118.30 |
| 1 | B | 850 | ASP | CB-CG-OD1 | 11.94 | 129.05 | 118.30 |
| 1 | B | 139 | PHE | CB-CG-CD2 | 11.88 | 129.11 | 120.80 |
| 1 | A | 310 | TYR | CB-CG-CD1 | -11.87 | 113.88 | 121.00 |
| 1 | B | 866 | ARG | NE-CZ-NH1 | 11.76 | 126.18 | 120.30 |
| 1 | B | 850 | ASP | CB-CG-OD2 | 11.73 | 128.86 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 123 | ARG | NE-CZ-NH2 | -11.70 | 114.45 | 120.30 |
| 1 | B | 123 | ARG | NE-CZ-NH2 | -11.60 | 114.50 | 120.30 |
| 1 | A | 155 | ASP | CB-CG-OD2 | -11.54 | 107.91 | 118.30 |
| 1 | B | 862 | ASP | CB-CG-OD2 | 11.51 | 128.66 | 118.30 |
| 1 | A | 514 | ASP | CB-CG-OD1 | -11.47 | 107.98 | 118.30 |
| 1 | B | 12 | ARG | NE-CZ-NH2 | -11.43 | 114.59 | 120.30 |
| 1 | B | 850 | ASP | OD1-CG-OD2 | -11.29 | 101.85 | 123.30 |
| 1 | B | 104 | ASP | CB-CG-OD2 | 11.19 | 128.37 | 118.30 |
| 1 | B | 657 | LEU | CB-CG-CD2 | 11.16 | 129.97 | 111.00 |
| 1 | B | 193 | GLU | OE1-CD-OE2 | 11.02 | 136.53 | 123.30 |
| 1 | B | 123 | ARG | NE-CZ-NH1 | 11.00 | 125.80 | 120.30 |
| 1 | A | 232 | LEU | CB-CG-CD1 | -10.97 | 92.34 | 111.00 |
| 1 | A | 478 | LEU | CB-CG-CD2 | -10.91 | 92.45 | 111.00 |
| 1 | B | 865 | PHE | N-CA-C | -10.84 | 81.72 | 111.00 |
| 1 | B | 399 | ASP | CB-CG-OD2 | 10.83 | 128.04 | 118.30 |
| 1 | B | 366 | ARG | NH1-CZ-NH2 | 10.81 | 131.29 | 119.40 |
| 1 | A | 497 | ASP | CB-CG-OD2 | 10.80 | 128.02 | 118.30 |
| 1 | B | 31 | ASP | CB-CG-OD1 | 10.77 | 127.99 | 118.30 |
| 1 | A | 31 | ASP | CB-CG-OD1 | 10.73 | 127.96 | 118.30 |
| 1 | A | 151 | ASP | CB-CG-OD2 | -10.71 | 108.66 | 118.30 |
| 1 | B | 216 | ASP | CB-CG-OD2 | 10.66 | 127.89 | 118.30 |
| 1 | A | 618 | LEU | CB-CG-CD2 | 10.53 | 128.90 | 111.00 |
| 1 | A | 339 | GLU | OE1-CD-OE2 | 10.46 | 135.85 | 123.30 |
| 1 | B | 872 | ASP | CB-CG-OD2 | 10.46 | 127.71 | 118.30 |
| 1 | B | 398 | ASP | CB-CG-OD2 | 10.40 | 127.67 | 118.30 |
| 1 | B | 402 | SER | C-N-CA | 10.36 | 147.60 | 121.70 |
| 1 | A | 862 | ASP | CB-CG-OD1 | 10.35 | 127.62 | 118.30 |
| 1 | A | 358 | THR | CA-CB-CG2 | -10.35 | 97.92 | 112.40 |
| 1 | A | 830 | LEU | CB-CG-CD2 | 10.30 | 128.51 | 111.00 |
| 1 | A | 513 | LEU | CB-CG-CD1 | -10.29 | 93.50 | 111.00 |
| 1 | B | 451 | ARG | NE-CZ-NH2 | 10.28 | 125.44 | 120.30 |
| 1 | A | 237 | LEU | CB-CG-CD2 | 10.19 | 128.33 | 111.00 |
| 1 | A | 332 | ILE | CG1-CB-CG2 | 10.18 | 133.80 | 111.40 |
| 1 | A | 165 | LEU | CB-CG-CD2 | 10.18 | 128.30 | 111.00 |
| 1 | A | 809 | ASP | CB-CG-OD2 | 10.16 | 127.45 | 118.30 |
| 1 | A | 211 | VAL | CB-CA-C | -10.15 | 92.12 | 111.40 |
| 1 | B | 428 | MET | CG-SD-CE | 10.12 | 116.40 | 100.20 |
| 1 | A | 88 | ILE | CG1-CB-CG2 | -10.12 | 89.14 | 111.40 |
| 1 | B | 362 | GLU | OE1-CD-OE2 | -10.12 | 111.16 | 123.30 |
| 1 | B | 58 | LEU | CA-CB-CG | 10.09 | 138.51 | 115.30 |
| 1 | B | 188 | VAL | CA-CB-CG1 | 10.08 | 126.03 | 110.90 |
| 1 | A | 165 | LEU | CA-CB-CG | -10.08 | 92.11 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 580 | ARG | NE-CZ-NH1 | 10.07 | 125.33 | 120.30 |
| 1 | A | 640 | LEU | CB-CG-CD2 | 10.04 | 128.07 | 111.00 |
| 1 | B | 396 | ASP | CB-CG-OD2 | 10.03 | 127.33 | 118.30 |
| 1 | B | 436 | TYR | CB-CG-CD1 | 9.98 | 126.99 | 121.00 |
| 1 | A | 522 | PRO | CA-C-O | -9.95 | 96.31 | 120.20 |
| 1 | A | 312 | ARG | NE-CZ-NH1 | -9.88 | 115.36 | 120.30 |
| 1 | B | 23 | ARG | NE-CZ-NH2 | -9.84 | 115.38 | 120.30 |
| 1 | A | 310 | TYR | CZ-CE2-CD2 | -9.83 | 110.95 | 119.80 |
| 1 | B | 446 | PRO | N-CD-CG | -9.77 | 88.55 | 103.20 |
| 1 | B | 36 | ARG | CG-CD-NE | 9.73 | 132.24 | 111.80 |
| 1 | A | 736 | ASP | CB-CG-OD2 | 9.72 | 127.05 | 118.30 |
| 1 | B | 315 | LEU | CB-CA-C | -9.66 | 91.84 | 110.20 |
| 1 | B | 862 | ASP | CB-CG-OD1 | -9.62 | 109.64 | 118.30 |
| 1 | B | 472 | VAL | CB-CA-C | -9.60 | 93.16 | 111.40 |
| 1 | A | 396 | ASP | OD1-CG-OD2 | -9.60 | 105.06 | 123.30 |
| 1 | A | 455 | LEU | CB-CG-CD1 | -9.59 | 94.69 | 111.00 |
| 1 | A | 339 | GLU | CG-CD-OE2 | -9.58 | 99.14 | 118.30 |
| 1 | A | 282 | ILE | CG1-CB-CG2 | -9.57 | 90.35 | 111.40 |
| 1 | B | 366 | ARG | NE-CZ-NH2 | -9.57 | 115.52 | 120.30 |
| 1 | A | 831 | ASN | CB-CA-C | 9.56 | 129.53 | 110.40 |
| 1 | A | 328 | PHE | O-C-N | -9.56 | 107.40 | 122.70 |
| 1 | B | 294 | LYS | CA-CB-CG | 9.56 | 134.43 | 113.40 |
| 1 | B | 587 | ASP | CB-CG-OD2 | 9.50 | 126.85 | 118.30 |
| 1 | A | 326 | MET | CG-SD-CE | 9.43 | 115.28 | 100.20 |
| 1 | A | 570 | ARG | NE-CZ-NH1 | 9.42 | 125.01 | 120.30 |
| 1 | B | 402 | SER | O-C-N | 9.37 | 137.69 | 122.70 |
| 1 | A | 812 | GLY | CA-C-O | -9.32 | 103.82 | 120.60 |
| 1 | A | 6 | MET | CG-SD-CE | -9.31 | 85.30 | 100.20 |
| 1 | A | 63 | LEU | CB-CG-CD1 | -9.30 | 95.18 | 111.00 |
| 1 | B | 208 | THR | CA-CB-CG2 | -9.30 | 99.39 | 112.40 |
| 1 | B | 449 | LEU | CB-CG-CD2 | 9.25 | 126.73 | 111.00 |
| 1 | B | 308 | ASP | CB-CG-OD2 | 9.25 | 126.63 | 118.30 |
| 1 | A | 682 | ASP | CB-CG-OD2 | 9.24 | 126.62 | 118.30 |
| 1 | B | 330 | ASP | CB-CG-OD1 | -9.24 | 109.98 | 118.30 |
| 1 | A | 185 | TYR | CD1-CE1-CZ | -9.23 | 111.49 | 119.80 |
| 1 | B | 315 | LEU | CB-CG-CD2 | 9.21 | 126.66 | 111.00 |
| 1 | A | 258 | LEU | CB-CG-CD1 | 9.17 | 126.59 | 111.00 |
| 1 | B | 344 | THR | OG1-CB-CG2 | -9.17 | 88.92 | 110.00 |
| 1 | A | 742 | ALA | N-CA-C | -9.16 | 86.27 | 111.00 |
| 1 | B | 647 | VAL | CG1-CB-CG2 | -9.15 | 96.26 | 110.90 |
| 1 | B | 469 | LEU | CB-CA-C | 9.12 | 127.53 | 110.20 |
| 1 | A | 216 | ASP | CB-CG-OD1 | 9.12 | 126.51 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 395 | ASP | CB-CG-OD2 | 9.11 | 126.50 | 118.30 |
| 1 | A | 367 | ARG | NE-CZ-NH1 | 9.08 | 124.84 | 120.30 |
| 1 | A | 803 | TYR | CA-C-O | 9.07 | 139.16 | 120.10 |
| 1 | B | 630 | ARG | NE-CZ-NH1 | -9.05 | 115.77 | 120.30 |
| 1 | B | 398 | ASP | O-C-N | -9.04 | 108.24 | 122.70 |
| 1 | B | 631 | MET | CA-CB-CG | 9.01 | 128.61 | 113.30 |
| 1 | B | 155 | ASP | CB-CG-OD1 | -9.00 | 110.20 | 118.30 |
| 1 | A | 233 | GLU | OE1-CD-OE2 | -8.82 | 112.71 | 123.30 |
| 1 | A | 362 | GLU | OE1-CD-OE2 | 8.81 | 133.88 | 123.30 |
| 1 | B | 181 | LEU | CB-CG-CD2 | -8.80 | 96.05 | 111.00 |
| 1 | A | 745 | LEU | CB-CG-CD2 | 8.79 | 125.95 | 111.00 |
| 1 | A | 36 | ARG | NE-CZ-NH1 | 8.77 | 124.69 | 120.30 |
| 1 | A | 18 | LEU | CB-CG-CD1 | 8.73 | 125.83 | 111.00 |
| 1 | B | 714 | ASN | CA-C-O | 8.72 | 138.41 | 120.10 |
| 1 | B | 433 | PHE | N-CA-CB | -8.71 | 94.93 | 110.60 |
| 1 | A | 665 | VAL | CA-CB-CG2 | -8.70 | 97.85 | 110.90 |
| 1 | B | 400 | TYR | N-CA-C | 8.70 | 134.49 | 111.00 |
| 1 | A | 682 | ASP | CB-CG-OD1 | -8.69 | 110.48 | 118.30 |
| 1 | B | 792 | LEU | CA-CB-CG | -8.68 | 95.35 | 115.30 |
| 1 | A | 591 | ASN | N-CA-C | -8.64 | 87.66 | 111.00 |
| 1 | A | 89 | VAL | CA-CB-CG1 | 8.61 | 123.81 | 110.90 |
| 1 | B | 697 | LEU | CB-CA-C | 8.59 | 126.52 | 110.20 |
| 1 | B | 291 | VAL | CG1-CB-CG2 | 8.56 | 124.60 | 110.90 |
| 1 | B | 601 | ILE | CG1-CB-CG2 | -8.54 | 92.62 | 111.40 |
| 1 | B | 331 | PHE | CB-CA-C | -8.52 | 93.36 | 110.40 |
| 1 | B | 485 | VAL | CA-CB-CG2 | -8.50 | 98.16 | 110.90 |
| 1 | A | 268 | ASP | CB-CG-OD2 | 8.46 | 125.91 | 118.30 |
| 1 | B | 430 | THR | OG1-CB-CG2 | -8.45 | 90.56 | 110.00 |
| 1 | B | 436 | TYR | CZ-CE2-CD2 | 8.44 | 127.39 | 119.80 |
| 1 | A | 605 | ARG | NE-CZ-NH2 | -8.43 | 116.08 | 120.30 |
| 1 | B | 682 | ASP | CB-CG-OD2 | 8.41 | 125.87 | 118.30 |
| 1 | A | 303 | GLU | CB-CG-CD | -8.40 | 91.53 | 114.20 |
| 1 | B | 331 | PHE | CB-CG-CD2 | -8.39 | 114.92 | 120.80 |
| 1 | A | 58 | LEU | CB-CG-CD2 | -8.38 | 96.76 | 111.00 |
| 1 | B | 629 | MET | CG-SD-CE | 8.38 | 113.60 | 100.20 |
| 1 | A | 447 | VAL | CB-CA-C | -8.37 | 95.49 | 111.40 |
| 1 | B | 583 | VAL | N-CA-C | -8.36 | 88.42 | 111.00 |
| 1 | A | 175 | GLU | CG-CD-OE2 | 8.35 | 135.01 | 118.30 |
| 1 | B | 436 | TYR | CB-CG-CD2 | -8.34 | 116.00 | 121.00 |
| 1 | B | 651 | ARG | NE-CZ-NH1 | 8.34 | 124.47 | 120.30 |
| 1 | A | 670 | ARG | NE-CZ-NH1 | -8.33 | 116.14 | 120.30 |
| 1 | A | 306 | LYS | CA-CB-CG | -8.32 | 95.08 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 240 | CYS | CA-CB-SG | -8.32 | 99.02 | 114.00 |
| 1 | A | 475 | ARG | NE-CZ-NH2 | -8.31 | 116.14 | 120.30 |
| 1 | B | 858 | LEU | N-CA-C | 8.28 | 133.35 | 111.00 |
| 1 | B | 724 | ARG | NE-CZ-NH2 | 8.27 | 124.43 | 120.30 |
| 1 | A | 319 | MET | C-N-CA | -8.26 | 101.04 | 121.70 |
| 1 | A | 547 | ASP | CB-CG-OD2 | 8.26 | 125.73 | 118.30 |
| 1 | B | 860 | ARG | NE-CZ-NH2 | -8.22 | 116.19 | 120.30 |
| 1 | B | 398 | ASP | N-CA-C | 8.22 | 133.19 | 111.00 |
| 1 | B | 641 | PRO | N-CD-CG | -8.20 | 90.90 | 103.20 |
| 1 | B | 319 | MET | CG-SD-CE | 8.18 | 113.29 | 100.20 |
| 1 | A | 354 | ARG | NE-CZ-NH1 | -8.17 | 116.22 | 120.30 |
| 1 | A | 442 | LEU | CA-CB-CG | 8.16 | 134.06 | 115.30 |
| 1 | B | 830 | LEU | CB-CG-CD1 | -8.15 | 97.14 | 111.00 |
| 1 | B | 32 | TYR | CB-CG-CD2 | 8.13 | 125.88 | 121.00 |
| 1 | A | 237 | LEU | CB-CG-CD1 | -8.10 | 97.23 | 111.00 |
| 1 | A | 427 | ASP | CB-CG-OD2 | 8.10 | 125.59 | 118.30 |
| 1 | B | 426 | ARG | NE-CZ-NH1 | -8.09 | 116.25 | 120.30 |
| 1 | B | 11 | ASP | CB-CG-OD2 | 8.09 | 125.58 | 118.30 |
| 1 | B | 644 | LEU | CA-CB-CG | -8.04 | 96.80 | 115.30 |
| 1 | B | 521 | LEU | CB-CG-CD1 | -8.03 | 97.35 | 111.00 |
| 1 | B | 398 | ASP | CA-C-O | -7.95 | 103.40 | 120.10 |
| 1 | A | 350 | SER | N-CA-CB | 7.95 | 122.42 | 110.50 |
| 1 | A | 585 | LEU | CB-CG-CD1 | -7.94 | 97.50 | 111.00 |
| 1 | B | 256 | LYS | CD-CE-NZ | 7.92 | 129.91 | 111.70 |
| 1 | A | 319 | MET | CG-SD-CE | 7.92 | 112.86 | 100.20 |
| 1 | A | 462 | GLN | O-C-N | -7.89 | 110.07 | 122.70 |
| 1 | B | 90 | ASP | CB-CA-C | 7.88 | 126.17 | 110.40 |
| 1 | A | 303 | GLU | N-CA-C | 7.85 | 132.20 | 111.00 |
| 1 | A | 702 | LEU | CA-C-O | -7.85 | 103.61 | 120.10 |
| 1 | A | 7 | LYS | CB-CG-CD | 7.84 | 131.98 | 111.60 |
| 1 | B | 619 | ASP | CB-CG-OD2 | 7.83 | 125.35 | 118.30 |
| 1 | A | 733 | LEU | CB-CG-CD2 | -7.81 | 97.72 | 111.00 |
| 1 | A | 350 | SER | O-C-N | 7.81 | 135.19 | 122.70 |
| 1 | B | 96 | ASP | CB-CG-OD2 | 7.80 | 125.32 | 118.30 |
| 1 | A | 159 | PRO | O-C-N | 7.78 | 135.15 | 122.70 |
| 1 | B | 440 | ARG | CB-CA-C | -7.77 | 94.87 | 110.40 |
| 1 | B | 436 | TYR | CE1-CZ-OH | 7.72 | 140.94 | 120.10 |
| 1 | B | 298 | SER | CA-CB-OG | -7.70 | 90.40 | 111.20 |
| 1 | B | 17 | GLY | N-CA-C | 7.69 | 132.32 | 113.10 |
| 1 | A | 772 | MET | CG-SD-CE | 7.69 | 112.50 | 100.20 |
| 1 | A | 803 | TYR | OH-CZ-CE2 | 7.68 | 140.85 | 120.10 |
| 1 | B | 44 | ALA | N-CA-CB | -7.65 | 99.39 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 104 | ASP | CB-CG-OD1 | -7.64 | 111.42 | 118.30 |
| 1 | A | 616 | PHE | CB-CG-CD1 | 7.61 | 126.13 | 120.80 |
| 1 | B | 36 | ARG | NH1-CZ-NH2 | -7.59 | 111.05 | 119.40 |
| 1 | B | 346 | ASP | CB-CG-OD2 | -7.59 | 111.47 | 118.30 |
| 1 | A | 809 | ASP | OD1-CG-OD2 | -7.58 | 108.89 | 123.30 |
| 1 | B | 675 | PHE | CB-CG-CD2 | 7.58 | 126.11 | 120.80 |
| 1 | B | 776 | MET | CB-CG-SD | -7.58 | 89.67 | 112.40 |
| 1 | A | 585 | LEU | CB-CG-CD2 | 7.57 | 123.87 | 111.00 |
| 1 | B | 93 | THR | CA-CB-CG2 | 7.56 | 122.99 | 112.40 |
| 1 | B | 161 | LYS | CD-CE-NZ | 7.54 | 129.05 | 111.70 |
| 1 | A | 389 | ILE | CB-CA-C | -7.54 | 96.52 | 111.60 |
| 1 | A | 499 | LEU | CB-CA-C | -7.54 | 95.87 | 110.20 |
| 1 | B | 882 | ASN | N-CA-C | -7.54 | 90.66 | 111.00 |
| 1 | A | 500 | LEU | CB-CG-CD2 | 7.53 | 123.79 | 111.00 |
| 1 | B | 388 | LYS | CB-CA-C | -7.52 | 95.35 | 110.40 |
| 1 | B | 69 | LYS | CD-CE-NZ | 7.52 | 129.00 | 111.70 |
| 1 | B | 830 | LEU | CA-CB-CG | 7.51 | 132.58 | 115.30 |
| 1 | B | 657 | LEU | CA-CB-CG | 7.50 | 132.56 | 115.30 |
| 1 | B | 16 | GLU | OE1-CD-OE2 | -7.50 | 114.31 | 123.30 |
| 1 | B | 108 | LEU | CA-CB-CG | -7.49 | 98.07 | 115.30 |
| 1 | A | 607 | ARG | NE-CZ-NH1 | -7.49 | 116.56 | 120.30 |
| 1 | A | 514 | ASP | CB-CG-OD2 | 7.48 | 125.03 | 118.30 |
| 1 | A | 340 | ILE | CB-CG1-CD1 | 7.47 | 134.82 | 113.90 |
| 1 | A | 872 | ASP | CB-CG-OD1 | -7.46 | 111.58 | 118.30 |
| 1 | B | 263 | ALA | CB-CA-C | -7.46 | 98.91 | 110.10 |
| 1 | A | 278 | ARG | CB-CA-C | -7.46 | 95.49 | 110.40 |
| 1 | A | 338 | LEU | CB-CG-CD1 | 7.45 | 123.66 | 111.00 |
| 1 | A | 350 | SER | N-CA-C | -7.43 | 90.95 | 111.00 |
| 1 | A | 175 | GLU | CA-CB-CG | 7.41 | 129.70 | 113.40 |
| 1 | A | 216 | ASP | OD1-CG-OD2 | -7.41 | 109.23 | 123.30 |
| 1 | A | 833 | HIS | N-CA-C | 7.40 | 130.97 | 111.00 |
| 1 | B | 651 | ARG | NE-CZ-NH2 | -7.39 | 116.60 | 120.30 |
| 1 | A | 151 | ASP | CB-CG-OD1 | 7.39 | 124.95 | 118.30 |
| 1 | A | 628 | GLU | CB-CG-CD | -7.39 | 94.24 | 114.20 |
| 1 | B | 121 | LEU | CB-CG-CD2 | -7.38 | 98.46 | 111.00 |
| 1 | A | 751 | LYS | CA-C-O | -7.37 | 104.63 | 120.10 |
| 1 | A | 620 | LYS | CB-CA-C | 7.37 | 125.13 | 110.40 |
| 1 | B | 862 | ASP | N-CA-C | -7.36 | 91.12 | 111.00 |
| 1 | A | 670 | ARG | CD-NE-CZ | -7.35 | 113.31 | 123.60 |
| 1 | A | 803 | TYR | CB-CG-CD2 | 7.34 | 125.41 | 121.00 |
| 1 | B | 151 | ASP | OD1-CG-OD2 | -7.34 | 109.35 | 123.30 |
| 1 | B | 267 | THR | O-C-N | -7.34 | 110.96 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 802 | ILE | CA-C-O | -7.34 | 104.69 | 120.10 |
| 1 | B | 65 | PRO | N-CD-CG | 7.33 | 114.20 | 103.20 |
| 1 | B | 0 | GLU | CA-C-O | -7.33 | 104.70 | 120.10 |
| 1 | A | 803 | TYR | CB-CG-CD1 | -7.33 | 116.60 | 121.00 |
| 1 | A | 165 | LEU | CB-CA-C | 7.29 | 124.05 | 110.20 |
| 1 | B | 92 | ALA | N-CA-CB | 7.29 | 120.31 | 110.10 |
| 1 | B | 233 | GLU | OE1-CD-OE2 | 7.29 | 132.05 | 123.30 |
| 1 | B | 348 | LEU | CB-CG-CD1 | 7.29 | 123.39 | 111.00 |
| 1 | B | 585 | LEU | CB-CG-CD1 | 7.27 | 123.36 | 111.00 |
| 1 | A | 12 | ARG | NE-CZ-NH1 | 7.27 | 123.94 | 120.30 |
| 1 | A | 759 | LEU | CB-CG-CD1 | -7.25 | 98.67 | 111.00 |
| 1 | B | 426 | ARG | NE-CZ-NH2 | 7.25 | 123.92 | 120.30 |
| 1 | A | 158 | LEU | CA-CB-CG | -7.24 | 98.66 | 115.30 |
| 1 | B | 139 | PHE | CB-CG-CD1 | -7.24 | 115.73 | 120.80 |
| 1 | A | 310 | TYR | CE1-CZ-OH | -7.23 | 100.57 | 120.10 |
| 1 | B | 391 | LEU | CB-CG-CD1 | 7.18 | 123.21 | 111.00 |
| 1 | A | 455 | LEU | CB-CG-CD2 | 7.18 | 123.21 | 111.00 |
| 1 | A | 440 | ARG | NE-CZ-NH1 | -7.15 | 116.72 | 120.30 |
| 1 | A | 758 | ASP | CB-CG-OD1 | 7.13 | 124.72 | 118.30 |
| 1 | B | 28 | LEU | CB-CG-CD1 | 7.13 | 123.13 | 111.00 |
| 1 | B | 674 | LEU | CB-CG-CD1 | 7.13 | 123.12 | 111.00 |
| 1 | A | 218 | GLN | C-N-CA | 7.12 | 139.51 | 121.70 |
| 1 | B | 155 | ASP | CB-CG-OD2 | 7.11 | 124.70 | 118.30 |
| 1 | B | 378 | PRO | N-CD-CG | -7.11 | 92.53 | 103.20 |
| 1 | B | 151 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | A | 861 | LEU | CB-CG-CD2 | -7.09 | 98.94 | 111.00 |
| 1 | B | 609 | TYR | N-CA-CB | 7.08 | 123.35 | 110.60 |
| 1 | B | 83 | SER | C-N-CA | -7.08 | 104.00 | 121.70 |
| 1 | B | 538 | THR | CB-CA-C | -7.07 | 92.51 | 111.60 |
| 1 | B | 746 | MET | CG-SD-CE | 7.05 | 111.48 | 100.20 |
| 1 | A | 691 | LEU | CB-CG-CD1 | 7.04 | 122.97 | 111.00 |
| 1 | A | 40 | LEU | CB-CG-CD2 | 7.04 | 122.96 | 111.00 |
| 1 | B | 278 | ARG | NE-CZ-NH2 | 7.04 | 123.82 | 120.30 |
| 1 | A | 860 | ARG | NE-CZ-NH2 | 7.03 | 123.81 | 120.30 |
| 1 | B | 89 | VAL | CA-CB-CG1 | 7.02 | 121.43 | 110.90 |
| 1 | B | 594 | LEU | CB-CG-CD2 | 7.01 | 122.91 | 111.00 |
| 1 | A | 351 | ARG | NE-CZ-NH2 | 7.01 | 123.80 | 120.30 |
| 1 | B | 340 | ILE | CG1-CB-CG2 | -7.00 | 96.00 | 111.40 |
| 1 | B | 164 | LYS | CD-CE-NZ | -7.00 | 95.61 | 111.70 |
| 1 | B | 98 | CYS | CA-CB-SG | 6.99 | 126.59 | 114.00 |
| 1 | B | 617 | ASP | CB-CA-C | -6.98 | 96.43 | 110.40 |
| 1 | B | 281 | LEU | CB-CG-CD2 | 6.97 | 122.85 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 825 | ALA | N-CA-CB | -6.97 | 100.34 | 110.10 |
| 1 | A | 702 | LEU | CA-CB-CG | 6.95 | 131.29 | 115.30 |
| 1 | A | 413 | LEU | CB-CG-CD2 | -6.95 | 99.19 | 111.00 |
| 1 | A | 655 | ASP | CB-CG-OD2 | 6.94 | 124.55 | 118.30 |
| 1 | A | 343 | LEU | CB-CG-CD2 | 6.94 | 122.79 | 111.00 |
| 1 | B | 449 | LEU | O-C-N | 6.93 | 133.79 | 122.70 |
| 1 | A | 601 | ILE | O-C-N | 6.93 | 133.78 | 122.70 |
| 1 | B | 461 | ALA | N-CA-CB | -6.92 | 100.42 | 110.10 |
| 1 | A | 631 | MET | CG-SD-CE | -6.92 | 89.13 | 100.20 |
| 1 | B | 199 | CYS | CA-CB-SG | -6.91 | 101.56 | 114.00 |
| 1 | A | 570 | ARG | NH1-CZ-NH2 | -6.91 | 111.80 | 119.40 |
| 1 | B | 389 | ILE | N-CA-C | -6.91 | 92.35 | 111.00 |
| 1 | B | 418 | ARG | NE-CZ-NH1 | -6.90 | 116.85 | 120.30 |
| 1 | A | 789 | PHE | N-CA-C | -6.90 | 92.38 | 111.00 |
| 1 | A | 237 | LEU | CA-CB-CG | -6.89 | 99.45 | 115.30 |
| 1 | B | 162 | ASP | CB-CG-OD2 | 6.88 | 124.50 | 118.30 |
| 1 | B | 159 | PRO | N-CD-CG | -6.88 | 92.88 | 103.20 |
| 1 | B | 200 | THR | OG1-CB-CG2 | -6.87 | 94.19 | 110.00 |
| 1 | A | 756 | HIS | N-CA-C | -6.87 | 92.45 | 111.00 |
| 1 | B | 396 | ASP | C-N-CA | 6.87 | 138.87 | 121.70 |
| 1 | B | 476 | ILE | CG1-CB-CG2 | -6.87 | 96.29 | 111.40 |
| 1 | B | 296 | PRO | N-CD-CG | -6.87 | 92.90 | 103.20 |
| 1 | B | 806 | PHE | CB-CG-CD2 | 6.87 | 125.61 | 120.80 |
| 1 | B | 808 | THR | O-C-N | -6.86 | 111.72 | 122.70 |
| 1 | A | 429 | GLU | CB-CA-C | 6.86 | 124.12 | 110.40 |
| 1 | A | 102 | LEU | CB-CG-CD2 | -6.86 | 99.34 | 111.00 |
| 1 | A | 358 | THR | OG1-CB-CG2 | -6.85 | 94.24 | 110.00 |
| 1 | A | 786 | PHE | N-CA-C | -6.85 | 92.50 | 111.00 |
| 1 | B | 580 | ARG | NE-CZ-NH2 | -6.85 | 116.88 | 120.30 |
| 1 | A | 768 | THR | N-CA-CB | -6.85 | 97.28 | 110.30 |
| 1 | A | 521 | LEU | CB-CG-CD1 | 6.85 | 122.64 | 111.00 |
| 1 | B | 811 | SER | CB-CA-C | 6.84 | 123.10 | 110.10 |
| 1 | A | 94 | ARG | NE-CZ-NH2 | -6.83 | 116.88 | 120.30 |
| 1 | B | 466 | PHE | CB-CA-C | -6.83 | 96.73 | 110.40 |
| 1 | A | 27 | TYR | CD1-CE1-CZ | -6.83 | 113.65 | 119.80 |
| 1 | A | 430 | THR | CA-CB-CG2 | 6.82 | 121.95 | 112.40 |
| 1 | B | 454 | PHE | CG-CD2-CE2 | 6.82 | 128.31 | 120.80 |
| 1 | A | 89 | VAL | CG1-CB-CG2 | -6.81 | 100.00 | 110.90 |
| 1 | B | 414 | MET | CG-SD-CE | -6.81 | 89.30 | 100.20 |
| 1 | A | 810 | ARG | NH1-CZ-NH2 | -6.81 | 111.91 | 119.40 |
| 1 | A | 324 | PHE | CB-CG-CD2 | -6.80 | 116.04 | 120.80 |
| 1 | B | 274 | TYR | CG-CD2-CE2 | 6.80 | 126.74 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 447 | VAL | CA-CB-CG1 | 6.79 | 121.09 | 110.90 |
| 1 | A | 356 | TRP | N-CA-C | -6.79 | 92.66 | 111.00 |
| 1 | A | 355 | ASN | N-CA-CB | -6.79 | 98.38 | 110.60 |
| 1 | A | 550 | ILE | C-N-CA | 6.78 | 138.66 | 121.70 |
| 1 | B | 866 | ARG | CA-CB-CG | 6.78 | 128.32 | 113.40 |
| 1 | B | 471 | GLU | OE1-CD-OE2 | -6.78 | 115.16 | 123.30 |
| 1 | A | 339 | GLU | N-CA-CB | -6.76 | 98.44 | 110.60 |
| 1 | A | 15 | ALA | CB-CA-C | -6.75 | 99.97 | 110.10 |
| 1 | A | 756 | HIS | CB-CA-C | 6.75 | 123.90 | 110.40 |
| 1 | A | 108 | LEU | CB-CG-CD2 | -6.74 | 99.53 | 111.00 |
| 1 | B | 63 | LEU | CB-CG-CD1 | 6.73 | 122.44 | 111.00 |
| 1 | A | 628 | GLU | N-CA-CB | -6.72 | 98.50 | 110.60 |
| 1 | A | 492 | PRO | N-CD-CG | -6.72 | 93.12 | 103.20 |
| 1 | B | 308 | ASP | N-CA-CB | -6.72 | 98.51 | 110.60 |
| 1 | A | 448 | HIS | N-CA-CB | 6.71 | 122.67 | 110.60 |
| 1 | B | 861 | LEU | CA-CB-CG | -6.70 | 99.88 | 115.30 |
| 1 | A | 2 | ALA | N-CA-C | -6.70 | 92.91 | 111.00 |
| 1 | A | 234 | ARG | NE-CZ-NH2 | 6.70 | 123.65 | 120.30 |
| 1 | A | 889 | LEU | CB-CG-CD2 | -6.70 | 99.61 | 111.00 |
| 1 | B | 233 | GLU | CG-CD-OE2 | -6.70 | 104.91 | 118.30 |
| 1 | B | 93 | THR | OG1-CB-CG2 | -6.69 | 94.62 | 110.00 |
| 1 | A | 96 | ASP | N-CA-C | -6.68 | 92.97 | 111.00 |
| 1 | B | 284 | MET | CG-SD-CE | 6.66 | 110.86 | 100.20 |
| 1 | B | 672 | GLU | OE1-CD-OE2 | 6.66 | 131.29 | 123.30 |
| 1 | A | 463 | SER | CB-CA-C | -6.66 | 97.45 | 110.10 |
| 1 | B | 139 | PHE | CG-CD1-CE1 | 6.66 | 128.12 | 120.80 |
| 1 | B | 290 | GLU | OE1-CD-OE2 | 6.65 | 131.28 | 123.30 |
| 1 | A | 303 | GLU | CG-CD-OE2 | -6.64 | 105.01 | 118.30 |
| 1 | A | 492 | PRO | CA-C-N | -6.64 | 102.59 | 117.20 |
| 1 | B | 670 | ARG | NE-CZ-NH2 | -6.64 | 116.98 | 120.30 |
| 1 | A | 634 | GLU | CG-CD-OE2 | 6.64 | 131.58 | 118.30 |
| 1 | B | 887 | LEU | CA-CB-CG | -6.63 | 100.05 | 115.30 |
| 1 | A | 104 | ASP | CB-CG-OD2 | 6.62 | 124.26 | 118.30 |
| 1 | B | 432 | GLY | O-C-N | 6.62 | 133.29 | 122.70 |
| 1 | A | 216 | ASP | CB-CG-OD2 | 6.62 | 124.26 | 118.30 |
| 1 | B | 724 | ARG | CD-NE-CZ | 6.62 | 132.86 | 123.60 |
| 1 | A | 522 | PRO | N-CA-C | 6.62 | 129.30 | 112.10 |
| 1 | A | 635 | ALA | CB-CA-C | -6.62 | 100.18 | 110.10 |
| 1 | A | 240 | CYS | CA-CB-SG | -6.61 | 102.11 | 114.00 |
| 1 | A | 831 | ASN | N-CA-CB | 6.59 | 122.46 | 110.60 |
| 1 | B | 62 | GLU | OE1-CD-OE2 | 6.59 | 131.21 | 123.30 |
| 1 | A | 630 | ARG | NE-CZ-NH2 | 6.58 | 123.59 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 830 | LEU | CB-CG-CD1 | -6.58 | 99.81 | 111.00 |
| 1 | A | 317 | VAL | CA-CB-CG2 | 6.58 | 120.76 | 110.90 |
| 1 | A | 232 | LEU | CA-CB-CG | 6.56 | 130.38 | 115.30 |
| 1 | A | 477 | ARG | NE-CZ-NH1 | -6.55 | 117.02 | 120.30 |
| 1 | B | 598 | GLU | CA-CB-CG | 6.55 | 127.82 | 113.40 |
| 1 | B | 390 | ARG | NE-CZ-NH1 | -6.55 | 117.02 | 120.30 |
| 1 | B | 436 | TYR | OH-CZ-CE2 | -6.54 | 102.44 | 120.10 |
| 1 | A | 612 | ILE | CG1-CB-CG2 | -6.54 | 97.02 | 111.40 |
| 1 | B | 291 | VAL | CB-CA-C | -6.54 | 98.98 | 111.40 |
| 1 | B | 6 | MET | N-CA-CB | 6.53 | 122.36 | 110.60 |
| 1 | B | 472 | VAL | CA-CB-CG1 | -6.53 | 101.11 | 110.90 |
| 1 | B | 396 | ASP | O-C-N | 6.53 | 133.14 | 122.70 |
| 1 | A | 447 | VAL | O-C-N | -6.52 | 112.27 | 122.70 |
| 1 | A | 28 | LEU | CB-CG-CD1 | -6.52 | 99.92 | 111.00 |
| 1 | A | 136 | ALA | N-CA-C | 6.52 | 128.59 | 111.00 |
| 1 | B | 477 | ARG | NE-CZ-NH2 | 6.51 | 123.56 | 120.30 |
| 1 | A | 312 | ARG | N-CA-C | -6.50 | 93.44 | 111.00 |
| 1 | B | 483 | TYR | CG-CD1-CE1 | 6.50 | 126.50 | 121.30 |
| 1 | A | 505 | GLU | CG-CD-OE1 | 6.50 | 131.30 | 118.30 |
| 1 | B | 133 | GLU | OE1-CD-OE2 | 6.50 | 131.09 | 123.30 |
| 1 | A | 477 | ARG | CD-NE-CZ | 6.49 | 132.69 | 123.60 |
| 1 | A | 319 | MET | N-CA-C | 6.49 | 128.52 | 111.00 |
| 1 | B | 185 | TYR | CB-CA-C | -6.48 | 97.43 | 110.40 |
| 1 | B | 121 | LEU | CA-CB-CG | 6.48 | 130.19 | 115.30 |
| 1 | A | 269 | ALA | O-C-N | 6.47 | 133.06 | 122.70 |
| 1 | A | 513 | LEU | CB-CG-CD2 | 6.47 | 122.01 | 111.00 |
| 1 | B | 628 | GLU | OE1-CD-OE2 | 6.47 | 131.07 | 123.30 |
| 1 | A | 205 | GLU | CA-CB-CG | 6.47 | 127.64 | 113.40 |
| 1 | B | 90 | ASP | CB-CG-OD2 | 6.47 | 124.12 | 118.30 |
| 1 | A | 820 | PRO | N-CD-CG | -6.46 | 93.50 | 103.20 |
| 1 | B | 200 | THR | CA-CB-CG2 | -6.46 | 103.35 | 112.40 |
| 1 | B | 890 | THR | OG1-CB-CG2 | -6.46 | 95.14 | 110.00 |
| 1 | A | 710 | MET | C-N-CA | 6.46 | 137.86 | 121.70 |
| 1 | B | 497 | ASP | CB-CG-OD2 | -6.46 | 112.49 | 118.30 |
| 1 | B | 321 | ASP | CB-CG-OD2 | 6.45 | 124.11 | 118.30 |
| 1 | A | 264 | TYR | CB-CG-CD1 | 6.45 | 124.87 | 121.00 |
| 1 | A | 266 | VAL | N-CA-C | -6.45 | 93.58 | 111.00 |
| 1 | B | 61 | LYS | CA-CB-CG | 6.45 | 127.59 | 113.40 |
| 1 | A | 672 | GLU | OE1-CD-OE2 | 6.45 | 131.04 | 123.30 |
| 1 | A | 404 | GLU | OE1-CD-OE2 | 6.44 | 131.03 | 123.30 |
| 1 | A | 278 | ARG | NE-CZ-NH2 | 6.44 | 123.52 | 120.30 |
| 1 | B | 389 | ILE | CB-CA-C | -6.44 | 98.72 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 215 | TYR | CG-CD1-CE1 | -6.43 | 116.15 | 121.30 |
| 1 | B | 364 | THR | CA-CB-CG2 | -6.43 | 103.40 | 112.40 |
| 1 | A | 242 | ILE | CG1-CB-CG2 | -6.43 | 97.26 | 111.40 |
| 1 | A | 460 | ARG | NH1-CZ-NH2 | 6.43 | 126.47 | 119.40 |
| 1 | B | 315 | LEU | CB-CG-CD1 | 6.41 | 121.90 | 111.00 |
| 1 | B | 193 | GLU | CG-CD-OE1 | -6.41 | 105.48 | 118.30 |
| 1 | A | 486 | VAL | O-C-N | 6.41 | 133.27 | 121.10 |
| 1 | A | 889 | LEU | O-C-N | -6.41 | 112.45 | 122.70 |
| 1 | A | 455 | LEU | CA-CB-CG | -6.40 | 100.57 | 115.30 |
| 1 | B | 18 | LEU | CB-CG-CD1 | -6.40 | 100.11 | 111.00 |
| 1 | A | 645 | HIS | N-CA-CB | 6.40 | 122.12 | 110.60 |
| 1 | B | 452 | ASP | CB-CG-OD1 | 6.39 | 124.05 | 118.30 |
| 1 | A | 76 | LYS | CD-CE-NZ | 6.39 | 126.39 | 111.70 |
| 1 | A | 193 | GLU | CB-CA-C | -6.38 | 97.63 | 110.40 |
| 1 | A | 434 | ALA | N-CA-CB | -6.38 | 101.17 | 110.10 |
| 1 | B | 242 | ILE | CG1-CB-CG2 | -6.38 | 97.37 | 111.40 |
| 1 | A | 128 | GLY | CA-C-O | -6.38 | 109.12 | 120.60 |
| 1 | A | 243 | ASN | N-CA-C | 6.37 | 128.21 | 111.00 |
| 1 | B | 23 | ARG | NE-CZ-NH1 | 6.37 | 123.48 | 120.30 |
| 1 | A | 233 | GLU | CA-CB-CG | 6.37 | 127.41 | 113.40 |
| 1 | B | 507 | LYS | CD-CE-NZ | 6.36 | 126.33 | 111.70 |
| 1 | B | 658 | ILE | O-C-N | 6.36 | 132.88 | 122.70 |
| 1 | B | 312 | ARG | CD-NE-CZ | 6.36 | 132.50 | 123.60 |
| 1 | A | 759 | LEU | C-N-CA | 6.36 | 137.59 | 121.70 |
| 1 | A | 570 | ARG | N-CA-C | -6.34 | 93.89 | 111.00 |
| 1 | B | 470 | ARG | N-CA-CB | -6.33 | 99.20 | 110.60 |
| 1 | B | 825 | ALA | CA-C-N | -6.33 | 103.28 | 117.20 |
| 1 | B | 477 | ARG | NE-CZ-NH1 | -6.31 | 117.14 | 120.30 |
| 1 | A | 297 | TRP | CB-CA-C | 6.31 | 123.02 | 110.40 |
| 1 | A | 324 | PHE | N-CA-CB | 6.30 | 121.94 | 110.60 |
| 1 | B | 131 | PHE | CZ-CE2-CD2 | -6.30 | 112.55 | 120.10 |
| 1 | B | 654 | ASP | CA-C-N | -6.29 | 103.36 | 117.20 |
| 1 | A | 640 | LEU | CB-CG-CD1 | -6.29 | 100.31 | 111.00 |
| 1 | B | 362 | GLU | CA-CB-CG | -6.28 | 99.59 | 113.40 |
| 1 | A | 110 | ALA | CB-CA-C | -6.27 | 100.69 | 110.10 |
| 1 | B | 336 | THR | OG1-CB-CG2 | -6.27 | 95.58 | 110.00 |
| 1 | B | 135 | TYR | CZ-CE2-CD2 | 6.26 | 125.43 | 119.80 |
| 1 | B | 451 | ARG | CA-CB-CG | 6.25 | 127.16 | 113.40 |
| 1 | B | 166 | VAL | CA-CB-CG2 | 6.25 | 120.27 | 110.90 |
| 1 | A | 588 | ARG | CA-C-O | 6.24 | 133.21 | 120.10 |
| 1 | A | 330 | ASP | CB-CG-OD2 | 6.24 | 123.92 | 118.30 |
| 1 | A | 486 | VAL | CA-C-O | -6.24 | 107.00 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 119 | THR | N-CA-CB | -6.23 | 98.46 | 110.30 |
| 1 | A | 591 | ASN | CB-CA-C | 6.23 | 122.86 | 110.40 |
| 1 | A | 609 | TYR | CG-CD2-CE2 | 6.23 | 126.29 | 121.30 |
| 1 | A | 387 | PHE | CG-CD1-CE1 | -6.22 | 113.95 | 120.80 |
| 1 | A | 637 | GLY | C-N-CA | -6.22 | 106.16 | 121.70 |
| 1 | A | 570 | ARG | CA-CB-CG | 6.21 | 127.07 | 113.40 |
| 1 | A | 617 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | B | 13 | GLU | N-CA-CB | 6.20 | 121.76 | 110.60 |
| 1 | A | 499 | LEU | CB-CG-CD2 | -6.19 | 100.48 | 111.00 |
| 1 | A | 587 | ASP | CB-CG-OD1 | -6.19 | 112.73 | 118.30 |
| 1 | A | 291 | VAL | CG1-CB-CG2 | 6.19 | 120.80 | 110.90 |
| 1 | B | 729 | LEU | CB-CA-C | 6.18 | 121.94 | 110.20 |
| 1 | B | 396 | ASP | CB-CG-OD1 | -6.17 | 112.74 | 118.30 |
| 1 | B | 681 | LEU | N-CA-C | 6.17 | 127.67 | 111.00 |
| 1 | A | 500 | LEU | N-CA-C | -6.17 | 94.34 | 111.00 |
| 1 | B | 151 | ASP | CB-CG-OD2 | 6.16 | 123.85 | 118.30 |
| 1 | B | 23 | ARG | CG-CD-NE | -6.15 | 98.88 | 111.80 |
| 1 | A | 112 | ALA | CB-CA-C | -6.14 | 100.89 | 110.10 |
| 1 | A | 114 | LEU | CA-CB-CG | 6.14 | 129.43 | 115.30 |
| 1 | B | 323 | GLU | OE1-CD-OE2 | 6.14 | 130.67 | 123.30 |
| 1 | A | 808 | THR | N-CA-CB | 6.14 | 121.97 | 110.30 |
| 1 | B | 32 | TYR | CG-CD2-CE2 | 6.13 | 126.21 | 121.30 |
| 1 | A | 616 | PHE | CZ-CE2-CD2 | 6.12 | 127.45 | 120.10 |
| 1 | B | 89 | VAL | CB-CA-C | -6.12 | 99.78 | 111.40 |
| 1 | B | 123 | ARG | CD-NE-CZ | -6.12 | 115.04 | 123.60 |
| 1 | B | 147 | GLY | CA-C-O | -6.12 | 109.59 | 120.60 |
| 1 | B | 349 | LYS | N-CA-C | -6.11 | 94.49 | 111.00 |
| 1 | B | 662 | ASP | CB-CG-OD2 | 6.10 | 123.79 | 118.30 |
| 1 | A | 697 | LEU | CA-CB-CG | -6.09 | 101.28 | 115.30 |
| 1 | B | 671 | LEU | CB-CG-CD1 | 6.09 | 121.36 | 111.00 |
| 1 | B | 124 | VAL | CG1-CB-CG2 | -6.09 | 101.15 | 110.90 |
| 1 | B | 323 | GLU | CG-CD-OE2 | -6.09 | 106.13 | 118.30 |
| 1 | A | 96 | ASP | CB-CG-OD2 | 6.08 | 123.78 | 118.30 |
| 1 | A | 100 | GLY | N-CA-C | 6.08 | 128.31 | 113.10 |
| 1 | A | 547 | ASP | CB-CG-OD1 | -6.08 | 112.83 | 118.30 |
| 1 | B | 232 | LEU | CA-CB-CG | 6.08 | 129.29 | 115.30 |
| 1 | A | 390 | ARG | N-CA-CB | -6.08 | 99.66 | 110.60 |
| 1 | A | 627 | TYR | CB-CG-CD1 | 6.08 | 124.65 | 121.00 |
| 1 | B | 277 | GLN | CB-CG-CD | 6.08 | 127.40 | 111.60 |
| 1 | B | 743 | THR | O-C-N | 6.07 | 132.41 | 122.70 |
| 1 | B | 627 | TYR | CG-CD2-CE2 | -6.07 | 116.44 | 121.30 |
| 1 | A | 284 | MET | CA-CB-CG | 6.07 | 123.61 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 114 | LEU | CA-C-O | -6.06 | 107.38 | 120.10 |
| 1 | B | 41 | GLU | CA-CB-CG | 6.05 | 126.72 | 113.40 |
| 1 | A | 780 | THR | OG1-CB-CG2 | -6.05 | 96.09 | 110.00 |
| 1 | B | 700 | SER | CA-C-N | -6.05 | 103.90 | 117.20 |
| 1 | A | 341 | CYS | CA-CB-SG | 6.04 | 124.87 | 114.00 |
| 1 | B | 475 | ARG | NE-CZ-NH2 | 6.04 | 123.32 | 120.30 |
| 1 | A | 310 | TYR | CD1-CG-CD2 | 6.03 | 124.53 | 117.90 |
| 1 | A | 507 | LYS | CD-CE-NZ | 6.02 | 125.55 | 111.70 |
| 1 | B | 221 | PRO | N-CD-CG | -6.02 | 94.18 | 103.20 |
| 1 | B | 297 | TRP | CA-CB-CG | 6.01 | 125.12 | 113.70 |
| 1 | B | 609 | TYR | CZ-CE2-CD2 | 6.01 | 125.21 | 119.80 |
| 1 | B | 490 | PHE | CB-CA-C | -6.00 | 98.39 | 110.40 |
| 1 | B | 76 | LYS | CD-CE-NZ | 6.00 | 125.50 | 111.70 |
| 1 | B | 700 | SER | O-C-N | 6.00 | 132.30 | 122.70 |
| 1 | A | 390 | ARG | NH1-CZ-NH2 | 6.00 | 126.00 | 119.40 |
| 1 | A | 333 | ARG | NE-CZ-NH2 | 5.99 | 123.29 | 120.30 |
| 1 | B | 838 | ILE | CA-C-O | -5.99 | 107.53 | 120.10 |
| 1 | B | 682 | ASP | N-CA-CB | -5.99 | 99.83 | 110.60 |
| 1 | B | 667 | CYS | C-N-CA | -5.98 | 106.74 | 121.70 |
| 1 | A | 202 | GLU | OE1-CD-OE2 | 5.98 | 130.48 | 123.30 |
| 1 | A | 329 | ARG | CB-CA-C | -5.98 | 98.43 | 110.40 |
| 1 | A | 830 | LEU | C-N-CA | -5.98 | 106.75 | 121.70 |
| 1 | B | 404 | GLU | OE1-CD-OE2 | 5.98 | 130.47 | 123.30 |
| 1 | A | 808 | THR | O-C-N | 5.97 | 132.26 | 122.70 |
| 1 | B | 91 | GLY | CA-C-O | -5.97 | 109.85 | 120.60 |
| 1 | A | 892 | TYR | CD1-CE1-CZ | -5.96 | 114.43 | 119.80 |
| 1 | B | 779 | ASP | CB-CG-OD1 | -5.96 | 112.94 | 118.30 |
| 1 | A | 516 | GLN | CB-CA-C | -5.96 | 98.49 | 110.40 |
| 1 | B | 428 | MET | CA-CB-CG | 5.95 | 123.42 | 113.30 |
| 1 | A | 809 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | A | 275 | GLN | O-C-N | -5.95 | 113.09 | 123.20 |
| 1 | A | 792 | LEU | CB-CA-C | -5.95 | 98.91 | 110.20 |
| 1 | A | 312 | ARG | NE-CZ-NH2 | 5.94 | 123.27 | 120.30 |
| 1 | B | 34 | THR | OG1-CB-CG2 | -5.94 | 96.34 | 110.00 |
| 1 | B | 399 | ASP | CB-CG-OD1 | -5.94 | 112.95 | 118.30 |
| 1 | B | 167 | PHE | CG-CD2-CE2 | 5.94 | 127.33 | 120.80 |
| 1 | B | 358 | THR | N-CA-C | 5.94 | 127.03 | 111.00 |
| 1 | A | 582 | MET | CG-SD-CE | -5.94 | 90.70 | 100.20 |
| 1 | B | 825 | ALA | C-N-CA | 5.93 | 136.53 | 121.70 |
| 1 | A | 393 | GLU | OE1-CD-OE2 | -5.93 | 116.18 | 123.30 |
| 1 | A | 876 | THR | N-CA-CB | 5.93 | 121.56 | 110.30 |
| 1 | B | 223 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 206 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | A | 578 | SER | CA-C-N | -5.92 | 104.18 | 117.20 |
| 1 | B | 602 | LEU | CB-CG-CD2 | 5.91 | 121.05 | 111.00 |
| 1 | B | 447 | VAL | O-C-N | -5.91 | 113.25 | 122.70 |
| 1 | A | 268 | ASP | CB-CG-OD1 | -5.91 | 112.98 | 118.30 |
| 1 | B | 402 | SER | N-CA-C | 5.91 | 126.95 | 111.00 |
| 1 | B | 410 | LEU | CB-CG-CD1 | 5.91 | 121.04 | 111.00 |
| 1 | B | 454 | PHE | CZ-CE2-CD2 | -5.90 | 113.02 | 120.10 |
| 1 | A | 328 | PHE | CA-C-N | 5.90 | 130.18 | 117.20 |
| 1 | B | 340 | ILE | CB-CG1-CD1 | 5.90 | 130.42 | 113.90 |
| 1 | B | 377 | TYR | CZ-CE2-CD2 | 5.90 | 125.11 | 119.80 |
| 1 | B | 18 | LEU | CB-CG-CD2 | 5.89 | 121.02 | 111.00 |
| 1 | B | 32 | TYR | CD1-CE1-CZ | 5.89 | 125.10 | 119.80 |
| 1 | B | 701 | VAL | CA-CB-CG1 | -5.88 | 102.08 | 110.90 |
| 1 | B | 107 | LEU | CA-CB-CG | -5.88 | 101.78 | 115.30 |
| 1 | B | 295 | GLY | N-CA-C | 5.88 | 127.79 | 113.10 |
| 1 | A | 53 | PRO | N-CA-CB | -5.87 | 96.14 | 102.60 |
| 1 | B | 443 | ALA | N-CA-CB | 5.86 | 118.31 | 110.10 |
| 1 | B | 193 | GLU | N-CA-C | -5.86 | 95.19 | 111.00 |
| 1 | A | 644 | LEU | CB-CG-CD1 | 5.85 | 120.95 | 111.00 |
| 1 | A | 166 | VAL | CA-CB-CG2 | -5.85 | 102.13 | 110.90 |
| 1 | A | 193 | GLU | OE1-CD-OE2 | 5.85 | 130.32 | 123.30 |
| 1 | A | 776 | MET | CB-CG-SD | -5.85 | 94.86 | 112.40 |
| 1 | B | 864 | MET | CA-CB-CG | -5.85 | 103.36 | 113.30 |
| 1 | A | 333 | ARG | N-CA-C | -5.84 | 95.23 | 111.00 |
| 1 | A | 491 | GLU | OE1-CD-OE2 | 5.84 | 130.31 | 123.30 |
| 1 | B | 241 | SER | O-C-N | 5.84 | 132.04 | 122.70 |
| 1 | B | 649 | VAL | CG1-CB-CG2 | -5.83 | 101.58 | 110.90 |
| 1 | A | 274 | TYR | CD1-CE1-CZ | 5.82 | 125.04 | 119.80 |
| 1 | A | 141 | PHE | CG-CD1-CE1 | -5.82 | 114.40 | 120.80 |
| 1 | A | 660 | ASP | CB-CG-OD2 | 5.82 | 123.54 | 118.30 |
| 1 | A | 281 | LEU | N-CA-C | -5.82 | 95.29 | 111.00 |
| 1 | A | 577 | GLU | OE1-CD-OE2 | -5.82 | 116.32 | 123.30 |
| 1 | B | 521 | LEU | N-CA-C | 5.82 | 126.71 | 111.00 |
| 1 | A | 510 | THR | CA-CB-CG2 | -5.82 | 104.25 | 112.40 |
| 1 | A | 107 | LEU | CB-CG-CD2 | -5.81 | 101.12 | 111.00 |
| 1 | B | 168 | VAL | CG1-CB-CG2 | 5.81 | 120.20 | 110.90 |
| 1 | A | 229 | LEU | N-CA-C | -5.81 | 95.31 | 111.00 |
| 1 | B | 806 | PHE | N-CA-C | -5.81 | 95.31 | 111.00 |
| 1 | A | 638 | PHE | CG-CD1-CE1 | 5.81 | 127.19 | 120.80 |
| 1 | B | 180 | LEU | CB-CG-CD2 | -5.81 | 101.12 | 111.00 |
| 1 | A | 115 | THR | O-C-N | -5.80 | 113.41 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 361 | TYR | CZ-CE2-CD2 | 5.80 | 125.03 | 119.80 |
| 1 | A | 803 | TYR | CE1-CZ-OH | -5.80 | 104.44 | 120.10 |
| 1 | B | 116 | LEU | CD1-CG-CD2 | -5.80 | 93.09 | 110.50 |
| 1 | B | 866 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | B | 114 | LEU | CB-CG-CD1 | -5.79 | 101.15 | 111.00 |
| 1 | A | 161 | LYS | CB-CG-CD | 5.78 | 126.63 | 111.60 |
| 1 | B | 76 | LYS | N-CA-CB | -5.78 | 100.19 | 110.60 |
| 1 | B | 48 | ASP | CB-CA-C | 5.78 | 121.95 | 110.40 |
| 1 | A | 429 | GLU | N-CA-CB | -5.77 | 100.21 | 110.60 |
| 1 | B | 95 | THR | OG1-CB-CG2 | -5.77 | 96.73 | 110.00 |
| 1 | B | 136 | ALA | N-CA-C | 5.77 | 126.58 | 111.00 |
| 1 | B | 508 | ALA | O-C-N | -5.77 | 113.39 | 123.20 |
| 1 | A | 775 | VAL | CB-CA-C | -5.77 | 100.44 | 111.40 |
| 1 | B | 349 | LYS | CB-CA-C | -5.77 | 98.86 | 110.40 |
| 1 | A | 311 | GLU | O-C-N | 5.76 | 131.92 | 122.70 |
| 1 | B | 418 | ARG | CA-CB-CG | 5.76 | 126.08 | 113.40 |
| 1 | A | 122 | HIS | CB-CA-C | -5.76 | 98.87 | 110.40 |
| 1 | A | 36 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 1 | A | 570 | ARG | NE-CZ-NH2 | 5.75 | 123.17 | 120.30 |
| 1 | B | 828 | PHE | CG-CD2-CE2 | -5.75 | 114.47 | 120.80 |
| 1 | B | 348 | LEU | N-CA-CB | 5.75 | 121.90 | 110.40 |
| 1 | B | 407 | CYS | N-CA-C | -5.75 | 95.49 | 111.00 |
| 1 | A | 619 | ASP | CB-CG-OD2 | 5.74 | 123.47 | 118.30 |
| 1 | A | 691 | LEU | N-CA-C | -5.74 | 95.50 | 111.00 |
| 1 | B | 303 | GLU | CB-CA-C | -5.73 | 98.93 | 110.40 |
| 1 | B | 624 | MET | CB-CA-C | 5.73 | 121.86 | 110.40 |
| 1 | B | 264 | TYR | CG-CD2-CE2 | -5.72 | 116.72 | 121.30 |
| 1 | A | 710 | MET | O-C-N | 5.71 | 131.84 | 122.70 |
| 1 | B | 289 | GLY | N-CA-C | 5.71 | 127.38 | 113.10 |
| 1 | B | 572 | ASN | N-CA-C | 5.71 | 126.40 | 111.00 |
| 1 | A | 820 | PRO | CA-C-O | 5.70 | 133.88 | 120.20 |
| 1 | B | 294 | LYS | CD-CE-NZ | 5.70 | 124.81 | 111.70 |
| 1 | B | 772 | MET | CG-SD-CE | -5.70 | 91.08 | 100.20 |
| 1 | A | 331 | PHE | CG-CD1-CE1 | -5.70 | 114.53 | 120.80 |
| 1 | A | 506 | LYS | CA-CB-CG | 5.70 | 125.93 | 113.40 |
| 1 | B | 77 | ARG | NE-CZ-NH2 | 5.69 | 123.15 | 120.30 |
| 1 | B | 162 | ASP | O-C-N | -5.69 | 113.52 | 123.20 |
| 1 | B | 625 | SER | N-CA-CB | 5.69 | 119.04 | 110.50 |
| 1 | B | 631 | MET | CB-CA-C | 5.69 | 121.78 | 110.40 |
| 1 | A | 757 | PRO | N-CD-CG | -5.69 | 94.67 | 103.20 |
| 1 | B | 159 | PRO | CA-CB-CG | -5.68 | 93.22 | 104.00 |
| 1 | B | 174 | ASN | O-C-N | 5.67 | 131.78 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 631 | MET | N-CA-CB | 5.67 | 120.81 | 110.60 |
| 1 | A | 96 | ASP | CB-CA-C | -5.67 | 99.06 | 110.40 |
| 1 | A | 192 | TYR | CB-CA-C | -5.66 | 99.07 | 110.40 |
| 1 | A | 185 | TYR | O-C-N | 5.66 | 131.76 | 122.70 |
| 1 | A | 324 | PHE | CB-CA-C | -5.66 | 99.08 | 110.40 |
| 1 | A | 470 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | B | 614 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | B | 340 | ILE | CA-CB-CG1 | -5.66 | 100.25 | 111.00 |
| 1 | B | 282 | ILE | CG1-CB-CG2 | -5.65 | 98.96 | 111.40 |
| 1 | B | 333 | ARG | CG-CD-NE | 5.65 | 123.67 | 111.80 |
| 1 | A | 638 | PHE | CD1-CE1-CZ | -5.65 | 113.32 | 120.10 |
| 1 | A | 195 | LEU | CB-CG-CD1 | -5.65 | 101.39 | 111.00 |
| 1 | A | 333 | ARG | CD-NE-CZ | 5.64 | 131.50 | 123.60 |
| 1 | A | 811 | SER | N-CA-CB | -5.64 | 102.04 | 110.50 |
| 1 | B | 145 | GLN | N-CA-CB | -5.64 | 100.45 | 110.60 |
| 1 | A | 831 | ASN | N-CA-C | -5.64 | 95.78 | 111.00 |
| 1 | A | 126 | PRO | O-C-N | 5.63 | 131.72 | 122.70 |
| 1 | B | 263 | ALA | N-CA-CB | 5.63 | 117.99 | 110.10 |
| 1 | B | 876 | THR | CA-CB-CG2 | -5.63 | 104.51 | 112.40 |
| 1 | B | 499 | LEU | N-CA-CB | -5.63 | 99.14 | 110.40 |
| 1 | A | 168 | VAL | CG1-CB-CG2 | -5.63 | 101.90 | 110.90 |
| 1 | A | 367 | ARG | NH1-CZ-NH2 | -5.63 | 113.21 | 119.40 |
| 1 | A | 204 | PHE | CB-CG-CD1 | -5.62 | 116.86 | 120.80 |
| 1 | A | 441 | GLU | OE1-CD-OE2 | -5.62 | 116.55 | 123.30 |
| 1 | B | 372 | GLY | N-CA-C | 5.62 | 127.16 | 113.10 |
| 1 | A | 281 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 1 | B | 513 | LEU | CB-CG-CD1 | 5.62 | 120.56 | 111.00 |
| 1 | B | 34 | THR | CA-CB-OG1 | -5.62 | 97.20 | 109.00 |
| 1 | B | 42 | ALA | CB-CA-C | -5.62 | 101.67 | 110.10 |
| 1 | A | 205 | GLU | CG-CD-OE2 | 5.62 | 129.53 | 118.30 |
| 1 | A | 185 | TYR | CE1-CZ-CE2 | 5.61 | 128.78 | 119.80 |
| 1 | B | 311 | GLU | C-N-CA | 5.61 | 135.74 | 121.70 |
| 1 | A | 180 | LEU | CB-CG-CD2 | -5.61 | 101.46 | 111.00 |
| 1 | B | 435 | VAL | CG1-CB-CG2 | -5.61 | 101.92 | 110.90 |
| 1 | A | 740 | VAL | CA-CB-CG2 | -5.60 | 102.50 | 110.90 |
| 1 | B | 131 | PHE | N-CA-CB | -5.60 | 100.52 | 110.60 |
| 1 | B | 333 | ARG | CA-CB-CG | -5.60 | 101.08 | 113.40 |
| 1 | B | 394 | VAL | O-C-N | 5.60 | 131.66 | 122.70 |
| 1 | A | 128 | GLY | CA-C-N | 5.60 | 129.51 | 117.20 |
| 1 | B | 296 | PRO | CB-CA-C | 5.60 | 125.99 | 112.00 |
| 1 | A | 766 | ILE | CG1-CB-CG2 | -5.59 | 99.09 | 111.40 |
| 1 | B | 828 | PHE | CG-CD1-CE1 | 5.59 | 126.95 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 808 | THR | C-N-CA | 5.59 | 135.68 | 121.70 |
| 1 | A | 821 | GLY | N-CA-C | -5.59 | 99.12 | 113.10 |
| 1 | A | 305 | ASN | N-CA-C | -5.59 | 95.91 | 111.00 |
| 1 | B | 12 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | B | 641 | PRO | CA-C-N | 5.59 | 129.49 | 117.20 |
| 1 | B | 93 | THR | N-CA-C | -5.58 | 95.92 | 111.00 |
| 1 | A | 389 | ILE | CA-CB-CG2 | -5.58 | 99.74 | 110.90 |
| 1 | A | 396 | ASP | CB-CG-OD2 | 5.58 | 123.32 | 118.30 |
| 1 | B | 573 | GLY | N-CA-C | -5.58 | 99.16 | 113.10 |
| 1 | A | 63 | LEU | CB-CG-CD2 | 5.57 | 120.47 | 111.00 |
| 1 | B | 733 | LEU | CA-C-O | -5.57 | 108.39 | 120.10 |
| 1 | B | 87 | PHE | CZ-CE2-CD2 | -5.57 | 113.42 | 120.10 |
| 1 | A | 666 | ARG | NE-CZ-NH1 | -5.56 | 117.52 | 120.30 |
| 1 | B | 359 | THR | OG1-CB-CG2 | -5.56 | 97.21 | 110.00 |
| 1 | B | 729 | LEU | CB-CG-CD1 | -5.56 | 101.55 | 111.00 |
| 1 | B | 660 | ASP | CB-CG-OD1 | 5.56 | 123.30 | 118.30 |
| 1 | B | 812 | GLY | CA-C-O | -5.56 | 110.59 | 120.60 |
| 1 | A | 854 | PHE | CB-CG-CD2 | -5.55 | 116.91 | 120.80 |
| 1 | B | 61 | LYS | CD-CE-NZ | 5.55 | 124.47 | 111.70 |
| 1 | B | 332 | ILE | CG1-CB-CG2 | 5.55 | 123.62 | 111.40 |
| 1 | B | 78 | PRO | CB-CG-CD | -5.55 | 84.86 | 106.50 |
| 1 | B | 340 | ILE | CA-CB-CG2 | 5.54 | 121.98 | 110.90 |
| 1 | A | 647 | VAL | CA-CB-CG2 | 5.54 | 119.20 | 110.90 |
| 1 | B | 728 | LYS | N-CA-C | -5.54 | 96.06 | 111.00 |
| 1 | B | 378 | PRO | N-CA-CB | 5.53 | 109.94 | 103.30 |
| 1 | A | 776 | MET | CA-CB-CG | 5.53 | 122.69 | 113.30 |
| 1 | B | 102 | LEU | CB-CG-CD1 | -5.53 | 101.61 | 111.00 |
| 1 | A | 204 | PHE | CD1-CE1-CZ | -5.52 | 113.48 | 120.10 |
| 1 | A | 382 | TRP | CA-CB-CG | -5.52 | 103.22 | 113.70 |
| 1 | A | 786 | PHE | N-CA-CB | 5.51 | 120.53 | 110.60 |
| 1 | A | 37 | ASN | N-CA-C | -5.51 | 96.12 | 111.00 |
| 1 | B | 631 | MET | CG-SD-CE | 5.51 | 109.02 | 100.20 |
| 1 | A | 852 | ASP | N-CA-C | -5.51 | 96.12 | 111.00 |
| 1 | B | 101 | ALA | CB-CA-C | 5.51 | 118.36 | 110.10 |
| 1 | B | 184 | ALA | CB-CA-C | -5.51 | 101.83 | 110.10 |
| 1 | A | 124 | VAL | CB-CA-C | -5.50 | 100.94 | 111.40 |
| 1 | A | 861 | LEU | N-CA-C | -5.50 | 96.14 | 111.00 |
| 1 | B | 124 | VAL | CA-CB-CG2 | 5.50 | 119.16 | 110.90 |
| 1 | A | 503 | PHE | CB-CA-C | -5.50 | 99.40 | 110.40 |
| 1 | B | 413 | LEU | CB-CG-CD2 | 5.50 | 120.35 | 111.00 |
| 1 | B | 473 | SER | CA-C-N | 5.50 | 129.31 | 117.20 |
| 1 | B | 195 | LEU | CB-CG-CD1 | 5.50 | 120.35 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 382 | TRP | CG-CD1-NE1 | 5.50 | 115.60 | 110.10 |
| 1 | B | 559 | LEU | O-C-N | 5.50 | 131.49 | 122.70 |
| 1 | A | 223 | ASP | CA-C-N | -5.49 | 105.12 | 117.20 |
| 1 | B | 605 | ARG | NE-CZ-NH2 | 5.49 | 123.05 | 120.30 |
| 1 | B | 377 | TYR | CA-C-O | 5.49 | 131.62 | 120.10 |
| 1 | A | 745 | LEU | CB-CG-CD1 | 5.48 | 120.32 | 111.00 |
| 1 | B | 312 | ARG | CB-CG-CD | 5.48 | 125.85 | 111.60 |
| 1 | B | 389 | ILE | N-CA-CB | 5.48 | 123.41 | 110.80 |
| 1 | B | 518 | GLN | CB-CA-C | -5.48 | 99.44 | 110.40 |
| 1 | B | 476 | ILE | CA-CB-CG1 | 5.48 | 121.41 | 111.00 |
| 1 | B | 303 | GLU | C-N-CA | 5.48 | 135.39 | 121.70 |
| 1 | A | 105 | SER | N-CA-CB | -5.47 | 102.29 | 110.50 |
| 1 | A | 163 | GLY | O-C-N | 5.47 | 131.45 | 122.70 |
| 1 | A | 23 | ARG | NE-CZ-NH1 | 5.47 | 123.03 | 120.30 |
| 1 | B | 744 | GLU | CG-CD-OE2 | -5.47 | 107.36 | 118.30 |
| 1 | B | 793 | TRP | CA-CB-CG | 5.47 | 124.09 | 113.70 |
| 1 | B | 493 | ASN | CB-CA-C | 5.47 | 121.33 | 110.40 |
| 1 | B | 848 | ASN | C-N-CA | 5.46 | 135.36 | 121.70 |
| 1 | B | 374 | CYS | CA-CB-SG | -5.46 | 104.17 | 114.00 |
| 1 | B | 51 | PHE | CZ-CE2-CD2 | 5.46 | 126.65 | 120.10 |
| 1 | B | 376 | ASN | CB-CG-OD1 | -5.46 | 110.68 | 121.60 |
| 1 | A | 319 | MET | O-C-N | -5.46 | 113.97 | 122.70 |
| 1 | A | 392 | GLU | N-CA-CB | -5.46 | 100.78 | 110.60 |
| 1 | A | 793 | TRP | CB-CA-C | -5.46 | 99.49 | 110.40 |
| 1 | A | 184 | ALA | N-CA-C | -5.45 | 96.29 | 111.00 |
| 1 | A | 588 | ARG | NE-CZ-NH1 | 5.44 | 123.02 | 120.30 |
| 1 | A | 127 | TYR | CG-CD1-CE1 | 5.44 | 125.65 | 121.30 |
| 1 | B | 264 | TYR | CB-CG-CD1 | -5.44 | 117.74 | 121.00 |
| 1 | B | 645 | HIS | N-CA-CB | 5.44 | 120.39 | 110.60 |
| 1 | A | 624 | MET | N-CA-CB | 5.43 | 120.38 | 110.60 |
| 1 | A | 134 | GLY | O-C-N | 5.43 | 131.39 | 122.70 |
| 1 | A | 442 | LEU | CA-C-O | -5.42 | 108.71 | 120.10 |
| 1 | A | 681 | LEU | CB-CG-CD1 | 5.42 | 120.22 | 111.00 |
| 1 | A | 336 | THR | OG1-CB-CG2 | -5.42 | 97.55 | 110.00 |
| 1 | B | 102 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 1 | A | 374 | CYS | O-C-N | -5.41 | 114.04 | 122.70 |
| 1 | B | 95 | THR | CA-CB-CG2 | 5.41 | 119.97 | 112.40 |
| 1 | B | 236 | SER | N-CA-CB | -5.41 | 102.39 | 110.50 |
| 1 | B | 193 | GLU | CA-C-O | -5.41 | 108.75 | 120.10 |
| 1 | B | 424 | PHE | C-N-CA | 5.41 | 133.65 | 122.30 |
| 1 | B | 579 | CYS | CB-CA-C | 5.40 | 121.19 | 110.40 |
| 1 | A | 433 | PHE | CG-CD2-CE2 | 5.39 | 126.73 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 398 | ASP | N-CA-CB | -5.39 | 100.90 | 110.60 |
| 1 | A | 652 | PHE | N-CA-C | 5.38 | 125.52 | 111.00 |
| 1 | A | 834 | ILE | N-CA-C | -5.38 | 96.49 | 111.00 |
| 1 | A | 291 | VAL | N-CA-CB | 5.37 | 123.32 | 111.50 |
| 1 | B | 348 | LEU | CB-CG-CD2 | 5.37 | 120.14 | 111.00 |
| 1 | B | 389 | ILE | CA-C-N | -5.37 | 105.38 | 117.20 |
| 1 | A | 436 | TYR | CG-CD1-CE1 | -5.37 | 117.00 | 121.30 |
| 1 | B | 385 | PRO | N-CD-CG | -5.37 | 95.14 | 103.20 |
| 1 | B | 329 | ARG | C-N-CA | 5.37 | 135.11 | 121.70 |
| 1 | A | 109 | ALA | CB-CA-C | 5.36 | 118.14 | 110.10 |
| 1 | A | 464 | GLU | N-CA-C | -5.36 | 96.52 | 111.00 |
| 1 | A | 646 | GLN | CG-CD-OE1 | -5.36 | 110.88 | 121.60 |
| 1 | A | 615 | LYS | CD-CE-NZ | 5.36 | 124.02 | 111.70 |
| 1 | B | 314 | GLN | CA-C-O | 5.34 | 131.32 | 120.10 |
| 1 | A | 871 | LEU | N-CA-CB | 5.34 | 121.09 | 110.40 |
| 1 | A | 746 | MET | CB-CG-SD | -5.34 | 96.38 | 112.40 |
| 1 | A | 701 | VAL | C-N-CA | 5.34 | 135.05 | 121.70 |
| 1 | A | 149 | TRP | CG-CD1-NE1 | -5.33 | 104.77 | 110.10 |
| 1 | A | 630 | ARG | CB-CA-C | 5.33 | 121.06 | 110.40 |
| 1 | A | 290 | GLU | CA-CB-CG | -5.33 | 101.68 | 113.40 |
| 1 | B | 109 | ALA | CA-C-N | -5.32 | 105.51 | 117.20 |
| 1 | B | 329 | ARG | CB-CG-CD | 5.31 | 125.41 | 111.60 |
| 1 | A | 453 | PHE | CD1-CE1-CZ | -5.31 | 113.73 | 120.10 |
| 1 | A | 243 | ASN | CB-CA-C | -5.30 | 99.79 | 110.40 |
| 1 | B | 745 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | A | 162 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 |
| 1 | A | 181 | LEU | CB-CA-C | -5.30 | 100.13 | 110.20 |
| 1 | A | 634 | GLU | CG-CD-OE1 | -5.30 | 107.70 | 118.30 |
| 1 | A | 797 | LYS | CD-CE-NZ | -5.30 | 99.51 | 111.70 |
| 1 | B | 860 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | A | 63 | LEU | C-N-CA | -5.29 | 111.18 | 122.30 |
| 1 | A | 375 | ARG | N-CA-CB | -5.29 | 101.07 | 110.60 |
| 1 | B | 349 | LYS | CB-CG-CD | -5.29 | 97.84 | 111.60 |
| 1 | B | 256 | LYS | N-CA-C | 5.29 | 125.28 | 111.00 |
| 1 | B | 118 | GLU | O-C-N | -5.29 | 114.24 | 122.70 |
| 1 | B | 441 | GLU | CA-C-N | -5.28 | 105.58 | 117.20 |
| 1 | B | 512 | GLU | CA-CB-CG | 5.28 | 125.02 | 113.40 |
| 1 | B | 388 | LYS | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | B | 143 | LEU | O-C-N | -5.27 | 114.26 | 122.70 |
| 1 | B | 402 | SER | CA-C-N | -5.27 | 105.60 | 117.20 |
| 1 | A | 242 | ILE | CA-CB-CG2 | 5.27 | 121.44 | 110.90 |
| 1 | B | 587 | ASP | N-CA-C | 5.27 | 125.23 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 388 | LYS | N-CA-C | 5.27 | 125.22 | 111.00 |
| 1 | B | 440 | ARG | NE-CZ-NH1 | 5.27 | 122.93 | 120.30 |
| 1 | B | 610 | LEU | CA-CB-CG | 5.27 | 127.41 | 115.30 |
| 1 | A | 218 | GLN | N-CA-CB | 5.26 | 120.07 | 110.60 |
| 1 | B | 524 | GLU | OE1-CD-OE2 | 5.26 | 129.61 | 123.30 |
| 1 | B | 377 | TYR | CA-C-N | -5.26 | 102.38 | 117.10 |
| 1 | B | 540 | PHE | CA-C-O | -5.26 | 109.06 | 120.10 |
| 1 | A | 188 | VAL | CG1-CB-CG2 | -5.25 | 102.50 | 110.90 |
| 1 | A | 862 | ASP | OD1-CG-OD2 | -5.25 | 113.32 | 123.30 |
| 1 | B | 188 | VAL | N-CA-C | -5.25 | 96.82 | 111.00 |
| 1 | A | 648 | ILE | CG1-CB-CG2 | -5.25 | 99.85 | 111.40 |
| 1 | B | 331 | PHE | CB-CG-CD1 | -5.25 | 117.13 | 120.80 |
| 1 | A | 323 | GLU | OE1-CD-OE2 | -5.24 | 117.01 | 123.30 |
| 1 | B | 872 | ASP | CB-CG-OD1 | -5.24 | 113.58 | 118.30 |
| 1 | B | 94 | ARG | C-N-CA | 5.24 | 134.79 | 121.70 |
| 1 | A | 384 | ASN | N-CA-CB | 5.24 | 120.02 | 110.60 |
| 1 | A | 237 | LEU | N-CA-CB | 5.23 | 120.87 | 110.40 |
| 1 | A | 448 | HIS | N-CA-C | 5.23 | 125.13 | 111.00 |
| 1 | B | 291 | VAL | CA-CB-CG1 | -5.23 | 103.05 | 110.90 |
| 1 | B | 416 | LYS | CD-CE-NZ | 5.23 | 123.74 | 111.70 |
| 1 | B | 770 | ARG | CA-C-N | 5.23 | 128.71 | 117.20 |
| 1 | A | 354 | ARG | CB-CA-C | 5.23 | 120.86 | 110.40 |
| 1 | A | 345 | PRO | CB-CG-CD | -5.23 | 86.11 | 106.50 |
| 1 | B | 499 | LEU | CB-CG-CD2 | 5.23 | 119.89 | 111.00 |
| 1 | A | 310 | TYR | OH-CZ-CE2 | 5.22 | 134.21 | 120.10 |
| 1 | A | 58 | LEU | CB-CG-CD1 | 5.22 | 119.88 | 111.00 |
| 1 | A | 823 | PHE | CG-CD2-CE2 | 5.22 | 126.54 | 120.80 |
| 1 | B | 345 | PRO | CA-N-CD | -5.22 | 104.19 | 111.50 |
| 1 | B | 337 | LYS | CA-CB-CG | -5.22 | 101.92 | 113.40 |
| 1 | B | 308 | ASP | CB-CA-C | 5.22 | 120.84 | 110.40 |
| 1 | A | 300 | ASN | N-CA-CB | -5.22 | 101.21 | 110.60 |
| 1 | A | 343 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 1 | A | 630 | ARG | N-CA-C | -5.21 | 96.95 | 111.00 |
| 1 | B | 117 | ASN | N-CA-CB | -5.20 | 101.24 | 110.60 |
| 1 | A | 296 | PRO | N-CD-CG | 5.20 | 111.00 | 103.20 |
| 1 | B | 58 | LEU | CB-CG-CD2 | -5.20 | 102.16 | 111.00 |
| 1 | B | 133 | GLU | C-N-CA | 5.20 | 133.21 | 122.30 |
| 1 | A | 711 | HIS | N-CA-CB | 5.19 | 119.95 | 110.60 |
| 1 | A | 855 | ILE | CB-CA-C | -5.19 | 101.22 | 111.60 |
| 1 | B | 480 | PRO | N-CD-CG | 5.19 | 110.98 | 103.20 |
| 1 | A | 40 | LEU | CD1-CG-CD2 | -5.19 | 94.94 | 110.50 |
| 1 | B | 671 | LEU | CB-CG-CD2 | -5.19 | 102.18 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 868 | PHE | CB-CG-CD1 | -5.18 | 117.17 | 120.80 |
| 1 | B | 858 | LEU | CB-CA-C | -5.18 | 100.35 | 110.20 |
| 1 | B | 31 | ASP | OD1-CG-OD2 | -5.18 | 113.45 | 123.30 |
| 1 | B | 336 | THR | N-CA-C | -5.18 | 97.00 | 111.00 |
| 1 | A | 49 | PRO | C-N-CA | -5.18 | 108.75 | 121.70 |
| 1 | B | 185 | TYR | CZ-CE2-CD2 | -5.18 | 115.14 | 119.80 |
| 1 | A | 93 | THR | CA-CB-CG2 | -5.18 | 105.15 | 112.40 |
| 1 | A | 810 | ARG | N-CA-CB | -5.18 | 101.28 | 110.60 |
| 1 | B | 876 | THR | OG1-CB-CG2 | -5.18 | 98.09 | 110.00 |
| 1 | A | 447 | VAL | C-N-CA | -5.18 | 108.76 | 121.70 |
| 1 | B | 148 | GLU | OE1-CD-OE2 | -5.18 | 117.09 | 123.30 |
| 1 | B | 426 | ARG | CA-CB-CG | 5.18 | 124.79 | 113.40 |
| 1 | A | 62 | GLU | O-C-N | 5.17 | 130.98 | 122.70 |
| 1 | B | 383 | VAL | O-C-N | 5.17 | 130.98 | 122.70 |
| 1 | A | 498 | PHE | CB-CG-CD2 | -5.17 | 117.18 | 120.80 |
| 1 | B | 426 | ARG | CB-CA-C | -5.17 | 100.07 | 110.40 |
| 1 | A | 123 | ARG | CA-CB-CG | 5.17 | 124.76 | 113.40 |
| 1 | A | 257 | ASN | C-N-CA | 5.16 | 134.61 | 121.70 |
| 1 | A | 69 | LYS | CD-CE-NZ | -5.16 | 99.83 | 111.70 |
| 1 | A | 331 | PHE | CB-CA-C | -5.16 | 100.08 | 110.40 |
| 1 | B | 684 | GLU | N-CA-C | 5.16 | 124.92 | 111.00 |
| 1 | B | 104 | ASP | OD1-CG-OD2 | -5.15 | 113.51 | 123.30 |
| 1 | B | 324 | PHE | CZ-CE2-CD2 | 5.15 | 126.28 | 120.10 |
| 1 | B | 450 | LYS | CD-CE-NZ | 5.15 | 123.55 | 111.70 |
| 1 | B | 141 | PHE | CZ-CE2-CD2 | 5.15 | 126.28 | 120.10 |
| 1 | B | 349 | LYS | O-C-N | 5.15 | 130.94 | 122.70 |
| 1 | B | 594 | LEU | CB-CG-CD1 | -5.14 | 102.26 | 111.00 |
| 1 | A | 308 | ASP | CB-CG-OD2 | -5.14 | 113.67 | 118.30 |
| 1 | A | 520 | ASN | N-CA-C | 5.14 | 124.87 | 111.00 |
| 1 | B | 320 | GLU | CA-CB-CG | -5.13 | 102.11 | 113.40 |
| 1 | B | 725 | GLN | N-CA-C | -5.13 | 97.14 | 111.00 |
| 1 | A | 684 | GLU | OE1-CD-OE2 | 5.13 | 129.46 | 123.30 |
| 1 | B | 333 | ARG | NE-CZ-NH2 | 5.13 | 122.87 | 120.30 |
| 1 | A | 85 | PRO | CA-N-CD | -5.13 | 104.31 | 111.50 |
| 1 | A | 167 | PHE | N-CA-C | 5.13 | 124.86 | 111.00 |
| 1 | A | 387 | PHE | CD1-CE1-CZ | 5.13 | 126.26 | 120.10 |
| 1 | B | 478 | LEU | CA-CB-CG | 5.13 | 127.10 | 115.30 |
| 1 | A | 429 | GLU | O-C-N | -5.13 | 114.49 | 122.70 |
| 1 | A | 212 | THR | N-CA-C | 5.13 | 124.85 | 111.00 |
| 1 | B | 743 | THR | C-N-CA | 5.13 | 134.52 | 121.70 |
| 1 | B | 611 | THR | N-CA-C | 5.13 | 124.84 | 111.00 |
| 1 | A | 143 | LEU | N-CA-CB | -5.12 | 100.15 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 341 | CYS | CA-CB-SG | -5.12 | 104.78 | 114.00 |
| 1 | A | 454 | PHE | CB-CG-CD1 | -5.12 | 117.22 | 120.80 |
| 1 | A | 381 | PHE | CB-CG-CD2 | -5.12 | 117.22 | 120.80 |
| 1 | B | 329 | ARG | CD-NE-CZ | 5.11 | 130.76 | 123.60 |
| 1 | A | 98 | CYS | CA-CB-SG | -5.11 | 104.81 | 114.00 |
| 1 | B | 67 | SER | N-CA-CB | 5.11 | 118.16 | 110.50 |
| 1 | B | 84 | ASN | CB-CA-C | 5.11 | 120.61 | 110.40 |
| 1 | A | 159 | PRO | CA-C-O | -5.11 | 107.95 | 120.20 |
| 1 | A | 330 | ASP | OD1-CG-OD2 | -5.10 | 113.60 | 123.30 |
| 1 | A | 317 | VAL | CG1-CB-CG2 | -5.10 | 102.74 | 110.90 |
| 1 | A | 860 | ARG | CB-CG-CD | 5.10 | 124.87 | 111.60 |
| 1 | A | 225 | TYR | CG-CD2-CE2 | -5.10 | 117.22 | 121.30 |
| 1 | B | 388 | LYS | CB-CG-CD | -5.10 | 98.34 | 111.60 |
| 1 | A | 281 | LEU | CB-CG-CD1 | 5.10 | 119.67 | 111.00 |
| 1 | B | 150 | VAL | CG1-CB-CG2 | -5.09 | 102.76 | 110.90 |
| 1 | A | 183 | LYS | CD-CE-NZ | 5.08 | 123.39 | 111.70 |
| 1 | B | 213 | GLU | CG-CD-OE2 | 5.08 | 128.47 | 118.30 |
| 1 | A | 153 | VAL | CA-CB-CG1 | 5.08 | 118.52 | 110.90 |
| 1 | B | 580 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 1 | A | 207 | PHE | CZ-CE2-CD2 | -5.08 | 114.00 | 120.10 |
| 1 | A | 403 | ARG | NE-CZ-NH1 | 5.08 | 122.84 | 120.30 |
| 1 | A | 608 | ASN | O-C-N | -5.08 | 114.58 | 122.70 |
| 1 | A | 602 | LEU | CB-CG-CD1 | 5.08 | 119.63 | 111.00 |
| 1 | B | 339 | GLU | N-CA-C | 5.08 | 124.70 | 111.00 |
| 1 | A | 647 | VAL | CA-CB-CG1 | 5.07 | 118.51 | 110.90 |
| 1 | A | 777 | ASP | CB-CG-OD2 | -5.07 | 113.74 | 118.30 |
| 1 | B | 391 | LEU | CB-CG-CD2 | -5.07 | 102.38 | 111.00 |
| 1 | B | 660 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 1 | B | 788 | GLU | N-CA-CB | 5.07 | 119.72 | 110.60 |
| 1 | B | 868 | PHE | O-C-N | -5.07 | 114.60 | 122.70 |
| 1 | A | 285 | ARG | N-CA-C | 5.06 | 124.67 | 111.00 |
| 1 | B | 195 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 1 | A | 462 | GLN | N-CA-CB | -5.06 | 101.49 | 110.60 |
| 1 | B | 345 | PRO | C-N-CA | 5.06 | 134.35 | 121.70 |
| 1 | B | 480 | PRO | CA-CB-CG | -5.06 | 94.39 | 104.00 |
| 1 | B | 789 | PHE | O-C-N | 5.06 | 130.79 | 122.70 |
| 1 | A | 468 | ASN | N-CA-CB | 5.06 | 119.70 | 110.60 |
| 1 | B | 610 | LEU | CB-CG-CD1 | 5.06 | 119.60 | 111.00 |
| 1 | A | 343 | LEU | CD1-CG-CD2 | -5.06 | 95.33 | 110.50 |
| 1 | A | 764 | PHE | CB-CG-CD1 | 5.05 | 124.34 | 120.80 |
| 1 | A | 93 | THR | C-N-CA | 5.05 | 134.33 | 121.70 |
| 1 | A | 623 | SER | N-CA-CB | -5.05 | 102.92 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | B | 343 | LEU | CA-CB-CG | -5.05 | 103.69 | 115.30 |
| 1 | B | 701 | VAL | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | B | 726 | PHE | CG-CD2-CE2 | 5.05 | 126.36 | 120.80 |
| 1 | A | 29 | ASN | CB-CA-C | 5.05 | 120.50 | 110.40 |
| 1 | B | 283 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | A | 808 | THR | CB-CA-C | -5.05 | 97.97 | 111.60 |
| 1 | A | 94 | ARG | N-CA-C | -5.04 | 97.39 | 111.00 |
| 1 | B | 217 | LEU | CB-CG-CD1 | -5.04 | 102.43 | 111.00 |
| 1 | A | 434 | ALA | CA-C-O | -5.04 | 109.52 | 120.10 |
| 1 | B | 237 | LEU | O-C-N | -5.04 | 114.64 | 122.70 |
| 1 | B | 362 | GLU | CB-CG-CD | 5.04 | 127.80 | 114.20 |
| 1 | B | 104 | ASP | CB-CA-C | 5.04 | 120.47 | 110.40 |
| 1 | A | 114 | LEU | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | A | 280 | ASN | CB-CG-OD1 | -5.03 | 111.53 | 121.60 |
| 1 | B | 191 | SER | N-CA-CB | 5.03 | 118.05 | 110.50 |
| 1 | B | 259 | VAL | CA-CB-CG2 | 5.03 | 118.45 | 110.90 |
| 1 | A | 285 | ARG | NH1-CZ-NH2 | 5.03 | 124.93 | 119.40 |
| 1 | A | 633 | ILE | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | B | 660 | ASP | OD1-CG-OD2 | -5.02 | 113.76 | 123.30 |
| 1 | A | 50 | ALA | CB-CA-C | 5.02 | 117.63 | 110.10 |
| 1 | A | 628 | GLU | OE1-CD-OE2 | 5.02 | 129.32 | 123.30 |
| 1 | A | 801 | GLY | CA-C-O | -5.02 | 111.57 | 120.60 |
| 1 | A | 35 | LEU | C-N-CA | -5.02 | 109.16 | 121.70 |
| 1 | B | 329 | ARG | CA-CB-CG | 5.02 | 124.43 | 113.40 |
| 1 | A | 469 | LEU | N-CA-CB | 5.01 | 120.43 | 110.40 |
| 1 | A | 105 | SER | O-C-N | -5.01 | 114.69 | 122.70 |
| 1 | B | 436 | TYR | CD1-CE1-CZ | -5.01 | 115.30 | 119.80 |
| 1 | A | 169 | HIS | N-CA-CB | -5.00 | 101.59 | 110.60 |
| 1 | B | 598 | GLU | CG-CD-OE2 | 5.00 | 128.31 | 118.30 |

There are no chirality outliers.

All (84) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 120 | ILE | Mainchain |
| 1 | A | 152 | VAL | Mainchain |
| 1 | A | 170 | SER | Peptide |
| 1 | A | 176 | PHE | Sidechain |
| 1 | A | 212 | THR | Mainchain |
| 1 | A | 218 | GLN | Mainchain,Peptide |
| 1 | A | 236 | SER | Mainchain |
| 1 | A | 24 | ALA | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 262 | HIS | Sidechain |
| 1 | A | 275 | GLN | Mainchain |
| 1 | A | 29 | ASN | Mainchain |
| 1 | A | 303 | GLU | Sidechain |
| 1 | A | 304 | TRP | Peptide |
| 1 | A | 319 | MET | Mainchain |
| 1 | A | 324 | PHE | Mainchain |
| 1 | A | 328 | PHE | Mainchain,Peptide |
| 1 | A | 356 | TRP | Mainchain |
| 1 | A | 371 | ALA | Mainchain |
| 1 | A | 386 | GLN | Mainchain |
| 1 | A | 402 | SER | Peptide |
| 1 | A | 415 | GLN | Sidechain |
| 1 | A | 434 | ALA | Mainchain |
| 1 | A | 466 | PHE | Sidechain |
| 1 | A | 473 | SER | Mainchain |
| 1 | A | 494 | LYS | Mainchain |
| 1 | A | 546 | ASP | Peptide |
| 1 | A | 549 | GLU | Peptide |
| 1 | A | 551 | SER | Peptide |
| 1 | A | 559 | LEU | Peptide |
| 1 | A | 570 | ARG | Peptide |
| 1 | A | 593 | LYS | Peptide |
| 1 | A | 598 | GLU | Peptide |
| 1 | A | 623 | SER | Peptide |
| 1 | A | 627 | TYR | Sidechain |
| 1 | A | 645 | HIS | Sidechain |
| 1 | A | 663 | ASN | Mainchain |
| 1 | A | 731 | VAL | Peptide |
| 1 | A | 802 | ILE | Peptide |
| 1 | A | 833 | HIS | Peptide |
| 1 | A | 834 | ILE | Peptide |
| 1 | A | 848 | ASN | Peptide |
| 1 | A | 99 | GLN | Mainchain,Peptide |
| 1 | B | 127 | TYR | Sidechain |
| 1 | B | 169 | HIS | Sidechain |
| 1 | B | 2 | ALA | Peptide |
| 1 | B | 215 | TYR | Sidechain |
| 1 | B | 225 | TYR | Sidechain |
| 1 | B | 294 | LYS | Peptide |
| 1 | B | 31 | ASP | Sidechain |
| 1 | B | 314 | GLN | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | B | 331 | PHE | Sidechain |
| 1 | B | 348 | LEU | Peptide |
| 1 | B | 38 | GLU | Mainchain |
| 1 | B | 398 | ASP | Mainchain |
| 1 | B | 399 | ASP | Mainchain,Peptide |
| 1 | B | 405 | SER | Peptide |
| 1 | B | 409 | PHE | Sidechain |
| 1 | B | 417 | HIS | Peptide |
| 1 | B | 43 | GLY | Peptide |
| 1 | B | 450 | LYS | Peptide |
| 1 | B | 469 | LEU | Mainchain |
| 1 | B | 538 | THR | Mainchain |
| 1 | B | 539 | LEU | Mainchain |
| 1 | B | 604 | ASN | Peptide |
| 1 | B | 621 | SER | Peptide |
| 1 | B | 638 | PHE | Sidechain |
| 1 | B | 64 | GLY | Peptide |
| 1 | B | 657 | LEU | Peptide |
| 1 | B | 700 | SER | Peptide |
| 1 | B | 738 | MET | Peptide |
| 1 | B | 785 | GLY | Peptide |
| 1 | B | 801 | GLY | Peptide |
| 1 | B | 806 | PHE | Peptide |
| 1 | B | 807 | GLU | Peptide |
| 1 | B | 821 | GLY | Peptide |
| 1 | B | 832 | GLN | Peptide |
| 1 | B | 860 | ARG | Peptide |
| 1 | B | 87 | PHE | Sidechain |
| 1 | B | 90 | ASP | Peptide |
| 1 | B | 92 | ALA | Peptide |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6053 | 0 | 5615 | 959 | 3 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | B | 6003 | 0 | 5477 | 969 | 1 |
| 2 | A | 172 | 0 | 0 | 53 | 1 |
| 2 | B | 140 | 0 | 0 | 45 | 1 |
| All | All | 12368 | 0 | 11092 | 1928 | 3 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 83.

All (1928) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:583:VAL:CB | 1:A:583:VAL:CA | 1.74 | 1.65 |
| 1:B:0:GLU:CA | 1:B:0:GLU:CB | 1.75 | 1.64 |
| 1:B:786:PHE:CA | 1:B:786:PHE:CB | 1.74 | 1.64 |
| 1:A:550:ILE:CB | 1:A:550:ILE:CA | 1.75 | 1.64 |
| 1:B:8:LEU:CD2 | 1:B:8:LEU:CG | 1.76 | 1.63 |
| 1:A:610:LEU:CD2 | 1:A:610:LEU:CG | 1.77 | 1.62 |
| 1:B:89:VAL:CB | 1:B:89:VAL:CA | 1.77 | 1.62 |
| 1:A:826:ALA:CB | 1:A:826:ALA:CA | 1.76 | 1.62 |
| 1:B:284:MET:CG | 1:B:284:MET:CB | 1.75 | 1.62 |
| 1:B:477:ARG:CG | 1:B:477:ARG:CB | 1.77 | 1.62 |
| 1:A:688:THR:CB | 1:A:688:THR:CG2 | 1.78 | 1.62 |
| 1:A:218:GLN:CA | 1:A:218:GLN:CB | 1.75 | 1.61 |
| 1:B:228:ILE:CB | 1:B:228:ILE:CG2 | 1.75 | 1.61 |
| 1:B:256:LYS:CG | 1:B:256:LYS:CB | 1.74 | 1.61 |
| 1:A:75:TRP:CB | 1:A:75:TRP:CG | 1.77 | 1.61 |
| 1:B:343:LEU:CD2 | 1:B:343:LEU:CG | 1.77 | 1.61 |
| 1:B:777:ASP:CB | 1:B:777:ASP:CA | 1.77 | 1.61 |
| 1:B:340:ILE:CD1 | 1:B:340:ILE:CG1 | 1.75 | 1.60 |
| 1:B:89:VAL:CG1 | 1:B:89:VAL:CB | 1.78 | 1.60 |
| 1:A:320:GLU:CB | 1:A:320:GLU:CA | 1.74 | 1.60 |
| 1:A:773:VAL:CG1 | 1:A:773:VAL:CB | 1.77 | 1.60 |
| 1:A:332:ILE:CB | 1:A:332:ILE:CG1 | 1.75 | 1.60 |
| 1:A:89:VAL:CB | 1:A:89:VAL:CG1 | 1.80 | 1.60 |
| 1:B:230:LYS:CE | 1:B:230:LYS:CD | 1.76 | 1.60 |
| 1:A:333:ARG:CD | 1:A:333:ARG:CG | 1.78 | 1.60 |
| 1:B:553:LYS:CA | 1:B:553:LYS:CB | 1.76 | 1.60 |
| 1:A:99:GLN:CB | 1:A:99:GLN:CA | 1.78 | 1.59 |
| 1:A:242:ILE:CD1 | 1:A:242:ILE:CG1 | 1.76 | 1.59 |
| 1:B:313:GLU:CB | 1:B:313:GLU:CG | 1.75 | 1.59 |
| 1:A:200:THR:CA | 1:A:200:THR:CB | 1.79 | 1.59 |
| 1:B:88:ILE:CG1 | 1:B:88:ILE:CD1 | 1.75 | 1.59 |
| 1:A:200:THR:CB | 1:A:200:THR:CG2 | 1.74 | 1.59 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:413:LEU:CD1 | 1:A:413:LEU:CG | 1.79 | 1.59 |
| 1:A:864:MET:CB | 1:A:864:MET:CA | 1.75 | 1.59 |
| 1:B:470:ARG:CB | 1:B:470:ARG:CG | 1.74 | 1.59 |
| 1:A:669:VAL:CB | 1:A:669:VAL:CG1 | 1.76 | 1.59 |
| 1:B:729:LEU:CG | 1:B:729:LEU:CD2 | 1.75 | 1.58 |
| 1:A:366:ARG:CG | 1:A:366:ARG:CD | 1.77 | 1.58 |
| 1:B:335:PHE:CA | 1:B:335:PHE:CB | 1.74 | 1.58 |
| 1:B:294:LYS:CG | 1:B:294:LYS:CD | 1.75 | 1.58 |
| 1:B:694:ILE:CB | 1:B:694:ILE:CA | 1.78 | 1.58 |
| 1:B:579:CYS:CB | 1:B:579:CYS:CA | 1.78 | 1.57 |
| 1:A:340:ILE:CB | 1:A:340:ILE:CG2 | 1.76 | 1.57 |
| 1:A:478:LEU:CD1 | 1:A:478:LEU:CG | 1.82 | 1.57 |
| 1:B:669:VAL:CA | 1:B:669:VAL:CB | 1.82 | 1.57 |
| 1:B:120:ILE:CG2 | 1:B:120:ILE:CB | 1.75 | 1.57 |
| 1:B:537:LYS:CG | 1:B:537:LYS:CD | 1.74 | 1.57 |
| 1:B:668:LEU:CG | 1:B:668:LEU:CD2 | 1.74 | 1.57 |
| 1:B:806:PHE:CB | 1:B:806:PHE:CG | 1.79 | 1.57 |
| 1:B:610:LEU:CD1 | 1:B:610:LEU:CG | 1.83 | 1.56 |
| 1:B:333:ARG:CD | 1:B:333:ARG:CG | 1.78 | 1.56 |
| 1:A:808:THR:CB | 1:A:808:THR:CG2 | 1.76 | 1.56 |
| 1:A:477:ARG:CD | 1:A:477:ARG:CG | 1.77 | 1.56 |
| 1:A:73:ILE:CD1 | 1:A:73:ILE:CG1 | 1.77 | 1.56 |
| 1:B:348:LEU:CD1 | 1:B:348:LEU:CG | 1.75 | 1.56 |
| 1:B:349:LYS:CE | 1:B:349:LYS:NZ | 1.68 | 1.56 |
| 1:A:772:MET:CB | 1:A:772:MET:CG | 1.78 | 1.56 |
| 1:A:883:ILE:CB | 1:A:883:ILE:CG2 | 1.76 | 1.56 |
| 1:A:340:ILE:CG1 | 1:A:340:ILE:CD1 | 1.78 | 1.55 |
| 1:A:7:LYS:CE | 1:A:7:LYS:CD | 1.78 | 1.55 |
| 1:B:345:PRO:CG | 1:B:345:PRO:CD | 1.78 | 1.55 |
| 1:B:277:GLN:CG | 1:B:277:GLN:CB | 1.76 | 1.55 |
| 1:A:831:ASN:CB | 1:A:831:ASN:CG | 1.75 | 1.55 |
| 1:B:677:ILE:CG1 | 1:B:677:ILE:CD1 | 1.75 | 1.54 |
| 1:B:780:THR:CG2 | 1:B:780:THR:CB | 1.79 | 1.54 |
| 1:B:740:VAL:CB | 1:B:740:VAL:CG1 | 1.76 | 1.54 |
| 1:A:602:LEU:CG | 1:A:602:LEU:CD1 | 1.80 | 1.54 |
| 1:B:142:GLN:CB | 1:B:142:GLN:CG | 1.84 | 1.54 |
| 1:B:164:LYS:CD | 1:B:164:LYS:CG | 1.80 | 1.54 |
| 1:A:494:LYS:CE | 1:A:494:LYS:NZ | 1.68 | 1.54 |
| 1:B:337:LYS:HZ2 | 1:B:337:LYS:CB | 1.05 | 1.54 |
| 1:B:690:GLN:CG | 1:B:690:GLN:CB | 1.84 | 1.54 |
| 1:A:883:ILE:CG1 | 1:A:883:ILE:CD1 | 1.80 | 1.53 |
| 1:A:227:ILE:CG1 | 1:A:227:ILE:CD1 | 1.79 | 1.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 1:A:428:MET:CB | 1:A:428:MET:CG | 1.83 | 1.53 |
| 1:A:317:VAL:CA | 1:A:317:VAL:CB | 1.84 | 1.53 |
| 1:B:456:ALA:C | 1:B:456:ALA:CA | 1.74 | 1.53 |
| 1:A:570:ARG:CB | 1:A:570:ARG:CG | 1.81 | 1.53 |
| 1:B:494:LYS:CE | 1:B:494:LYS:CD | 1.77 | 1.53 |
| 1:B:883:ILE:CA | 1:B:883:ILE:CB | 1.81 | 1.52 |
| 1:B:26:LYS:CG | 1:B:26:LYS:CB | 1.77 | 1.52 |
| 1:A:388:LYS:NZ | 1:A:388:LYS:CE | 1.68 | 1.52 |
| 1:A:618:LEU:CD2 | 1:A:618:LEU:CG | 1.82 | 1.52 |
| 1:A:219:LYS:CG | 1:A:219:LYS:CD | 1.87 | 1.52 |
| 1:B:90:ASP:CB | 1:B:90:ASP:CG | 1.77 | 1.52 |
| 1:A:757:PRO:CG | 1:A:757:PRO:CD | 1.82 | 1.51 |
| 1:A:671:LEU:CA | 1:A:671:LEU:CB | 1.89 | 1.51 |
| 1:A:270:LYS:NZ | 1:A:270:LYS:CE | 1.73 | 1.50 |
| 1:A:26:LYS:NZ | 1:A:26:LYS:CE | 1.73 | 1.50 |
| 1:B:136:ALA:CA | 1:B:136:ALA:N | 1.67 | 1.50 |
| 1:A:450:LYS:NZ | 1:A:450:LYS:CE | 1.67 | 1.50 |
| 1:A:115:THR:CB | 1:A:115:THR:CG2 | 1.87 | 1.50 |
| 1:B:226:GLN:CG | 1:B:226:GLN:CD | 1.80 | 1.50 |
| 1:B:69:LYS:CG | 1:B:69:LYS:CB | 1.87 | 1.50 |
| 1:B:572:ASN:C | 1:B:572:ASN:CA | 1.77 | 1.50 |
| 1:B:480:PRO:CB | 1:B:480:PRO:CG | 1.80 | 1.50 |
| 1:B:824:GLU:CB | 1:B:824:GLU:CA | 1.86 | 1.49 |
| 1:B:440:ARG:CD | 1:B:440:ARG:CG | 1.86 | 1.49 |
| 1:A:218:GLN:CG | 1:A:218:GLN:CB | 1.87 | 1.49 |
| 1:A:174:ASN:CG | 1:A:174:ASN:CB | 1.78 | 1.48 |
| 1:A:615:LYS:CE | 1:A:615:LYS:NZ | 1.74 | 1.48 |
| 1:A:639:LYS:CE | 1:A:639:LYS:NZ | 1.77 | 1.48 |
| 1:B:341:CYS:SG | 1:B:341:CYS:CB | 2.02 | 1.48 |
| 1:B:346:ASP:CG | 1:B:346:ASP:CB | 1.78 | 1.47 |
| 1:B:643:GLN:CG | 1:B:643:GLN:CD | 1.78 | 1.47 |
| 1:A:652:PHE:CE1 | 1:A:667:CYS:HB2 | 1.46 | 1.47 |
| 1:A:452:ASP:CG | 1:A:452:ASP:CB | 1.82 | 1.47 |
| 1:A:120:ILE:CD1 | 1:A:120:ILE:CG1 | 1.89 | 1.46 |
| 1:B:312:ARG:CG | 1:B:312:ARG:CD | 1.90 | 1.46 |
| 1:B:284:MET:CE | 1:B:284:MET:SD | 2.03 | 1.46 |
| 1:A:631:MET:SD | 1:A:631:MET:CG | 2.02 | 1.46 |
| 1:A:6:MET:CE | 1:A:6:MET:SD | 2.04 | 1.46 |
| 1:B:746:MET:CE | 1:B:746:MET:SD | 2.04 | 1.46 |
| 1:A:680:GLN:CB | 1:A:680:GLN:CA | 1.92 | 1.46 |
| 1:A:731:VAL:HG21 | 1:A:733:LEU:CD1 | 1.46 | 1.46 |
| 1:B:319:MET:CE | 1:B:319:MET:SD | 2.04 | 1.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:869:ARG:CB | 1:B:869:ARG:CA | 1.92 | 1.45 |
| 1:B:316:ARG:CB | 1:B:316:ARG:CA | 1.93 | 1.44 |
| 1:A:582:MET:SD | 1:A:582:MET:CE | 2.03 | 1.44 |
| 1:B:837:MET:SD | 1:B:837:MET:CE | 2.05 | 1.43 |
| 1:B:67:SER:CB | 1:B:67:SER:CA | 1.96 | 1.42 |
| 1:A:414:MET:CE | 1:A:414:MET:SD | 2.06 | 1.42 |
| 1:A:891:MET:SD | 1:A:891:MET:CE | 2.09 | 1.40 |
| 1:B:582:MET:SD | 1:B:582:MET:CE | 2.10 | 1.40 |
| 1:B:332:ILE:CG2 | 1:B:332:ILE:CB | 1.98 | 1.39 |
| 1:A:337:LYS:NZ | 1:A:337:LYS:CE | 1.85 | 1.38 |
| 1:A:65:PRO:CB | 1:A:65:PRO:CG | 1.87 | 1.34 |
| 1:A:731:VAL:CG2 | 1:A:733:LEU:HD12 | 1.56 | 1.33 |
| 1:B:631:MET:CE | 1:B:631:MET:SD | 2.16 | 1.33 |
| 1:A:6:MET:CG | 1:A:6:MET:SD | 2.21 | 1.27 |
| 1:B:6:MET:SD | 1:B:6:MET:CE | 2.23 | 1.26 |
| 1:A:428:MET:CG | 1:A:428:MET:SD | 2.23 | 1.25 |
| 1:B:469:LEU:HD12 | 1:B:470:ARG:N | 1.49 | 1.24 |
| 1:B:6:MET:SD | 1:B:6:MET:CG | 2.26 | 1.23 |
| 1:B:296:PRO:HG3 | 2:B:946:HOH:O | 1.40 | 1.20 |
| 1:B:772:MET:CE | 1:B:772:MET:SD | 2.32 | 1.18 |
| 1:B:86:GLN:HG3 | 1:B:89:VAL:CG2 | 1.73 | 1.18 |
| 1:A:63:LEU:HD12 | 1:A:70:THR:HG23 | 1.18 | 1.18 |
| 1:B:440:ARG:HG2 | 1:B:441:GLU:N | 1.54 | 1.17 |
| 1:B:343:LEU:CD1 | 1:B:343:LEU:H | 1.52 | 1.15 |
| 1:A:710:MET:N | 2:A:1030:HOH:O | 1.80 | 1.14 |
| 1:A:258:LEU:HD22 | 1:A:258:LEU:C | 1.67 | 1.14 |
| 1:B:337:LYS:NZ | 1:B:337:LYS:HB3 | 1.06 | 1.14 |
| 1:A:327:SER:H | 1:A:329:ARG:NH1 | 1.46 | 1.12 |
| 1:B:21:HIS:HE1 | 1:B:123:ARG:HG2 | 1.10 | 1.11 |
| 1:A:63:LEU:HD12 | 1:A:70:THR:CG2 | 1.82 | 1.09 |
| 1:A:468:ASN:HB3 | 2:A:905:HOH:O | 1.49 | 1.09 |
| 1:B:295:GLY:HA3 | 1:B:298:SER:O | 1.52 | 1.09 |
| 1:B:651:ARG:CZ | 1:B:670:ARG:NH2 | 2.16 | 1.09 |
| 1:A:447:VAL:HG11 | 2:A:926:HOH:O | 1.53 | 1.09 |
| 1:A:631:MET:SD | 1:A:631:MET:CE | 2.41 | 1.08 |
| 1:B:538:THR:HG22 | 1:B:539:LEU:H | 1.13 | 1.08 |
| 1:A:698:SER:O | 1:A:701:VAL:N | 1.85 | 1.08 |
| 1:B:69:LYS:NZ | 1:B:69:LYS:CB | 2.16 | 1.08 |
| 1:B:343:LEU:N | 1:B:343:LEU:HD12 | 1.67 | 1.07 |
| 1:B:440:ARG:CG | 1:B:441:GLU:H | 1.67 | 1.07 |
| 1:B:805:ARG:N | 1:B:811:SER:HG | 1.49 | 1.07 |
| 1:B:850:ASP:O | 1:B:851:PHE:CB | 2.02 | 1.07 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:576:LEU:O | 1:B:578:SER:N | 1.88 | 1.06 |
| 1:B:308:ASP:OD1 | 1:B:308:ASP:N | 1.87 | 1.06 |
| 1:A:75:TRP:CZ3 | 1:A:159:PRO:HG3 | 1.90 | 1.06 |
| 1:A:306:LYS:HG3 | 1:A:307:VAL:N | 1.47 | 1.05 |
| 1:B:330:ASP:C | 1:B:330:ASP:OD1 | 1.90 | 1.04 |
| 1:B:389:ILE:H | 1:B:389:ILE:HD12 | 1.18 | 1.04 |
| 1:B:86:GLN:HG3 | 1:B:89:VAL:HG23 | 1.34 | 1.04 |
| 1:A:599:PHE:CD2 | 1:A:599:PHE:O | 2.10 | 1.03 |
| 1:B:440:ARG:HG2 | 1:B:441:GLU:H | 0.89 | 1.03 |
| 1:B:525:LYS:HB3 | 1:B:525:LYS:NZ | 1.72 | 1.03 |
| 1:A:665:VAL:O | 1:A:669:VAL:HG23 | 1.59 | 1.03 |
| 1:B:364:THR:OG1 | 1:B:646:GLN:NE2 | 1.92 | 1.02 |
| 1:B:651:ARG:CZ | 1:B:670:ARG:CZ | 2.37 | 1.02 |
| 1:A:652:PHE:CE1 | 1:A:667:CYS:CB | 2.43 | 1.02 |
| 1:B:429:GLU:O | 1:B:468:ASN:HB2 | 1.60 | 1.02 |
| 1:A:223:ASP:O | 1:A:227:ILE:HD12 | 1.58 | 1.01 |
| 1:B:538:THR:O | 1:B:539:LEU:HB2 | 1.59 | 1.01 |
| 1:A:832:GLN:OE1 | 1:A:832:GLN:C | 2.00 | 1.01 |
| 1:B:69:LYS:HB3 | 1:B:69:LYS:NZ | 1.74 | 1.01 |
| 1:B:740:VAL:HG12 | 1:B:741:SER:H | 1.26 | 1.00 |
| 1:A:596:LEU:O | 2:A:995:HOH:O | 1.78 | 1.00 |
| 1:A:155:ASP:C | 1:A:155:ASP:OD2 | 1.95 | 1.00 |
| 1:B:850:ASP:O | 1:B:851:PHE:HB2 | 1.20 | 1.00 |
| 1:B:21:HIS:CE1 | 1:B:123:ARG:HG2 | 1.96 | 1.00 |
| 1:B:784:LEU:HB3 | 1:B:788:GLU:O | 1.63 | 0.99 |
| 1:A:106:TRP:CH2 | 1:A:198:GLY:HA3 | 1.98 | 0.99 |
| 1:B:651:ARG:HG3 | 2:B:914:HOH:O | 1.61 | 0.99 |
| 1:A:731:VAL:HG11 | 1:A:733:LEU:HD11 | 1.44 | 0.99 |
| 1:A:702:LEU:HD21 | 2:A:1036:HOH:O | 1.63 | 0.99 |
| 1:B:773:VAL:HA | 1:B:784:LEU:HD21 | 1.45 | 0.99 |
| 1:B:61:LYS:H | 1:B:65:PRO:HD2 | 1.28 | 0.98 |
| 1:B:670:ARG:HA | 1:B:673:ILE:HD12 | 1.42 | 0.98 |
| 1:A:256:LYS:CD | 1:A:258:LEU:HD21 | 1.92 | 0.98 |
| 1:B:343:LEU:HD12 | 1:B:343:LEU:H | 0.81 | 0.98 |
| 1:A:256:LYS:HD3 | 1:A:258:LEU:HD11 | 1.42 | 0.98 |
| 1:A:689:ILE:C | 1:A:689:ILE:HD12 | 1.83 | 0.97 |
| 1:B:69:LYS:HZ3 | 1:B:69:LYS:HB3 | 1.27 | 0.97 |
| 1:B:525:LYS:HB3 | 1:B:525:LYS:HZ2 | 1.28 | 0.96 |
| 1:B:331:PHE:N | 1:B:331:PHE:CD2 | 2.20 | 0.96 |
| 1:B:469:LEU:HD12 | 1:B:470:ARG:H | 1.22 | 0.96 |
| 1:B:375:ARG:HH11 | 1:B:375:ARG:HB2 | 1.30 | 0.95 |
| 1:B:389:ILE:N | 1:B:389:ILE:HD12 | 1.75 | 0.95 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:465:HIS:ND1 | 1:A:465:HIS:N | 2.13 | 0.95 |
| 1:A:619:ASP:O | 1:A:620:LYS:C | 2.03 | 0.95 |
| 1:A:270:LYS:HB2 | 1:A:325:TRP:CH2 | 2.02 | 0.95 |
| 1:B:839:ILE:O | 1:B:843:SER:N | 2.00 | 0.95 |
| 1:A:270:LYS:HB2 | 1:A:325:TRP:HH2 | 1.29 | 0.94 |
| 1:A:77:ARG:HG2 | 1:A:156:ASP:OD2 | 1.66 | 0.94 |
| 1:B:4:ILE:HD11 | 1:B:889:LEU:HA | 1.49 | 0.94 |
| 1:A:256:LYS:HD3 | 1:A:258:LEU:HD21 | 1.48 | 0.94 |
| 1:B:579:CYS:O | 1:B:583:VAL:HG12 | 1.66 | 0.93 |
| 1:A:881:VAL:HG12 | 1:A:885:GLU:OE2 | 1.67 | 0.93 |
| 1:A:75:TRP:CH2 | 1:A:159:PRO:HG3 | 2.03 | 0.93 |
| 1:B:440:ARG:CG | 1:B:440:ARG:HH21 | 1.80 | 0.93 |
| 1:B:585:LEU:HG | 1:B:586:MET:HE2 | 1.50 | 0.93 |
| 1:B:538:THR:O | 1:B:539:LEU:CB | 2.16 | 0.93 |
| 1:A:218:GLN:HA | 1:A:218:GLN:CB | 1.99 | 0.92 |
| 1:B:256:LYS:HB3 | 1:B:256:LYS:NZ | 1.82 | 0.92 |
| 1:A:332:ILE:HB | 1:A:332:ILE:CG1 | 1.98 | 0.92 |
| 1:B:740:VAL:HG21 | 1:B:789:PHE:HD1 | 1.35 | 0.92 |
| 1:A:306:LYS:HG3 | 1:A:307:VAL:H | 1.26 | 0.91 |
| 1:A:4:ILE:HD12 | 1:A:5:ALA:N | 1.85 | 0.91 |
| 1:A:228:ILE:O | 1:A:232:LEU:HD23 | 1.71 | 0.91 |
| 1:B:795:ASN:O | 1:B:799:TRP:CD1 | 2.23 | 0.91 |
| 1:B:337:LYS:HZ3 | 1:B:337:LYS:HB3 | 1.32 | 0.91 |
| 1:A:395:ASP:H | 1:A:406:GLY:HA3 | 1.30 | 0.91 |
| 1:B:4:ILE:CD1 | 1:B:889:LEU:HA | 2.00 | 0.91 |
| 1:A:30:GLN:HE22 | 1:A:187:LYS:NZ | 1.67 | 0.90 |
| 1:B:390:ARG:HG2 | 1:B:390:ARG:HH11 | 1.36 | 0.90 |
| 1:B:88:ILE:HG23 | 1:B:88:ILE:O | 1.69 | 0.90 |
| 1:A:336:THR:HG23 | 1:A:337:LYS:N | 1.86 | 0.90 |
| 1:A:13:GLU:O | 1:A:16:GLU:N | 2.05 | 0.90 |
| 1:B:701:VAL:HG13 | 1:B:860:ARG:HH11 | 1.33 | 0.90 |
| 1:B:468:ASN:O | 1:B:468:ASN:OD1 | 1.90 | 0.90 |
| 1:B:607:ARG:HH21 | 1:B:607:ARG:HB3 | 1.37 | 0.90 |
| 1:A:13:GLU:O | 1:A:16:GLU:HG2 | 1.72 | 0.89 |
| 1:A:73:ILE:HD11 | 2:A:1032:HOH:O | 1.70 | 0.89 |
| 1:B:343:LEU:CD2 | 1:B:343:LEU:CB | 2.50 | 0.89 |
| 1:A:305:ASN:HD22 | 1:A:306:LYS:N | 1.71 | 0.89 |
| 1:A:822:ALA:HA | 1:A:825:ALA:HB3 | 1.54 | 0.89 |
| 1:B:116:LEU:HD11 | 1:B:287:PRO:HG3 | 1.53 | 0.88 |
| 1:A:254:THR:N | 2:A:1011:HOH:O | 2.05 | 0.88 |
| 1:B:626:ALA:HB1 | 1:B:649:VAL:HG22 | 1.56 | 0.88 |
| 1:B:667:CYS:O | 1:B:668:LEU:C | 2.09 | 0.88 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:327:SER:H | 1:A:329:ARG:HH11 | 1.21 | 0.87 |
| 1:A:618:LEU:CD2 | 1:A:618:LEU:HG | 2.01 | 0.87 |
| 1:B:517:ILE:H | 1:B:517:ILE:HD12 | 1.36 | 0.87 |
| 1:B:438:VAL:HG22 | 1:B:484:ILE:CD1 | 2.04 | 0.87 |
| 1:A:132:GLN:O | 1:A:133:GLU:C | 2.12 | 0.87 |
| 1:B:89:VAL:CB | 1:B:89:VAL:C | 2.42 | 0.87 |
| 1:A:389:ILE:HG22 | 1:A:390:ARG:N | 1.88 | 0.87 |
| 1:B:479:PRO:O | 1:B:483:TYR:OH | 1.92 | 0.86 |
| 1:A:358:THR:O | 1:A:359:THR:HG23 | 1.75 | 0.86 |
| 1:A:327:SER:N | 1:A:329:ARG:NH1 | 2.22 | 0.86 |
| 1:B:69:LYS:HZ2 | 1:B:69:LYS:CB | 1.86 | 0.86 |
| 1:B:790:LYS:O | 1:B:791:TYR:C | 2.13 | 0.86 |
| 1:A:63:LEU:CD1 | 1:A:70:THR:HG23 | 2.05 | 0.86 |
| 1:B:651:ARG:NH1 | 1:B:670:ARG:NH1 | 2.23 | 0.86 |
| 1:B:469:LEU:C | 1:B:469:LEU:HD12 | 1.93 | 0.85 |
| 1:B:629:MET:SD | 1:B:633:ILE:HD11 | 2.16 | 0.85 |
| 1:B:822:ALA:O | 1:B:825:ALA:HB3 | 1.74 | 0.85 |
| 1:B:331:PHE:HD2 | 1:B:331:PHE:N | 1.70 | 0.85 |
| 1:A:558:ILE:HG22 | 1:A:559:LEU:N | 1.89 | 0.85 |
| 1:B:554:GLU:O | 1:B:557:THR:HB | 1.76 | 0.85 |
| 1:B:499:LEU:HD23 | 2:B:948:HOH:O | 1.76 | 0.85 |
| 1:B:120:ILE:CG2 | 1:B:120:ILE:CG1 | 2.54 | 0.85 |
| 1:A:853:ASN:N | 1:A:853:ASN:HD22 | 1.73 | 0.85 |
| 1:B:8:LEU:HD13 | 1:B:885:GLU:HG2 | 1.59 | 0.85 |
| 1:B:95:THR:OG1 | 1:B:97:ILE:HG22 | 1.77 | 0.85 |
| 1:A:822:ALA:CA | 1:A:825:ALA:HB3 | 2.06 | 0.85 |
| 1:A:388:LYS:HZ1 | 1:A:482:GLU:CD | 1.81 | 0.84 |
| 1:B:658:ILE:CG2 | 1:B:658:ILE:O | 2.25 | 0.84 |
| 1:B:538:THR:HG22 | 1:B:539:LEU:N | 1.90 | 0.84 |
| 1:A:611:THR:O | 1:A:611:THR:HG22 | 1.75 | 0.84 |
| 1:B:670:ARG:O | 1:B:674:LEU:HD22 | 1.77 | 0.84 |
| 1:B:724:ARG:HB2 | 1:B:724:ARG:HH21 | 1.41 | 0.84 |
| 1:A:358:THR:HG22 | 1:A:359:THR:N | 1.92 | 0.84 |
| 1:B:537:LYS:HB2 | 1:B:537:LYS:HZ2 | 1.42 | 0.84 |
| 1:B:97:ILE:HD11 | 1:B:108:LEU:CD1 | 2.08 | 0.84 |
| 1:A:832:GLN:CD | 1:A:833:HIS:H | 1.79 | 0.84 |
| 1:A:329:ARG:HD2 | 1:A:333:ARG:HH12 | 1.42 | 0.83 |
| 1:A:296:PRO:CG | 1:A:304:TRP:HB2 | 2.07 | 0.83 |
| 1:A:296:PRO:O | 1:A:297:TRP:HB2 | 1.79 | 0.83 |
| 1:A:731:VAL:CG2 | 1:A:733:LEU:CD1 | 2.34 | 0.83 |
| 1:A:478:LEU:HG | 1:A:478:LEU:CD1 | 2.08 | 0.83 |
| 1:A:31:ASP:C | 1:A:31:ASP:OD2 | 2.14 | 0.83 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:831:ASN:HB3 | 1:B:833:HIS:CB | 2.08 | 0.83 |
| 1:A:766:ILE:HD11 | 2:A:967:HOH:O | 1.77 | 0.83 |
| 1:A:756:HIS:CB | 1:A:757:PRO:HD2 | 2.06 | 0.83 |
| 1:B:86:GLN:HG3 | 1:B:89:VAL:HG21 | 1.59 | 0.83 |
| 1:A:89:VAL:CG2 | 1:A:89:VAL:CG1 | 2.56 | 0.83 |
| 1:A:41:GLU:OE2 | 2:A:974:HOH:O | 1.97 | 0.83 |
| 1:B:135:TYR:C | 1:B:136:ALA:CA | 2.47 | 0.82 |
| 1:A:13:GLU:HA | 1:A:13:GLU:OE1 | 1.77 | 0.82 |
| 1:A:748:ILE:HG23 | 1:A:749:LEU:HD22 | 1.61 | 0.82 |
| 1:B:469:LEU:CD1 | 1:B:470:ARG:H | 1.92 | 0.82 |
| 1:A:582:MET:HB3 | 1:A:602:LEU:HD11 | 1.62 | 0.82 |
| 1:B:242:ILE:HD13 | 1:B:243:ASN:N | 1.94 | 0.82 |
| 1:A:301:SER:O | 1:A:302:TYR:O | 1.98 | 0.82 |
| 1:B:296:PRO:HB3 | 2:B:946:HOH:O | 1.79 | 0.82 |
| 1:B:364:THR:HG1 | 1:B:646:GLN:HE22 | 1.26 | 0.82 |
| 1:A:519:ALA:HB2 | 1:A:675:PHE:CE1 | 2.15 | 0.82 |
| 1:B:801:GLY:O | 2:B:975:HOH:O | 1.97 | 0.82 |
| 1:B:8:LEU:O | 1:B:9:ALA:C | 2.17 | 0.82 |
| 1:A:198:GLY:O | 1:A:199:CYS:HB2 | 1.80 | 0.82 |
| 1:B:524:GLU:N | 1:B:524:GLU:OE1 | 2.12 | 0.82 |
| 1:A:822:ALA:C | 1:A:825:ALA:HB3 | 2.00 | 0.82 |
| 1:B:492:PRO:HB2 | 1:B:493:ASN:ND2 | 1.95 | 0.82 |
| 1:A:799:TRP:CH2 | 1:A:858:LEU:O | 2.32 | 0.82 |
| 1:B:343:LEU:CD2 | 1:B:343:LEU:CD1 | 2.58 | 0.81 |
| 1:A:429:GLU:OE1 | 1:A:494:LYS:NZ | 2.12 | 0.81 |
| 1:B:86:GLN:CG | 1:B:89:VAL:CG2 | 2.57 | 0.81 |
| 1:A:821:GLY:HA3 | 2:A:1015:HOH:O | 1.81 | 0.81 |
| 1:B:223:ASP:O | 1:B:227:ILE:HG13 | 1.80 | 0.81 |
| 1:A:106:TRP:CZ2 | 1:A:198:GLY:HA3 | 2.14 | 0.81 |
| 1:A:366:ARG:CD | 1:A:366:ARG:CB | 2.58 | 0.81 |
| 1:B:430:THR:HA | 1:B:468:ASN:HB2 | 1.62 | 0.81 |
| 1:B:390:ARG:HG2 | 1:B:390:ARG:NH1 | 1.91 | 0.81 |
| 1:A:221:PRO:HB2 | 1:A:223:ASP:OD2 | 1.79 | 0.81 |
| 1:A:808:THR:O | 1:A:808:THR:CG2 | 2.29 | 0.81 |
| 1:B:651:ARG:NH2 | 1:B:670:ARG:CZ | 2.42 | 0.81 |
| 1:B:457:ASN:H | 1:B:457:ASN:HD22 | 1.29 | 0.81 |
| 1:A:100:GLY:HA3 | 1:A:103:GLY:HA3 | 1.61 | 0.81 |
| 1:A:665:VAL:HG23 | 1:A:666:ARG:N | 1.96 | 0.81 |
| 1:B:144:TRP:CZ2 | 1:B:147:GLY:HA2 | 2.16 | 0.81 |
| 1:B:555:LEU:O | 1:B:556:GLN:C | 2.18 | 0.81 |
| 1:A:832:GLN:CD | 1:A:833:HIS:N | 2.34 | 0.81 |
| 1:B:440:ARG:HG2 | 1:B:440:ARG:HH21 | 1.44 | 0.81 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:832:GLN:OE1 | 1:A:832:GLN:CA | 2.29 | 0.81 |
| 1:A:825:ALA:HB2 | 2:A:912:HOH:O | 1.80 | 0.80 |
| 1:B:572:ASN:HA | 1:B:572:ASN:C | 2.00 | 0.80 |
| 1:A:256:LYS:HD2 | 1:A:258:LEU:HD21 | 1.64 | 0.80 |
| 1:A:4:ILE:HD12 | 1:A:4:ILE:C | 1.99 | 0.80 |
| 1:B:80:GLU:O | 1:B:81:LEU:HD23 | 1.82 | 0.80 |
| 1:B:211:VAL:HG12 | 1:B:341:CYS:HB2 | 1.64 | 0.80 |
| 1:A:50:ALA:C | 1:A:52:PRO:HD3 | 2.02 | 0.80 |
| 1:B:653:ALA:O | 2:B:1022:HOH:O | 1.98 | 0.80 |
| 1:A:651:ARG:NH1 | 1:A:651:ARG:O | 2.15 | 0.79 |
| 1:B:677:ILE:O | 1:B:681:LEU:HG | 1.83 | 0.79 |
| 1:B:740:VAL:HG21 | 1:B:789:PHE:CD1 | 2.17 | 0.79 |
| 1:A:329:ARG:HG2 | 1:A:329:ARG:NH2 | 1.96 | 0.79 |
| 1:A:99:GLN:CB | 1:A:99:GLN:C | 2.48 | 0.79 |
| 1:A:258:LEU:CD2 | 1:A:258:LEU:C | 2.46 | 0.79 |
| 1:A:739:GLU:N | 2:A:979:HOH:O | 2.05 | 0.79 |
| 1:B:525:LYS:NZ | 1:B:525:LYS:CB | 2.45 | 0.79 |
| 1:B:264:TYR:HE2 | 1:B:286:ASN:HB2 | 1.48 | 0.79 |
| 1:A:808:THR:O | 1:A:808:THR:HG23 | 1.81 | 0.79 |
| 1:A:652:PHE:HE1 | 1:A:667:CYS:HB2 | 1.45 | 0.79 |
| 1:A:258:LEU:H | 1:A:258:LEU:CD1 | 1.96 | 0.79 |
| 1:A:365:TRP:CZ2 | 1:A:488:SER:HA | 2.18 | 0.79 |
| 1:A:211:VAL:HG23 | 1:A:211:VAL:O | 1.81 | 0.79 |
| 1:A:682:ASP:OD1 | 1:A:685:ASN:HA | 1.83 | 0.79 |
| 1:A:217:LEU:O | 1:A:220:ALA:HB2 | 1.83 | 0.79 |
| 1:A:605:ARG:NH1 | 2:A:1034:HOH:O | 2.07 | 0.78 |
| 1:A:832:GLN:OE1 | 1:A:833:HIS:N | 2.15 | 0.78 |
| 1:A:13:GLU:HA | 1:A:16:GLU:HG2 | 1.65 | 0.78 |
| 1:B:69:LYS:HZ2 | 1:B:69:LYS:HB2 | 1.46 | 0.78 |
| 1:B:576:LEU:O | 1:B:579:CYS:N | 2.17 | 0.78 |
| 1:B:277:GLN:CG | 1:B:277:GLN:CA | 2.60 | 0.78 |
| 1:B:89:VAL:O | 1:B:89:VAL:HB | 1.84 | 0.78 |
| 1:B:170:SER:O | 1:B:172:GLN:N | 2.17 | 0.78 |
| 1:B:136:ALA:HA | 1:B:136:ALA:N | 1.94 | 0.78 |
| 1:B:553:LYS:CB | 1:B:553:LYS:HA | 2.12 | 0.78 |
| 1:B:17:GLY:O | 1:B:20:SER:OG | 2.01 | 0.78 |
| 1:A:158:LEU:HB3 | 1:A:165:LEU:HD11 | 1.66 | 0.78 |
| 1:B:309:PRO:O | 1:B:313:GLU:OE1 | 2.02 | 0.78 |
| 1:B:651:ARG:NE | 1:B:670:ARG:NH2 | 2.32 | 0.78 |
| 1:B:69:LYS:CE | 1:B:69:LYS:CB | 2.62 | 0.78 |
| 1:B:313:GLU:CA | 1:B:313:GLU:CG | 2.62 | 0.77 |
| 1:A:594:LEU:O | 1:A:598:GLU:OE2 | 2.01 | 0.77 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:323:GLU:OE2 | 1:B:323:GLU:HA | 1.84 | 0.77 |
| 1:A:832:GLN:N | 2:A:919:HOH:O | 2.16 | 0.77 |
| 1:B:439:PRO:HB2 | 1:B:440:ARG:HD3 | 1.65 | 0.77 |
| 1:B:601:ILE:HD12 | 2:B:987:HOH:O | 1.82 | 0.77 |
| 1:A:493:ASN:ND2 | 1:A:627:TYR:OH | 2.18 | 0.77 |
| 1:B:25:ILE:CD1 | 1:B:148:GLU:OE1 | 2.32 | 0.77 |
| 1:A:373:GLY:HA3 | 1:A:492:PRO:HG3 | 1.65 | 0.77 |
| 1:B:8:LEU:CD2 | 1:B:8:LEU:HG | 2.10 | 0.77 |
| 1:B:576:LEU:O | 1:B:577:GLU:C | 2.22 | 0.77 |
| 1:B:61:LYS:HG3 | 1:B:65:PRO:O | 1.84 | 0.77 |
| 1:A:306:LYS:O | 1:A:307:VAL:C | 2.22 | 0.77 |
| 1:B:61:LYS:HG3 | 1:B:66:ASN:HB2 | 1.65 | 0.77 |
| 1:A:13:GLU:CA | 1:A:16:GLU:HG2 | 2.15 | 0.77 |
| 1:B:701:VAL:CG1 | 1:B:860:ARG:HG2 | 2.15 | 0.77 |
| 1:A:386:GLN:HB3 | 1:A:513:LEU:HB3 | 1.67 | 0.77 |
| 1:A:822:ALA:HA | 1:A:825:ALA:CB | 2.14 | 0.77 |
| 1:B:601:ILE:HD13 | 1:B:604:ASN:ND2 | 1.99 | 0.77 |
| 1:A:122:HIS:HA | 1:A:125:VAL:O | 1.84 | 0.77 |
| 1:B:202:GLU:CB | 1:B:470:ARG:HH11 | 1.98 | 0.77 |
| 1:B:328:PHE:O | 1:B:331:PHE:CE2 | 2.38 | 0.77 |
| 1:B:796:ILE:O | 1:B:799:TRP:HB2 | 1.85 | 0.76 |
| 1:B:361:TYR:O | 1:B:499:LEU:HA | 1.85 | 0.76 |
| 1:B:161:LYS:O | 1:B:163:GLY:N | 2.18 | 0.76 |
| 1:B:795:ASN:O | 1:B:799:TRP:CG | 2.38 | 0.76 |
| 1:B:86:GLN:CG | 1:B:89:VAL:HG23 | 2.14 | 0.76 |
| 1:B:740:VAL:CG1 | 1:B:741:SER:H | 1.98 | 0.76 |
| 1:B:430:THR:HA | 1:B:468:ASN:CB | 2.14 | 0.76 |
| 1:A:350:SER:C | 1:A:352:THR:H | 1.88 | 0.76 |
| 1:A:68:SER:O | 1:A:69:LYS:C | 2.24 | 0.76 |
| 1:B:537:LYS:CB | 1:B:537:LYS:NZ | 2.48 | 0.76 |
| 1:A:114:LEU:HD13 | 1:A:121:LEU:HD23 | 1.67 | 0.76 |
| 1:A:314:GLN:HG3 | 1:A:315:LEU:N | 1.99 | 0.76 |
| 1:B:607:ARG:CB | 1:B:607:ARG:HH21 | 1.99 | 0.76 |
| 1:B:106:TRP:CZ3 | 1:B:107:LEU:HD12 | 2.21 | 0.76 |
| 1:A:293:TRP:O | 1:A:295:GLY:N | 2.18 | 0.76 |
| 1:B:35:LEU:HD13 | 1:B:46:PHE:CE1 | 2.21 | 0.75 |
| 1:B:348:LEU:CD1 | 1:B:348:LEU:CD2 | 2.64 | 0.75 |
| 1:A:333:ARG:O | 1:A:334:GLU:HB2 | 1.86 | 0.75 |
| 1:B:470:ARG:CG | 1:B:470:ARG:CA | 2.64 | 0.75 |
| 1:B:729:LEU:CD1 | 1:B:729:LEU:CD2 | 2.63 | 0.75 |
| 1:A:84:ASN:O | 1:A:84:ASN:OD1 | 2.03 | 0.75 |
| 1:A:13:GLU:C | 1:A:16:GLU:HG2 | 2.06 | 0.75 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:731:VAL:HG21 | 1:A:733:LEU:CG | 2.15 | 0.75 |
| 1:A:205:GLU:HG2 | 1:A:210:GLY:O | 1.85 | 0.75 |
| 1:B:294:LYS:CB | 1:B:294:LYS:CD | 2.65 | 0.75 |
| 1:A:75:TRP:CZ3 | 1:A:159:PRO:CG | 2.68 | 0.75 |
| 1:A:329:ARG:NH2 | 1:A:329:ARG:CG | 2.48 | 0.75 |
| 1:A:306:LYS:CG | 1:A:307:VAL:N | 2.40 | 0.75 |
| 1:B:25:ILE:HD11 | 1:B:148:GLU:OE1 | 1.87 | 0.75 |
| 1:B:98:CYS:SG | 1:B:171:ALA:HB2 | 2.28 | 0.74 |
| 1:A:655:ASP:HB2 | 1:A:656:GLU:OE1 | 1.87 | 0.74 |
| 1:A:296:PRO:HG2 | 1:A:304:TRP:HB2 | 1.70 | 0.74 |
| 1:A:411:LEU:HD11 | 1:A:485:VAL:HG21 | 1.69 | 0.74 |
| 1:B:820:PRO:HB2 | 1:B:822:ALA:H | 1.51 | 0.74 |
| 1:A:44:ALA:HA | 2:A:966:HOH:O | 1.87 | 0.74 |
| 1:A:317:VAL:HB | 1:A:317:VAL:CA | 2.15 | 0.74 |
| 1:B:585:LEU:CG | 1:B:586:MET:HE2 | 2.18 | 0.74 |
| 1:B:212:THR:CB | 1:B:340:ILE:HD13 | 2.17 | 0.74 |
| 1:A:326:MET:SD | 1:A:330:ASP:HB2 | 2.28 | 0.74 |
| 1:A:300:ASN:N | 1:A:300:ASN:ND2 | 2.36 | 0.74 |
| 1:A:329:ARG:O | 1:A:329:ARG:CG | 2.36 | 0.74 |
| 1:B:457:ASN:H | 1:B:457:ASN:ND2 | 1.86 | 0.74 |
| 1:B:466:PHE:CD2 | 1:B:490:PHE:HD1 | 2.05 | 0.74 |
| 1:A:652:PHE:CD1 | 1:A:667:CYS:HB2 | 2.23 | 0.73 |
| 1:B:88:ILE:HD11 | 1:B:121:LEU:HD21 | 1.70 | 0.73 |
| 1:B:97:ILE:HD11 | 1:B:108:LEU:HD11 | 1.70 | 0.73 |
| 1:A:821:GLY:CA | 2:A:1015:HOH:O | 2.37 | 0.73 |
| 1:B:802:ILE:O | 1:B:802:ILE:CG2 | 2.35 | 0.73 |
| 1:B:228:ILE:CG1 | 1:B:228:ILE:CG2 | 2.65 | 0.73 |
| 1:A:329:ARG:HD2 | 1:A:333:ARG:NH1 | 2.04 | 0.73 |
| 1:B:469:LEU:CD1 | 1:B:470:ARG:N | 2.40 | 0.73 |
| 1:A:610:LEU:CD2 | 1:A:610:LEU:CB | 2.65 | 0.73 |
| 1:B:204:PHE:HB3 | 1:B:340:ILE:HG13 | 1.69 | 0.73 |
| 1:A:307:VAL:HA | 2:A:909:HOH:O | 1.88 | 0.73 |
| 1:A:652:PHE:CZ | 1:A:667:CYS:HB2 | 2.17 | 0.73 |
| 1:A:395:ASP:N | 1:A:406:GLY:HA3 | 2.03 | 0.73 |
| 1:A:731:VAL:HG11 | 1:A:733:LEU:CD1 | 2.19 | 0.73 |
| 1:B:106:TRP:CZ3 | 1:B:107:LEU:CD1 | 2.72 | 0.73 |
| 1:B:88:ILE:CB | 1:B:88:ILE:CD1 | 2.66 | 0.73 |
| 1:A:517:ILE:HD12 | 1:A:883:ILE:HG23 | 1.71 | 0.72 |
| 1:A:293:TRP:NE1 | 2:A:1024:HOH:O | 2.21 | 0.72 |
| 1:A:380:THR:O | 1:A:382:TRP:N | 2.22 | 0.72 |
| 1:A:228:ILE:HG12 | 1:A:337:LYS:NZ | 2.04 | 0.72 |
| 1:A:731:VAL:HG23 | 1:A:733:LEU:H | 1.55 | 0.72 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:61:LYS:N | 1:B:65:PRO:HD2 | 2.04 | 0.72 |
| 1:A:808:THR:C | 1:A:808:THR:CG2 | 2.57 | 0.72 |
| 1:A:230:LYS:NZ | 1:A:233:GLU:OE1 | 2.22 | 0.72 |
| 1:B:383:VAL:CG1 | 1:B:383:VAL:O | 2.37 | 0.72 |
| 1:A:602:LEU:CD1 | 1:A:602:LEU:CD2 | 2.67 | 0.72 |
| 1:B:438:VAL:HG22 | 1:B:484:ILE:HD11 | 1.71 | 0.72 |
| 1:B:27:TYR:CE2 | 1:B:28:LEU:HD12 | 2.25 | 0.72 |
| 1:A:158:LEU:O | 1:A:160:THR:HG23 | 1.90 | 0.72 |
| 1:B:556:GLN:O | 1:B:557:THR:C | 2.29 | 0.72 |
| 1:B:670:ARG:O | 1:B:674:LEU:CD2 | 2.37 | 0.71 |
| 1:B:330:ASP:O | 1:B:330:ASP:OD1 | 2.08 | 0.71 |
| 1:B:729:LEU:HG | 1:B:729:LEU:CD2 | 2.12 | 0.71 |
| 1:B:120:ILE:CG2 | 1:B:120:ILE:CA | 2.65 | 0.71 |
| 1:B:521:LEU:HD11 | 1:B:638:PHE:CZ | 2.26 | 0.71 |
| 1:B:447:VAL:CB | 1:B:513:LEU:CD1 | 2.69 | 0.71 |
| 1:A:414:MET:HB2 | 2:A:901:HOH:O | 1.89 | 0.71 |
| 1:B:49:PRO:HG2 | 2:B:935:HOH:O | 1.89 | 0.71 |
| 1:A:610:LEU:HG | 1:A:610:LEU:CD2 | 2.13 | 0.71 |
| 1:A:89:VAL:H | 1:A:175:GLU:CD | 1.93 | 0.71 |
| 1:B:874:ASN:O | 1:B:876:THR:N | 2.24 | 0.71 |
| 1:A:883:ILE:CG1 | 1:A:883:ILE:CG2 | 2.66 | 0.71 |
| 1:A:519:ALA:HB2 | 1:A:675:PHE:CZ | 2.24 | 0.71 |
| 1:B:339:GLU:OE2 | 1:B:339:GLU:N | 2.22 | 0.71 |
| 1:B:836:SER:OG | 2:B:953:HOH:O | 2.07 | 0.71 |
| 1:A:97:ILE:HD13 | 1:A:108:LEU:HD12 | 1.72 | 0.71 |
| 1:B:778:SER:C | 1:B:779:ASP:OD1 | 2.29 | 0.71 |
| 1:A:756:HIS:CG | 1:A:757:PRO:HD2 | 2.26 | 0.71 |
| 1:B:443:ALA:HB3 | 2:B:894:HOH:O | 1.89 | 0.71 |
| 1:A:158:LEU:CB | 1:A:165:LEU:HD11 | 2.21 | 0.71 |
| 1:B:390:ARG:HD2 | 1:B:482:GLU:HG2 | 1.72 | 0.71 |
| 1:B:538:THR:CG2 | 1:B:539:LEU:H | 1.98 | 0.71 |
| 1:B:810:ARG:O | 1:B:811:SER:HB2 | 1.91 | 0.71 |
| 1:A:599:PHE:C | 1:A:599:PHE:CD2 | 2.64 | 0.71 |
| 1:A:611:THR:O | 1:A:611:THR:CG2 | 2.38 | 0.71 |
| 1:B:238:LEU:HD12 | 1:B:238:LEU:N | 2.06 | 0.71 |
| 1:B:607:ARG:O | 1:B:610:LEU:HG | 1.91 | 0.70 |
| 1:A:31:ASP:OD2 | 1:A:32:TYR:N | 2.24 | 0.70 |
| 1:A:96:ASP:HB2 | 1:A:171:ALA:H | 1.55 | 0.70 |
| 1:B:537:LYS:CG | 1:B:537:LYS:CE | 2.69 | 0.70 |
| 1:A:242:ILE:HG13 | 1:A:242:ILE:O | 1.90 | 0.70 |
| 1:A:199:CYS:SG | 1:A:202:GLU:HG3 | 2.31 | 0.70 |
| 1:B:784:LEU:HD12 | 1:B:784:LEU:N | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:860:ARG:HD2 | 2:A:1023:HOH:O | 1.90 | 0.70 |
| 1:A:105:SER:O | 1:A:106:TRP:C | 2.28 | 0.70 |
| 1:A:30:GLN:HE22 | 1:A:187:LYS:HZ3 | 1.38 | 0.70 |
| 1:B:661:PHE:O | 1:B:665:VAL:HG13 | 1.92 | 0.70 |
| 1:A:808:THR:CA | 1:A:808:THR:CG2 | 2.70 | 0.70 |
| 1:A:428:MET:CE | 2:A:970:HOH:O | 2.38 | 0.70 |
| 1:B:525:LYS:HB3 | 1:B:525:LYS:HZ3 | 1.57 | 0.70 |
| 1:B:874:ASN:O | 1:B:875:GLY:C | 2.30 | 0.70 |
| 1:B:146:PHE:HB3 | 1:B:416:LYS:HG2 | 1.72 | 0.70 |
| 1:B:697:LEU:HA | 1:B:700:SER:OG | 1.92 | 0.70 |
| 1:A:290:GLU:CD | 1:A:290:GLU:H | 1.92 | 0.70 |
| 1:A:157:LEU:C | 1:A:158:LEU:HG | 2.11 | 0.70 |
| 1:A:336:THR:CG2 | 1:A:337:LYS:N | 2.55 | 0.70 |
| 1:A:350:SER:O | 1:A:352:THR:CG2 | 2.40 | 0.70 |
| 1:B:89:VAL:CG1 | 1:B:89:VAL:HB | 2.14 | 0.70 |
| 1:B:740:VAL:HG12 | 1:B:741:SER:N | 2.06 | 0.70 |
| 1:B:264:TYR:CE2 | 1:B:286:ASN:HB2 | 2.26 | 0.70 |
| 1:B:318:LYS:O | 1:B:320:GLU:N | 2.25 | 0.70 |
| 1:B:256:LYS:HB3 | 1:B:256:LYS:HZ2 | 1.57 | 0.69 |
| 1:B:296:PRO:HD2 | 2:B:912:HOH:O | 1.91 | 0.69 |
| 1:A:833:HIS:CD2 | 1:A:833:HIS:C | 2.64 | 0.69 |
| 1:B:430:THR:O | 1:B:489:THR:HA | 1.92 | 0.69 |
| 1:A:467:ILE:HG22 | 1:A:468:ASN:H | 1.56 | 0.69 |
| 1:B:376:ASN:C | 1:B:378:PRO:HD3 | 2.12 | 0.69 |
| 1:B:605:ARG:HG2 | 1:B:605:ARG:HH21 | 1.56 | 0.69 |
| 1:B:537:LYS:CB | 1:B:537:LYS:CD | 2.69 | 0.69 |
| 1:A:364:THR:HG22 | 1:A:497:ASP:OD1 | 1.92 | 0.69 |
| 1:B:656:GLU:OE2 | 1:B:656:GLU:HA | 1.89 | 0.69 |
| 1:B:123:ARG:NH1 | 1:B:346:ASP:OD1 | 2.25 | 0.69 |
| 1:A:224:LEU:HD22 | 1:A:228:ILE:HG13 | 1.73 | 0.69 |
| 1:A:296:PRO:HB3 | 2:A:962:HOH:O | 1.92 | 0.69 |
| 1:B:389:ILE:HG23 | 1:B:510:THR:HG22 | 1.74 | 0.69 |
| 1:A:30:GLN:HE22 | 1:A:187:LYS:HZ1 | 1.37 | 0.69 |
| 1:B:86:GLN:CG | 1:B:89:VAL:HG21 | 2.21 | 0.69 |
| 1:A:451:ARG:HH11 | 1:A:451:ARG:HG2 | 1.57 | 0.69 |
| 1:B:517:ILE:H | 1:B:517:ILE:CD1 | 2.02 | 0.69 |
| 1:B:601:ILE:HA | 1:B:604:ASN:HD22 | 1.55 | 0.69 |
| 1:A:155:ASP:OD2 | 1:A:157:LEU:N | 2.20 | 0.69 |
| 1:A:309:PRO:HA | 2:A:949:HOH:O | 1.92 | 0.69 |
| 1:B:291:VAL:CG2 | 1:B:292:GLU:H | 2.05 | 0.69 |
| 1:B:256:LYS:CG | 1:B:256:LYS:CA | 2.70 | 0.69 |
| 1:A:578:SER:O | 1:A:582:MET:HG3 | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:135:TYR:O | 1:B:136:ALA:HB3 | 1.93 | 0.69 |
| 1:A:688:THR:CA | 1:A:688:THR:CG2 | 2.68 | 0.69 |
| 1:B:337:LYS:NZ | 1:B:337:LYS:CB | 1.90 | 0.69 |
| 1:A:551:SER:C | 1:A:552:VAL:O | 2.32 | 0.69 |
| 1:A:329:ARG:HH21 | 1:A:329:ARG:CG | 2.05 | 0.68 |
| 1:B:605:ARG:NH2 | 1:B:672:GLU:OE2 | 2.26 | 0.68 |
| 1:B:651:ARG:HD2 | 1:B:893:SER:OXT | 1.94 | 0.68 |
| 1:B:172:GLN:HA | 1:B:172:GLN:OE1 | 1.93 | 0.68 |
| 1:A:320:GLU:N | 1:A:320:GLU:CB | 2.54 | 0.68 |
| 1:B:62:GLU:HB3 | 1:B:193:GLU:OE1 | 1.92 | 0.68 |
| 1:A:373:GLY:O | 1:A:384:ASN:ND2 | 2.26 | 0.68 |
| 1:B:376:ASN:O | 1:B:378:PRO:HD3 | 1.93 | 0.68 |
| 1:A:780:THR:HG22 | 1:A:780:THR:O | 1.93 | 0.68 |
| 1:A:692:ASP:OD1 | 1:A:692:ASP:C | 2.32 | 0.68 |
| 1:A:731:VAL:CG1 | 1:A:733:LEU:HD11 | 2.21 | 0.68 |
| 1:B:424:PHE:CZ | 1:B:711:HIS:HA | 2.29 | 0.68 |
| 1:B:224:LEU:O | 1:B:224:LEU:HD22 | 1.94 | 0.68 |
| 1:A:614:ARG:HH12 | 1:A:620:LYS:HB3 | 1.59 | 0.68 |
| 1:B:202:GLU:CB | 1:B:470:ARG:NH1 | 2.57 | 0.68 |
| 1:B:656:GLU:C | 1:B:657:LEU:HG | 2.14 | 0.68 |
| 1:B:369:SER:O | 1:B:383:VAL:CG1 | 2.42 | 0.68 |
| 1:B:745:LEU:HD23 | 1:B:769:CYS:HB3 | 1.74 | 0.68 |
| 1:A:477:ARG:CD | 1:A:477:ARG:CB | 2.70 | 0.67 |
| 1:A:13:GLU:CA | 1:A:13:GLU:OE1 | 2.41 | 0.67 |
| 1:B:802:ILE:O | 1:B:802:ILE:HG22 | 1.94 | 0.67 |
| 1:B:270:LYS:O | 1:B:281:LEU:HB2 | 1.94 | 0.67 |
| 1:B:296:PRO:CB | 2:B:946:HOH:O | 2.30 | 0.67 |
| 1:B:492:PRO:CB | 1:B:493:ASN:ND2 | 2.57 | 0.67 |
| 1:B:881:VAL:HG23 | 1:B:882:ASN:N | 2.06 | 0.67 |
| 1:B:582:MET:SD | 1:B:606:ILE:HD11 | 2.33 | 0.67 |
| 1:B:106:TRP:HZ3 | 1:B:107:LEU:HD12 | 1.59 | 0.67 |
| 1:B:341:CYS:CA | 1:B:341:CYS:SG | 2.82 | 0.67 |
| 1:A:413:LEU:CB | 1:A:413:LEU:CD1 | 2.72 | 0.67 |
| 1:B:777:ASP:CB | 1:B:777:ASP:C | 2.63 | 0.67 |
| 1:A:32:TYR:HE1 | 1:A:138:ILE:O | 1.77 | 0.67 |
| 1:B:784:LEU:O | 1:B:785:GLY:O | 2.12 | 0.67 |
| 1:B:838:ILE:HG23 | 1:B:839:ILE:N | 2.10 | 0.67 |
| 1:A:47:GLN:HA | 1:A:47:GLN:OE1 | 1.95 | 0.67 |
| 1:B:343:LEU:HB2 | 1:B:345:PRO:HD2 | 1.75 | 0.67 |
| 1:A:631:MET:SD | 1:A:631:MET:CB | 2.83 | 0.67 |
| 1:A:756:HIS:CD2 | 1:A:757:PRO:HD2 | 2.30 | 0.67 |
| 1:A:185:TYR:OH | 1:A:206:ASP:OD2 | 2.11 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:23:ARG:NH1 | 1:B:23:ARG:HG2 | 2.10 | 0.67 |
| 1:B:332:ILE:CG2 | 1:B:332:ILE:C | 2.63 | 0.67 |
| 1:A:832:GLN:HA | 1:A:832:GLN:OE1 | 1.95 | 0.67 |
| 1:B:212:THR:OG1 | 1:B:340:ILE:HD13 | 1.95 | 0.67 |
| 1:B:97:ILE:HD11 | 1:B:108:LEU:HD12 | 1.77 | 0.67 |
| 1:A:283:ARG:NH1 | 1:A:319:MET:HB2 | 2.09 | 0.67 |
| 1:A:629:MET:HG2 | 1:A:659:ILE:HD12 | 1.75 | 0.67 |
| 1:B:25:ILE:HG22 | 1:B:26:LYS:N | 2.10 | 0.66 |
| 1:A:440:ARG:HG2 | 1:A:441:GLU:N | 2.09 | 0.66 |
| 1:A:219:LYS:HA | 1:A:219:LYS:CD | 2.26 | 0.66 |
| 1:B:295:GLY:CA | 1:B:298:SER:O | 2.37 | 0.66 |
| 1:B:552:VAL:O | 1:B:555:LEU:N | 2.29 | 0.66 |
| 1:B:724:ARG:HB3 | 2:B:1002:HOH:O | 1.94 | 0.66 |
| 1:A:350:SER:O | 1:A:352:THR:HG22 | 1.93 | 0.66 |
| 1:B:51:PHE:CE1 | 1:B:187:LYS:HA | 2.30 | 0.66 |
| 1:A:514:ASP:OD1 | 1:A:515:ASP:N | 2.28 | 0.66 |
| 1:B:98:CYS:SG | 1:B:169:HIS:NE2 | 2.69 | 0.66 |
| 1:A:293:TRP:CZ2 | 2:A:1024:HOH:O | 2.46 | 0.66 |
| 1:A:748:ILE:HG23 | 1:A:749:LEU:CD2 | 2.25 | 0.66 |
| 1:A:213:GLU:OE1 | 1:A:475:ARG:NH2 | 2.28 | 0.66 |
| 1:B:792:LEU:HG | 1:B:792:LEU:O | 1.95 | 0.66 |
| 1:B:308:ASP:OD1 | 2:B:907:HOH:O | 2.13 | 0.66 |
| 1:B:446:PRO:HG2 | 2:B:894:HOH:O | 1.96 | 0.66 |
| 1:A:551:SER:O | 1:A:552:VAL:O | 2.13 | 0.66 |
| 1:A:273:THR:H | 1:A:312:ARG:HH21 | 1.42 | 0.66 |
| 1:A:335:PHE:C | 1:A:335:PHE:CD1 | 2.69 | 0.66 |
| 1:A:620:LYS:HE2 | 2:A:1022:HOH:O | 1.94 | 0.66 |
| 1:B:284:MET:SD | 1:B:284:MET:CB | 2.82 | 0.66 |
| 1:B:98:CYS:SG | 1:B:169:HIS:CE1 | 2.89 | 0.66 |
| 1:A:628:GLU:OE1 | 1:A:631:MET:SD | 2.54 | 0.66 |
| 1:B:411:LEU:HD13 | 1:B:502:PHE:CE1 | 2.31 | 0.66 |
| 1:A:855:ILE:CG2 | 1:A:855:ILE:O | 2.42 | 0.66 |
| 1:A:333:ARG:CB | 1:A:333:ARG:CD | 2.73 | 0.66 |
| 1:A:205:GLU:OE1 | 1:A:471:GLU:OE2 | 2.13 | 0.66 |
| 1:B:291:VAL:HG23 | 1:B:292:GLU:N | 2.11 | 0.66 |
| 1:B:284:MET:O | 1:B:323:GLU:OE2 | 2.13 | 0.66 |
| 1:B:283:ARG:HH21 | 1:B:325:TRP:HE1 | 1.44 | 0.66 |
| 1:B:613:PHE:CE1 | 1:B:624:MET:HG2 | 2.30 | 0.65 |
| 1:B:237:LEU:N | 1:B:237:LEU:HD23 | 2.11 | 0.65 |
| 1:A:219:LYS:HA | 1:A:219:LYS:HD3 | 1.78 | 0.65 |
| 1:B:429:GLU:C | 1:B:468:ASN:HD22 | 1.99 | 0.65 |
| 1:A:514:ASP:OD2 | 1:A:642:CYS:N | 2.24 | 0.65 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:883:ILE:HG22 | 2:B:929:HOH:O | 1.95 | 0.65 |
| 1:B:365:TRP:O | 1:B:495:GLU:HA | 1.97 | 0.65 |
| 1:A:330:ASP:OD2 | 2:A:921:HOH:O | 2.14 | 0.65 |
| 1:B:27:TYR:CD2 | 1:B:28:LEU:HD12 | 2.31 | 0.65 |
| 1:A:135:TYR:CG | 1:A:136:ALA:N | 2.62 | 0.65 |
| 1:B:215:TYR:HB2 | 1:B:337:LYS:NZ | 2.12 | 0.65 |
| 1:B:658:ILE:O | 1:B:658:ILE:HG22 | 1.96 | 0.65 |
| 1:A:403:ARG:HG2 | 1:A:477:ARG:CZ | 2.27 | 0.65 |
| 1:A:51:PHE:CG | 1:A:187:LYS:HG3 | 2.32 | 0.65 |
| 1:B:701:VAL:HG13 | 1:B:860:ARG:CG | 2.26 | 0.65 |
| 1:B:223:ASP:OD2 | 1:B:223:ASP:C | 2.29 | 0.65 |
| 1:B:712:TYR:O | 1:B:713:SER:O | 2.15 | 0.65 |
| 1:A:301:SER:O | 1:A:302:TYR:C | 2.36 | 0.65 |
| 1:B:256:LYS:HZ3 | 1:B:256:LYS:HB3 | 1.61 | 0.64 |
| 1:A:59:GLY:HA3 | 1:A:193:GLU:CD | 2.18 | 0.64 |
| 1:B:862:ASP:OD1 | 1:B:866:ARG:NE | 2.31 | 0.64 |
| 1:A:273:THR:H | 1:A:312:ARG:HD2 | 1.62 | 0.64 |
| 1:A:291:VAL:HG23 | 1:A:292:GLU:N | 2.11 | 0.64 |
| 1:A:669:VAL:CA | 1:A:669:VAL:CG1 | 2.73 | 0.64 |
| 1:A:229:LEU:O | 1:A:231:ALA:N | 2.29 | 0.64 |
| 1:A:731:VAL:HG23 | 1:A:733:LEU:N | 2.11 | 0.64 |
| 1:A:430:THR:HA | 1:A:467:ILE:O | 1.97 | 0.64 |
| 1:A:573:GLY:O | 1:A:574:PHE:O | 2.16 | 0.64 |
| 1:B:430:THR:OG1 | 1:B:468:ASN:HB3 | 1.98 | 0.64 |
| 1:B:487:PRO:O | 1:B:488:SER:HB3 | 1.96 | 0.64 |
| 1:A:358:THR:O | 1:A:359:THR:CG2 | 2.45 | 0.64 |
| 1:A:329:ARG:HG3 | 1:A:329:ARG:O | 1.98 | 0.64 |
| 1:A:228:ILE:HG12 | 1:A:337:LYS:HZ3 | 1.61 | 0.64 |
| 1:A:689:ILE:HD12 | 1:A:690:GLN:N | 2.13 | 0.64 |
| 1:A:599:PHE:HD2 | 1:A:599:PHE:O | 1.80 | 0.64 |
| 1:A:803:TYR:HA | 1:A:822:ALA:HB2 | 1.79 | 0.64 |
| 1:B:291:VAL:CG2 | 1:B:292:GLU:N | 2.58 | 0.64 |
| 1:B:424:PHE:HA | 1:B:426:ARG:HH21 | 1.63 | 0.64 |
| 1:A:86:GLN:HB3 | 1:A:89:VAL:CG2 | 2.28 | 0.64 |
| 1:A:337:LYS:CD | 1:A:337:LYS:NZ | 2.59 | 0.64 |
| 1:B:839:ILE:HD12 | 1:B:840:ARG:CB | 2.28 | 0.64 |
| 1:B:429:GLU:C | 1:B:468:ASN:HB2 | 2.17 | 0.64 |
| 1:A:13:GLU:O | 1:A:16:GLU:CG | 2.44 | 0.64 |
| 1:B:343:LEU:HD22 | 2:B:990:HOH:O | 1.96 | 0.64 |
| 1:A:414:MET:CB | 2:A:901:HOH:O | 2.46 | 0.64 |
| 1:B:4:ILE:HD13 | 1:B:889:LEU:HA | 1.80 | 0.64 |
| 1:A:256:LYS:HD3 | 1:A:258:LEU:CD1 | 2.22 | 0.64 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:83:SER:O | 1:A:84:ASN:HB3 | 1.96 | 0.64 |
| 1:B:296:PRO:CD | 2:B:912:HOH:O | 2.46 | 0.64 |
| 1:A:27:TYR:CD2 | 1:A:28:LEU:HG | 2.32 | 0.64 |
| 1:B:440:ARG:NH2 | 1:B:440:ARG:CG | 2.59 | 0.64 |
| 1:A:389:ILE:HD11 | 1:A:502:PHE:HE2 | 1.62 | 0.64 |
| 1:B:795:ASN:O | 1:B:799:TRP:HB2 | 1.98 | 0.64 |
| 1:A:314:GLN:HG3 | 1:A:315:LEU:H | 1.63 | 0.64 |
| 1:A:520:ASN:OD1 | 1:A:520:ASN:N | 2.28 | 0.64 |
| 1:A:435:VAL:CG1 | 1:A:461:ALA:HB3 | 2.28 | 0.64 |
| 1:A:772:MET:CG | 1:A:772:MET:CA | 2.71 | 0.64 |
| 1:A:428:MET:HB2 | 2:A:910:HOH:O | 1.97 | 0.64 |
| 1:B:464:GLU:HG2 | 1:B:464:GLU:O | 1.98 | 0.64 |
| 1:B:328:PHE:CE2 | 1:B:331:PHE:CZ | 2.86 | 0.63 |
| 1:A:499:LEU:HB3 | 2:A:901:HOH:O | 1.98 | 0.63 |
| 1:A:358:THR:HG22 | 1:A:359:THR:H | 1.63 | 0.63 |
| 1:B:195:LEU:O | 1:B:195:LEU:HD22 | 1.97 | 0.63 |
| 1:A:74:LYS:O | 1:A:160:THR:OG1 | 2.07 | 0.63 |
| 1:A:272:VAL:HA | 1:A:312:ARG:HD2 | 1.78 | 0.63 |
| 1:B:328:PHE:O | 1:B:331:PHE:HE2 | 1.82 | 0.63 |
| 1:A:731:VAL:HG21 | 1:A:733:LEU:HD12 | 0.70 | 0.63 |
| 1:A:365:TRP:CE2 | 1:A:488:SER:HA | 2.33 | 0.63 |
| 1:A:656:GLU:N | 1:A:656:GLU:OE1 | 2.31 | 0.63 |
| 1:B:335:PHE:CG | 1:B:335:PHE:CA | 2.78 | 0.63 |
| 1:B:610:LEU:CD1 | 1:B:610:LEU:HG | 2.19 | 0.63 |
| 1:A:258:LEU:H | 1:A:258:LEU:HD13 | 1.63 | 0.63 |
| 1:A:177:TRP:CD2 | 1:A:178:SER:N | 2.67 | 0.63 |
| 1:B:303:GLU:OE2 | 1:B:304:TRP:N | 2.32 | 0.63 |
| 1:A:94:ARG:CD | 2:A:1049:HOH:O | 2.46 | 0.63 |
| 1:A:87:PHE:CD2 | 1:A:88:ILE:HG22 | 2.33 | 0.63 |
| 1:A:51:PHE:N | 1:A:52:PRO:HD3 | 2.14 | 0.63 |
| 1:A:669:VAL:CG2 | 1:A:669:VAL:CG1 | 2.72 | 0.63 |
| 1:A:665:VAL:O | 1:A:666:ARG:C | 2.34 | 0.62 |
| 1:B:25:ILE:HD13 | 1:B:148:GLU:OE1 | 1.99 | 0.62 |
| 1:A:388:LYS:NZ | 1:A:482:GLU:OE1 | 2.32 | 0.62 |
| 1:B:69:LYS:CA | 1:B:69:LYS:CG | 2.76 | 0.62 |
| 1:B:27:TYR:CE2 | 1:B:28:LEU:CD1 | 2.82 | 0.62 |
| 1:B:701:VAL:HG11 | 1:B:860:ARG:HG2 | 1.81 | 0.62 |
| 1:B:427:ASP:HB3 | 2:B:1003:HOH:O | 1.97 | 0.62 |
| 1:B:74:LYS:HA | 2:B:1000:HOH:O | 1.98 | 0.62 |
| 1:B:597:VAL:O | 1:B:600:ASN:HB3 | 1.99 | 0.62 |
| 1:A:193:GLU:O | 1:A:195:LEU:N | 2.33 | 0.62 |
| 1:A:204:PHE:CD1 | 1:A:340:ILE:HD11 | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:883:ILE:CB | 1:A:883:ILE:CD1 | 2.76 | 0.62 |
| 1:B:726:PHE:CD2 | 1:B:726:PHE:N | 2.62 | 0.62 |
| 1:A:874:ASN:O | 1:A:876:THR:N | 2.32 | 0.62 |
| 1:B:651:ARG:NH1 | 1:B:670:ARG:CZ | 2.58 | 0.62 |
| 1:A:403:ARG:HG2 | 1:A:477:ARG:NE | 2.14 | 0.62 |
| 1:A:216:ASP:HB3 | 1:A:219:LYS:HB3 | 1.80 | 0.62 |
| 1:B:103:GLY:HA3 | 2:B:903:HOH:O | 2.00 | 0.62 |
| 1:B:724:ARG:HH21 | 1:B:724:ARG:CB | 2.10 | 0.62 |
| 1:A:328:PHE:CZ | 1:A:331:PHE:HZ | 2.18 | 0.62 |
| 1:A:582:MET:CE | 1:A:582:MET:CG | 2.78 | 0.62 |
| 1:A:172:GLN:O | 1:A:174:ASN:ND2 | 2.33 | 0.62 |
| 1:A:389:ILE:CG2 | 1:A:390:ARG:N | 2.60 | 0.62 |
| 1:A:855:ILE:HG22 | 1:A:855:ILE:O | 1.99 | 0.62 |
| 1:A:87:PHE:HD2 | 1:A:88:ILE:HG22 | 1.64 | 0.62 |
| 1:B:453:PHE:CZ | 1:B:457:ASN:OD1 | 2.53 | 0.62 |
| 1:A:327:SER:H | 1:A:329:ARG:HH12 | 1.40 | 0.62 |
| 1:A:448:HIS:CD2 | 1:A:630:ARG:NH2 | 2.67 | 0.62 |
| 1:B:616:PHE:CE1 | 1:B:628:GLU:HB3 | 2.35 | 0.62 |
| 1:A:328:PHE:CZ | 1:A:331:PHE:CZ | 2.87 | 0.62 |
| 1:B:786:PHE:N | 1:B:786:PHE:CB | 2.56 | 0.62 |
| 1:A:826:ALA:CB | 1:A:826:ALA:C | 2.63 | 0.62 |
| 1:A:773:VAL:CG2 | 1:A:773:VAL:CG1 | 2.74 | 0.62 |
| 1:A:63:LEU:CD1 | 1:A:70:THR:CG2 | 2.67 | 0.62 |
| 1:A:242:ILE:O | 1:A:242:ILE:CG1 | 2.48 | 0.62 |
| 1:B:337:LYS:HB3 | 1:B:337:LYS:HZ2 | 0.46 | 0.62 |
| 1:B:440:ARG:CD | 1:B:440:ARG:CB | 2.77 | 0.62 |
| 1:A:82:LEU:O | 1:A:84:ASN:N | 2.32 | 0.62 |
| 1:B:377:TYR:N | 1:B:378:PRO:HD3 | 2.12 | 0.62 |
| 1:B:379:ALA:HB2 | 2:B:1012:HOH:O | 2.00 | 0.62 |
| 1:A:75:TRP:CG | 1:A:75:TRP:CA | 2.80 | 0.62 |
| 1:A:7:LYS:CG | 1:A:7:LYS:CE | 2.76 | 0.62 |
| 1:A:833:HIS:HD2 | 1:A:833:HIS:C | 2.03 | 0.62 |
| 1:B:883:ILE:C | 1:B:883:ILE:CB | 2.63 | 0.62 |
| 1:A:553:LYS:O | 1:A:554:GLU:HB2 | 1.99 | 0.62 |
| 1:B:778:SER:O | 1:B:779:ASP:OD1 | 2.17 | 0.61 |
| 1:B:740:VAL:CA | 1:B:740:VAL:CG1 | 2.76 | 0.61 |
| 1:A:759:LEU:CD1 | 1:A:812:GLY:O | 2.48 | 0.61 |
| 1:A:307:VAL:O | 1:A:308:ASP:HB2 | 1.98 | 0.61 |
| 1:A:199:CYS:HB3 | 1:A:202:GLU:HG3 | 1.83 | 0.61 |
| 1:B:88:ILE:CD1 | 1:B:121:LEU:HD21 | 2.30 | 0.61 |
| 1:B:677:ILE:CB | 1:B:677:ILE:CD1 | 2.73 | 0.61 |
| 1:A:629:MET:O | 1:A:630:ARG:C | 2.38 | 0.61 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:B:649:VAL:O | 1:B:650:ALA:C | 2.37 | 0.61 |
| 1:A:701:VAL:O | 1:A:701:VAL:HG13 | 2.00 | 0.61 |
| 1:A:35:LEU:O | 1:A:36:ARG:C | 2.36 | 0.61 |
| 1:B:49:PRO:CG | 2:B:935:HOH:O | 2.46 | 0.61 |
| 1:A:772:MET:CB | 1:A:772:MET:SD | 2.87 | 0.61 |
| 1:A:306:LYS:CG | 1:A:307:VAL:H | 2.05 | 0.61 |
| 1:A:653:ALA:HA | 1:A:659:ILE:HG12 | 1.82 | 0.61 |
| 1:A:327:SER:CB | 1:A:329:ARG:HH11 | 2.14 | 0.61 |
| 1:A:640:LEU:O | 1:A:645:HIS:NE2 | 2.33 | 0.61 |
| 1:B:161:LYS:O | 1:B:162:ASP:C | 2.36 | 0.61 |
| 1:B:861:LEU:O | 1:B:862:ASP:O | 2.19 | 0.61 |
| 1:A:739:GLU:O | 1:A:739:GLU:CD | 2.38 | 0.61 |
| 1:B:519:ALA:HB2 | 1:B:675:PHE:CE2 | 2.36 | 0.61 |
| 1:A:451:ARG:NH1 | 1:A:451:ARG:HG2 | 2.16 | 0.61 |
| 1:A:680:GLN:O | 1:A:682:ASP:N | 2.33 | 0.61 |
| 1:B:883:ILE:N | 1:B:883:ILE:CB | 2.62 | 0.61 |
| 1:A:228:ILE:O | 1:A:229:LEU:O | 2.19 | 0.61 |
| 1:B:60:PHE:CE2 | 1:B:193:GLU:HG2 | 2.36 | 0.61 |
| 1:A:140:HIS:HB3 | 1:A:153:VAL:HG23 | 1.83 | 0.61 |
| 1:B:579:CYS:HA | 1:B:579:CYS:CB | 2.17 | 0.61 |
| 1:A:746:MET:O | 1:A:746:MET:HG2 | 2.01 | 0.61 |
| 1:B:798:LYS:O | 1:B:802:ILE:HG13 | 2.00 | 0.61 |
| 1:B:434:ALA:HA | 1:B:462:GLN:HB3 | 1.83 | 0.61 |
| 1:B:89:VAL:O | 1:B:89:VAL:CB | 2.44 | 0.60 |
| 1:A:327:SER:HB3 | 1:A:329:ARG:HH11 | 1.66 | 0.60 |
| 1:B:668:LEU:CD2 | 1:B:668:LEU:CB | 2.72 | 0.60 |
| 1:A:672:GLU:HA | 1:A:672:GLU:OE2 | 1.99 | 0.60 |
| 1:B:853:ASN:O | 1:B:857:CYS:N | 2.31 | 0.60 |
| 1:B:8:LEU:CB | 1:B:8:LEU:CD2 | 2.76 | 0.60 |
| 1:A:155:ASP:OD2 | 1:A:156:ASP:N | 2.32 | 0.60 |
| 1:A:193:GLU:C | 1:A:195:LEU:H | 2.05 | 0.60 |
| 1:B:892:TYR:O | 1:B:893:SER:CB | 2.50 | 0.60 |
| 1:A:60:PHE:CD2 | 1:A:193:GLU:OE1 | 2.53 | 0.60 |
| 1:A:293:TRP:CE2 | 2:A:1024:HOH:O | 2.54 | 0.60 |
| 1:B:723:GLU:C | 1:B:726:PHE:HD2 | 2.04 | 0.60 |
| 1:A:731:VAL:CB | 1:A:733:LEU:CD1 | 2.79 | 0.60 |
| 1:A:860:ARG:NH1 | 1:A:860:ARG:CB | 2.63 | 0.60 |
| 1:B:358:THR:O | 1:B:359:THR:HG23 | 2.02 | 0.60 |
| 1:A:549:GLU:O | 1:A:595:GLY:HA2 | 2.01 | 0.60 |
| 1:B:574:PHE:CE1 | 1:B:661:PHE:HE1 | 2.20 | 0.60 |
| 1:A:602:LEU:O | 1:A:605:ARG:HB2 | 2.02 | 0.60 |
| 1:B:225:TYR:CE1 | 1:B:280:ASN:ND2 | 2.69 | 0.60 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:297:TRP:CD1 | 1:A:297:TRP:O | 2.55 | 0.60 |
| 1:B:277:GLN:HA | 1:B:277:GLN:HE21 | 1.66 | 0.60 |
| 1:A:94:ARG:HD2 | 2:A:1049:HOH:O | 2.01 | 0.60 |
| 1:B:582:MET:SD | 1:B:602:LEU:HD21 | 2.42 | 0.60 |
| 1:B:493:ASN:N | 1:B:493:ASN:HD22 | 2.00 | 0.60 |
| 1:A:494:LYS:NZ | 1:A:494:LYS:CD | 2.60 | 0.60 |
| 1:B:866:ARG:HH11 | 1:B:866:ARG:HG3 | 1.67 | 0.60 |
| 1:A:413:LEU:CD2 | 1:A:413:LEU:CD1 | 2.73 | 0.60 |
| 1:B:457:ASN:HD22 | 1:B:457:ASN:N | 1.93 | 0.60 |
| 1:A:614:ARG:HH12 | 1:A:620:LYS:HE3 | 1.67 | 0.60 |
| 1:A:860:ARG:NH1 | 1:A:860:ARG:HB3 | 2.15 | 0.60 |
| 1:A:759:LEU:HD12 | 1:A:812:GLY:HA2 | 1.84 | 0.59 |
| 1:A:365:TRP:O | 1:A:495:GLU:HA | 2.02 | 0.59 |
| 1:A:122:HIS:CD2 | 1:A:127:TYR:CE2 | 2.90 | 0.59 |
| 1:A:26:LYS:O | 1:A:27:TYR:C | 2.40 | 0.59 |
| 1:B:701:VAL:CG1 | 1:B:860:ARG:CG | 2.80 | 0.59 |
| 1:A:290:GLU:N | 1:A:290:GLU:CD | 2.55 | 0.59 |
| 1:A:270:LYS:CD | 1:A:270:LYS:NZ | 2.63 | 0.59 |
| 1:B:670:ARG:HA | 1:B:673:ILE:CD1 | 2.27 | 0.59 |
| 1:B:524:GLU:CD | 1:B:524:GLU:N | 2.53 | 0.59 |
| 1:A:100:GLY:HA2 | 1:A:167:PHE:HA | 1.85 | 0.59 |
| 1:A:273:THR:N | 1:A:312:ARG:HH21 | 1.99 | 0.59 |
| 1:B:585:LEU:HD11 | 1:B:672:GLU:HG2 | 1.83 | 0.59 |
| 1:A:224:LEU:O | 1:A:228:ILE:HG13 | 2.02 | 0.59 |
| 1:B:212:THR:OG1 | 1:B:340:ILE:CD1 | 2.51 | 0.59 |
| 1:A:692:ASP:OD1 | 1:A:694:ILE:N | 2.35 | 0.59 |
| 1:A:240:CYS:O | 1:A:263:ALA:O | 2.20 | 0.59 |
| 1:B:369:SER:O | 1:B:383:VAL:HG13 | 2.01 | 0.59 |
| 1:B:4:ILE:O | 1:B:6:MET:N | 2.36 | 0.59 |
| 1:A:122:HIS:CA | 1:A:125:VAL:O | 2.50 | 0.59 |
| 1:B:656:GLU:O | 1:B:657:LEU:HG | 2.03 | 0.59 |
| 1:B:415:GLN:HE22 | 1:B:428:MET:HB3 | 1.68 | 0.59 |
| 1:A:87:PHE:HA | 1:A:131:PHE:HE1 | 1.66 | 0.59 |
| 1:B:773:VAL:CA | 1:B:784:LEU:HD21 | 2.27 | 0.59 |
| 1:B:242:ILE:HG23 | 1:B:242:ILE:O | 2.02 | 0.59 |
| 1:A:360:PHE:HB2 | 1:A:499:LEU:HD11 | 1.83 | 0.59 |
| 1:A:23:ARG:HH11 | 1:A:23:ARG:HG2 | 1.68 | 0.59 |
| 1:B:506:LYS:O | 1:B:507:LYS:C | 2.32 | 0.59 |
| 1:A:824:GLU:N | 1:A:828:PHE:O | 2.36 | 0.58 |
| 1:A:228:ILE:O | 1:A:232:LEU:CD2 | 2.47 | 0.58 |
| 1:B:140:HIS:HD2 | 1:B:151:ASP:OD1 | 1.85 | 0.58 |
| 1:A:864:MET:CB | 1:A:864:MET:C | 2.69 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:221:PRO:C | 1:A:223:ASP:H | 2.05 | 0.58 |
| 1:B:670:ARG:CA | 1:B:673:ILE:HD12 | 2.25 | 0.58 |
| 1:B:226:GLN:HG3 | 2:B:955:HOH:O | 2.02 | 0.58 |
| 1:A:619:ASP:O | 1:A:620:LYS:O | 2.21 | 0.58 |
| 1:B:291:VAL:HG23 | 1:B:292:GLU:H | 1.68 | 0.58 |
| 1:A:610:LEU:CD2 | 1:A:610:LEU:HA | 2.34 | 0.58 |
| 1:B:410:LEU:HB2 | 1:B:503:PHE:HB2 | 1.86 | 0.58 |
| 1:A:340:ILE:CG1 | 1:A:340:ILE:CG2 | 2.79 | 0.58 |
| 1:B:740:VAL:CG1 | 1:B:740:VAL:HB | 2.16 | 0.58 |
| 1:A:499:LEU:HG | 1:A:501:ARG:HD2 | 1.85 | 0.58 |
| 1:A:487:PRO:O | 1:A:488:SER:HB3 | 2.02 | 0.58 |
| 1:B:766:ILE:O | 1:B:769:CYS:N | 2.34 | 0.58 |
| 1:B:296:PRO:HG2 | 1:B:304:TRP:CG | 2.38 | 0.58 |
| 1:A:263:ALA:CB | 1:A:288:TRP:HZ3 | 2.17 | 0.58 |
| 1:A:196:SER:O | 1:A:197:GLY:C | 2.42 | 0.58 |
| 1:B:97:ILE:HG12 | 1:B:98:CYS:N | 2.17 | 0.58 |
| 1:B:272:VAL:HB | 1:B:311:GLU:HG3 | 1.85 | 0.58 |
| 1:B:595:GLY:O | 1:B:599:PHE:HB2 | 2.04 | 0.58 |
| 1:A:306:LYS:O | 1:A:307:VAL:O | 2.22 | 0.58 |
| 1:B:574:PHE:HE1 | 1:B:661:PHE:CE1 | 2.22 | 0.58 |
| 1:B:867:ALA:O | 1:B:869:ARG:N | 2.37 | 0.58 |
| 1:B:658:ILE:HG23 | 1:B:658:ILE:O | 2.04 | 0.58 |
| 1:B:525:LYS:HZ3 | 1:B:525:LYS:CB | 2.14 | 0.58 |
| 1:A:17:GLY:O | 1:A:18:LEU:C | 2.34 | 0.58 |
| 1:B:48:ASP:HB2 | 1:B:155:ASP:OD1 | 2.04 | 0.58 |
| 1:B:274:TYR:O | 1:B:275:GLN:C | 2.40 | 0.58 |
| 1:B:855:ILE:CB | 2:B:974:HOH:O | 2.51 | 0.58 |
| 1:A:309:PRO:O | 1:A:311:GLU:N | 2.36 | 0.58 |
| 1:B:335:PHE:CB | 1:B:335:PHE:C | 2.70 | 0.58 |
| 1:B:694:ILE:HB | 1:B:694:ILE:CA | 2.18 | 0.58 |
| 1:A:233:GLU:O | 1:A:353:LEU:CB | 2.52 | 0.58 |
| 1:B:831:ASN:O | 1:B:833:HIS:C | 2.42 | 0.58 |
| 1:B:46:PHE:CD2 | 1:B:138:ILE:HD12 | 2.39 | 0.58 |
| 1:A:317:VAL:CB | 1:A:317:VAL:C | 2.69 | 0.57 |
| 1:B:694:ILE:CG1 | 1:B:694:ILE:CA | 2.78 | 0.57 |
| 1:B:484:ILE:HD12 | 1:B:513:LEU:HD22 | 1.85 | 0.57 |
| 1:A:316:ARG:CB | 2:A:1007:HOH:O | 2.52 | 0.57 |
| 1:B:668:LEU:CD2 | 1:B:668:LEU:CD1 | 2.79 | 0.57 |
| 1:B:330:ASP:C | 1:B:332:ILE:H | 2.06 | 0.57 |
| 1:A:428:MET:CB | 2:A:910:HOH:O | 2.52 | 0.57 |
| 1:B:66:ASN:HD22 | 1:B:66:ASN:N | 2.00 | 0.57 |
| 1:A:464:GLU:O | 1:A:465:HIS:O | 2.22 | 0.57 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:460:ARG:O | 1:B:461:ALA:HB2 | 2.03 | 0.57 |
| 1:A:237:LEU:C | 1:A:238:LEU:HD12 | 2.25 | 0.57 |
| 1:B:806:PHE:O | 1:B:807:GLU:HB3 | 2.04 | 0.57 |
| 1:B:328:PHE:O | 1:B:328:PHE:CG | 2.56 | 0.57 |
| 1:A:183:LYS:O | 1:A:187:LYS:HB2 | 2.05 | 0.57 |
| 1:B:316:ARG:O | 1:B:317:VAL:C | 2.42 | 0.57 |
| 1:B:523:ASP:O | 1:B:524:GLU:C | 2.41 | 0.57 |
| 1:B:197:GLY:O | 1:B:198:GLY:C | 2.43 | 0.57 |
| 1:A:305:ASN:C | 1:A:305:ASN:HD22 | 2.06 | 0.57 |
| 1:B:537:LYS:HB2 | 1:B:537:LYS:NZ | 2.09 | 0.57 |
| 1:A:651:ARG:C | 1:A:651:ARG:HH11 | 2.08 | 0.57 |
| 1:B:376:ASN:N | 1:B:376:ASN:OD1 | 2.22 | 0.57 |
| 1:B:69:LYS:HZ3 | 1:B:69:LYS:CB | 1.95 | 0.57 |
| 1:B:537:LYS:CB | 1:B:537:LYS:HZ2 | 2.07 | 0.57 |
| 1:A:219:LYS:CD | 1:A:219:LYS:CB | 2.78 | 0.57 |
| 1:B:624:MET:O | 1:B:658:ILE:HG13 | 2.05 | 0.57 |
| 1:B:388:LYS:NZ | 1:B:482:GLU:HB3 | 2.19 | 0.57 |
| 1:B:797:LYS:O | 1:B:800:GLN:HB3 | 2.04 | 0.57 |
| 1:B:200:THR:HG23 | 1:B:201:SER:N | 2.19 | 0.57 |
| 1:B:323:GLU:CA | 1:B:323:GLU:OE2 | 2.47 | 0.57 |
| 1:B:21:HIS:CD2 | 1:B:142:GLN:HE22 | 2.23 | 0.57 |
| 1:B:332:ILE:CG2 | 1:B:332:ILE:CA | 2.79 | 0.57 |
| 1:A:327:SER:OG | 1:A:329:ARG:CZ | 2.53 | 0.57 |
| 1:A:230:LYS:HE3 | 1:A:505:GLU:CD | 2.25 | 0.57 |
| 1:B:40:LEU:HD13 | 1:B:136:ALA:HB2 | 1.87 | 0.57 |
| 1:B:69:LYS:NZ | 1:B:69:LYS:HB2 | 2.06 | 0.57 |
| 1:B:106:TRP:CZ3 | 1:B:107:LEU:HD13 | 2.40 | 0.57 |
| 1:A:860:ARG:CZ | 1:A:860:ARG:HB3 | 2.35 | 0.57 |
| 1:A:291:VAL:CG2 | 1:A:292:GLU:N | 2.67 | 0.57 |
| 1:A:238:LEU:CD1 | 1:A:238:LEU:N | 2.68 | 0.56 |
| 1:B:519:ALA:HB2 | 1:B:675:PHE:CD2 | 2.40 | 0.56 |
| 1:A:552:VAL:HA | 1:A:592:GLY:O | 2.05 | 0.56 |
| 1:B:221:PRO:O | 1:B:224:LEU:HB2 | 2.05 | 0.56 |
| 1:B:678:PHE:HD2 | 1:B:886:TRP:CD1 | 2.23 | 0.56 |
| 1:B:789:PHE:C | 1:B:789:PHE:CD2 | 2.79 | 0.56 |
| 1:B:8:LEU:CD1 | 1:B:885:GLU:HB3 | 2.35 | 0.56 |
| 1:B:8:LEU:HD13 | 1:B:885:GLU:CG | 2.34 | 0.56 |
| 1:A:307:VAL:HG12 | 2:A:909:HOH:O | 2.05 | 0.56 |
| 1:A:305:ASN:H | 1:A:305:ASN:ND2 | 2.03 | 0.56 |
| 1:B:430:THR:CA | 1:B:468:ASN:HB2 | 2.33 | 0.56 |
| 1:B:440:ARG:CG | 1:B:441:GLU:N | 2.30 | 0.56 |
| 1:B:835:TYR:O | 1:B:837:MET:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:383:VAL:HG12 | 1:B:383:VAL:O | 2.05 | 0.56 |
| 1:B:810:ARG:O | 1:B:811:SER:CB | 2.52 | 0.56 |
| 1:B:601:ILE:HD13 | 1:B:604:ASN:CG | 2.24 | 0.56 |
| 1:A:740:VAL:O | 1:A:783:LYS:HA | 2.06 | 0.56 |
| 1:B:807:GLU:HG3 | 1:B:808:THR:N | 2.19 | 0.56 |
| 1:A:256:LYS:HA | 1:A:258:LEU:CD1 | 2.35 | 0.56 |
| 1:B:238:LEU:CD1 | 1:B:238:LEU:N | 2.69 | 0.56 |
| 1:A:435:VAL:HG11 | 1:A:461:ALA:HB3 | 1.87 | 0.56 |
| 1:B:313:GLU:HA | 1:B:315:LEU:HD12 | 1.87 | 0.56 |
| 1:A:366:ARG:O | 1:A:367:ARG:C | 2.39 | 0.56 |
| 1:B:582:MET:CG | 1:B:582:MET:CE | 2.83 | 0.56 |
| 1:A:602:LEU:O | 1:A:603:TRP:C | 2.43 | 0.56 |
| 1:A:278:ARG:CG | 1:A:279:VAL:H | 2.18 | 0.56 |
| 1:A:296:PRO:O | 1:A:297:TRP:CB | 2.48 | 0.56 |
| 1:B:672:GLU:O | 1:B:673:ILE:C | 2.44 | 0.56 |
| 1:B:521:LEU:CD2 | 1:B:636:ALA:O | 2.54 | 0.56 |
| 1:A:388:LYS:NZ | 1:A:482:GLU:CD | 2.57 | 0.56 |
| 1:A:414:MET:CG | 1:A:414:MET:CE | 2.81 | 0.56 |
| 1:B:96:ASP:OD2 | 1:B:170:SER:OG | 2.11 | 0.56 |
| 1:B:88:ILE:O | 1:B:88:ILE:CG2 | 2.41 | 0.56 |
| 1:B:624:MET:O | 1:B:658:ILE:CG1 | 2.53 | 0.56 |
| 1:A:484:ILE:CD1 | 1:A:486:VAL:HG23 | 2.36 | 0.56 |
| 1:A:462:GLN:O | 1:A:463:SER:C | 2.43 | 0.56 |
| 1:A:698:SER:O | 1:A:700:SER:N | 2.38 | 0.56 |
| 1:B:97:ILE:CD1 | 1:B:108:LEU:HD11 | 2.35 | 0.56 |
| 1:B:780:THR:HA | 1:B:892:TYR:CZ | 2.41 | 0.56 |
| 1:B:690:GLN:CG | 1:B:690:GLN:CA | 2.80 | 0.56 |
| 1:B:867:ALA:C | 1:B:869:ARG:N | 2.55 | 0.56 |
| 1:A:435:VAL:HG13 | 1:A:460:ARG:O | 2.05 | 0.56 |
| 1:B:609:TYR:CD2 | 1:B:665:VAL:HB | 2.41 | 0.56 |
| 1:B:651:ARG:NH1 | 1:B:670:ARG:HH12 | 2.02 | 0.56 |
| 1:B:120:ILE:CG2 | 1:B:120:ILE:C | 2.74 | 0.56 |
| 1:A:450:LYS:HE3 | 1:A:631:MET:HG2 | 1.87 | 0.56 |
| 1:A:758:ASP:O | 1:A:759:LEU:C | 2.43 | 0.56 |
| 1:B:389:ILE:HD13 | 1:B:483:TYR:HB2 | 1.87 | 0.56 |
| 1:B:605:ARG:CZ | 1:B:672:GLU:OE2 | 2.55 | 0.55 |
| 1:A:808:THR:C | 1:A:808:THR:HG23 | 2.23 | 0.55 |
| 1:B:135:TYR:O | 1:B:136:ALA:CA | 2.54 | 0.55 |
| 1:B:868:PHE:CE2 | 1:B:879:ILE:HG12 | 2.41 | 0.55 |
| 1:B:555:LEU:O | 1:B:556:GLN:O | 2.23 | 0.55 |
| 1:A:655:ASP:C | 1:A:656:GLU:OE1 | 2.45 | 0.55 |
| 1:A:177:TRP:CG | 1:A:178:SER:N | 2.74 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:696:TRP:O | 1:B:700:SER:OG | 2.23 | 0.55 |
| 1:B:395:ASP:O | 1:B:396:ASP:C | 2.44 | 0.55 |
| 1:A:610:LEU:HD22 | 1:A:610:LEU:HA | 1.88 | 0.55 |
| 1:A:624:MET:HB3 | 1:A:659:ILE:O | 2.06 | 0.55 |
| 1:A:278:ARG:NH2 | 2:A:929:HOH:O | 2.38 | 0.55 |
| 1:B:87:PHE:CE1 | 1:B:180:LEU:HD12 | 2.40 | 0.55 |
| 1:A:800:GLN:HG3 | 1:A:851:PHE:HE1 | 1.70 | 0.55 |
| 1:A:204:PHE:HE2 | 1:A:237:LEU:HD12 | 1.71 | 0.55 |
| 1:B:669:VAL:CB | 1:B:669:VAL:C | 2.71 | 0.55 |
| 1:B:361:TYR:O | 1:B:500:LEU:N | 2.39 | 0.55 |
| 1:A:380:THR:O | 1:A:381:PHE:C | 2.41 | 0.55 |
| 1:B:426:ARG:HG2 | 2:B:1029:HOH:O | 2.05 | 0.55 |
| 1:B:370:THR:HA | 1:B:383:VAL:HG12 | 1.87 | 0.55 |
| 1:A:520:ASN:C | 1:A:521:LEU:HG | 2.27 | 0.55 |
| 1:B:723:GLU:O | 1:B:726:PHE:HD2 | 1.89 | 0.55 |
| 1:A:349:LYS:HA | 2:A:1006:HOH:O | 2.06 | 0.55 |
| 1:B:787:GLU:C | 1:B:789:PHE:H | 2.10 | 0.55 |
| 1:B:457:ASN:ND2 | 1:B:457:ASN:N | 2.48 | 0.55 |
| 1:B:724:ARG:O | 1:B:724:ARG:NH2 | 2.40 | 0.55 |
| 1:B:667:CYS:O | 1:B:668:LEU:O | 2.24 | 0.55 |
| 1:A:757:PRO:O | 1:A:758:ASP:CB | 2.55 | 0.55 |
| 1:B:701:VAL:CG1 | 1:B:860:ARG:HD3 | 2.37 | 0.55 |
| 1:B:507:LYS:HD2 | 1:B:507:LYS:H | 1.72 | 0.55 |
| 1:A:773:VAL:CG1 | 1:A:773:VAL:CA | 2.76 | 0.55 |
| 1:B:493:ASN:ND2 | 1:B:493:ASN:N | 2.55 | 0.55 |
| 1:A:680:GLN:C | 1:A:682:ASP:H | 2.10 | 0.55 |
| 1:B:795:ASN:O | 1:B:799:TRP:CB | 2.55 | 0.55 |
| 1:A:655:ASP:CB | 1:A:656:GLU:OE1 | 2.55 | 0.55 |
| 1:A:591:ASN:ND2 | 1:A:592:GLY:H | 2.05 | 0.55 |
| 1:B:274:TYR:CE2 | 1:B:275:GLN:HG3 | 2.41 | 0.55 |
| 1:A:332:ILE:CA | 1:A:332:ILE:CG1 | 2.80 | 0.55 |
| 1:A:204:PHE:CE2 | 1:A:237:LEU:HD12 | 2.41 | 0.55 |
| 1:A:340:ILE:HB | 1:A:340:ILE:CG2 | 2.18 | 0.55 |
| 1:B:447:VAL:CB | 1:B:513:LEU:HD12 | 2.36 | 0.55 |
| 1:B:168:VAL:HB | 1:B:182:GLU:OE2 | 2.07 | 0.55 |
| 1:A:872:ASP:O | 1:A:872:ASP:CG | 2.44 | 0.55 |
| 1:B:0:GLU:CB | 1:B:0:GLU:C | 2.68 | 0.54 |
| 1:A:785:GLY:HA3 | 1:A:788:GLU:OE1 | 2.07 | 0.54 |
| 1:A:583:VAL:C | 1:A:583:VAL:CB | 2.66 | 0.54 |
| 1:B:258:LEU:O | 1:B:259:VAL:HG22 | 2.08 | 0.54 |
| 1:A:254:THR:HG23 | 1:A:255:PHE:H | 1.72 | 0.54 |
| 1:A:880:GLN:C | 1:A:881:VAL:HG22 | 2.28 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:370:THR:HA | 1:A:383:VAL:O | 2.06 | 0.54 |
| 1:B:273:THR:H | 1:B:311:GLU:HG2 | 1.72 | 0.54 |
| 1:A:613:PHE:CZ | 1:A:622:GLY:O | 2.61 | 0.54 |
| 1:A:776:MET:HE1 | 1:A:791:TYR:CD2 | 2.42 | 0.54 |
| 1:B:212:THR:CB | 1:B:340:ILE:CD1 | 2.85 | 0.54 |
| 1:B:775:VAL:HG12 | 1:B:893:SER:HB2 | 1.89 | 0.54 |
| 1:A:428:MET:HE2 | 2:A:970:HOH:O | 2.04 | 0.54 |
| 1:B:102:LEU:HD22 | 1:B:161:LYS:HE2 | 1.90 | 0.54 |
| 1:B:867:ALA:O | 1:B:868:PHE:C | 2.44 | 0.54 |
| 1:B:28:LEU:C | 1:B:30:GLN:H | 2.09 | 0.54 |
| 1:B:872:ASP:O | 1:B:873:LYS:C | 2.45 | 0.54 |
| 1:A:366:ARG:NE | 1:A:366:ARG:CG | 2.64 | 0.54 |
| 1:B:583:VAL:O | 1:B:584:ASN:CB | 2.53 | 0.54 |
| 1:A:394:VAL:HG12 | 1:A:407:CYS:SG | 2.47 | 0.54 |
| 1:A:831:ASN:O | 1:A:832:GLN:O | 2.25 | 0.54 |
| 1:A:227:ILE:CB | 1:A:227:ILE:CD1 | 2.79 | 0.54 |
| 1:A:290:GLU:N | 1:A:290:GLU:OE2 | 2.33 | 0.54 |
| 1:A:683:PRO:O | 1:A:685:ASN:N | 2.40 | 0.54 |
| 1:A:731:VAL:CG1 | 1:A:733:LEU:CD1 | 2.82 | 0.54 |
| 1:A:358:THR:CG2 | 1:A:359:THR:N | 2.67 | 0.54 |
| 1:B:286:ASN:HD22 | 1:B:290:GLU:H | 1.55 | 0.54 |
| 1:B:427:ASP:CB | 2:B:1003:HOH:O | 2.54 | 0.54 |
| 1:B:89:VAL:CG2 | 1:B:89:VAL:CA | 2.81 | 0.54 |
| 1:A:193:GLU:C | 1:A:195:LEU:N | 2.58 | 0.54 |
| 1:B:521:LEU:HD22 | 1:B:636:ALA:O | 2.08 | 0.54 |
| 1:A:4:ILE:CD1 | 1:A:4:ILE:C | 2.74 | 0.54 |
| 1:B:712:TYR:CA | 2:B:956:HOH:O | 2.56 | 0.54 |
| 1:A:75:TRP:CH2 | 1:A:159:PRO:CG | 2.86 | 0.54 |
| 1:A:575:SER:O | 1:A:578:SER:N | 2.41 | 0.54 |
| 1:B:135:TYR:O | 1:B:136:ALA:CB | 2.56 | 0.54 |
| 1:B:439:PRO:HB2 | 1:B:440:ARG:CD | 2.36 | 0.54 |
| 1:B:447:VAL:CB | 1:B:513:LEU:HD11 | 2.38 | 0.54 |
| 1:A:3:GLY:HA2 | 1:A:777:ASP:O | 2.08 | 0.54 |
| 1:B:502:PHE:CG | 1:B:510:THR:HG21 | 2.43 | 0.54 |
| 1:A:745:LEU:HD12 | 1:A:749:LEU:CD2 | 2.37 | 0.54 |
| 1:A:758:ASP:O | 1:A:759:LEU:HB3 | 2.08 | 0.54 |
| 1:A:13:GLU:HA | 1:A:16:GLU:CG | 2.37 | 0.54 |
| 1:A:386:GLN:CB | 1:A:513:LEU:HB3 | 2.36 | 0.54 |
| 1:B:146:PHE:HA | 1:B:414:MET:HE2 | 1.90 | 0.54 |
| 1:A:273:THR:N | 1:A:312:ARG:HD2 | 2.22 | 0.54 |
| 1:B:206:ASP:OD1 | 1:B:206:ASP:N | 2.38 | 0.54 |
| 1:B:651:ARG:NH2 | 1:B:670:ARG:NE | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:115:THR:CG2 | 1:A:115:THR:CA | 2.80 | 0.54 |
| 1:B:524:GLU:CD | 1:B:524:GLU:H | 2.12 | 0.54 |
| 1:B:862:ASP:O | 1:B:864:MET:N | 2.40 | 0.54 |
| 1:A:61:LYS:O | 1:A:62:GLU:CB | 2.56 | 0.53 |
| 1:B:390:ARG:HD2 | 1:B:482:GLU:CG | 2.38 | 0.53 |
| 1:B:370:THR:HA | 1:B:383:VAL:CG1 | 2.38 | 0.53 |
| 1:B:831:ASN:O | 1:B:834:ILE:N | 2.40 | 0.53 |
| 1:A:642:CYS:O | 1:A:646:GLN:HG3 | 2.08 | 0.53 |
| 1:B:99:GLN:NE2 | 1:B:105:SER:HB3 | 2.23 | 0.53 |
| 1:A:824:GLU:CA | 1:A:828:PHE:O | 2.56 | 0.53 |
| 1:B:256:LYS:O | 1:B:258:LEU:N | 2.41 | 0.53 |
| 1:A:604:ASN:O | 1:A:605:ARG:C | 2.46 | 0.53 |
| 1:A:135:TYR:CD2 | 1:A:136:ALA:N | 2.77 | 0.53 |
| 1:A:188:VAL:HG23 | 1:A:189:ASN:N | 2.23 | 0.53 |
| 1:B:789:PHE:C | 1:B:789:PHE:HD2 | 2.11 | 0.53 |
| 1:A:576:LEU:HA | 1:A:579:CYS:HB2 | 1.90 | 0.53 |
| 1:A:430:THR:HG22 | 1:A:490:PHE:HB2 | 1.90 | 0.53 |
| 1:B:820:PRO:HD2 | 1:B:822:ALA:HB3 | 1.90 | 0.53 |
| 1:A:484:ILE:HD13 | 1:A:486:VAL:HG23 | 1.89 | 0.53 |
| 1:B:430:THR:H | 1:B:494:LYS:NZ | 2.06 | 0.53 |
| 1:B:390:ARG:NH1 | 1:B:390:ARG:CG | 2.58 | 0.53 |
| 1:B:438:VAL:HG23 | 1:B:482:GLU:O | 2.09 | 0.53 |
| 1:B:701:VAL:HG12 | 1:B:860:ARG:HD3 | 1.89 | 0.53 |
| 1:A:81:LEU:HD23 | 1:A:81:LEU:O | 2.09 | 0.53 |
| 1:A:665:VAL:HG23 | 1:A:666:ARG:H | 1.70 | 0.53 |
| 1:B:701:VAL:HG13 | 1:B:860:ARG:NH1 | 2.15 | 0.53 |
| 1:A:436:TYR:HB2 | 1:A:484:ILE:CG2 | 2.39 | 0.53 |
| 1:A:826:ALA:N | 1:A:826:ALA:CB | 2.66 | 0.53 |
| 1:B:114:LEU:O | 1:B:121:LEU:HD12 | 2.08 | 0.53 |
| 1:A:864:MET:CB | 1:A:864:MET:N | 2.67 | 0.53 |
| 1:A:677:ILE:CG2 | 1:A:681:LEU:HD12 | 2.39 | 0.53 |
| 1:B:213:GLU:O | 1:B:339:GLU:OE2 | 2.26 | 0.53 |
| 1:B:574:PHE:CE1 | 1:B:661:PHE:CE1 | 2.96 | 0.53 |
| 1:A:478:LEU:CB | 1:A:478:LEU:CD1 | 2.79 | 0.53 |
| 1:B:429:GLU:HB3 | 1:B:494:LYS:CE | 2.38 | 0.53 |
| 1:B:438:VAL:HG22 | 1:B:484:ILE:HD13 | 1.85 | 0.53 |
| 1:A:690:GLN:CG | 1:A:690:GLN:O | 2.57 | 0.53 |
| 1:A:610:LEU:CD2 | 1:A:610:LEU:CA | 2.87 | 0.53 |
| 1:B:113:SER:C | 1:B:115:THR:H | 2.11 | 0.53 |
| 1:B:215:TYR:HB2 | 1:B:337:LYS:HZ1 | 1.73 | 0.53 |
| 1:B:453:PHE:CE2 | 1:B:457:ASN:OD1 | 2.62 | 0.53 |
| 1:B:701:VAL:HG13 | 1:B:860:ARG:HG2 | 1.86 | 0.53 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:160:THR:OG1 | 1:B:165:LEU:HD23 | 2.08 | 0.53 |
| 1:A:633:ILE:HD11 | 1:A:648:ILE:HD13 | 1.90 | 0.53 |
| 1:A:571:THR:HG22 | 1:A:572:ASN:N | 2.24 | 0.53 |
| 1:B:124:VAL:O | 1:B:126:PRO:HD3 | 2.08 | 0.53 |
| 1:A:307:VAL:O | 1:A:308:ASP:CB | 2.56 | 0.53 |
| 1:A:327:SER:CB | 1:A:329:ARG:NH1 | 2.72 | 0.53 |
| 1:B:440:ARG:N | 1:B:440:ARG:HD3 | 2.24 | 0.53 |
| 1:A:468:ASN:CB | 2:A:905:HOH:O | 2.29 | 0.53 |
| 1:B:501:ARG:HD2 | 2:B:948:HOH:O | 2.08 | 0.53 |
| 1:B:601:ILE:HG21 | 2:B:987:HOH:O | 2.09 | 0.53 |
| 1:B:186:ALA:O | 1:B:187:LYS:C | 2.43 | 0.53 |
| 1:B:366:ARG:N | 1:B:370:THR:OG1 | 2.42 | 0.53 |
| 1:B:374:CYS:SG | 1:B:376:ASN:OD1 | 2.67 | 0.53 |
| 1:B:677:ILE:HG22 | 1:B:681:LEU:HD12 | 1.91 | 0.52 |
| 1:B:779:ASP:O | 1:B:780:THR:C | 2.46 | 0.52 |
| 1:A:759:LEU:HD12 | 1:A:812:GLY:O | 2.10 | 0.52 |
| 1:A:218:GLN:CD | 1:A:218:GLN:CB | 2.75 | 0.52 |
| 1:B:335:PHE:CD1 | 1:B:336:THR:HB | 2.44 | 0.52 |
| 1:B:670:ARG:HG3 | 1:B:674:LEU:HD21 | 1.90 | 0.52 |
| 1:A:748:ILE:HG23 | 1:A:749:LEU:N | 2.24 | 0.52 |
| 1:A:573:GLY:O | 1:A:574:PHE:C | 2.45 | 0.52 |
| 1:A:872:ASP:O | 1:A:872:ASP:OD2 | 2.26 | 0.52 |
| 1:A:343:LEU:H | 1:A:343:LEU:HD12 | 1.74 | 0.52 |
| 1:A:356:TRP:HA | 1:A:356:TRP:CE3 | 2.43 | 0.52 |
| 1:A:630:ARG:HG3 | 1:A:645:HIS:CE1 | 2.44 | 0.52 |
| 1:A:613:PHE:HZ | 1:A:622:GLY:O | 1.93 | 0.52 |
| 1:A:660:ASP:O | 1:A:664:PHE:HB2 | 2.09 | 0.52 |
| 1:B:740:VAL:CG1 | 1:B:741:SER:N | 2.69 | 0.52 |
| 1:B:800:GLN:HA | 1:B:851:PHE:HZ | 1.74 | 0.52 |
| 1:A:853:ASN:ND2 | 1:A:853:ASN:N | 2.52 | 0.52 |
| 1:B:508:ALA:O | 1:B:509:GLY:C | 2.42 | 0.52 |
| 1:B:384:ASN:HB3 | 1:B:385:PRO:CD | 2.39 | 0.52 |
| 1:B:153:VAL:O | 1:B:153:VAL:HG12 | 2.09 | 0.52 |
| 1:B:540:PHE:O | 1:B:540:PHE:CD1 | 2.62 | 0.52 |
| 1:B:113:SER:C | 1:B:115:THR:N | 2.63 | 0.52 |
| 1:B:296:PRO:HD2 | 1:B:304:TRP:HB3 | 1.91 | 0.52 |
| 1:B:674:LEU:O | 1:B:678:PHE:HB2 | 2.10 | 0.52 |
| 1:A:675:PHE:O | 1:A:676:LYS:C | 2.47 | 0.52 |
| 1:A:124:VAL:HG13 | 1:A:142:GLN:O | 2.10 | 0.52 |
| 1:B:8:LEU:O | 1:B:10:LYS:N | 2.43 | 0.52 |
| 1:B:258:LEU:O | 1:B:259:VAL:CG2 | 2.58 | 0.52 |
| 1:A:255:PHE:CB | 1:A:333:ARG:CG | 2.88 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:330:ASP:C | 1:B:332:ILE:N | 2.64 | 0.52 |
| 1:B:387:PHE:HB2 | 1:B:485:VAL:HG13 | 1.91 | 0.52 |
| 1:B:197:GLY:O | 1:B:198:GLY:O | 2.28 | 0.52 |
| 1:A:78:PRO:HB3 | 1:A:176:PHE:CZ | 2.45 | 0.52 |
| 1:A:297:TRP:O | 1:A:298:SER:OG | 2.19 | 0.52 |
| 1:A:517:ILE:HG23 | 1:A:640:LEU:CD2 | 2.40 | 0.52 |
| 1:B:790:LYS:O | 1:B:793:TRP:N | 2.43 | 0.52 |
| 1:B:435:VAL:HA | 1:B:484:ILE:O | 2.10 | 0.52 |
| 1:A:739:GLU:O | 1:A:739:GLU:OE1 | 2.26 | 0.52 |
| 1:B:274:TYR:CD2 | 1:B:275:GLN:HG3 | 2.44 | 0.52 |
| 1:A:306:LYS:HE3 | 1:A:307:VAL:H | 1.74 | 0.52 |
| 1:A:467:ILE:HG22 | 1:A:468:ASN:N | 2.24 | 0.52 |
| 1:A:372:GLY:O | 1:A:380:THR:OG1 | 2.05 | 0.52 |
| 1:B:585:LEU:CD2 | 1:B:586:MET:CE | 2.89 | 0.52 |
| 1:B:328:PHE:CE2 | 1:B:331:PHE:CE2 | 2.98 | 0.52 |
| 1:A:695:SER:O | 1:A:696:TRP:C | 2.47 | 0.52 |
| 1:B:519:ALA:HB2 | 1:B:675:PHE:CZ | 2.45 | 0.51 |
| 1:A:302:TYR:O | 1:A:303:GLU:HB3 | 2.10 | 0.51 |
| 1:A:350:SER:O | 1:A:352:THR:HG23 | 2.09 | 0.51 |
| 1:A:63:LEU:O | 1:A:70:THR:HG21 | 2.09 | 0.51 |
| 1:A:236:SER:C | 1:A:238:LEU:CD1 | 2.79 | 0.51 |
| 1:B:806:PHE:CD1 | 1:B:806:PHE:CB | 2.80 | 0.51 |
| 1:A:695:SER:O | 1:A:697:LEU:N | 2.43 | 0.51 |
| 1:A:343:LEU:O | 1:A:344:THR:C | 2.45 | 0.51 |
| 1:A:81:LEU:CD2 | 1:A:81:LEU:O | 2.57 | 0.51 |
| 1:B:605:ARG:HG2 | 1:B:605:ARG:NH2 | 2.25 | 0.51 |
| 1:B:208:THR:O | 1:B:346:ASP:OD1 | 2.28 | 0.51 |
| 1:B:161:LYS:C | 1:B:163:GLY:H | 2.13 | 0.51 |
| 1:B:524:GLU:O | 1:B:526:VAL:N | 2.43 | 0.51 |
| 1:B:377:TYR:C | 1:B:379:ALA:H | 2.13 | 0.51 |
| 1:A:135:TYR:O | 1:A:136:ALA:HB3 | 2.10 | 0.51 |
| 1:A:773:VAL:HG11 | 1:A:782:GLY:O | 2.11 | 0.51 |
| 1:B:643:GLN:NE2 | 1:B:643:GLN:CG | 2.66 | 0.51 |
| 1:B:65:PRO:O | 1:B:66:ASN:HB2 | 2.10 | 0.51 |
| 1:A:490:PHE:CD2 | 1:A:490:PHE:C | 2.84 | 0.51 |
| 1:A:314:GLN:CG | 1:A:315:LEU:N | 2.72 | 0.51 |
| 1:A:37:ASN:C | 1:A:39:CYS:H | 2.14 | 0.51 |
| 1:A:267:THR:OG1 | 1:A:319:MET:CE | 2.59 | 0.51 |
| 1:B:694:ILE:HA | 1:B:694:ILE:CB | 2.21 | 0.51 |
| 1:A:4:ILE:HD11 | 1:A:889:LEU:HD23 | 1.92 | 0.51 |
| 1:A:746:MET:SD | 1:A:766:ILE:N | 2.83 | 0.51 |
| 1:A:121:LEU:O | 1:A:121:LEU:HD22 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:435:VAL:O | 1:A:460:ARG:O | 2.27 | 0.51 |
| 1:B:404:GLU:OE1 | 1:B:404:GLU:HA | 2.09 | 0.51 |
| 1:B:660:ASP:OD1 | 1:B:663:ASN:OD1 | 2.29 | 0.51 |
| 1:B:579:CYS:CB | 1:B:579:CYS:N | 2.69 | 0.51 |
| 1:B:429:GLU:CA | 1:B:468:ASN:HD22 | 2.24 | 0.51 |
| 1:A:219:LYS:CD | 1:A:219:LYS:CA | 2.88 | 0.51 |
| 1:A:335:PHE:CD1 | 1:A:335:PHE:O | 2.63 | 0.51 |
| 1:B:526:VAL:HB | 2:B:950:HOH:O | 2.11 | 0.51 |
| 1:B:784:LEU:N | 1:B:784:LEU:CD1 | 2.73 | 0.51 |
| 1:B:610:LEU:HB3 | 1:B:661:PHE:CE2 | 2.46 | 0.51 |
| 1:A:238:LEU:HD12 | 1:A:238:LEU:N | 2.24 | 0.51 |
| 1:B:493:ASN:ND2 | 1:B:627:TYR:OH | 2.44 | 0.51 |
| 1:B:161:LYS:C | 1:B:163:GLY:N | 2.62 | 0.51 |
| 1:B:800:GLN:HA | 1:B:851:PHE:CZ | 2.46 | 0.51 |
| 1:B:430:THR:CA | 1:B:468:ASN:CB | 2.89 | 0.51 |
| 1:A:395:ASP:OD1 | 1:A:408:SER:HB3 | 2.11 | 0.51 |
| 1:B:450:LYS:O | 1:B:454:PHE:CD1 | 2.64 | 0.51 |
| 1:A:154:VAL:HG22 | 1:A:155:ASP:H | 1.76 | 0.51 |
| 1:A:139:PHE:HE1 | 1:A:156:ASP:HB3 | 1.75 | 0.51 |
| 1:A:329:ARG:HG3 | 1:A:333:ARG:HH11 | 1.76 | 0.51 |
| 1:B:470:ARG:CB | 1:B:470:ARG:CD | 2.81 | 0.51 |
| 1:A:414:MET:CE | 1:A:471:GLU:OE1 | 2.59 | 0.51 |
| 1:A:467:ILE:CD1 | 1:A:472:VAL:HG22 | 2.40 | 0.51 |
| 1:B:601:ILE:CG2 | 2:B:987:HOH:O | 2.58 | 0.51 |
| 1:B:95:THR:HG22 | 1:B:287:PRO:C | 2.31 | 0.51 |
| 1:B:236:SER:C | 1:B:237:LEU:HD23 | 2.31 | 0.51 |
| 1:B:660:ASP:HB2 | 2:B:1011:HOH:O | 2.11 | 0.51 |
| 1:B:412:ALA:HB2 | 1:B:473:SER:HB2 | 1.92 | 0.51 |
| 1:A:199:CYS:CB | 1:A:202:GLU:HG3 | 2.41 | 0.50 |
| 1:A:200:THR:CB | 1:A:200:THR:C | 2.68 | 0.50 |
| 1:A:216:ASP:OD1 | 1:A:335:PHE:CZ | 2.65 | 0.50 |
| 1:B:272:VAL:O | 1:B:278:ARG:HA | 2.12 | 0.50 |
| 1:B:89:VAL:N | 1:B:175:GLU:OE2 | 2.44 | 0.50 |
| 1:B:652:PHE:HE1 | 1:B:891:MET:HE3 | 1.76 | 0.50 |
| 1:B:142:GLN:CB | 1:B:142:GLN:NE2 | 2.75 | 0.50 |
| 1:A:757:PRO:O | 1:A:758:ASP:HB2 | 2.12 | 0.50 |
| 1:A:122:HIS:CG | 1:A:127:TYR:CE2 | 3.00 | 0.50 |
| 1:A:291:VAL:CG2 | 1:A:292:GLU:H | 2.24 | 0.50 |
| 1:B:507:LYS:HD2 | 2:B:934:HOH:O | 2.10 | 0.50 |
| 1:A:407:CYS:HB2 | 1:A:478:LEU:O | 2.11 | 0.50 |
| 1:B:640:LEU:HD21 | 1:B:671:LEU:HD11 | 1.93 | 0.50 |
| 1:A:6:MET:CE | 1:A:6:MET:CG | 2.88 | 0.50 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:800:GLN:HG3 | 1:A:851:PHE:CE1 | 2.46 | 0.50 |
| 1:A:117:ASN:OD1 | 1:A:119:THR:HB | 2.12 | 0.50 |
| 1:B:400:TYR:CG | 1:B:401:ASP:N | 2.80 | 0.50 |
| 1:B:477:ARG:CB | 1:B:477:ARG:CD | 2.81 | 0.50 |
| 1:B:694:ILE:C | 1:B:694:ILE:CB | 2.75 | 0.50 |
| 1:B:208:THR:HA | 2:B:908:HOH:O | 2.11 | 0.50 |
| 1:B:226:GLN:CD | 1:B:226:GLN:CB | 2.72 | 0.50 |
| 1:B:4:ILE:O | 1:B:5:ALA:C | 2.49 | 0.50 |
| 1:A:853:ASN:O | 1:A:857:CYS:HB2 | 2.11 | 0.50 |
| 1:B:398:ASP:HB2 | 2:B:964:HOH:O | 2.10 | 0.50 |
| 1:A:77:ARG:O | 1:A:81:LEU:HD13 | 2.12 | 0.50 |
| 1:A:97:ILE:HG12 | 1:A:98:CYS:H | 1.75 | 0.50 |
| 1:A:746:MET:CG | 1:A:746:MET:O | 2.55 | 0.50 |
| 1:A:365:TRP:CZ2 | 1:A:488:SER:CA | 2.91 | 0.50 |
| 1:A:340:ILE:CG2 | 1:A:340:ILE:CA | 2.78 | 0.50 |
| 1:B:677:ILE:O | 1:B:681:LEU:N | 2.39 | 0.50 |
| 1:B:521:LEU:HB3 | 1:B:522:PRO:HD2 | 1.93 | 0.50 |
| 1:A:881:VAL:HG12 | 1:A:885:GLU:HB2 | 1.92 | 0.50 |
| 1:A:13:GLU:O | 1:A:14:ALA:C | 2.49 | 0.50 |
| 1:B:225:TYR:CE1 | 1:B:280:ASN:CG | 2.84 | 0.50 |
| 1:A:644:LEU:O | 1:A:648:ILE:HG13 | 2.12 | 0.50 |
| 1:A:37:ASN:C | 1:A:39:CYS:N | 2.65 | 0.50 |
| 1:B:400:TYR:CD1 | 1:B:401:ASP:N | 2.78 | 0.50 |
| 1:B:256:LYS:HE3 | 1:B:293:TRP:HA | 1.94 | 0.50 |
| 1:B:366:ARG:HA | 1:B:495:GLU:HG2 | 1.94 | 0.50 |
| 1:B:616:PHE:O | 1:B:624:MET:HB3 | 2.11 | 0.50 |
| 1:B:443:ALA:CB | 2:B:894:HOH:O | 2.54 | 0.50 |
| 1:B:603:TRP:O | 1:B:603:TRP:CD1 | 2.65 | 0.50 |
| 1:A:168:VAL:O | 1:A:169:HIS:HB3 | 2.11 | 0.50 |
| 1:B:456:ALA:C | 1:B:456:ALA:HA | 2.12 | 0.50 |
| 1:A:272:VAL:CA | 1:A:312:ARG:HD2 | 2.41 | 0.50 |
| 1:A:320:GLU:C | 1:A:320:GLU:CB | 2.73 | 0.49 |
| 1:B:651:ARG:NH1 | 1:B:891:MET:HA | 2.27 | 0.49 |
| 1:B:439:PRO:C | 1:B:440:ARG:HD3 | 2.32 | 0.49 |
| 1:B:60:PHE:CD2 | 1:B:60:PHE:N | 2.79 | 0.49 |
| 1:A:741:SER:C | 1:A:743:THR:N | 2.55 | 0.49 |
| 1:A:489:THR:OG1 | 1:A:491:GLU:O | 2.30 | 0.49 |
| 1:A:771:SER:OG | 1:A:893:SER:O | 2.29 | 0.49 |
| 1:A:27:TYR:HB2 | 1:A:150:VAL:CG1 | 2.42 | 0.49 |
| 1:A:698:SER:C | 1:A:700:SER:N | 2.65 | 0.49 |
| 1:B:838:ILE:CG2 | 1:B:839:ILE:N | 2.75 | 0.49 |
| 1:A:309:PRO:O | 1:A:310:TYR:C | 2.49 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:461:ALA:C | 1:B:462:GLN:HG3 | 2.31 | 0.49 |
| 1:A:231:ALA:O | 1:A:234:ARG:HB2 | 2.13 | 0.49 |
| 1:B:6:MET:SD | 1:B:870:SER:OG | 2.59 | 0.49 |
| 1:A:350:SER:C | 1:A:352:THR:N | 2.63 | 0.49 |
| 1:A:314:GLN:CG | 1:A:315:LEU:H | 2.25 | 0.49 |
| 1:B:230:LYS:HB3 | 1:B:234:ARG:NH2 | 2.28 | 0.49 |
| 1:A:105:SER:O | 1:A:108:LEU:HB2 | 2.11 | 0.49 |
| 1:A:200:THR:CA | 1:A:200:THR:CG2 | 2.87 | 0.49 |
| 1:A:120:ILE:HD13 | 1:A:237:LEU:HD21 | 1.94 | 0.49 |
| 1:B:669:VAL:O | 1:B:673:ILE:HG13 | 2.12 | 0.49 |
| 1:A:5:ALA:C | 1:A:7:LYS:H | 2.15 | 0.49 |
| 1:A:51:PHE:HB2 | 1:A:187:LYS:HG3 | 1.93 | 0.49 |
| 1:A:621:SER:OG | 1:A:623:SER:HB2 | 2.13 | 0.49 |
| 1:A:633:ILE:CD1 | 1:A:648:ILE:HD13 | 2.42 | 0.49 |
| 1:A:606:ILE:O | 1:A:609:TYR:N | 2.45 | 0.49 |
| 1:A:168:VAL:HB | 1:A:182:GLU:OE2 | 2.12 | 0.49 |
| 1:B:142:GLN:CB | 1:B:142:GLN:CD | 2.72 | 0.49 |
| 1:A:619:ASP:O | 1:A:621:SER:N | 2.44 | 0.49 |
| 1:B:424:PHE:HZ | 1:B:711:HIS:HA | 1.74 | 0.49 |
| 1:A:85:PRO:HB2 | 1:A:131:PHE:CG | 2.48 | 0.49 |
| 1:B:303:GLU:HG2 | 1:B:303:GLU:O | 2.03 | 0.49 |
| 1:B:161:LYS:HG3 | 1:B:166:VAL:HG11 | 1.94 | 0.49 |
| 1:B:724:ARG:HB2 | 1:B:724:ARG:NH2 | 2.19 | 0.49 |
| 1:A:35:LEU:HD22 | 1:A:46:PHE:CE1 | 2.48 | 0.49 |
| 1:A:83:SER:O | 1:A:84:ASN:CB | 2.59 | 0.49 |
| 1:A:664:PHE:CZ | 1:A:668:LEU:HD11 | 2.48 | 0.49 |
| 1:B:14:ALA:O | 1:B:17:GLY:N | 2.46 | 0.49 |
| 1:A:228:ILE:O | 1:A:229:LEU:C | 2.51 | 0.49 |
| 1:B:146:PHE:HA | 1:B:414:MET:CE | 2.42 | 0.49 |
| 1:A:769:CYS:O | 1:A:770:ARG:C | 2.49 | 0.49 |
| 1:B:585:LEU:CD2 | 1:B:586:MET:HE2 | 2.43 | 0.49 |
| 1:A:628:GLU:O | 1:A:629:MET:C | 2.51 | 0.49 |
| 1:A:832:GLN:CD | 1:A:832:GLN:C | 2.70 | 0.49 |
| 1:B:25:ILE:CG2 | 1:B:26:LYS:N | 2.75 | 0.49 |
| 1:B:6:MET:SD | 1:B:6:MET:HA | 2.52 | 0.49 |
| 1:A:734:ALA:O | 1:A:736:ASP:N | 2.45 | 0.49 |
| 1:A:304:TRP:CE2 | 1:A:313:GLU:OE2 | 2.65 | 0.49 |
| 1:B:585:LEU:HD23 | 1:B:586:MET:CE | 2.43 | 0.49 |
| 1:B:158:LEU:HB2 | 1:B:165:LEU:HD21 | 1.94 | 0.49 |
| 1:B:160:THR:HG1 | 1:B:165:LEU:HD23 | 1.78 | 0.49 |
| 1:B:0:GLU:HA | 1:B:0:GLU:CB | 2.19 | 0.48 |
| 1:B:212:THR:HB | 1:B:340:ILE:CD1 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:824:GLU:CB | 1:B:824:GLU:HA | 2.24 | 0.48 |
| 1:A:695:SER:O | 1:A:698:SER:N | 2.46 | 0.48 |
| 1:A:350:SER:HB3 | 1:A:352:THR:HG22 | 1.95 | 0.48 |
| 1:A:114:LEU:CD1 | 1:A:121:LEU:HD23 | 2.41 | 0.48 |
| 1:A:225:TYR:HB2 | 1:A:328:PHE:CE2 | 2.48 | 0.48 |
| 1:B:57:SER:O | 1:B:191:SER:HB2 | 2.12 | 0.48 |
| 1:A:106:TRP:HZ2 | 1:A:195:LEU:O | 1.97 | 0.48 |
| 1:A:256:LYS:CA | 1:A:258:LEU:HD13 | 2.44 | 0.48 |
| 1:A:358:THR:C | 1:A:359:THR:HG23 | 2.31 | 0.48 |
| 1:B:106:TRP:HZ2 | 1:B:195:LEU:O | 1.97 | 0.48 |
| 1:A:47:GLN:OE1 | 1:A:47:GLN:CA | 2.53 | 0.48 |
| 1:B:595:GLY:O | 1:B:599:PHE:CB | 2.61 | 0.48 |
| 1:A:25:ILE:O | 1:A:151:ASP:N | 2.46 | 0.48 |
| 1:B:340:ILE:HG13 | 1:B:340:ILE:CD1 | 2.20 | 0.48 |
| 1:B:537:LYS:CG | 1:B:537:LYS:NZ | 2.75 | 0.48 |
| 1:A:335:PHE:HD1 | 1:A:336:THR:HB | 1.78 | 0.48 |
| 1:B:731:VAL:HG11 | 1:B:739:GLU:O | 2.13 | 0.48 |
| 1:B:730:PHE:O | 1:B:732:GLN:N | 2.46 | 0.48 |
| 1:A:308:ASP:OD2 | 1:A:313:GLU:HG3 | 2.14 | 0.48 |
| 1:A:665:VAL:O | 1:A:666:ARG:O | 2.30 | 0.48 |
| 1:B:585:LEU:HG | 1:B:586:MET:CE | 2.35 | 0.48 |
| 1:B:789:PHE:O | 1:B:792:LEU:HB3 | 2.13 | 0.48 |
| 1:A:519:ALA:CB | 1:A:675:PHE:CE1 | 2.91 | 0.48 |
| 1:B:227:ILE:O | 1:B:228:ILE:C | 2.47 | 0.48 |
| 1:A:281:LEU:HA | 1:A:327:SER:HA | 1.95 | 0.48 |
| 1:B:142:GLN:CB | 1:B:142:GLN:HE21 | 2.26 | 0.48 |
| 1:B:330:ASP:OD1 | 1:B:331:PHE:N | 2.44 | 0.48 |
| 1:A:470:ARG:O | 1:A:471:GLU:O | 2.32 | 0.48 |
| 1:B:697:LEU:HA | 1:B:700:SER:HG | 1.78 | 0.48 |
| 1:A:792:LEU:O | 1:A:792:LEU:HD12 | 2.14 | 0.48 |
| 1:B:684:GLU:O | 1:B:685:ASN:C | 2.52 | 0.48 |
| 1:A:319:MET:CG | 1:A:320:GLU:N | 2.76 | 0.48 |
| 1:A:305:ASN:HD22 | 1:A:306:LYS:H | 1.54 | 0.48 |
| 1:B:729:LEU:HD22 | 2:B:1027:HOH:O | 2.14 | 0.48 |
| 1:B:634:GLU:HA | 1:B:638:PHE:O | 2.13 | 0.48 |
| 1:A:831:ASN:CB | 1:A:831:ASN:ND2 | 2.67 | 0.48 |
| 1:B:453:PHE:CD2 | 1:B:453:PHE:C | 2.86 | 0.48 |
| 1:B:572:ASN:CA | 1:B:573:GLY:N | 2.70 | 0.48 |
| 1:A:258:LEU:HD13 | 1:A:258:LEU:N | 2.28 | 0.48 |
| 1:B:828:PHE:CG | 1:B:861:LEU:HD23 | 2.48 | 0.48 |
| 1:B:415:GLN:NE2 | 1:B:428:MET:HB3 | 2.28 | 0.48 |
| 1:B:382:TRP:HB3 | 1:B:451:ARG:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:760:LYS:CA | 1:A:760:LYS:HE3 | 2.42 | 0.48 |
| 1:A:154:VAL:HG22 | 1:A:155:ASP:N | 2.29 | 0.48 |
| 1:A:258:LEU:N | 1:A:258:LEU:CD1 | 2.73 | 0.48 |
| 1:A:857:CYS:C | 1:A:859:VAL:H | 2.16 | 0.48 |
| 1:B:99:GLN:HE22 | 1:B:105:SER:HB3 | 1.79 | 0.48 |
| 1:A:824:GLU:C | 1:A:826:ALA:H | 2.17 | 0.48 |
| 1:A:267:THR:OG1 | 1:A:319:MET:HE3 | 2.14 | 0.48 |
| 1:A:105:SER:O | 1:A:106:TRP:O | 2.32 | 0.48 |
| 1:A:66:ASN:O | 1:A:67:SER:O | 2.32 | 0.48 |
| 1:A:391:LEU:HB3 | 1:A:407:CYS:HB3 | 1.96 | 0.48 |
| 1:B:100:GLY:HA3 | 1:B:166:VAL:O | 2.13 | 0.48 |
| 1:A:176:PHE:O | 1:A:179:ALA:HB3 | 2.13 | 0.48 |
| 1:A:887:LEU:HD23 | 1:A:887:LEU:HA | 1.65 | 0.48 |
| 1:A:105:SER:O | 1:A:108:LEU:CB | 2.62 | 0.48 |
| 1:A:97:ILE:HD13 | 1:A:108:LEU:CD1 | 2.42 | 0.48 |
| 1:B:21:HIS:HD2 | 1:B:142:GLN:HE22 | 1.59 | 0.48 |
| 1:B:430:THR:HG23 | 1:B:468:ASN:HB3 | 1.96 | 0.48 |
| 1:A:467:ILE:CD1 | 1:A:472:VAL:CG2 | 2.92 | 0.48 |
| 1:B:145:GLN:O | 1:B:146:PHE:C | 2.51 | 0.48 |
| 1:A:686:THR:HG21 | 2:A:977:HOH:O | 2.14 | 0.48 |
| 1:A:850:ASP:OD2 | 2:A:935:HOH:O | 2.20 | 0.48 |
| 1:B:284:MET:CA | 1:B:284:MET:CG | 2.80 | 0.48 |
| 1:A:579:CYS:HA | 1:A:582:MET:HE3 | 1.96 | 0.48 |
| 1:A:403:ARG:HB3 | 1:A:477:ARG:HD2 | 1.96 | 0.47 |
| 1:A:30:GLN:NE2 | 1:A:187:LYS:NZ | 2.49 | 0.47 |
| 1:B:383:VAL:HG13 | 1:B:383:VAL:O | 2.13 | 0.47 |
| 1:B:616:PHE:CZ | 1:B:631:MET:O | 2.67 | 0.47 |
| 1:B:525:LYS:O | 1:B:526:VAL:O | 2.31 | 0.47 |
| 1:A:358:THR:CG2 | 1:A:359:THR:H | 2.25 | 0.47 |
| 1:A:146:PHE:HB3 | 1:A:416:LYS:HG2 | 1.96 | 0.47 |
| 1:B:116:LEU:CD1 | 1:B:287:PRO:HG3 | 2.34 | 0.47 |
| 1:B:537:LYS:CB | 1:B:537:LYS:HZ3 | 2.25 | 0.47 |
| 1:B:369:SER:O | 1:B:383:VAL:HG11 | 2.13 | 0.47 |
| 1:B:83:SER:O | 1:B:85:PRO:HD3 | 2.14 | 0.47 |
| 1:B:109:ALA:O | 1:B:113:SER:HB3 | 2.14 | 0.47 |
| 1:A:306:LYS:CE | 1:A:307:VAL:H | 2.26 | 0.47 |
| 1:A:60:PHE:O | 1:A:61:LYS:CB | 2.62 | 0.47 |
| 1:A:242:ILE:CB | 1:A:242:ILE:CD1 | 2.75 | 0.47 |
| 1:B:764:PHE:CE1 | 1:B:851:PHE:O | 2.66 | 0.47 |
| 1:B:412:ALA:CB | 1:B:473:SER:HB2 | 2.43 | 0.47 |
| 1:B:282:ILE:HG22 | 1:B:326:MET:HG3 | 1.96 | 0.47 |
| 1:A:773:VAL:O | 1:A:774:ALA:C | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:304:TRP:CE2 | 1:B:312:ARG:HD3 | 2.50 | 0.47 |
| 1:B:349:LYS:CG | 1:B:350:SER:N | 2.77 | 0.47 |
| 1:B:868:PHE:HZ | 1:B:878:GLN:HA | 1.80 | 0.47 |
| 1:A:743:THR:O | 1:A:747:ASN:OD1 | 2.32 | 0.47 |
| 1:B:242:ILE:CG2 | 1:B:242:ILE:O | 2.62 | 0.47 |
| 1:B:12:ARG:HH21 | 1:B:885:GLU:CD | 2.18 | 0.47 |
| 1:B:228:ILE:CG2 | 1:B:228:ILE:CA | 2.84 | 0.47 |
| 1:A:304:TRP:CZ2 | 1:A:317:VAL:HG13 | 2.50 | 0.47 |
| 1:A:327:SER:N | 1:A:329:ARG:HH12 | 2.06 | 0.47 |
| 1:B:585:LEU:CD1 | 1:B:672:GLU:HG2 | 2.43 | 0.47 |
| 1:B:342:ASN:ND2 | 1:B:346:ASP:OD2 | 2.47 | 0.47 |
| 1:A:576:LEU:O | 1:A:580:ARG:CB | 2.63 | 0.47 |
| 1:B:388:LYS:HZ3 | 1:B:482:GLU:HB3 | 1.78 | 0.47 |
| 1:A:258:LEU:O | 1:A:258:LEU:HD22 | 2.09 | 0.47 |
| 1:B:451:ARG:HD2 | 2:B:902:HOH:O | 2.14 | 0.47 |
| 1:A:862:ASP:OD2 | 1:A:862:ASP:C | 2.50 | 0.47 |
| 1:A:821:GLY:C | 1:A:823:PHE:H | 2.18 | 0.47 |
| 1:A:756:HIS:HB2 | 1:A:757:PRO:HD2 | 1.94 | 0.47 |
| 1:B:364:THR:HG1 | 1:B:646:GLN:NE2 | 1.95 | 0.47 |
| 1:B:764:PHE:HE1 | 1:B:851:PHE:O | 1.97 | 0.47 |
| 1:B:389:ILE:CD1 | 1:B:389:ILE:N | 2.54 | 0.47 |
| 1:B:524:GLU:O | 1:B:525:LYS:C | 2.52 | 0.47 |
| 1:A:803:TYR:N | 1:A:822:ALA:HB1 | 2.29 | 0.47 |
| 1:A:32:TYR:HB2 | 1:A:153:VAL:CG2 | 2.44 | 0.47 |
| 1:B:377:TYR:O | 1:B:379:ALA:N | 2.47 | 0.47 |
| 1:B:82:LEU:O | 1:B:83:SER:C | 2.52 | 0.47 |
| 1:A:93:THR:HB | 1:A:321:ASP:OD2 | 2.15 | 0.47 |
| 1:A:296:PRO:HG3 | 1:A:304:TRP:HB2 | 1.93 | 0.47 |
| 1:B:241:SER:OG | 1:B:336:THR:HG22 | 2.14 | 0.47 |
| 1:B:328:PHE:CZ | 1:B:331:PHE:CE2 | 3.02 | 0.47 |
| 1:B:517:ILE:CG2 | 1:B:883:ILE:HG13 | 2.43 | 0.47 |
| 1:A:617:ASP:O | 1:A:618:LEU:C | 2.53 | 0.47 |
| 1:A:229:LEU:O | 1:A:232:LEU:N | 2.47 | 0.47 |
| 1:A:228:ILE:HG12 | 1:A:337:LYS:HZ1 | 1.78 | 0.47 |
| 1:A:822:ALA:HA | 2:A:912:HOH:O | 2.14 | 0.47 |
| 1:A:368:GLY:HA2 | 1:A:627:TYR:CE1 | 2.49 | 0.47 |
| 1:A:553:LYS:C | 1:A:555:LEU:N | 2.67 | 0.47 |
| 1:A:263:ALA:HB2 | 1:A:288:TRP:HZ3 | 1.78 | 0.47 |
| 1:A:453:PHE:C | 1:A:453:PHE:CD2 | 2.88 | 0.47 |
| 1:A:820:PRO:HD2 | 2:A:928:HOH:O | 2.14 | 0.47 |
| 1:B:112:ALA:O | 1:B:115:THR:HB | 2.14 | 0.47 |
| 1:A:669:VAL:O | 1:A:670:ARG:C | 2.52 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:224:LEU:HD22 | 1:A:224:LEU:O | 2.15 | 0.47 |
| 1:A:50:ALA:O | 1:A:52:PRO:HD3 | 2.13 | 0.47 |
| 1:B:375:ARG:CB | 1:B:375:ARG:HH11 | 2.15 | 0.47 |
| 1:A:146:PHE:CD1 | 1:A:416:LYS:HA | 2.50 | 0.47 |
| 1:A:96:ASP:C | 1:A:97:ILE:O | 2.50 | 0.47 |
| 1:A:120:ILE:CD1 | 1:A:237:LEU:HD21 | 2.45 | 0.47 |
| 1:B:670:ARG:HG3 | 1:B:674:LEU:CD2 | 2.45 | 0.47 |
| 1:B:332:ILE:HG22 | 1:B:333:ARG:N | 2.29 | 0.47 |
| 1:B:789:PHE:O | 1:B:789:PHE:HD2 | 1.98 | 0.47 |
| 1:B:626:ALA:CB | 1:B:649:VAL:HG22 | 2.37 | 0.47 |
| 1:B:538:THR:CG2 | 1:B:539:LEU:N | 2.58 | 0.47 |
| 1:A:23:ARG:O | 1:A:24:ALA:C | 2.53 | 0.47 |
| 1:B:108:LEU:HD12 | 1:B:108:LEU:HA | 1.58 | 0.46 |
| 1:B:675:PHE:O | 1:B:678:PHE:HB3 | 2.15 | 0.46 |
| 1:B:136:ALA:CB | 1:B:136:ALA:N | 2.67 | 0.46 |
| 1:B:411:LEU:CD1 | 1:B:502:PHE:CE1 | 2.98 | 0.46 |
| 1:A:386:GLN:HB3 | 1:A:513:LEU:CB | 2.41 | 0.46 |
| 1:A:112:ALA:C | 1:A:114:LEU:H | 2.19 | 0.46 |
| 1:A:608:ASN:O | 1:A:609:TYR:C | 2.44 | 0.46 |
| 1:A:98:CYS:SG | 1:A:169:HIS:CE1 | 3.08 | 0.46 |
| 1:A:478:LEU:HA | 1:A:478:LEU:HD23 | 1.36 | 0.46 |
| 1:B:585:LEU:O | 1:B:586:MET:O | 2.33 | 0.46 |
| 1:B:453:PHE:O | 1:B:453:PHE:CD2 | 2.67 | 0.46 |
| 1:A:411:LEU:HD22 | 1:A:433:PHE:CE1 | 2.50 | 0.46 |
| 1:A:100:GLY:HA3 | 1:A:103:GLY:CA | 2.39 | 0.46 |
| 1:A:386:GLN:O | 1:A:387:PHE:CG | 2.69 | 0.46 |
| 1:B:327:SER:OG | 1:B:329:ARG:HB2 | 2.15 | 0.46 |
| 1:A:67:SER:O | 1:A:68:SER:C | 2.52 | 0.46 |
| 1:A:758:ASP:O | 1:A:759:LEU:CB | 2.58 | 0.46 |
| 1:A:48:ASP:OD2 | 1:A:187:LYS:HE3 | 2.15 | 0.46 |
| 1:A:571:THR:CG2 | 1:A:572:ASN:H | 2.29 | 0.46 |
| 1:B:511:GLN:CB | 2:B:899:HOH:O | 2.63 | 0.46 |
| 1:B:284:MET:HB2 | 1:B:324:PHE:CZ | 2.51 | 0.46 |
| 1:B:476:ILE:HG22 | 1:B:478:LEU:HG | 1.98 | 0.46 |
| 1:A:320:GLU:O | 1:A:321:ASP:C | 2.54 | 0.46 |
| 1:B:230:LYS:CD | 1:B:230:LYS:NZ | 2.68 | 0.46 |
| 1:A:670:ARG:O | 1:A:673:ILE:N | 2.48 | 0.46 |
| 1:A:579:CYS:HA | 1:A:582:MET:CE | 2.46 | 0.46 |
| 1:A:46:PHE:CD2 | 1:A:138:ILE:HD12 | 2.51 | 0.46 |
| 1:B:242:ILE:C | 1:B:242:ILE:HD13 | 2.35 | 0.46 |
| 1:B:692:ASP:O | 1:B:693:LEU:C | 2.53 | 0.46 |
| 1:B:521:LEU:HB3 | 1:B:522:PRO:CD | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:90:ASP:OD1 | 1:B:92:ALA:O | 2.34 | 0.46 |
| 1:B:193:GLU:O | 1:B:196:SER:OG | 2.24 | 0.46 |
| 1:A:693:LEU:HA | 1:A:868:PHE:CE2 | 2.50 | 0.46 |
| 1:A:487:PRO:O | 1:A:488:SER:CB | 2.57 | 0.46 |
| 1:B:723:GLU:C | 1:B:726:PHE:CD2 | 2.87 | 0.46 |
| 1:A:585:LEU:HD11 | 1:A:605:ARG:NH2 | 2.30 | 0.46 |
| 1:A:600:ASN:C | 1:A:602:LEU:N | 2.68 | 0.46 |
| 1:A:51:PHE:CB | 1:A:187:LYS:HG3 | 2.46 | 0.46 |
| 1:B:279:VAL:HG23 | 1:B:281:LEU:HD23 | 1.98 | 0.46 |
| 1:A:686:THR:CG2 | 2:A:977:HOH:O | 2.63 | 0.46 |
| 1:A:829:HIS:CE1 | 2:A:917:HOH:O | 2.69 | 0.46 |
| 1:A:66:ASN:O | 1:A:67:SER:C | 2.52 | 0.46 |
| 1:B:652:PHE:HE1 | 1:B:891:MET:CE | 2.28 | 0.46 |
| 1:A:429:GLU:CG | 1:A:494:LYS:HE3 | 2.46 | 0.46 |
| 1:A:96:ASP:O | 1:A:97:ILE:O | 2.33 | 0.46 |
| 1:B:636:ALA:CB | 1:B:668:LEU:HD13 | 2.46 | 0.46 |
| 1:B:430:THR:HA | 1:B:468:ASN:HB3 | 1.97 | 0.46 |
| 1:A:652:PHE:CD1 | 1:A:667:CYS:CB | 2.94 | 0.46 |
| 1:A:698:SER:C | 1:A:700:SER:H | 2.17 | 0.46 |
| 1:A:748:ILE:HG23 | 1:A:749:LEU:H | 1.81 | 0.46 |
| 1:A:284:MET:HE2 | 1:A:326:MET:SD | 2.56 | 0.46 |
| 1:A:656:GLU:CD | 1:A:656:GLU:N | 2.70 | 0.46 |
| 1:B:228:ILE:O | 1:B:232:LEU:HD23 | 2.16 | 0.46 |
| 1:B:340:ILE:HG12 | 1:B:340:ILE:CD1 | 2.20 | 0.46 |
| 1:A:88:ILE:HA | 1:A:175:GLU:CG | 2.45 | 0.46 |
| 1:B:390:ARG:HH11 | 1:B:390:ARG:CG | 2.07 | 0.46 |
| 1:A:693:LEU:HA | 1:A:868:PHE:CZ | 2.51 | 0.46 |
| 1:B:110:ALA:HA | 1:B:204:PHE:CE2 | 2.51 | 0.46 |
| 1:A:327:SER:OG | 1:A:329:ARG:NE | 2.49 | 0.46 |
| 1:B:576:LEU:O | 1:B:578:SER:CA | 2.62 | 0.46 |
| 1:B:673:ILE:HG22 | 1:B:677:ILE:CD1 | 2.46 | 0.46 |
| 1:B:780:THR:CG2 | 1:B:780:THR:OG1 | 2.55 | 0.46 |
| 1:A:677:ILE:HG22 | 1:A:678:PHE:N | 2.29 | 0.46 |
| 1:A:467:ILE:HD12 | 1:A:472:VAL:CG2 | 2.45 | 0.46 |
| 1:B:328:PHE:CD2 | 1:B:331:PHE:CE2 | 3.05 | 0.45 |
| 1:A:450:LYS:HB3 | 1:A:451:ARG:H | 1.62 | 0.45 |
| 1:A:232:LEU:HA | 1:A:232:LEU:HD13 | 1.76 | 0.45 |
| 1:A:30:GLN:NE2 | 1:A:187:LYS:HZ3 | 2.09 | 0.45 |
| 1:B:552:VAL:O | 1:B:554:GLU:N | 2.49 | 0.45 |
| 1:B:89:VAL:CG1 | 1:B:89:VAL:CG2 | 2.88 | 0.45 |
| 1:B:66:ASN:O | 1:B:67:SER:O | 2.34 | 0.45 |
| 1:B:805:ARG:N | 1:B:811:SER:OG | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:552:VAL:C | 1:B:554:GLU:N | 2.69 | 0.45 |
| 1:A:745:LEU:HD12 | 1:A:749:LEU:HD21 | 1.99 | 0.45 |
| 1:B:696:TRP:O | 1:B:700:SER:CB | 2.63 | 0.45 |
| 1:A:60:PHE:N | 1:A:64:GLY:HA3 | 2.31 | 0.45 |
| 1:A:576:LEU:CA | 1:A:579:CYS:HB2 | 2.46 | 0.45 |
| 1:A:731:VAL:HG23 | 1:A:732:GLN:N | 2.31 | 0.45 |
| 1:A:268:ASP:HB3 | 1:A:283:ARG:HB3 | 1.97 | 0.45 |
| 1:A:305:ASN:ND2 | 1:A:305:ASN:N | 2.64 | 0.45 |
| 1:A:63:LEU:C | 1:A:193:GLU:OE2 | 2.54 | 0.45 |
| 1:B:583:VAL:O | 1:B:584:ASN:HB2 | 2.16 | 0.45 |
| 1:B:20:SER:O | 1:B:21:HIS:C | 2.53 | 0.45 |
| 1:A:757:PRO:HG3 | 2:A:1029:HOH:O | 2.16 | 0.45 |
| 1:A:26:LYS:HD3 | 1:A:26:LYS:HA | 1.67 | 0.45 |
| 1:A:27:TYR:O | 1:A:30:GLN:HG3 | 2.17 | 0.45 |
| 1:A:273:THR:OG1 | 1:A:312:ARG:NH2 | 2.49 | 0.45 |
| 1:A:872:ASP:HB2 | 1:A:879:ILE:HG22 | 1.97 | 0.45 |
| 1:A:361:TYR:OH | 1:A:510:THR:C | 2.54 | 0.45 |
| 1:B:12:ARG:O | 1:B:16:GLU:HG3 | 2.17 | 0.45 |
| 1:B:576:LEU:C | 1:B:578:SER:N | 2.67 | 0.45 |
| 1:B:681:LEU:O | 1:B:683:PRO:HD2 | 2.15 | 0.45 |
| 1:B:61:LYS:O | 1:B:62:GLU:HB2 | 2.15 | 0.45 |
| 1:A:414:MET:HE3 | 1:A:471:GLU:OE1 | 2.17 | 0.45 |
| 1:B:656:GLU:O | 1:B:657:LEU:CB | 2.64 | 0.45 |
| 1:A:21:HIS:ND1 | 2:A:1060:HOH:O | 2.05 | 0.45 |
| 1:A:388:LYS:NZ | 1:A:482:GLU:HG2 | 2.32 | 0.45 |
| 1:B:796:ILE:O | 1:B:799:TRP:CB | 2.62 | 0.45 |
| 1:B:856:SER:C | 1:B:858:LEU:N | 2.69 | 0.45 |
| 1:B:831:ASN:C | 1:B:833:HIS:N | 2.69 | 0.45 |
| 1:B:256:LYS:HB3 | 1:B:256:LYS:CE | 2.46 | 0.45 |
| 1:B:476:ILE:HG22 | 1:B:477:ARG:N | 2.32 | 0.45 |
| 1:A:283:ARG:HB2 | 1:A:325:TRP:CE2 | 2.51 | 0.45 |
| 1:A:223:ASP:C | 1:A:227:ILE:HD12 | 2.32 | 0.45 |
| 1:B:135:TYR:CG | 1:B:136:ALA:N | 2.83 | 0.45 |
| 1:A:433:PHE:HE2 | 1:A:472:VAL:HG12 | 1.82 | 0.45 |
| 1:B:799:TRP:HZ2 | 1:B:828:PHE:HE1 | 1.64 | 0.45 |
| 1:B:822:ALA:O | 1:B:825:ALA:CB | 2.56 | 0.45 |
| 1:A:739:GLU:HA | 2:A:979:HOH:O | 2.17 | 0.45 |
| 1:A:21:HIS:NE2 | 1:A:123:ARG:O | 2.50 | 0.45 |
| 1:A:68:SER:OG | 1:A:69:LYS:N | 2.50 | 0.45 |
| 1:A:665:VAL:C | 1:A:669:VAL:HG23 | 2.32 | 0.45 |
| 1:A:883:ILE:CA | 1:A:883:ILE:CG2 | 2.84 | 0.45 |
| 1:A:604:ASN:HD22 | 1:A:604:ASN:N | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:411:LEU:C | 1:A:411:LEU:HD23 | 2.37 | 0.45 |
| 1:B:828:PHE:HZ | 1:B:862:ASP:OD1 | 2.00 | 0.45 |
| 1:B:557:THR:HG22 | 1:B:558:ILE:N | 2.32 | 0.45 |
| 1:A:743:THR:O | 1:A:744:GLU:C | 2.55 | 0.45 |
| 1:A:571:THR:HG22 | 1:A:572:ASN:H | 1.81 | 0.45 |
| 1:A:760:LYS:HA | 1:A:760:LYS:HE3 | 1.99 | 0.45 |
| 1:B:871:LEU:N | 1:B:871:LEU:HD12 | 2.31 | 0.45 |
| 1:A:828:PHE:CD1 | 1:A:828:PHE:N | 2.85 | 0.45 |
| 1:A:58:LEU:O | 1:A:63:LEU:HG | 2.16 | 0.45 |
| 1:A:212:THR:HG21 | 1:A:340:ILE:HD12 | 1.99 | 0.45 |
| 1:B:676:LYS:O | 1:B:677:ILE:C | 2.55 | 0.45 |
| 1:B:69:LYS:HG2 | 1:B:102:LEU:CD1 | 2.47 | 0.45 |
| 1:B:502:PHE:CB | 1:B:510:THR:HG21 | 2.47 | 0.45 |
| 1:A:352:THR:OG1 | 1:A:352:THR:O | 2.34 | 0.45 |
| 1:A:656:GLU:O | 1:A:657:LEU:CB | 2.65 | 0.45 |
| 1:B:696:TRP:CE3 | 1:B:700:SER:HB3 | 2.52 | 0.45 |
| 1:A:878:GLN:HE21 | 1:A:878:GLN:HB3 | 1.52 | 0.45 |
| 1:B:651:ARG:CZ | 1:B:670:ARG:HH22 | 2.23 | 0.45 |
| 1:B:328:PHE:CD2 | 1:B:331:PHE:CZ | 3.04 | 0.45 |
| 1:A:32:TYR:HB2 | 1:A:153:VAL:HG23 | 1.98 | 0.45 |
| 1:B:461:ALA:C | 1:B:462:GLN:CG | 2.83 | 0.45 |
| 1:B:404:GLU:C | 1:B:405:SER:OG | 2.56 | 0.45 |
| 1:A:193:GLU:O | 1:A:194:ALA:C | 2.56 | 0.44 |
| 1:B:581:SER:C | 1:B:583:VAL:H | 2.21 | 0.44 |
| 1:B:21:HIS:CE1 | 1:B:123:ARG:NE | 2.85 | 0.44 |
| 1:B:430:THR:H | 1:B:494:LYS:HZ1 | 1.65 | 0.44 |
| 1:A:803:TYR:CD2 | 1:A:803:TYR:C | 2.88 | 0.44 |
| 1:A:521:LEU:N | 1:A:522:PRO:CD | 2.79 | 0.44 |
| 1:B:598:GLU:H | 1:B:598:GLU:CD | 2.20 | 0.44 |
| 1:B:48:ASP:CB | 1:B:155:ASP:OD1 | 2.65 | 0.44 |
| 1:B:87:PHE:HE1 | 1:B:180:LEU:HD12 | 1.82 | 0.44 |
| 1:A:355:ASN:O | 1:A:356:TRP:CB | 2.63 | 0.44 |
| 1:A:78:PRO:HB3 | 1:A:176:PHE:CE2 | 2.52 | 0.44 |
| 1:A:10:LYS:HD2 | 1:A:10:LYS:N | 2.32 | 0.44 |
| 1:B:156:ASP:N | 1:B:156:ASP:OD2 | 2.49 | 0.44 |
| 1:A:94:ARG:N | 1:A:321:ASP:OD2 | 2.50 | 0.44 |
| 1:A:106:TRP:CZ3 | 1:A:198:GLY:HA3 | 2.49 | 0.44 |
| 1:A:618:LEU:H | 1:A:618:LEU:HD23 | 1.82 | 0.44 |
| 1:A:682:ASP:HB2 | 1:A:689:ILE:HG22 | 1.99 | 0.44 |
| 1:B:628:GLU:O | 1:B:631:MET:N | 2.45 | 0.44 |
| 1:A:491:GLU:HG3 | 1:A:491:GLU:H | 1.55 | 0.44 |
| 1:B:212:THR:CG2 | 1:B:212:THR:O | 2.62 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:585:LEU:HB3 | 1:B:586:MET:H | 1.54 | 0.44 |
| 1:B:328:PHE:CG | 1:B:331:PHE:HE2 | 2.35 | 0.44 |
| 1:B:388:LYS:NZ | 1:B:388:LYS:HB2 | 2.32 | 0.44 |
| 1:B:642:CYS:O | 1:B:643:GLN:C | 2.51 | 0.44 |
| 1:B:867:ALA:C | 1:B:869:ARG:H | 2.19 | 0.44 |
| 1:A:389:ILE:HD11 | 1:A:485:VAL:HG11 | 1.99 | 0.44 |
| 1:A:284:MET:O | 1:A:323:GLU:O | 2.35 | 0.44 |
| 1:B:614:ARG:HD2 | 1:B:614:ARG:HA | 1.56 | 0.44 |
| 1:A:135:TYR:OH | 1:A:156:ASP:OD1 | 2.27 | 0.44 |
| 1:B:113:SER:HA | 1:B:116:LEU:HD13 | 1.99 | 0.44 |
| 1:A:270:LYS:CB | 1:A:325:TRP:CH2 | 2.89 | 0.44 |
| 1:A:88:ILE:HA | 1:A:175:GLU:HG2 | 1.99 | 0.44 |
| 1:A:89:VAL:N | 1:A:175:GLU:OE1 | 2.49 | 0.44 |
| 1:B:651:ARG:CZ | 1:B:891:MET:HA | 2.48 | 0.44 |
| 1:B:453:PHE:O | 1:B:457:ASN:OD1 | 2.35 | 0.44 |
| 1:A:759:LEU:CD1 | 1:A:812:GLY:HA2 | 2.46 | 0.44 |
| 1:A:433:PHE:CE2 | 1:A:463:SER:HB3 | 2.53 | 0.44 |
| 1:B:697:LEU:CA | 1:B:700:SER:HG | 2.29 | 0.44 |
| 1:B:459:SER:HB2 | 1:B:461:ALA:H | 1.82 | 0.44 |
| 1:A:207:PHE:C | 1:A:208:THR:HG23 | 2.37 | 0.44 |
| 1:A:355:ASN:O | 1:A:356:TRP:HB2 | 2.18 | 0.44 |
| 1:A:505:GLU:O | 1:A:505:GLU:CG | 2.66 | 0.44 |
| 1:B:438:VAL:HG12 | 1:B:439:PRO:HD2 | 2.00 | 0.44 |
| 1:A:731:VAL:CG2 | 1:A:733:LEU:CG | 2.88 | 0.44 |
| 1:B:613:PHE:CD2 | 1:B:613:PHE:C | 2.91 | 0.44 |
| 1:B:861:LEU:O | 1:B:862:ASP:C | 2.50 | 0.44 |
| 1:B:80:GLU:O | 1:B:81:LEU:CD2 | 2.61 | 0.44 |
| 1:A:386:GLN:HB2 | 1:A:513:LEU:O | 2.18 | 0.44 |
| 1:A:23:ARG:HH11 | 1:A:23:ARG:CG | 2.31 | 0.44 |
| 1:A:677:ILE:O | 1:A:678:PHE:C | 2.52 | 0.44 |
| 1:A:502:PHE:CD1 | 1:A:502:PHE:N | 2.85 | 0.44 |
| 1:A:114:LEU:HD13 | 1:A:121:LEU:CD2 | 2.44 | 0.44 |
| 1:B:36:ARG:O | 1:B:37:ASN:C | 2.54 | 0.44 |
| 1:A:313:GLU:O | 1:A:313:GLU:CG | 2.63 | 0.44 |
| 1:B:584:ASN:HD22 | 1:B:584:ASN:HA | 1.62 | 0.44 |
| 1:A:626:ALA:O | 1:A:628:GLU:N | 2.51 | 0.44 |
| 1:B:883:ILE:CA | 1:B:883:ILE:CG1 | 2.82 | 0.44 |
| 1:B:28:LEU:C | 1:B:30:GLN:N | 2.71 | 0.44 |
| 1:A:553:LYS:C | 1:A:555:LEU:H | 2.21 | 0.44 |
| 1:A:208:THR:O | 1:A:343:LEU:HD11 | 2.18 | 0.44 |
| 1:A:200:THR:CB | 1:A:200:THR:N | 2.69 | 0.44 |
| 1:B:582:MET:HG2 | 1:B:602:LEU:HD21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:3:GLY:O | 1:B:778:SER:OG | 2.21 | 0.44 |
| 1:A:27:TYR:CE2 | 1:A:28:LEU:HG | 2.53 | 0.44 |
| 1:B:382:TRP:O | 1:B:448:HIS:HE1 | 2.00 | 0.44 |
| 1:B:321:ASP:O | 1:B:322:GLY:C | 2.57 | 0.44 |
| 1:A:319:MET:SD | 1:A:322:GLY:O | 2.76 | 0.44 |
| 1:A:94:ARG:HD3 | 2:A:1049:HOH:O | 2.13 | 0.44 |
| 1:A:281:LEU:HD21 | 1:A:297:TRP:CZ2 | 2.53 | 0.44 |
| 1:B:651:ARG:CD | 1:B:893:SER:OXT | 2.64 | 0.44 |
| 1:B:342:ASN:CG | 1:B:346:ASP:OD2 | 2.56 | 0.44 |
| 1:B:277:GLN:HA | 1:B:277:GLN:NE2 | 2.32 | 0.44 |
| 1:B:100:GLY:N | 2:B:903:HOH:O | 2.48 | 0.44 |
| 1:A:677:ILE:O | 1:A:679:LYS:N | 2.50 | 0.44 |
| 1:B:318:LYS:O | 1:B:320:GLU:HG2 | 2.18 | 0.44 |
| 1:A:795:ASN:O | 1:A:796:ILE:C | 2.52 | 0.44 |
| 1:B:293:TRP:CD1 | 1:B:324:PHE:CD1 | 3.06 | 0.43 |
| 1:A:94:ARG:C | 1:A:95:THR:OG1 | 2.56 | 0.43 |
| 1:B:365:TRP:CZ2 | 1:B:488:SER:HA | 2.53 | 0.43 |
| 1:B:644:LEU:HA | 1:B:647:VAL:HG22 | 1.98 | 0.43 |
| 1:A:13:GLU:O | 1:A:16:GLU:CA | 2.66 | 0.43 |
| 1:A:117:ASN:OD1 | 1:A:117:ASN:C | 2.57 | 0.43 |
| 1:A:631:MET:HB2 | 1:A:631:MET:SD | 2.57 | 0.43 |
| 1:B:837:MET:CG | 1:B:837:MET:CE | 2.93 | 0.43 |
| 1:A:803:TYR:CA | 1:A:822:ALA:HB2 | 2.46 | 0.43 |
| 1:B:28:LEU:O | 1:B:30:GLN:N | 2.51 | 0.43 |
| 1:B:697:LEU:CA | 1:B:700:SER:OG | 2.66 | 0.43 |
| 1:A:435:VAL:HG13 | 1:A:461:ALA:HB3 | 2.00 | 0.43 |
| 1:B:230:LYS:CE | 1:B:230:LYS:CG | 2.86 | 0.43 |
| 1:B:610:LEU:CD1 | 1:B:610:LEU:CD2 | 2.86 | 0.43 |
| 1:B:349:LYS:HG2 | 1:B:350:SER:N | 2.34 | 0.43 |
| 1:B:792:LEU:HD12 | 1:B:792:LEU:HA | 1.94 | 0.43 |
| 1:A:228:ILE:CG1 | 1:A:337:LYS:NZ | 2.77 | 0.43 |
| 1:A:225:TYR:CZ | 1:A:280:ASN:HB3 | 2.54 | 0.43 |
| 1:A:874:ASN:O | 1:A:875:GLY:C | 2.51 | 0.43 |
| 1:A:157:LEU:O | 1:A:158:LEU:HG | 2.17 | 0.43 |
| 1:A:255:PHE:CB | 1:A:333:ARG:HG2 | 2.48 | 0.43 |
| 1:A:833:HIS:CD2 | 1:A:834:ILE:N | 2.87 | 0.43 |
| 1:A:679:LYS:O | 1:A:682:ASP:O | 2.36 | 0.43 |
| 1:B:60:PHE:CE2 | 1:B:193:GLU:CG | 3.01 | 0.43 |
| 1:A:403:ARG:CG | 1:A:477:ARG:NE | 2.81 | 0.43 |
| 1:A:293:TRP:CH2 | 1:A:326:MET:CB | 3.01 | 0.43 |
| 1:A:63:LEU:HD12 | 1:A:70:THR:HG21 | 1.88 | 0.43 |
| 1:B:312:ARG:NE | 1:B:312:ARG:CG | 2.74 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:312:ARG:HG2 | 1:B:313:GLU:OE1 | 2.19 | 0.43 |
| 1:B:729:LEU:CB | 1:B:729:LEU:CD2 | 2.84 | 0.43 |
| 1:B:674:LEU:HD22 | 1:B:674:LEU:H | 1.82 | 0.43 |
| 1:B:746:MET:HE3 | 2:B:965:HOH:O | 2.18 | 0.43 |
| 1:A:411:LEU:CD1 | 1:A:485:VAL:HG21 | 2.45 | 0.43 |
| 1:A:701:VAL:O | 1:A:701:VAL:CG1 | 2.64 | 0.43 |
| 1:A:881:VAL:CG1 | 1:A:885:GLU:HB2 | 2.48 | 0.43 |
| 1:B:701:VAL:CG1 | 1:B:860:ARG:CD | 2.97 | 0.43 |
| 1:A:741:SER:O | 1:A:742:ALA:C | 2.56 | 0.43 |
| 1:A:484:ILE:CD1 | 1:A:486:VAL:CG2 | 2.97 | 0.43 |
| 1:A:291:VAL:HG23 | 1:A:292:GLU:H | 1.83 | 0.43 |
| 1:A:824:GLU:CB | 1:A:829:HIS:HA | 2.48 | 0.43 |
| 1:A:75:TRP:CE3 | 1:A:159:PRO:HG3 | 2.48 | 0.43 |
| 1:A:309:PRO:C | 1:A:311:GLU:N | 2.72 | 0.43 |
| 1:A:69:LYS:HB2 | 1:A:69:LYS:HE3 | 1.76 | 0.43 |
| 1:A:51:PHE:N | 1:A:52:PRO:CD | 2.82 | 0.43 |
| 1:B:387:PHE:CD2 | 1:B:387:PHE:N | 2.86 | 0.43 |
| 1:A:370:THR:O | 1:A:384:ASN:HA | 2.19 | 0.43 |
| 1:B:595:GLY:HA3 | 1:B:598:GLU:OE1 | 2.18 | 0.43 |
| 1:A:831:ASN:C | 2:A:919:HOH:O | 2.54 | 0.43 |
| 1:B:100:GLY:HA3 | 1:B:167:PHE:HA | 2.01 | 0.43 |
| 1:B:646:GLN:O | 1:B:647:VAL:C | 2.56 | 0.43 |
| 1:A:293:TRP:CE3 | 1:A:295:GLY:O | 2.71 | 0.43 |
| 1:B:200:THR:H | 1:B:200:THR:HG22 | 1.28 | 0.43 |
| 1:B:285:ARG:HA | 1:B:322:GLY:O | 2.18 | 0.43 |
| 1:B:215:TYR:HB2 | 1:B:337:LYS:HZ3 | 1.83 | 0.43 |
| 1:A:633:ILE:O | 1:A:636:ALA:HB3 | 2.18 | 0.43 |
| 1:B:282:ILE:HD13 | 1:B:282:ILE:HG21 | 1.72 | 0.43 |
| 1:A:54:VAL:HB | 1:A:55:SER:H | 1.48 | 0.43 |
| 1:A:144:TRP:CZ2 | 1:A:147:GLY:HA2 | 2.54 | 0.43 |
| 1:B:115:THR:O | 1:B:116:LEU:C | 2.56 | 0.43 |
| 1:A:140:HIS:HB3 | 1:A:153:VAL:CG2 | 2.49 | 0.43 |
| 1:A:668:LEU:HD23 | 1:A:668:LEU:HA | 1.72 | 0.43 |
| 1:A:393:GLU:HB2 | 1:A:506:LYS:HG2 | 2.01 | 0.43 |
| 1:B:617:ASP:CG | 1:B:617:ASP:O | 2.47 | 0.43 |
| 1:B:204:PHE:CB | 1:B:340:ILE:HG13 | 2.44 | 0.42 |
| 1:B:21:HIS:CE1 | 2:B:945:HOH:O | 2.71 | 0.42 |
| 1:A:517:ILE:HG23 | 1:A:640:LEU:HD23 | 2.00 | 0.42 |
| 1:A:693:LEU:O | 1:A:697:LEU:HG | 2.18 | 0.42 |
| 1:A:543:LEU:CB | 1:A:596:LEU:CB | 2.97 | 0.42 |
| 1:B:862:ASP:CG | 1:B:866:ARG:HE | 2.21 | 0.42 |
| 1:B:860:ARG:NH1 | 1:B:860:ARG:HG3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:273:THR:H | 1:A:312:ARG:NH2 | 2.14 | 0.42 |
| 1:A:800:GLN:CG | 1:A:851:PHE:HE1 | 2.32 | 0.42 |
| 1:A:775:VAL:HG12 | 1:A:776:MET:N | 2.29 | 0.42 |
| 1:B:8:LEU:C | 1:B:10:LYS:N | 2.73 | 0.42 |
| 1:B:577:GLU:O | 1:B:578:SER:O | 2.37 | 0.42 |
| 1:B:624:MET:O | 1:B:658:ILE:HD11 | 2.19 | 0.42 |
| 1:B:18:LEU:HD12 | 1:B:18:LEU:HA | 1.80 | 0.42 |
| 1:A:129:GLN:OE1 | 1:A:139:PHE:HB3 | 2.20 | 0.42 |
| 1:B:211:VAL:HG13 | 1:B:212:THR:N | 2.26 | 0.42 |
| 1:A:98:CYS:O | 1:A:99:GLN:C | 2.58 | 0.42 |
| 1:B:585:LEU:CD2 | 1:B:586:MET:HE3 | 2.49 | 0.42 |
| 1:A:758:ASP:O | 1:A:759:LEU:O | 2.37 | 0.42 |
| 1:B:484:ILE:HD12 | 1:B:513:LEU:CD2 | 2.48 | 0.42 |
| 1:B:644:LEU:HD23 | 1:B:647:VAL:HG21 | 2.02 | 0.42 |
| 1:A:599:PHE:HD2 | 1:A:599:PHE:C | 2.17 | 0.42 |
| 1:B:242:ILE:HD13 | 1:B:243:ASN:CB | 2.49 | 0.42 |
| 1:A:386:GLN:HG2 | 1:A:484:ILE:HD11 | 2.02 | 0.42 |
| 1:A:240:CYS:SG | 1:A:266:VAL:HG23 | 2.60 | 0.42 |
| 1:A:329:ARG:HH21 | 1:A:333:ARG:NH1 | 2.17 | 0.42 |
| 1:A:97:ILE:O | 1:A:98:CYS:CB | 2.64 | 0.42 |
| 1:A:237:LEU:HB2 | 1:A:340:ILE:HG12 | 2.01 | 0.42 |
| 1:A:174:ASN:CG | 1:A:174:ASN:H | 2.23 | 0.42 |
| 1:B:613:PHE:HZ | 1:B:623:SER:CA | 2.33 | 0.42 |
| 1:B:485:VAL:HG11 | 1:B:502:PHE:HZ | 1.84 | 0.42 |
| 1:A:599:PHE:CG | 1:A:599:PHE:O | 2.67 | 0.42 |
| 1:A:109:ALA:HB2 | 1:A:262:HIS:O | 2.19 | 0.42 |
| 1:B:284:MET:O | 1:B:323:GLU:HA | 2.19 | 0.42 |
| 1:B:313:GLU:OE1 | 1:B:313:GLU:N | 2.52 | 0.42 |
| 1:B:670:ARG:O | 1:B:673:ILE:HB | 2.20 | 0.42 |
| 1:A:578:SER:C | 1:A:582:MET:HG3 | 2.40 | 0.42 |
| 1:B:626:ALA:C | 1:B:628:GLU:H | 2.23 | 0.42 |
| 1:A:614:ARG:NH1 | 1:A:620:LYS:HB3 | 2.31 | 0.42 |
| 1:B:858:LEU:C | 1:B:860:ARG:N | 2.70 | 0.42 |
| 1:B:558:ILE:O | 1:B:559:LEU:C | 2.58 | 0.42 |
| 1:A:503:PHE:N | 1:A:503:PHE:CD1 | 2.87 | 0.42 |
| 1:B:340:ILE:HG23 | 1:B:340:ILE:CD1 | 2.50 | 0.42 |
| 1:A:311:GLU:C | 1:A:313:GLU:H | 2.22 | 0.42 |
| 1:A:327:SER:N | 1:A:329:ARG:HH11 | 1.99 | 0.42 |
| 1:A:59:GLY:HA3 | 1:A:193:GLU:OE2 | 2.19 | 0.42 |
| 1:A:429:GLU:CD | 1:A:494:LYS:HE3 | 2.40 | 0.42 |
| 1:A:678:PHE:CE2 | 1:A:689:ILE:HG12 | 2.54 | 0.42 |
| 1:B:525:LYS:HG2 | 1:B:525:LYS:H | 1.51 | 0.42 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:827:GLY:O | 1:B:828:PHE:CD2 | 2.72 | 0.42 |
| 1:A:100:GLY:C | 1:A:103:GLY:H | 2.23 | 0.42 |
| 1:A:84:ASN:C | 1:A:84:ASN:OD1 | 2.58 | 0.42 |
| 1:A:204:PHE:HE2 | 1:A:237:LEU:CD1 | 2.33 | 0.42 |
| 1:B:671:LEU:O | 1:B:674:LEU:HB2 | 2.19 | 0.42 |
| 1:B:772:MET:CE | 1:B:772:MET:CG | 2.96 | 0.42 |
| 1:B:856:SER:O | 1:B:858:LEU:N | 2.52 | 0.42 |
| 1:B:663:ASN:O | 1:B:664:PHE:C | 2.58 | 0.42 |
| 1:B:2:ALA:CB | 2:B:999:HOH:O | 2.67 | 0.42 |
| 1:B:579:CYS:HA | 1:B:582:MET:HB2 | 2.00 | 0.42 |
| 1:A:403:ARG:HB3 | 1:A:477:ARG:CD | 2.50 | 0.42 |
| 1:B:492:PRO:C | 1:B:494:LYS:H | 2.21 | 0.42 |
| 1:A:680:GLN:C | 1:A:682:ASP:N | 2.71 | 0.42 |
| 1:A:256:LYS:CA | 1:A:258:LEU:CD1 | 2.97 | 0.42 |
| 1:A:741:SER:O | 1:A:745:LEU:N | 2.44 | 0.42 |
| 1:B:172:GLN:OE1 | 1:B:172:GLN:CA | 2.66 | 0.42 |
| 1:B:696:TRP:O | 1:B:700:SER:N | 2.53 | 0.42 |
| 1:A:349:LYS:CG | 1:A:349:LYS:O | 2.68 | 0.42 |
| 1:A:77:ARG:HG3 | 1:A:157:LEU:HD12 | 2.02 | 0.42 |
| 1:B:503:PHE:CD1 | 1:B:503:PHE:N | 2.88 | 0.42 |
| 1:B:313:GLU:CG | 1:B:313:GLU:HA | 2.47 | 0.42 |
| 1:B:681:LEU:C | 1:B:683:PRO:CD | 2.88 | 0.42 |
| 1:B:677:ILE:HG22 | 1:B:681:LEU:CD1 | 2.50 | 0.42 |
| 1:B:487:PRO:O | 1:B:488:SER:CB | 2.58 | 0.42 |
| 1:B:766:ILE:HG23 | 1:B:767:ASP:N | 2.34 | 0.42 |
| 1:A:77:ARG:CG | 1:A:156:ASP:OD2 | 2.53 | 0.42 |
| 1:B:682:ASP:N | 1:B:683:PRO:CD | 2.83 | 0.42 |
| 1:B:892:TYR:O | 1:B:893:SER:HB2 | 2.20 | 0.42 |
| 1:B:61:LYS:CG | 1:B:66:ASN:HB2 | 2.42 | 0.42 |
| 1:B:366:ARG:HH11 | 1:B:366:ARG:HD3 | 1.39 | 0.42 |
| 1:B:625:SER:O | 1:B:626:ALA:C | 2.55 | 0.42 |
| 1:A:256:LYS:C | 1:A:258:LEU:HD13 | 2.41 | 0.42 |
| 1:A:32:TYR:O | 1:A:36:ARG:N | 2.53 | 0.42 |
| 1:A:874:ASN:C | 1:A:876:THR:N | 2.72 | 0.42 |
| 1:B:197:GLY:C | 1:B:198:GLY:O | 2.58 | 0.42 |
| 1:B:33:GLU:OE1 | 1:B:37:ASN:OD1 | 2.38 | 0.42 |
| 1:A:809:ASP:O | 1:A:810:ARG:C | 2.58 | 0.42 |
| 1:A:715:ILE:HD12 | 1:A:715:ILE:HA | 1.60 | 0.42 |
| 1:A:93:THR:CB | 1:A:321:ASP:OD2 | 2.67 | 0.41 |
| 1:A:236:SER:C | 1:A:238:LEU:HD12 | 2.40 | 0.41 |
| 1:B:100:GLY:HA3 | 1:B:167:PHE:CA | 2.50 | 0.41 |
| 1:B:12:ARG:O | 1:B:15:ALA:HB3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:688:THR:N | 1:A:688:THR:CG2 | 2.82 | 0.41 |
| 1:A:256:LYS:HD3 | 1:A:258:LEU:CD2 | 2.34 | 0.41 |
| 1:A:745:LEU:HD12 | 1:A:749:LEU:HD23 | 2.01 | 0.41 |
| 1:A:374:CYS:C | 1:A:381:PHE:CD1 | 2.94 | 0.41 |
| 1:B:692:ASP:C | 1:B:692:ASP:OD1 | 2.57 | 0.41 |
| 1:B:113:SER:OG | 1:B:204:PHE:HE2 | 2.04 | 0.41 |
| 1:B:206:ASP:CG | 1:B:470:ARG:HH22 | 2.24 | 0.41 |
| 1:B:610:LEU:HA | 1:B:661:PHE:HE2 | 1.84 | 0.41 |
| 1:A:517:ILE:HG12 | 1:A:641:PRO:CD | 2.50 | 0.41 |
| 1:A:229:LEU:O | 1:A:230:LYS:C | 2.57 | 0.41 |
| 1:A:854:PHE:O | 1:A:857:CYS:HB3 | 2.20 | 0.41 |
| 1:B:35:LEU:HD13 | 1:B:46:PHE:CZ | 2.51 | 0.41 |
| 1:A:364:THR:CG2 | 1:A:497:ASP:OD1 | 2.65 | 0.41 |
| 1:B:179:ALA:O | 1:B:182:GLU:HB3 | 2.19 | 0.41 |
| 1:A:632:ALA:O | 1:A:633:ILE:C | 2.58 | 0.41 |
| 1:A:663:ASN:O | 1:A:664:PHE:O | 2.38 | 0.41 |
| 1:A:285:ARG:O | 1:A:287:PRO:HD3 | 2.19 | 0.41 |
| 1:B:174:ASN:HD22 | 1:B:174:ASN:HA | 1.41 | 0.41 |
| 1:B:321:ASP:O | 1:B:323:GLU:N | 2.54 | 0.41 |
| 1:A:88:ILE:O | 1:A:89:VAL:HG22 | 2.19 | 0.41 |
| 1:A:189:ASN:OD1 | 1:A:195:LEU:CD2 | 2.68 | 0.41 |
| 1:A:67:SER:O | 1:A:70:THR:N | 2.51 | 0.41 |
| 1:A:600:ASN:C | 1:A:602:LEU:H | 2.22 | 0.41 |
| 1:A:223:ASP:CG | 1:A:227:ILE:HD11 | 2.41 | 0.41 |
| 1:B:453:PHE:CE1 | 1:B:457:ASN:OD1 | 2.73 | 0.41 |
| 1:A:224:LEU:HD21 | 1:A:337:LYS:HZ1 | 1.86 | 0.41 |
| 1:B:644:LEU:HA | 1:B:647:VAL:CG2 | 2.49 | 0.41 |
| 1:A:380:THR:C | 1:A:382:TRP:N | 2.73 | 0.41 |
| 1:A:856:SER:O | 1:A:860:ARG:HG3 | 2.20 | 0.41 |
| 1:A:823:PHE:O | 1:A:826:ALA:N | 2.52 | 0.41 |
| 1:B:673:ILE:O | 1:B:676:LYS:N | 2.53 | 0.41 |
| 1:B:449:LEU:HD13 | 1:B:453:PHE:CD1 | 2.55 | 0.41 |
| 1:B:456:ALA:CA | 1:B:457:ASN:N | 2.66 | 0.41 |
| 1:B:856:SER:C | 1:B:858:LEU:H | 2.24 | 0.41 |
| 1:B:35:LEU:HD13 | 1:B:46:PHE:HE1 | 1.80 | 0.41 |
| 1:A:349:LYS:O | 1:A:349:LYS:HG3 | 2.20 | 0.41 |
| 1:B:78:PRO:CD | 1:B:156:ASP:HB2 | 2.51 | 0.41 |
| 1:B:211:VAL:HG11 | 1:B:410:LEU:HD23 | 2.02 | 0.41 |
| 1:B:294:LYS:CE | 1:B:294:LYS:CG | 2.87 | 0.41 |
| 1:A:616:PHE:HD2 | 1:A:628:GLU:HG2 | 1.86 | 0.41 |
| 1:B:430:THR:N | 1:B:468:ASN:HB2 | 2.35 | 0.41 |
| 1:A:224:LEU:O | 1:A:228:ILE:N | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:172:GLN:O | 1:A:174:ASN:N | 2.53 | 0.41 |
| 1:A:689:ILE:O | 1:A:689:ILE:HD12 | 2.19 | 0.41 |
| 1:B:581:SER:O | 1:B:583:VAL:N | 2.54 | 0.41 |
| 1:A:415:GLN:HE22 | 1:A:428:MET:HB3 | 1.86 | 0.41 |
| 1:A:177:TRP:CE3 | 1:A:178:SER:N | 2.89 | 0.41 |
| 1:A:393:GLU:OE1 | 1:A:506:LYS:HG3 | 2.20 | 0.41 |
| 1:B:632:ALA:O | 1:B:635:ALA:HB3 | 2.20 | 0.41 |
| 1:B:256:LYS:CD | 1:B:256:LYS:CB | 2.80 | 0.41 |
| 1:B:95:THR:HG23 | 1:B:288:TRP:CD1 | 2.56 | 0.41 |
| 1:A:61:LYS:O | 1:A:62:GLU:HB2 | 2.21 | 0.41 |
| 1:B:429:GLU:OE2 | 1:B:494:LYS:HB3 | 2.21 | 0.41 |
| 1:A:435:VAL:CG1 | 1:A:461:ALA:O | 2.69 | 0.41 |
| 1:A:196:SER:O | 1:A:197:GLY:O | 2.38 | 0.41 |
| 1:A:775:VAL:O | 1:A:775:VAL:CG1 | 2.62 | 0.41 |
| 1:A:571:THR:CG2 | 1:A:572:ASN:N | 2.84 | 0.41 |
| 1:B:141:PHE:CD2 | 1:B:181:LEU:HD12 | 2.56 | 0.41 |
| 1:A:479:PRO:O | 1:A:480:PRO:C | 2.51 | 0.41 |
| 1:A:824:GLU:C | 1:A:826:ALA:N | 2.74 | 0.41 |
| 1:B:284:MET:HB2 | 1:B:324:PHE:CE2 | 2.56 | 0.41 |
| 1:B:113:SER:HA | 1:B:116:LEU:CD1 | 2.51 | 0.41 |
| 1:A:88:ILE:HD13 | 1:A:88:ILE:HG21 | 1.40 | 0.41 |
| 1:B:335:PHE:CG | 1:B:335:PHE:C | 2.94 | 0.41 |
| 1:B:574:PHE:CZ | 1:B:606:ILE:HD13 | 2.55 | 0.41 |
| 1:A:640:LEU:O | 1:A:645:HIS:CD2 | 2.74 | 0.41 |
| 1:B:456:ALA:O | 1:B:457:ASN:C | 2.58 | 0.41 |
| 1:A:756:HIS:O | 1:A:757:PRO:O | 2.39 | 0.41 |
| 1:B:131:PHE:HA | 1:B:135:TYR:CD1 | 2.56 | 0.41 |
| 1:B:40:LEU:CD1 | 1:B:136:ALA:HB2 | 2.50 | 0.41 |
| 1:A:677:ILE:C | 1:A:679:LYS:N | 2.74 | 0.41 |
| 1:B:647:VAL:HG23 | 1:B:648:ILE:N | 2.36 | 0.41 |
| 1:A:697:LEU:HD23 | 1:A:697:LEU:HA | 1.66 | 0.41 |
| 1:B:739:GLU:OE2 | 1:B:785:GLY:HA2 | 2.21 | 0.41 |
| 1:B:773:VAL:CB | 1:B:784:LEU:HD11 | 2.51 | 0.41 |
| 1:B:499:LEU:O | 2:B:948:HOH:O | 2.22 | 0.41 |
| 1:A:328:PHE:C | 1:A:330:ASP:H | 2.24 | 0.41 |
| 1:A:10:LYS:HE3 | 2:A:1021:HOH:O | 2.21 | 0.41 |
| 1:B:37:ASN:HA | 1:B:37:ASN:HD22 | 1.56 | 0.41 |
| 1:A:449:LEU:H | 1:A:449:LEU:HG | 1.55 | 0.41 |
| 1:A:852:ASP:C | 1:A:852:ASP:OD2 | 2.59 | 0.41 |
| 1:B:651:ARG:HH12 | 1:B:670:ARG:NH1 | 2.09 | 0.41 |
| 1:A:628:GLU:C | 1:A:630:ARG:N | 2.73 | 0.41 |
| 1:A:388:LYS:HZ2 | 1:A:482:GLU:HG2 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:413:LEU:O | 1:B:471:GLU:HA | 2.21 | 0.41 |
| 1:A:620:LYS:HB3 | 1:A:620:LYS:HE3 | 1.67 | 0.41 |
| 1:B:853:ASN:HB3 | 1:B:854:PHE:H | 1.71 | 0.41 |
| 1:A:64:GLY:HA3 | 1:A:65:PRO:HD3 | 1.89 | 0.40 |
| 1:B:583:VAL:HG23 | 1:B:594:LEU:HD13 | 2.02 | 0.40 |
| 1:B:120:ILE:HD11 | 1:B:342:ASN:HD21 | 1.86 | 0.40 |
| 1:A:625:SER:O | 1:A:626:ALA:C | 2.54 | 0.40 |
| 1:A:223:ASP:CG | 1:A:227:ILE:CD1 | 2.90 | 0.40 |
| 1:B:456:ALA:O | 1:B:457:ASN:O | 2.38 | 0.40 |
| 1:B:492:PRO:HB2 | 1:B:493:ASN:CG | 2.42 | 0.40 |
| 1:A:353:LEU:C | 1:A:354:ARG:HG2 | 2.42 | 0.40 |
| 1:B:438:VAL:CG2 | 1:B:484:ILE:HD11 | 2.47 | 0.40 |
| 1:B:768:THR:O | 1:B:772:MET:HG3 | 2.21 | 0.40 |
| 1:B:797:LYS:O | 1:B:800:GLN:CB | 2.68 | 0.40 |
| 1:B:696:TRP:CD2 | 1:B:700:SER:HB3 | 2.56 | 0.40 |
| 1:A:440:ARG:HH21 | 1:A:440:ARG:HD2 | 1.71 | 0.40 |
| 1:A:479:PRO:HA | 1:A:480:PRO:HD3 | 1.90 | 0.40 |
| 1:B:409:PHE:N | 1:B:409:PHE:CD2 | 2.88 | 0.40 |
| 1:A:829:HIS:HE1 | 2:A:917:HOH:O | 2.04 | 0.40 |
| 1:B:97:ILE:HD13 | 1:B:97:ILE:HG23 | 1.72 | 0.40 |
| 1:B:790:LYS:O | 1:B:792:LEU:N | 2.51 | 0.40 |
| 1:B:487:PRO:O | 1:B:487:PRO:HG2 | 2.20 | 0.40 |
| 1:B:76:LYS:HD2 | 1:B:81:LEU:HD21 | 2.02 | 0.40 |
| 1:B:875:GLY:C | 1:B:877:GLY:H | 2.22 | 0.40 |
| 1:B:719:GLU:N | 1:B:719:GLU:CD | 2.75 | 0.40 |
| 1:A:159:PRO:C | 1:A:160:THR:CG2 | 2.89 | 0.40 |
| 1:A:450:LYS:CE | 1:A:631:MET:HG2 | 2.49 | 0.40 |
| 1:A:831:ASN:CA | 2:A:919:HOH:O | 2.68 | 0.40 |
| 1:B:242:ILE:CD1 | 1:B:243:ASN:N | 2.74 | 0.40 |
| 1:A:268:ASP:CG | 1:A:269:ALA:H | 2.19 | 0.40 |
| 1:A:63:LEU:HB3 | 1:A:193:GLU:HG3 | 2.03 | 0.40 |
| 1:A:415:GLN:NE2 | 1:A:428:MET:HB3 | 2.37 | 0.40 |
| 1:A:756:HIS:CD2 | 1:A:757:PRO:CD | 3.00 | 0.40 |
| 1:B:390:ARG:NH1 | 1:B:392:GLU:OE1 | 2.53 | 0.40 |
| 1:B:440:ARG:N | 1:B:440:ARG:CD | 2.85 | 0.40 |
| 1:B:369:SER:OG | 1:B:646:GLN:HG2 | 2.21 | 0.40 |
| 1:A:674:LEU:O | 1:A:675:PHE:C | 2.57 | 0.40 |
| 1:B:27:TYR:CE2 | 1:B:28:LEU:HD11 | 2.56 | 0.40 |
| 1:B:291:VAL:H | 1:B:291:VAL:HG22 | 1.30 | 0.40 |
| 1:A:89:VAL:N | 1:A:175:GLU:CD | 2.68 | 0.40 |
| 1:A:87:PHE:HB2 | 1:A:131:PHE:CE1 | 2.57 | 0.40 |
| 1:A:189:ASN:OD1 | 1:A:195:LEU:HD21 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:468:ASN:O | 1:B:468:ASN:CG | 2.58 | 0.40 |
| 1:B:492:PRO:O | 1:B:494:LYS:N | 2.55 | 0.40 |
| 1:B:413:LEU:HD22 | 1:B:487:PRO:HB2 | 2.02 | 0.40 |
| 1:B:648:ILE:HG22 | 1:B:649:VAL:N | 2.37 | 0.40 |
| 1:A:766:ILE:HD13 | 1:A:766:ILE:HG21 | 1.52 | 0.40 |
| 1:A:263:ALA:HB2 | 1:A:288:TRP:CZ3 | 2.56 | 0.40 |

All (3) 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 | Distance(Å) | Clash(Å) |
|-----------------|-----------------------|-------------|----------|
| 1:A:457:ASN:OD1 | 2:B:1033:HOH:O[1_454] | 1.56 | 0.64 |
| 1:A:442:LEU:CD2 | 2:A:922:HOH:O[1_455] | 1.95 | 0.25 |
| 1:A:300:ASN:OD1 | 1:B:303:GLU:N[2_656] | 2.08 | 0.12 |

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 | 747/900 (83%) | 500 (67%) | 143 (19%) | 104 (14%) | 0 | 1 |
| 1 | B | 748/900 (83%) | 497 (66%) | 146 (20%) | 105 (14%) | 0 | 1 |
| All | All | 1495/1800 (83%) | 997 (67%) | 289 (19%) | 209 (14%) | 0 | 1 |

All (209) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 54 | VAL |
| 1 | A | 60 | PHE |
| 1 | A | 63 | LEU |
| 1 | A | 67 | SER |
| 1 | A | 83 | SER |
| 1 | A | 84 | ASN |
| 1 | A | 101 | ALA |
| 1 | A | 135 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 199 | CYS |
| 1 | A | 219 | LYS |
| 1 | A | 255 | PHE |
| 1 | A | 279 | VAL |
| 1 | A | 297 | TRP |
| 1 | A | 302 | TYR |
| 1 | A | 307 | VAL |
| 1 | A | 324 | PHE |
| 1 | A | 353 | LEU |
| 1 | A | 356 | TRP |
| 1 | A | 381 | PHE |
| 1 | A | 403 | ARG |
| 1 | A | 406 | GLY |
| 1 | A | 465 | HIS |
| 1 | A | 471 | GLU |
| 1 | A | 548 | MET |
| 1 | A | 550 | ILE |
| 1 | A | 552 | VAL |
| 1 | A | 574 | PHE |
| 1 | A | 586 | MET |
| 1 | A | 620 | LYS |
| 1 | A | 624 | MET |
| 1 | A | 627 | TYR |
| 1 | A | 678 | PHE |
| 1 | A | 681 | LEU |
| 1 | A | 685 | ASN |
| 1 | A | 714 | ASN |
| 1 | A | 735 | GLY |
| 1 | A | 750 | ASN |
| 1 | A | 757 | PRO |
| 1 | A | 758 | ASP |
| 1 | A | 832 | GLN |
| 1 | A | 833 | HIS |
| 1 | A | 834 | ILE |
| 1 | A | 835 | TYR |
| 1 | A | 849 | MET |
| 1 | A | 875 | GLY |
| 1 | B | 15 | ALA |
| 1 | B | 62 | GLU |
| 1 | B | 67 | SER |
| 1 | B | 92 | ALA |
| 1 | B | 135 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 162 | ASP |
| 1 | B | 171 | ALA |
| 1 | B | 175 | GLU |
| 1 | B | 198 | GLY |
| 1 | B | 263 | ALA |
| 1 | B | 295 | GLY |
| 1 | B | 304 | TRP |
| 1 | B | 317 | VAL |
| 1 | B | 320 | GLU |
| 1 | B | 322 | GLY |
| 1 | B | 346 | ASP |
| 1 | B | 398 | ASP |
| 1 | B | 400 | TYR |
| 1 | B | 403 | ARG |
| 1 | B | 428 | MET |
| 1 | B | 440 | ARG |
| 1 | B | 441 | GLU |
| 1 | B | 456 | ALA |
| 1 | B | 457 | ASN |
| 1 | B | 465 | HIS |
| 1 | B | 467 | ILE |
| 1 | B | 539 | LEU |
| 1 | B | 558 | ILE |
| 1 | B | 574 | PHE |
| 1 | B | 577 | GLU |
| 1 | B | 586 | MET |
| 1 | B | 617 | ASP |
| 1 | B | 618 | LEU |
| 1 | B | 620 | LYS |
| 1 | B | 647 | VAL |
| 1 | B | 654 | ASP |
| 1 | B | 657 | LEU |
| 1 | B | 713 | SER |
| 1 | B | 725 | GLN |
| 1 | B | 731 | VAL |
| 1 | B | 808 | THR |
| 1 | B | 810 | ARG |
| 1 | B | 833 | HIS |
| 1 | B | 839 | ILE |
| 1 | B | 850 | ASP |
| 1 | B | 851 | PHE |
| 1 | B | 863 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 875 | GLY |
| 1 | A | 4 | ILE |
| 1 | A | 14 | ALA |
| 1 | A | 15 | ALA |
| 1 | A | 99 | GLN |
| 1 | A | 173 | GLY |
| 1 | A | 174 | ASN |
| 1 | A | 263 | ALA |
| 1 | A | 264 | TYR |
| 1 | A | 313 | GLU |
| 1 | A | 317 | VAL |
| 1 | A | 326 | MET |
| 1 | A | 334 | GLU |
| 1 | A | 349 | LYS |
| 1 | A | 404 | GLU |
| 1 | A | 461 | ALA |
| 1 | A | 559 | LEU |
| 1 | A | 606 | ILE |
| 1 | A | 618 | LEU |
| 1 | A | 664 | PHE |
| 1 | A | 809 | ASP |
| 1 | A | 810 | ARG |
| 1 | B | 5 | ALA |
| 1 | B | 61 | LYS |
| 1 | B | 81 | LEU |
| 1 | B | 97 | ILE |
| 1 | B | 172 | GLN |
| 1 | B | 262 | HIS |
| 1 | B | 268 | ASP |
| 1 | B | 334 | GLU |
| 1 | B | 396 | ASP |
| 1 | B | 461 | ALA |
| 1 | B | 515 | ASP |
| 1 | B | 525 | LYS |
| 1 | B | 552 | VAL |
| 1 | B | 576 | LEU |
| 1 | B | 585 | LEU |
| 1 | B | 627 | TYR |
| 1 | B | 632 | ALA |
| 1 | B | 648 | ILE |
| 1 | B | 673 | ILE |
| 1 | B | 684 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 785 | GLY |
| 1 | B | 807 | GLU |
| 1 | B | 811 | SER |
| 1 | B | 836 | SER |
| 1 | B | 837 | MET |
| 1 | B | 857 | CYS |
| 1 | B | 873 | LYS |
| 1 | A | 42 | ALA |
| 1 | A | 61 | LYS |
| 1 | A | 69 | LYS |
| 1 | A | 79 | THR |
| 1 | A | 98 | CYS |
| 1 | A | 108 | LEU |
| 1 | A | 194 | ALA |
| 1 | A | 229 | LEU |
| 1 | A | 318 | LYS |
| 1 | A | 351 | ARG |
| 1 | A | 440 | ARG |
| 1 | A | 441 | GLU |
| 1 | B | 56 | HIS |
| 1 | B | 316 | ARG |
| 1 | B | 448 | HIS |
| 1 | B | 490 | PHE |
| 1 | B | 551 | SER |
| 1 | B | 582 | MET |
| 1 | B | 822 | ALA |
| 1 | B | 849 | MET |
| 1 | B | 853 | ASN |
| 1 | A | 13 | GLU |
| 1 | A | 24 | ALA |
| 1 | A | 278 | ARG |
| 1 | A | 316 | ARG |
| 1 | A | 329 | ARG |
| 1 | A | 517 | ILE |
| 1 | A | 543 | LEU |
| 1 | A | 626 | ALA |
| 1 | A | 699 | PHE |
| 1 | A | 731 | VAL |
| 1 | A | 749 | LEU |
| 1 | A | 825 | ALA |
| 1 | B | 69 | LYS |
| 1 | B | 319 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 393 | GLU |
| 1 | B | 453 | PHE |
| 1 | B | 557 | THR |
| 1 | B | 605 | ARG |
| 1 | B | 630 | ARG |
| 1 | B | 646 | GLN |
| 1 | B | 770 | ARG |
| 1 | B | 798 | LYS |
| 1 | B | 806 | PHE |
| 1 | B | 829 | HIS |
| 1 | B | 868 | PHE |
| 1 | A | 90 | ASP |
| 1 | A | 97 | ILE |
| 1 | A | 100 | GLY |
| 1 | A | 557 | THR |
| 1 | A | 575 | SER |
| 1 | A | 683 | PRO |
| 1 | A | 870 | SER |
| 1 | B | 14 | ALA |
| 1 | B | 732 | GLN |
| 1 | B | 794 | ASN |
| 1 | B | 823 | PHE |
| 1 | A | 677 | ILE |
| 1 | B | 88 | ILE |
| 1 | B | 447 | VAL |
| 1 | A | 521 | LEU |
| 1 | A | 701 | VAL |
| 1 | A | 592 | GLY |
| 1 | A | 802 | ILE |
| 1 | B | 740 | VAL |
| 1 | A | 291 | VAL |
| 1 | B | 54 | VAL |
| 1 | A | 89 | VAL |

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 | 606/782 (78%) | 459 (76%) | 147 (24%) | 1 | 3 |
| 1 | B | 584/782 (75%) | 429 (74%) | 155 (26%) | 1 | 2 |
| All | All | 1190/1564 (76%) | 888 (75%) | 302 (25%) | 1 | 2 |

All (302) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | MET |
| 1 | A | 7 | LYS |
| 1 | A | 10 | LYS |
| 1 | A | 12 | ARG |
| 1 | A | 13 | GLU |
| 1 | A | 22 | GLU |
| 1 | A | 29 | ASN |
| 1 | A | 30 | GLN |
| 1 | A | 36 | ARG |
| 1 | A | 38 | GLU |
| 1 | A | 41 | GLU |
| 1 | A | 52 | PRO |
| 1 | A | 53 | PRO |
| 1 | A | 55 | SER |
| 1 | A | 57 | SER |
| 1 | A | 66 | ASN |
| 1 | A | 67 | SER |
| 1 | A | 69 | LYS |
| 1 | A | 70 | THR |
| 1 | A | 81 | LEU |
| 1 | A | 85 | PRO |
| 1 | A | 88 | ILE |
| 1 | A | 89 | VAL |
| 1 | A | 90 | ASP |
| 1 | A | 96 | ASP |
| 1 | A | 98 | CYS |
| 1 | A | 108 | LEU |
| 1 | A | 115 | THR |
| 1 | A | 116 | LEU |
| 1 | A | 121 | LEU |
| 1 | A | 132 | GLN |
| 1 | A | 144 | TRP |
| 1 | A | 151 | ASP |
| 1 | A | 153 | VAL |
| 1 | A | 155 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 162 | ASP |
| 1 | A | 165 | LEU |
| 1 | A | 174 | ASN |
| 1 | A | 191 | SER |
| 1 | A | 201 | SER |
| 1 | A | 204 | PHE |
| 1 | A | 211 | VAL |
| 1 | A | 218 | GLN |
| 1 | A | 219 | LYS |
| 1 | A | 224 | LEU |
| 1 | A | 229 | LEU |
| 1 | A | 230 | LYS |
| 1 | A | 242 | ILE |
| 1 | A | 258 | LEU |
| 1 | A | 264 | TYR |
| 1 | A | 275 | GLN |
| 1 | A | 278 | ARG |
| 1 | A | 284 | MET |
| 1 | A | 296 | PRO |
| 1 | A | 300 | ASN |
| 1 | A | 305 | ASN |
| 1 | A | 306 | LYS |
| 1 | A | 310 | TYR |
| 1 | A | 317 | VAL |
| 1 | A | 324 | PHE |
| 1 | A | 325 | TRP |
| 1 | A | 329 | ARG |
| 1 | A | 330 | ASP |
| 1 | A | 332 | ILE |
| 1 | A | 334 | GLU |
| 1 | A | 335 | PHE |
| 1 | A | 336 | THR |
| 1 | A | 343 | LEU |
| 1 | A | 344 | THR |
| 1 | A | 352 | THR |
| 1 | A | 354 | ARG |
| 1 | A | 355 | ASN |
| 1 | A | 356 | TRP |
| 1 | A | 388 | LYS |
| 1 | A | 393 | GLU |
| 1 | A | 394 | VAL |
| 1 | A | 408 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 428 | MET |
| 1 | A | 429 | GLU |
| 1 | A | 442 | LEU |
| 1 | A | 447 | VAL |
| 1 | A | 465 | HIS |
| 1 | A | 467 | ILE |
| 1 | A | 468 | ASN |
| 1 | A | 470 | ARG |
| 1 | A | 484 | ILE |
| 1 | A | 487 | PRO |
| 1 | A | 497 | ASP |
| 1 | A | 499 | LEU |
| 1 | A | 506 | LYS |
| 1 | A | 507 | LYS |
| 1 | A | 511 | GLN |
| 1 | A | 512 | GLU |
| 1 | A | 513 | LEU |
| 1 | A | 521 | LEU |
| 1 | A | 558 | ILE |
| 1 | A | 584 | ASN |
| 1 | A | 598 | GLU |
| 1 | A | 599 | PHE |
| 1 | A | 605 | ARG |
| 1 | A | 610 | LEU |
| 1 | A | 612 | ILE |
| 1 | A | 620 | LYS |
| 1 | A | 625 | SER |
| 1 | A | 628 | GLU |
| 1 | A | 630 | ARG |
| 1 | A | 639 | LYS |
| 1 | A | 643 | GLN |
| 1 | A | 647 | VAL |
| 1 | A | 656 | GLU |
| 1 | A | 658 | ILE |
| 1 | A | 666 | ARG |
| 1 | A | 667 | CYS |
| 1 | A | 672 | GLU |
| 1 | A | 674 | LEU |
| 1 | A | 690 | GLN |
| 1 | A | 701 | VAL |
| 1 | A | 711 | HIS |
| 1 | A | 714 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 715 | ILE |
| 1 | A | 744 | GLU |
| 1 | A | 748 | ILE |
| 1 | A | 751 | LYS |
| 1 | A | 759 | LEU |
| 1 | A | 760 | LYS |
| 1 | A | 766 | ILE |
| 1 | A | 767 | ASP |
| 1 | A | 775 | VAL |
| 1 | A | 777 | ASP |
| 1 | A | 788 | GLU |
| 1 | A | 810 | ARG |
| 1 | A | 832 | GLN |
| 1 | A | 833 | HIS |
| 1 | A | 848 | ASN |
| 1 | A | 849 | MET |
| 1 | A | 852 | ASP |
| 1 | A | 853 | ASN |
| 1 | A | 860 | ARG |
| 1 | A | 865 | PHE |
| 1 | A | 871 | LEU |
| 1 | A | 874 | ASN |
| 1 | A | 876 | THR |
| 1 | A | 878 | GLN |
| 1 | A | 880 | GLN |
| 1 | A | 881 | VAL |
| 1 | A | 882 | ASN |
| 1 | A | 884 | GLN |
| 1 | B | 7 | LYS |
| 1 | B | 20 | SER |
| 1 | B | 28 | LEU |
| 1 | B | 33 | GLU |
| 1 | B | 36 | ARG |
| 1 | B | 38 | GLU |
| 1 | B | 41 | GLU |
| 1 | B | 49 | PRO |
| 1 | B | 54 | VAL |
| 1 | B | 60 | PHE |
| 1 | B | 61 | LYS |
| 1 | B | 62 | GLU |
| 1 | B | 66 | ASN |
| 1 | B | 68 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 69 | LYS |
| 1 | B | 70 | THR |
| 1 | B | 78 | PRO |
| 1 | B | 79 | THR |
| 1 | B | 84 | ASN |
| 1 | B | 86 | GLN |
| 1 | B | 90 | ASP |
| 1 | B | 97 | ILE |
| 1 | B | 111 | ILE |
| 1 | B | 113 | SER |
| 1 | B | 118 | GLU |
| 1 | B | 153 | VAL |
| 1 | B | 154 | VAL |
| 1 | B | 159 | PRO |
| 1 | B | 164 | LYS |
| 1 | B | 172 | GLN |
| 1 | B | 174 | ASN |
| 1 | B | 181 | LEU |
| 1 | B | 185 | TYR |
| 1 | B | 188 | VAL |
| 1 | B | 195 | LEU |
| 1 | B | 200 | THR |
| 1 | B | 223 | ASP |
| 1 | B | 224 | LEU |
| 1 | B | 229 | LEU |
| 1 | B | 234 | ARG |
| 1 | B | 237 | LEU |
| 1 | B | 242 | ILE |
| 1 | B | 256 | LYS |
| 1 | B | 265 | SER |
| 1 | B | 277 | GLN |
| 1 | B | 278 | ARG |
| 1 | B | 279 | VAL |
| 1 | B | 291 | VAL |
| 1 | B | 296 | PRO |
| 1 | B | 298 | SER |
| 1 | B | 303 | GLU |
| 1 | B | 304 | TRP |
| 1 | B | 305 | ASN |
| 1 | B | 308 | ASP |
| 1 | B | 313 | GLU |
| 1 | B | 315 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 321 | ASP |
| 1 | B | 329 | ARG |
| 1 | B | 331 | PHE |
| 1 | B | 335 | PHE |
| 1 | B | 337 | LYS |
| 1 | B | 339 | GLU |
| 1 | B | 343 | LEU |
| 1 | B | 346 | ASP |
| 1 | B | 348 | LEU |
| 1 | B | 350 | SER |
| 1 | B | 359 | THR |
| 1 | B | 364 | THR |
| 1 | B | 375 | ARG |
| 1 | B | 376 | ASN |
| 1 | B | 378 | PRO |
| 1 | B | 388 | LYS |
| 1 | B | 389 | ILE |
| 1 | B | 390 | ARG |
| 1 | B | 394 | VAL |
| 1 | B | 396 | ASP |
| 1 | B | 398 | ASP |
| 1 | B | 399 | ASP |
| 1 | B | 401 | ASP |
| 1 | B | 405 | SER |
| 1 | B | 409 | PHE |
| 1 | B | 410 | LEU |
| 1 | B | 414 | MET |
| 1 | B | 418 | ARG |
| 1 | B | 427 | ASP |
| 1 | B | 429 | GLU |
| 1 | B | 438 | VAL |
| 1 | B | 440 | ARG |
| 1 | B | 450 | LYS |
| 1 | B | 451 | ARG |
| 1 | B | 455 | LEU |
| 1 | B | 457 | ASN |
| 1 | B | 462 | GLN |
| 1 | B | 464 | GLU |
| 1 | B | 468 | ASN |
| 1 | B | 472 | VAL |
| 1 | B | 490 | PHE |
| 1 | B | 493 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 494 | LYS |
| 1 | B | 507 | LYS |
| 1 | B | 512 | GLU |
| 1 | B | 517 | ILE |
| 1 | B | 521 | LEU |
| 1 | B | 524 | GLU |
| 1 | B | 525 | LYS |
| 1 | B | 526 | VAL |
| 1 | B | 537 | LYS |
| 1 | B | 572 | ASN |
| 1 | B | 580 | ARG |
| 1 | B | 584 | ASN |
| 1 | B | 598 | GLU |
| 1 | B | 607 | ARG |
| 1 | B | 614 | ARG |
| 1 | B | 616 | PHE |
| 1 | B | 628 | GLU |
| 1 | B | 629 | MET |
| 1 | B | 630 | ARG |
| 1 | B | 631 | MET |
| 1 | B | 640 | LEU |
| 1 | B | 642 | CYS |
| 1 | B | 643 | GLN |
| 1 | B | 648 | ILE |
| 1 | B | 655 | ASP |
| 1 | B | 656 | GLU |
| 1 | B | 657 | LEU |
| 1 | B | 670 | ARG |
| 1 | B | 674 | LEU |
| 1 | B | 684 | GLU |
| 1 | B | 688 | THR |
| 1 | B | 690 | GLN |
| 1 | B | 691 | LEU |
| 1 | B | 699 | PHE |
| 1 | B | 701 | VAL |
| 1 | B | 702 | LEU |
| 1 | B | 724 | ARG |
| 1 | B | 726 | PHE |
| 1 | B | 739 | GLU |
| 1 | B | 741 | SER |
| 1 | B | 775 | VAL |
| 1 | B | 779 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 781 | THR |
| 1 | B | 784 | LEU |
| 1 | B | 789 | PHE |
| 1 | B | 790 | LYS |
| 1 | B | 797 | LYS |
| 1 | B | 806 | PHE |
| 1 | B | 831 | ASN |
| 1 | B | 837 | MET |
| 1 | B | 851 | PHE |
| 1 | B | 853 | ASN |
| 1 | B | 854 | PHE |
| 1 | B | 857 | CYS |
| 1 | B | 860 | ARG |
| 1 | B | 866 | ARG |
| 1 | B | 893 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 30 | GLN |
| 1 | A | 37 | ASN |
| 1 | A | 84 | ASN |
| 1 | A | 132 | GLN |
| 1 | A | 142 | GLN |
| 1 | A | 174 | ASN |
| 1 | A | 275 | GLN |
| 1 | A | 300 | ASN |
| 1 | A | 305 | ASN |
| 1 | A | 355 | ASN |
| 1 | A | 448 | HIS |
| 1 | A | 462 | GLN |
| 1 | A | 493 | ASN |
| 1 | A | 591 | ASN |
| 1 | A | 604 | ASN |
| 1 | A | 690 | GLN |
| 1 | A | 711 | HIS |
| 1 | A | 714 | ASN |
| 1 | A | 756 | HIS |
| 1 | A | 795 | ASN |
| 1 | A | 800 | GLN |
| 1 | A | 829 | HIS |
| 1 | A | 833 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 853 | ASN |
| 1 | A | 878 | GLN |
| 1 | A | 884 | GLN |
| 1 | A | 888 | GLN |
| 1 | B | 21 | HIS |
| 1 | B | 37 | ASN |
| 1 | B | 47 | GLN |
| 1 | B | 66 | ASN |
| 1 | B | 99 | GLN |
| 1 | B | 140 | HIS |
| 1 | B | 142 | GLN |
| 1 | B | 174 | ASN |
| 1 | B | 243 | ASN |
| 1 | B | 257 | ASN |
| 1 | B | 277 | GLN |
| 1 | B | 280 | ASN |
| 1 | B | 286 | ASN |
| 1 | B | 342 | ASN |
| 1 | B | 437 | GLN |
| 1 | B | 457 | ASN |
| 1 | B | 468 | ASN |
| 1 | B | 493 | ASN |
| 1 | B | 556 | GLN |
| 1 | B | 584 | ASN |
| 1 | B | 604 | ASN |
| 1 | B | 646 | GLN |
| 1 | B | 663 | ASN |
| 1 | B | 831 | ASN |
| 1 | B | 853 | ASN |
| 1 | B | 874 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 | 783/900 (87%) | -0.41 | 11 (1%) 72 72 | 16, 49, 81, 98 | 0 |
| 1 | B | 788/900 (87%) | -0.32 | 16 (2%) 62 63 | 17, 51, 84, 102 | 0 |
| All | All | 1571/1800 (87%) | -0.36 | 27 (1%) 67 68 | 16, 50, 83, 102 | 0 |

All (27) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 587 | ASP | 4.5 |
| 1 | A | 550 | ILE | 4.5 |
| 1 | B | 596 | LEU | 3.9 |
| 1 | B | 402 | SER | 3.6 |
| 1 | B | 843 | SER | 3.6 |
| 1 | B | 742 | ALA | 3.6 |
| 1 | A | 70 | THR | 3.4 |
| 1 | B | 400 | TYR | 3.3 |
| 1 | B | 394 | VAL | 3.3 |
| 1 | B | 712 | TYR | 3.0 |
| 1 | B | 594 | LEU | 3.0 |
| 1 | B | 714 | ASN | 2.9 |
| 1 | A | 596 | LEU | 2.9 |
| 1 | B | 403 | ARG | 2.6 |
| 1 | B | 823 | PHE | 2.5 |
| 1 | B | 799 | TRP | 2.4 |
| 1 | A | 812 | GLY | 2.3 |
| 1 | B | 398 | ASP | 2.2 |
| 1 | A | 522 | PRO | 2.1 |
| 1 | B | 765 | GLY | 2.1 |
| 1 | A | 595 | GLY | 2.1 |
| 1 | A | 546 | ASP | 2.1 |
| 1 | A | 711 | HIS | 2.1 |
| 1 | B | 622 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 549 | GLU | 2.0 |
| 1 | A | 75 | TRP | 2.0 |
| 1 | A | 85 | PRO | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.