



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:15 PM GMT

PDB ID : 4HHB
Title : THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT
1.74 ANGSTROMS RESOLUTION
Authors : Fermi, G.; Perutz, M.F.
Deposited on : 1984-03-07
Resolution : 1.74 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

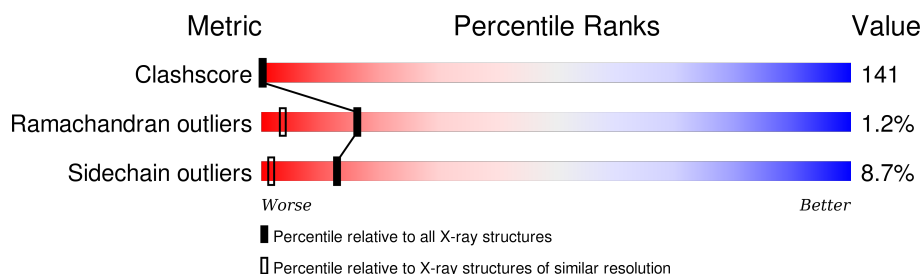
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 Å.

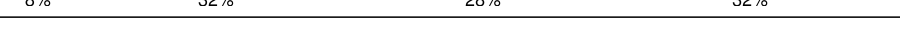
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 2570 (1.76-1.72) |
| Ramachandran outliers | 100387 | 2544 (1.76-1.72) |
| Sidechain outliers | 100360 | 2544 (1.76-1.72) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 141 |  |
| 1 | C | 141 |  |
| 2 | B | 146 |  |
| 2 | D | 146 |  |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called HEMOGLOBIN (DEOXY) (ALPHA CHAIN).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1069 | 685 | 187 | 194 | 3 | | | |
| 1 | C | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1069 | 685 | 187 | 194 | 3 | | | |

- Molecule 2 is a protein called HEMOGLOBIN (DEOXY) (BETA CHAIN).

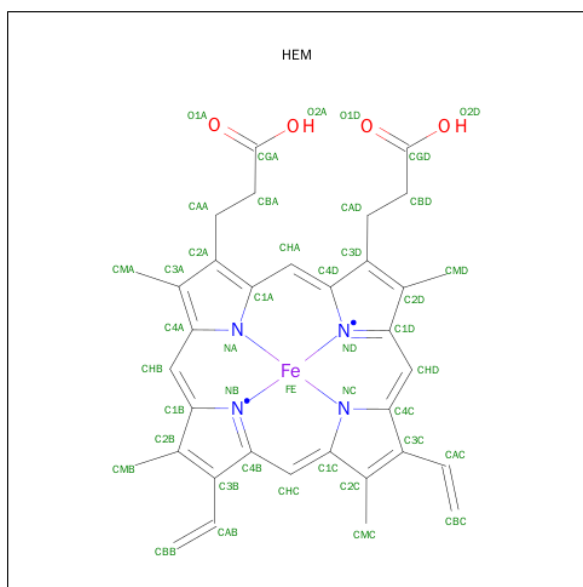
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 724 | 195 | 201 | 3 | | | |
| 2 | D | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1123 | 724 | 195 | 201 | 3 | | | |

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3 | D | 1 | Total P 1 1 | 0 | 0 |
| 3 | B | 1 | Total P 1 1 | 0 | 0 |

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 4 | A | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 4 | B | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 4 | C | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 4 | D | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5 | A | 56 | Total O 56 56 | 0 | 0 |
| 5 | B | 57 | Total O 57 57 | 0 | 0 |
| 5 | C | 59 | Total O 59 59 | 0 | 0 |

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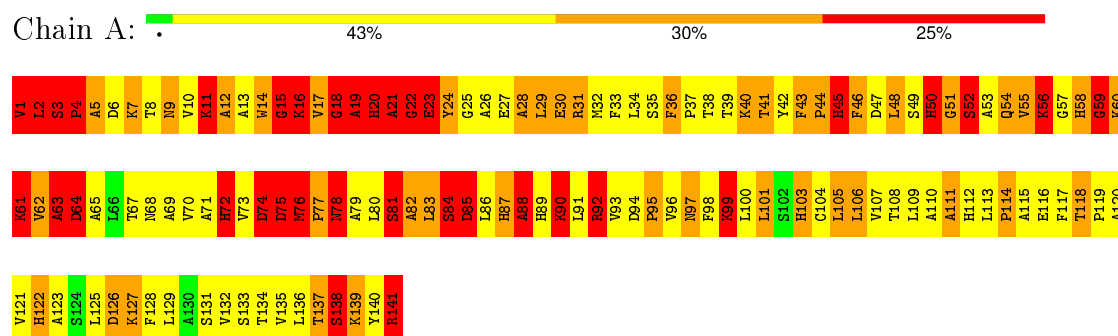
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | D | 49 | Total | O | 0 | 0 |
| | | | 49 | 49 | | |

3 Residue-property plots

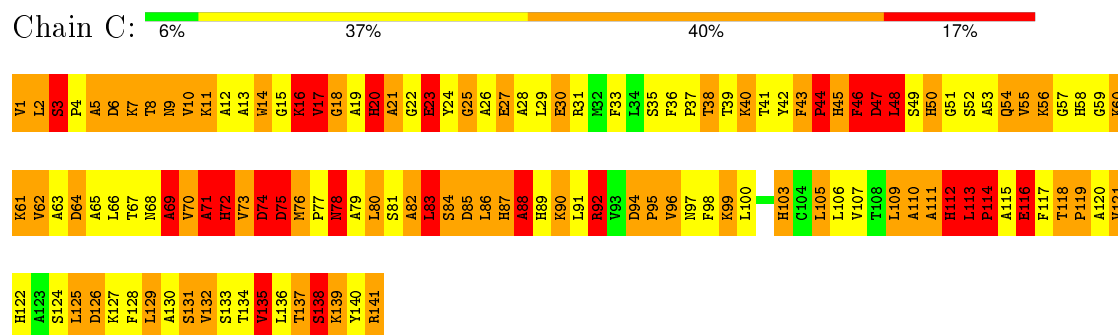
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

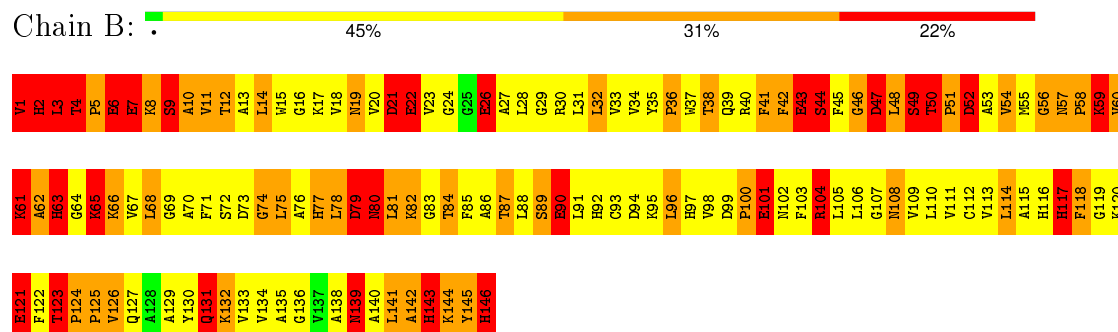
• Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)



• Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)

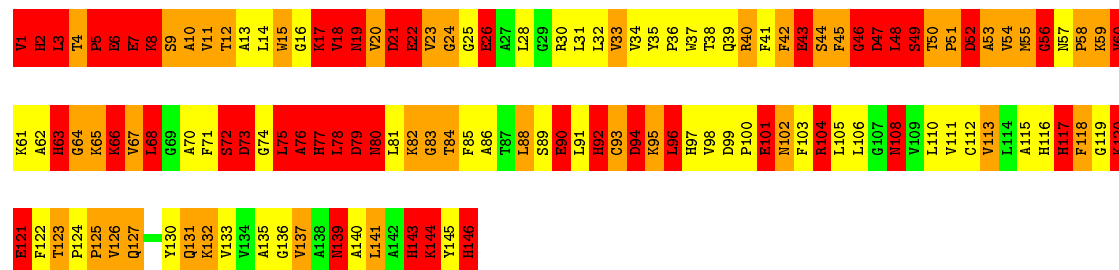


• Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)



- Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)

Chain D: 8% 32% 28% 32%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 63.15Å 83.59Å 53.80Å 90.00° 99.34° 90.00° | Depositor |
| Resolution (Å) | (Not available) – 1.74 | Depositor |
| % Data completeness (in resolution range) | (Not available) ((Not available)-1.74) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | unknown | Depositor |
| R, R_{free} | 0.135 , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 4779 | wwPDB-VP |
| Average B, all atoms (Å ²) | 24.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PO4

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 | 8.18 | 370/1097 (33.7%) | 6.34 | 444/1491 (29.8%) |
| 1 | C | 8.79 | 358/1097 (32.6%) | 7.51 | 407/1491 (27.3%) |
| 2 | B | 10.84 | 417/1153 (36.2%) | 6.61 | 446/1566 (28.5%) |
| 2 | D | 10.60 | 436/1153 (37.8%) | 7.98 | 526/1566 (33.6%) |
| All | All | 9.70 | 1581/4500 (35.1%) | 7.15 | 1823/6114 (29.8%) |

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 | 1 | 51 |
| 1 | C | 2 | 45 |
| 2 | B | 2 | 49 |
| 2 | D | 5 | 62 |
| All | All | 10 | 207 |

All (1581) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2 | B | 26 | GLU | CD-OE1 | 143.13 | 2.83 | 1.25 |
| 1 | C | 92 | ARG | NE-CZ | 126.10 | 2.96 | 1.33 |
| 2 | D | 6 | GLU | CD-OE2 | 121.79 | 2.59 | 1.25 |
| 2 | B | 26 | GLU | CD-OE2 | 106.90 | 2.43 | 1.25 |
| 1 | C | 23 | GLU | CD-OE1 | 101.97 | 2.37 | 1.25 |
| 2 | D | 104 | ARG | NE-CZ | 96.15 | 2.58 | 1.33 |
| 1 | A | 92 | ARG | NE-CZ | 95.65 | 2.57 | 1.33 |
| 2 | B | 22 | GLU | CD-OE2 | 78.69 | 2.12 | 1.25 |
| 2 | B | 104 | ARG | NE-CZ | 61.72 | 2.13 | 1.33 |
| 2 | D | 90 | GLU | CG-CD | 60.86 | 2.43 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 43 | GLU | CG-CD | 60.66 | 2.42 | 1.51 |
| 2 | D | 22 | GLU | CG-CD | 58.05 | 2.39 | 1.51 |
| 2 | B | 121 | GLU | CD-OE1 | 56.01 | 1.87 | 1.25 |
| 2 | D | 52 | ASP | CG-OD2 | 51.95 | 2.44 | 1.25 |
| 2 | D | 2 | HIS | CG-ND1 | 49.81 | 2.48 | 1.38 |
| 2 | B | 104 | ARG | CZ-NH2 | 49.80 | 1.97 | 1.33 |
| 2 | D | 26 | GLU | CD-OE1 | 48.92 | 1.79 | 1.25 |
| 1 | A | 60 | LYS | CE-NZ | 47.93 | 2.68 | 1.49 |
| 1 | A | 90 | LYS | CE-NZ | 47.25 | 2.67 | 1.49 |
| 2 | B | 22 | GLU | CD-OE1 | 46.75 | 1.77 | 1.25 |
| 1 | C | 1 | VAL | CB-CG2 | 45.68 | 2.48 | 1.52 |
| 2 | B | 65 | LYS | CE-NZ | 44.03 | 2.59 | 1.49 |
| 2 | D | 73 | ASP | CG-OD2 | 43.88 | 2.26 | 1.25 |
| 1 | C | 1 | VAL | N-CA | 43.63 | 2.33 | 1.46 |
| 1 | C | 116 | GLU | CB-CG | 42.97 | 2.33 | 1.52 |
| 1 | C | 23 | GLU | CG-CD | 42.51 | 2.15 | 1.51 |
| 1 | A | 23 | GLU | CD-OE1 | 42.41 | 1.72 | 1.25 |
| 2 | B | 104 | ARG | CZ-NH1 | 42.02 | 1.87 | 1.33 |
| 1 | C | 92 | ARG | CZ-NH1 | 41.72 | 1.87 | 1.33 |
| 2 | D | 26 | GLU | CD-OE2 | 41.28 | 1.71 | 1.25 |
| 1 | C | 30 | GLU | CD-OE2 | -41.18 | 0.80 | 1.25 |
| 2 | B | 2 | HIS | CG-CD2 | 41.11 | 2.05 | 1.35 |
| 1 | C | 138 | SER | CA-CB | 40.95 | 2.14 | 1.52 |
| 2 | D | 22 | GLU | CB-CG | -40.05 | 0.76 | 1.52 |
| 2 | D | 132 | LYS | CE-NZ | 39.97 | 2.48 | 1.49 |
| 1 | A | 75 | ASP | CB-CG | -39.80 | 0.68 | 1.51 |
| 1 | A | 138 | SER | CA-CB | 39.62 | 2.12 | 1.52 |
| 2 | D | 43 | GLU | CB-CG | -38.94 | 0.78 | 1.52 |
| 2 | D | 5 | PRO | CA-CB | 38.90 | 2.31 | 1.53 |
| 1 | A | 23 | GLU | CG-CD | 38.85 | 2.10 | 1.51 |
| 2 | D | 58 | PRO | CG-CD | -38.65 | 0.23 | 1.50 |
| 2 | B | 117 | HIS | CD2-NE2 | 37.97 | 2.21 | 1.42 |
| 1 | A | 78 | ASN | CG-OD1 | 37.90 | 2.07 | 1.24 |
| 2 | B | 6 | GLU | CD-OE1 | 37.86 | 1.67 | 1.25 |
| 2 | B | 6 | GLU | CG-CD | 36.95 | 2.07 | 1.51 |
| 2 | D | 20 | VAL | CB-CG2 | 36.90 | 2.30 | 1.52 |
| 2 | B | 121 | GLU | CG-CD | 36.90 | 2.07 | 1.51 |
| 2 | B | 2 | HIS | CB-CG | -36.83 | 0.83 | 1.50 |
| 2 | B | 139 | ASN | CB-CG | -36.83 | 0.66 | 1.51 |
| 2 | B | 43 | GLU | CD-OE1 | -36.77 | 0.85 | 1.25 |
| 2 | B | 90 | GLU | CG-CD | 36.68 | 2.06 | 1.51 |
| 2 | D | 101 | GLU | CG-CD | 36.62 | 2.06 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 92 | ARG | CZ-NH2 | -36.39 | 0.85 | 1.33 |
| 2 | D | 82 | LYS | CD-CE | 36.28 | 2.42 | 1.51 |
| 1 | C | 56 | LYS | CD-CE | 35.42 | 2.39 | 1.51 |
| 2 | D | 90 | GLU | CD-OE1 | 35.18 | 1.64 | 1.25 |
| 2 | B | 65 | LYS | CB-CG | -34.95 | 0.58 | 1.52 |
| 2 | D | 26 | GLU | CB-CG | 34.81 | 2.18 | 1.52 |
| 2 | D | 47 | ASP | CA-C | 34.66 | 2.43 | 1.52 |
| 1 | C | 23 | GLU | CD-OE2 | -34.47 | 0.87 | 1.25 |
| 2 | B | 82 | LYS | CE-NZ | 34.42 | 2.35 | 1.49 |
| 2 | B | 66 | LYS | CD-CE | 34.36 | 2.37 | 1.51 |
| 1 | A | 75 | ASP | CG-OD2 | 34.26 | 2.04 | 1.25 |
| 2 | B | 59 | LYS | CD-CE | 34.19 | 2.36 | 1.51 |
| 2 | B | 101 | GLU | CG-CD | 33.84 | 2.02 | 1.51 |
| 2 | B | 65 | LYS | CD-CE | 33.62 | 2.35 | 1.51 |
| 2 | B | 2 | HIS | ND1-CE1 | 33.32 | 2.18 | 1.34 |
| 1 | C | 1 | VAL | CB-CG1 | 33.07 | 2.22 | 1.52 |
| 2 | D | 121 | GLU | CG-CD | 32.89 | 2.01 | 1.51 |
| 1 | A | 30 | GLU | CG-CD | 32.43 | 2.00 | 1.51 |
| 2 | B | 82 | LYS | CD-CE | -32.40 | 0.70 | 1.51 |
| 2 | D | 120 | LYS | CE-NZ | 32.27 | 2.29 | 1.49 |
| 2 | D | 79 | ASP | CG-OD1 | 32.20 | 1.99 | 1.25 |
| 2 | B | 2 | HIS | CD2-NE2 | 32.02 | 2.09 | 1.42 |
| 2 | D | 79 | ASP | CG-OD2 | 31.85 | 1.98 | 1.25 |
| 1 | A | 81 | SER | CA-CB | 31.84 | 2.00 | 1.52 |
| 2 | D | 43 | GLU | CD-OE1 | 31.82 | 1.60 | 1.25 |
| 2 | B | 8 | LYS | CE-NZ | 31.50 | 2.27 | 1.49 |
| 2 | D | 47 | ASP | N-CA | 31.42 | 2.09 | 1.46 |
| 2 | D | 2 | HIS | CA-CB | 30.88 | 2.21 | 1.53 |
| 2 | B | 146 | HIS | CB-CG | 30.49 | 2.04 | 1.50 |
| 2 | D | 6 | GLU | CB-CG | -30.44 | 0.94 | 1.52 |
| 2 | D | 66 | LYS | CD-CE | 30.42 | 2.27 | 1.51 |
| 2 | D | 6 | GLU | CG-CD | 30.34 | 1.97 | 1.51 |
| 2 | D | 43 | GLU | CD-OE2 | 30.30 | 1.58 | 1.25 |
| 2 | B | 90 | GLU | CD-OE1 | -30.12 | 0.92 | 1.25 |
| 1 | C | 99 | LYS | CD-CE | 30.11 | 2.26 | 1.51 |
| 2 | D | 6 | GLU | CA-C | 30.01 | 2.31 | 1.52 |
| 1 | A | 127 | LYS | CB-CG | -29.93 | 0.71 | 1.52 |
| 1 | C | 30 | GLU | CG-CD | 29.51 | 1.96 | 1.51 |
| 2 | B | 49 | SER | C-O | 29.47 | 1.79 | 1.23 |
| 1 | A | 92 | ARG | CG-CD | 29.45 | 2.25 | 1.51 |
| 2 | D | 2 | HIS | CG-CD2 | 29.45 | 1.85 | 1.35 |
| 2 | D | 143 | HIS | CG-CD2 | 29.09 | 1.85 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | C | 99 | LYS | CB-CG | -28.97 | 0.74 | 1.52 |
| 1 | C | 16 | LYS | CD-CE | 28.72 | 2.23 | 1.51 |
| 1 | A | 99 | LYS | CE-NZ | 28.60 | 2.20 | 1.49 |
| 2 | B | 65 | LYS | CG-CD | 28.60 | 2.49 | 1.52 |
| 2 | B | 12 | THR | CB-CG2 | -28.55 | 0.58 | 1.52 |
| 2 | D | 6 | GLU | CD-OE1 | -28.52 | 0.94 | 1.25 |
| 2 | B | 77 | HIS | CG-CD2 | 28.39 | 1.84 | 1.35 |
| 2 | D | 3 | LEU | C-O | 28.24 | 1.77 | 1.23 |
| 2 | D | 65 | LYS | CD-CE | 27.80 | 2.20 | 1.51 |
| 1 | A | 61 | LYS | CD-CE | -27.73 | 0.81 | 1.51 |
| 2 | B | 139 | ASN | CG-ND2 | 27.55 | 2.01 | 1.32 |
| 2 | B | 6 | GLU | CD-OE2 | -27.46 | 0.95 | 1.25 |
| 1 | A | 15 | GLY | C-O | 27.29 | 1.67 | 1.23 |
| 2 | D | 144 | LYS | CE-NZ | 27.14 | 2.16 | 1.49 |
| 1 | A | 78 | ASN | CB-CG | -27.09 | 0.88 | 1.51 |
| 2 | D | 146 | HIS | ND1-CE1 | -27.02 | 0.67 | 1.34 |
| 2 | D | 43 | GLU | CG-CD | 26.84 | 1.92 | 1.51 |
| 1 | C | 92 | ARG | CZ-NH2 | -26.47 | 0.98 | 1.33 |
| 1 | C | 40 | LYS | CD-CE | -26.26 | 0.85 | 1.51 |
| 2 | D | 26 | GLU | CG-CD | 25.76 | 1.90 | 1.51 |
| 2 | B | 143 | HIS | ND1-CE1 | 25.75 | 1.99 | 1.34 |
| 2 | D | 45 | PHE | C-N | -25.51 | 0.87 | 1.33 |
| 2 | B | 117 | HIS | CG-ND1 | 25.44 | 1.94 | 1.38 |
| 1 | A | 17 | VAL | C-O | -25.43 | 0.75 | 1.23 |
| 2 | D | 2 | HIS | CE1-NE2 | 25.33 | 1.91 | 1.32 |
| 2 | B | 6 | GLU | CB-CG | -25.27 | 1.04 | 1.52 |
| 2 | B | 7 | GLU | CA-CB | -25.13 | 0.98 | 1.53 |
| 2 | B | 1 | VAL | C-O | 24.89 | 1.70 | 1.23 |
| 2 | D | 2 | HIS | CB-CG | -24.75 | 1.05 | 1.50 |
| 1 | A | 75 | ASP | CG-OD1 | 24.71 | 1.82 | 1.25 |
| 1 | A | 49 | SER | CB-OG | -24.50 | 1.10 | 1.42 |
| 2 | B | 5 | PRO | N-CD | 24.22 | 1.81 | 1.47 |
| 2 | D | 20 | VAL | CA-CB | 24.21 | 2.05 | 1.54 |
| 2 | B | 8 | LYS | CB-CG | -24.20 | 0.87 | 1.52 |
| 1 | C | 49 | SER | CB-OG | -24.15 | 1.10 | 1.42 |
| 2 | D | 121 | GLU | CD-OE1 | 24.11 | 1.52 | 1.25 |
| 2 | D | 76 | ALA | N-CA | 24.06 | 1.94 | 1.46 |
| 1 | A | 96 | VAL | CB-CG2 | -24.05 | 1.02 | 1.52 |
| 2 | B | 1 | VAL | CB-CG1 | 24.01 | 2.03 | 1.52 |
| 2 | B | 1 | VAL | C-N | -23.87 | 0.79 | 1.34 |
| 2 | B | 43 | GLU | CD-OE2 | 23.53 | 1.51 | 1.25 |
| 1 | C | 46 | PHE | CD2-CE2 | -23.52 | 0.92 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 47 | ASP | CG-OD2 | 23.25 | 1.78 | 1.25 |
| 1 | C | 90 | LYS | CE-NZ | 23.11 | 2.06 | 1.49 |
| 2 | B | 121 | GLU | CB-CG | -22.88 | 1.08 | 1.52 |
| 2 | B | 2 | HIS | CG-ND1 | 22.82 | 1.89 | 1.38 |
| 2 | D | 121 | GLU | CB-CG | -22.68 | 1.09 | 1.52 |
| 2 | B | 22 | GLU | CG-CD | 22.64 | 1.85 | 1.51 |
| 1 | C | 92 | ARG | CD-NE | -22.63 | 1.07 | 1.46 |
| 2 | D | 77 | HIS | ND1-CE1 | 22.61 | 1.91 | 1.34 |
| 2 | B | 45 | PHE | CG-CD2 | -22.55 | 1.04 | 1.38 |
| 2 | D | 2 | HIS | ND1-CE1 | 22.27 | 1.90 | 1.34 |
| 2 | D | 50 | THR | CA-CB | 22.26 | 2.11 | 1.53 |
| 2 | B | 49 | SER | CB-OG | 22.20 | 1.71 | 1.42 |
| 2 | D | 104 | ARG | CD-NE | 22.18 | 1.84 | 1.46 |
| 2 | D | 77 | HIS | CD2-NE2 | 22.18 | 1.88 | 1.42 |
| 1 | C | 56 | LYS | CG-CD | 21.99 | 2.27 | 1.52 |
| 2 | D | 65 | LYS | CG-CD | 21.96 | 2.27 | 1.52 |
| 2 | B | 58 | PRO | N-CD | 21.93 | 1.78 | 1.47 |
| 1 | A | 14 | TRP | CG-CD1 | 21.88 | 1.67 | 1.36 |
| 1 | A | 50 | HIS | CA-CB | 21.85 | 2.02 | 1.53 |
| 2 | D | 5 | PRO | N-CA | 21.80 | 1.84 | 1.47 |
| 2 | B | 2 | HIS | CA-CB | 21.68 | 2.01 | 1.53 |
| 1 | A | 85 | ASP | CG-OD1 | -21.66 | 0.75 | 1.25 |
| 1 | A | 18 | GLY | CA-C | 21.65 | 1.86 | 1.51 |
| 1 | A | 21 | ALA | CA-C | 21.59 | 2.09 | 1.52 |
| 2 | B | 1 | VAL | CA-C | 21.57 | 2.09 | 1.52 |
| 2 | D | 21 | ASP | CA-C | -21.48 | 0.97 | 1.52 |
| 1 | C | 15 | GLY | C-O | 21.34 | 1.57 | 1.23 |
| 2 | D | 146 | HIS | CG-ND1 | 21.18 | 1.85 | 1.38 |
| 1 | C | 60 | LYS | CE-NZ | 21.16 | 2.02 | 1.49 |
| 1 | A | 72 | HIS | CG-ND1 | 21.11 | 1.85 | 1.38 |
| 1 | A | 64 | ASP | CB-CG | 21.03 | 1.96 | 1.51 |
| 1 | A | 85 | ASP | CG-OD2 | 20.96 | 1.73 | 1.25 |
| 2 | D | 8 | LYS | CD-CE | 20.93 | 2.03 | 1.51 |
| 2 | B | 49 | SER | CA-CB | 20.58 | 1.83 | 1.52 |
| 1 | C | 14 | TRP | CZ3-CH2 | 20.53 | 1.72 | 1.40 |
| 1 | A | 50 | HIS | C-N | -20.39 | 0.96 | 1.33 |
| 2 | B | 144 | LYS | CE-NZ | 20.24 | 1.99 | 1.49 |
| 2 | B | 42 | PHE | CG-CD1 | 20.19 | 1.69 | 1.38 |
| 2 | D | 139 | ASN | CG-OD1 | 20.14 | 1.68 | 1.24 |
| 2 | D | 42 | PHE | CG-CD1 | 20.11 | 1.69 | 1.38 |
| 2 | D | 95 | LYS | CE-NZ | 20.00 | 1.99 | 1.49 |
| 2 | B | 144 | LYS | CD-CE | 19.96 | 2.01 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 75 | ASP | CA-CB | 19.91 | 1.97 | 1.53 |
| 2 | B | 146 | HIS | ND1-CE1 | 19.85 | 1.84 | 1.34 |
| 2 | D | 17 | LYS | CE-NZ | 19.82 | 1.98 | 1.49 |
| 1 | A | 22 | GLY | CA-C | -19.78 | 1.20 | 1.51 |
| 2 | D | 9 | SER | CB-OG | -19.77 | 1.16 | 1.42 |
| 1 | A | 96 | VAL | CB-CG1 | -19.71 | 1.11 | 1.52 |
| 1 | A | 74 | ASP | CG-OD1 | -19.67 | 0.80 | 1.25 |
| 1 | C | 61 | LYS | CE-NZ | 19.65 | 1.98 | 1.49 |
| 2 | D | 13 | ALA | CA-CB | -19.60 | 1.11 | 1.52 |
| 1 | A | 84 | SER | CA-CB | 19.59 | 1.82 | 1.52 |
| 1 | C | 22 | GLY | CA-C | -19.50 | 1.20 | 1.51 |
| 2 | D | 4 | THR | C-N | -19.46 | 0.97 | 1.34 |
| 1 | A | 24 | TYR | CE1-CZ | -19.36 | 1.13 | 1.38 |
| 2 | D | 80 | ASN | CG-OD1 | 19.27 | 1.66 | 1.24 |
| 2 | D | 7 | GLU | CD-OE1 | 19.26 | 1.46 | 1.25 |
| 2 | D | 46 | GLY | CA-C | 19.23 | 1.82 | 1.51 |
| 1 | C | 114 | PRO | CA-C | 19.07 | 1.91 | 1.52 |
| 2 | D | 1 | VAL | CA-C | 19.05 | 2.02 | 1.52 |
| 2 | D | 95 | LYS | CG-CD | 18.98 | 2.17 | 1.52 |
| 2 | D | 7 | GLU | CB-CG | 18.89 | 1.88 | 1.52 |
| 2 | B | 45 | PHE | CE1-CZ | -18.81 | 1.01 | 1.37 |
| 1 | A | 139 | LYS | CE-NZ | 18.78 | 1.96 | 1.49 |
| 1 | C | 72 | HIS | CG-ND1 | 18.76 | 1.80 | 1.38 |
| 2 | B | 44 | SER | CB-OG | -18.63 | 1.18 | 1.42 |
| 2 | D | 66 | LYS | CE-NZ | 18.57 | 1.95 | 1.49 |
| 2 | D | 47 | ASP | CA-CB | 18.49 | 1.94 | 1.53 |
| 1 | A | 14 | TRP | CD2-CE2 | 18.40 | 1.63 | 1.41 |
| 2 | B | 79 | ASP | CG-OD2 | 18.34 | 1.67 | 1.25 |
| 2 | B | 146 | HIS | CG-ND1 | -18.29 | 0.98 | 1.38 |
| 2 | D | 82 | LYS | CE-NZ | 18.27 | 1.94 | 1.49 |
| 1 | C | 84 | SER | CB-OG | -18.21 | 1.18 | 1.42 |
| 1 | A | 15 | GLY | C-N | -18.19 | 0.92 | 1.34 |
| 1 | A | 11 | LYS | CD-CE | 18.16 | 1.96 | 1.51 |
| 1 | C | 116 | GLU | CD-OE2 | 18.14 | 1.45 | 1.25 |
| 1 | C | 112 | HIS | CG-ND1 | 18.10 | 1.78 | 1.38 |
| 2 | B | 9 | SER | N-CA | -18.09 | 1.10 | 1.46 |
| 2 | D | 8 | LYS | CE-NZ | 18.03 | 1.94 | 1.49 |
| 1 | A | 14 | TRP | NE1-CE2 | -18.00 | 1.14 | 1.37 |
| 2 | D | 101 | GLU | CD-OE2 | 17.94 | 1.45 | 1.25 |
| 2 | B | 40 | ARG | CZ-NH2 | 17.86 | 1.56 | 1.33 |
| 1 | A | 74 | ASP | C-N | -17.86 | 0.93 | 1.34 |
| 2 | B | 117 | HIS | CG-CD2 | 17.86 | 1.66 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | C | 84 | SER | CA-CB | 17.82 | 1.79 | 1.52 |
| 1 | C | 139 | LYS | CD-CE | 17.80 | 1.95 | 1.51 |
| 2 | D | 53 | ALA | C-O | -17.74 | 0.89 | 1.23 |
| 1 | C | 20 | HIS | ND1-CE1 | 17.71 | 1.79 | 1.34 |
| 1 | A | 99 | LYS | CD-CE | 17.55 | 1.95 | 1.51 |
| 2 | B | 9 | SER | CA-CB | 17.51 | 1.79 | 1.52 |
| 2 | D | 76 | ALA | CA-C | -17.40 | 1.07 | 1.52 |
| 2 | B | 59 | LYS | CE-NZ | 17.34 | 1.92 | 1.49 |
| 1 | A | 46 | PHE | CG-CD2 | -17.27 | 1.12 | 1.38 |
| 2 | D | 22 | GLU | CD-OE1 | 17.19 | 1.44 | 1.25 |
| 2 | D | 78 | LEU | CG-CD2 | -17.10 | 0.88 | 1.51 |
| 1 | C | 11 | LYS | CE-NZ | 17.09 | 1.91 | 1.49 |
| 1 | A | 60 | LYS | CD-CE | 17.00 | 1.93 | 1.51 |
| 1 | A | 67 | THR | CB-OG1 | -16.96 | 1.09 | 1.43 |
| 1 | A | 37 | PRO | N-CD | -16.94 | 1.24 | 1.47 |
| 1 | C | 74 | ASP | C-O | -16.90 | 0.91 | 1.23 |
| 2 | D | 58 | PRO | N-CD | 16.84 | 1.71 | 1.47 |
| 2 | D | 1 | VAL | CB-CG2 | -16.76 | 1.17 | 1.52 |
| 2 | B | 76 | ALA | C-O | -16.68 | 0.91 | 1.23 |
| 2 | D | 83 | GLY | C-O | 16.67 | 1.50 | 1.23 |
| 2 | B | 5 | PRO | N-CA | -16.64 | 1.19 | 1.47 |
| 2 | D | 20 | VAL | CB-CG1 | -16.62 | 1.18 | 1.52 |
| 1 | A | 17 | VAL | CA-C | 16.61 | 1.96 | 1.52 |
| 1 | A | 116 | GLU | CD-OE2 | 16.55 | 1.43 | 1.25 |
| 2 | D | 19 | ASN | CG-OD1 | 16.47 | 1.60 | 1.24 |
| 1 | A | 16 | LYS | CD-CE | 16.40 | 1.92 | 1.51 |
| 2 | D | 2 | HIS | C-O | 16.37 | 1.54 | 1.23 |
| 1 | C | 105 | LEU | CG-CD2 | 16.34 | 2.12 | 1.51 |
| 2 | D | 144 | LYS | CD-CE | -16.26 | 1.10 | 1.51 |
| 2 | B | 117 | HIS | ND1-CE1 | 16.21 | 1.75 | 1.34 |
| 2 | D | 117 | HIS | CG-ND1 | 16.13 | 1.74 | 1.38 |
| 2 | B | 87 | THR | CA-CB | 16.13 | 1.95 | 1.53 |
| 2 | B | 79 | ASP | CB-CG | -16.08 | 1.18 | 1.51 |
| 2 | B | 124 | PRO | N-CD | 16.08 | 1.70 | 1.47 |
| 2 | D | 59 | LYS | CG-CD | -16.07 | 0.97 | 1.52 |
| 2 | B | 146 | HIS | CG-CD2 | 16.06 | 1.63 | 1.35 |
| 2 | D | 43 | GLU | CA-CB | -16.02 | 1.18 | 1.53 |
| 2 | D | 66 | LYS | CG-CD | 15.99 | 2.06 | 1.52 |
| 1 | C | 90 | LYS | CD-CE | 15.99 | 1.91 | 1.51 |
| 2 | D | 73 | ASP | C-N | 15.96 | 1.61 | 1.33 |
| 1 | A | 99 | LYS | CB-CG | -15.95 | 1.09 | 1.52 |
| 2 | B | 74 | GLY | C-N | 15.91 | 1.70 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 145 | TYR | C-N | -15.90 | 0.97 | 1.34 |
| 2 | B | 139 | ASN | CG-OD1 | 15.86 | 1.58 | 1.24 |
| 2 | D | 43 | GLU | CA-C | 15.86 | 1.94 | 1.52 |
| 2 | B | 132 | LYS | CE-NZ | 15.84 | 1.88 | 1.49 |
| 1 | A | 56 | LYS | CG-CD | 15.83 | 2.06 | 1.52 |
| 1 | C | 72 | HIS | CG-CD2 | 15.72 | 1.62 | 1.35 |
| 2 | B | 40 | ARG | NE-CZ | 15.64 | 1.53 | 1.33 |
| 1 | C | 72 | HIS | CB-CG | -15.59 | 1.22 | 1.50 |
| 2 | D | 66 | LYS | CB-CG | -15.54 | 1.10 | 1.52 |
| 1 | A | 131 | SER | CB-OG | -15.53 | 1.22 | 1.42 |
| 1 | A | 137 | THR | CB-CG2 | -15.50 | 1.01 | 1.52 |
| 2 | D | 1 | VAL | N-CA | 15.50 | 1.77 | 1.46 |
| 2 | D | 19 | ASN | CG-ND2 | 15.49 | 1.71 | 1.32 |
| 2 | B | 21 | ASP | CB-CG | 15.47 | 1.84 | 1.51 |
| 2 | B | 145 | TYR | CD2-CE2 | 15.46 | 1.62 | 1.39 |
| 1 | A | 99 | LYS | CG-CD | -15.38 | 1.00 | 1.52 |
| 2 | D | 12 | THR | CA-CB | 15.36 | 1.93 | 1.53 |
| 2 | D | 117 | HIS | CE1-NE2 | -15.32 | 0.97 | 1.32 |
| 1 | C | 16 | LYS | CB-CG | 15.31 | 1.93 | 1.52 |
| 2 | D | 130 | TYR | CE1-CZ | 15.31 | 1.58 | 1.38 |
| 1 | C | 82 | ALA | C-N | 15.31 | 1.69 | 1.34 |
| 2 | D | 52 | ASP | N-CA | 15.28 | 1.76 | 1.46 |
| 2 | B | 87 | THR | CB-CG2 | 15.27 | 2.02 | 1.52 |
| 2 | D | 41 | PHE | CE1-CZ | -15.25 | 1.08 | 1.37 |
| 1 | A | 84 | SER | CB-OG | -15.24 | 1.22 | 1.42 |
| 2 | B | 59 | LYS | CG-CD | -15.22 | 1.00 | 1.52 |
| 1 | A | 14 | TRP | CB-CG | -15.21 | 1.22 | 1.50 |
| 1 | C | 70 | VAL | C-N | -15.11 | 0.99 | 1.34 |
| 1 | A | 44 | PRO | CA-C | 15.08 | 1.83 | 1.52 |
| 2 | B | 1 | VAL | CA-CB | 15.08 | 1.86 | 1.54 |
| 1 | A | 50 | HIS | CG-CD2 | 15.03 | 1.61 | 1.35 |
| 1 | A | 17 | VAL | C-N | 14.96 | 1.59 | 1.33 |
| 2 | D | 59 | LYS | CD-CE | 14.89 | 1.88 | 1.51 |
| 1 | C | 114 | PRO | N-CA | 14.86 | 1.72 | 1.47 |
| 1 | A | 3 | SER | C-N | 14.86 | 1.62 | 1.34 |
| 1 | C | 14 | TRP | CG-CD1 | 14.86 | 1.57 | 1.36 |
| 1 | A | 23 | GLU | CD-OE2 | 14.85 | 1.42 | 1.25 |
| 1 | C | 25 | GLY | C-O | 14.78 | 1.47 | 1.23 |
| 2 | D | 80 | ASN | N-CA | 14.77 | 1.75 | 1.46 |
| 1 | A | 1 | VAL | N-CA | -14.73 | 1.16 | 1.46 |
| 2 | D | 73 | ASP | CA-CB | 14.72 | 1.86 | 1.53 |
| 1 | C | 78 | ASN | CA-C | -14.71 | 1.14 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 20 | HIS | CG-ND1 | 14.65 | 1.71 | 1.38 |
| 1 | A | 137 | THR | CA-CB | 14.64 | 1.91 | 1.53 |
| 2 | D | 21 | ASP | CG-OD1 | 14.59 | 1.58 | 1.25 |
| 1 | C | 7 | LYS | N-CA | 14.55 | 1.75 | 1.46 |
| 2 | B | 108 | ASN | CB-CG | 14.55 | 1.84 | 1.51 |
| 2 | D | 117 | HIS | CG-CD2 | 14.54 | 1.60 | 1.35 |
| 1 | C | 72 | HIS | CA-CB | 14.52 | 1.85 | 1.53 |
| 2 | B | 143 | HIS | CG-ND1 | 14.50 | 1.70 | 1.38 |
| 1 | C | 68 | ASN | CG-OD1 | -14.47 | 0.92 | 1.24 |
| 2 | D | 21 | ASP | C-O | 14.42 | 1.50 | 1.23 |
| 2 | D | 8 | LYS | CA-CB | 14.40 | 1.85 | 1.53 |
| 2 | D | 73 | ASP | CG-OD1 | 14.40 | 1.58 | 1.25 |
| 1 | A | 52 | SER | N-CA | 14.37 | 1.75 | 1.46 |
| 1 | A | 16 | LYS | CG-CD | 14.35 | 2.01 | 1.52 |
| 2 | D | 55 | MET | CA-C | 14.33 | 1.90 | 1.52 |
| 2 | B | 44 | SER | C-O | 14.33 | 1.50 | 1.23 |
| 1 | A | 14 | TRP | CE2-CZ2 | -14.28 | 1.15 | 1.39 |
| 2 | B | 145 | TYR | CE1-CZ | 14.27 | 1.57 | 1.38 |
| 1 | A | 1 | VAL | CA-CB | 14.26 | 1.84 | 1.54 |
| 1 | C | 118 | THR | C-N | -14.24 | 1.07 | 1.34 |
| 2 | B | 125 | PRO | N-CD | 14.17 | 1.67 | 1.47 |
| 1 | C | 139 | LYS | CE-NZ | 14.16 | 1.84 | 1.49 |
| 2 | D | 15 | TRP | CD2-CE2 | 14.15 | 1.58 | 1.41 |
| 1 | C | 37 | PRO | N-CD | -14.10 | 1.28 | 1.47 |
| 1 | A | 74 | ASP | CG-OD2 | 14.07 | 1.57 | 1.25 |
| 2 | D | 125 | PRO | N-CD | 14.06 | 1.67 | 1.47 |
| 2 | B | 90 | GLU | CA-CB | 14.03 | 1.84 | 1.53 |
| 2 | D | 108 | ASN | CB-CG | 14.03 | 1.83 | 1.51 |
| 2 | D | 117 | HIS | CB-CG | -14.02 | 1.24 | 1.50 |
| 2 | D | 80 | ASN | CA-CB | -13.95 | 1.16 | 1.53 |
| 2 | B | 81 | LEU | C-N | 13.94 | 1.66 | 1.34 |
| 1 | C | 1 | VAL | CA-CB | -13.93 | 1.25 | 1.54 |
| 1 | A | 2 | LEU | C-N | -13.92 | 1.02 | 1.34 |
| 2 | D | 40 | ARG | CZ-NH1 | -13.85 | 1.15 | 1.33 |
| 2 | B | 66 | LYS | N-CA | -13.84 | 1.18 | 1.46 |
| 1 | C | 14 | TRP | CD2-CE2 | 13.72 | 1.57 | 1.41 |
| 2 | D | 30 | ARG | CD-NE | -13.72 | 1.23 | 1.46 |
| 2 | B | 102 | ASN | CG-OD1 | -13.68 | 0.93 | 1.24 |
| 2 | D | 76 | ALA | C-O | 13.68 | 1.49 | 1.23 |
| 2 | D | 79 | ASP | CB-CG | -13.68 | 1.23 | 1.51 |
| 2 | D | 18 | VAL | CA-CB | -13.62 | 1.26 | 1.54 |
| 2 | B | 130 | TYR | CD2-CE2 | 13.59 | 1.59 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 74 | ASP | CB-CG | 13.56 | 1.80 | 1.51 |
| 2 | B | 143 | HIS | CB-CG | 13.55 | 1.74 | 1.50 |
| 1 | A | 1 | VAL | CB-CG2 | -13.50 | 1.24 | 1.52 |
| 2 | B | 1 | VAL | CB-CG2 | -13.43 | 1.24 | 1.52 |
| 1 | C | 131 | SER | CA-CB | 13.40 | 1.73 | 1.52 |
| 1 | A | 50 | HIS | C-O | 13.39 | 1.48 | 1.23 |
| 2 | B | 80 | ASN | N-CA | 13.38 | 1.73 | 1.46 |
| 1 | A | 127 | LYS | CG-CD | 13.37 | 1.97 | 1.52 |
| 1 | A | 56 | LYS | CD-CE | 13.35 | 1.84 | 1.51 |
| 2 | B | 7 | GLU | CB-CG | 13.35 | 1.77 | 1.52 |
| 1 | A | 90 | LYS | CD-CE | 13.26 | 1.84 | 1.51 |
| 1 | A | 14 | TRP | CA-CB | 13.22 | 1.83 | 1.53 |
| 1 | A | 92 | ARG | CZ-NH1 | 13.20 | 1.50 | 1.33 |
| 2 | B | 9 | SER | CA-C | 13.17 | 1.87 | 1.52 |
| 2 | D | 95 | LYS | C-N | 13.07 | 1.64 | 1.34 |
| 1 | C | 7 | LYS | CA-C | -13.07 | 1.19 | 1.52 |
| 2 | B | 76 | ALA | C-N | 13.06 | 1.64 | 1.34 |
| 2 | B | 40 | ARG | CZ-NH1 | -13.03 | 1.16 | 1.33 |
| 2 | D | 20 | VAL | CA-C | -13.01 | 1.19 | 1.52 |
| 2 | D | 49 | SER | CA-C | 12.97 | 1.86 | 1.52 |
| 1 | C | 68 | ASN | C-O | 12.97 | 1.48 | 1.23 |
| 1 | C | 50 | HIS | CG-ND1 | 12.96 | 1.67 | 1.38 |
| 1 | A | 26 | ALA | N-CA | -12.93 | 1.20 | 1.46 |
| 2 | D | 48 | LEU | N-CA | 12.93 | 1.72 | 1.46 |
| 2 | D | 18 | VAL | CB-CG2 | 12.93 | 1.79 | 1.52 |
| 1 | C | 14 | TRP | CD2-CE3 | -12.91 | 1.21 | 1.40 |
| 1 | A | 106 | LEU | CB-CG | -12.90 | 1.15 | 1.52 |
| 2 | B | 5 | PRO | CA-C | 12.89 | 1.78 | 1.52 |
| 2 | B | 40 | ARG | CD-NE | -12.88 | 1.24 | 1.46 |
| 2 | B | 46 | GLY | C-O | 12.86 | 1.44 | 1.23 |
| 1 | A | 20 | HIS | CE1-NE2 | -12.85 | 1.03 | 1.32 |
| 2 | D | 126 | VAL | CA-CB | 12.84 | 1.81 | 1.54 |
| 2 | B | 66 | LYS | CE-NZ | 12.82 | 1.81 | 1.49 |
| 1 | A | 33 | PHE | CE2-CZ | -12.79 | 1.13 | 1.37 |
| 1 | C | 72 | HIS | CA-C | -12.77 | 1.19 | 1.52 |
| 1 | A | 71 | ALA | CA-C | -12.75 | 1.19 | 1.52 |
| 1 | A | 24 | TYR | CE2-CZ | 12.71 | 1.55 | 1.38 |
| 1 | A | 134 | THR | CB-OG1 | -12.71 | 1.17 | 1.43 |
| 1 | C | 140 | TYR | CG-CD1 | -12.71 | 1.22 | 1.39 |
| 2 | B | 89 | SER | CB-OG | 12.69 | 1.58 | 1.42 |
| 2 | B | 6 | GLU | C-O | 12.67 | 1.47 | 1.23 |
| 2 | D | 21 | ASP | CB-CG | 12.67 | 1.78 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 31 | ARG | CD-NE | 12.67 | 1.68 | 1.46 |
| 2 | D | 44 | SER | CB-OG | -12.66 | 1.25 | 1.42 |
| 2 | B | 71 | PHE | C-N | -12.62 | 1.05 | 1.34 |
| 2 | B | 73 | ASP | CA-C | -12.59 | 1.20 | 1.52 |
| 1 | C | 7 | LYS | CG-CD | 12.56 | 1.95 | 1.52 |
| 1 | A | 140 | TYR | CE1-CZ | -12.50 | 1.22 | 1.38 |
| 2 | B | 2 | HIS | CE1-NE2 | 12.49 | 1.61 | 1.32 |
| 1 | A | 56 | LYS | C-N | 12.49 | 1.55 | 1.33 |
| 2 | D | 50 | THR | N-CA | 12.46 | 1.71 | 1.46 |
| 2 | D | 139 | ASN | CA-CB | -12.45 | 1.20 | 1.53 |
| 2 | B | 8 | LYS | C-O | 12.45 | 1.47 | 1.23 |
| 1 | C | 75 | ASP | N-CA | 12.44 | 1.71 | 1.46 |
| 1 | A | 19 | ALA | C-O | 12.42 | 1.47 | 1.23 |
| 2 | B | 43 | GLU | CA-CB | -12.40 | 1.26 | 1.53 |
| 2 | D | 54 | VAL | CB-CG2 | -12.40 | 1.26 | 1.52 |
| 2 | B | 52 | ASP | CB-CG | 12.37 | 1.77 | 1.51 |
| 1 | C | 118 | THR | CB-CG2 | -12.37 | 1.11 | 1.52 |
| 2 | D | 40 | ARG | C-O | 12.33 | 1.46 | 1.23 |
| 2 | B | 80 | ASN | CG-OD1 | 12.30 | 1.51 | 1.24 |
| 1 | A | 77 | PRO | CA-C | -12.30 | 1.28 | 1.52 |
| 1 | A | 76 | MET | CB-CG | -12.23 | 1.12 | 1.51 |
| 2 | B | 74 | GLY | N-CA | -12.23 | 1.27 | 1.46 |
| 2 | D | 36 | PRO | N-CD | -12.23 | 1.30 | 1.47 |
| 1 | A | 46 | PHE | CB-CG | -12.22 | 1.30 | 1.51 |
| 1 | C | 73 | VAL | CA-CB | 12.21 | 1.80 | 1.54 |
| 2 | D | 77 | HIS | CE1-NE2 | -12.21 | 1.04 | 1.32 |
| 1 | A | 45 | HIS | C-N | 12.21 | 1.62 | 1.34 |
| 1 | C | 4 | PRO | N-CA | -12.21 | 1.26 | 1.47 |
| 1 | A | 59 | GLY | CA-C | -12.20 | 1.32 | 1.51 |
| 1 | C | 140 | TYR | CE2-CZ | -12.17 | 1.22 | 1.38 |
| 2 | D | 73 | ASP | CA-C | -12.16 | 1.21 | 1.52 |
| 2 | B | 2 | HIS | CA-C | 12.14 | 1.84 | 1.52 |
| 1 | A | 24 | TYR | CB-CG | 12.14 | 1.69 | 1.51 |
| 1 | A | 73 | VAL | CA-C | -12.14 | 1.21 | 1.52 |
| 2 | D | 94 | ASP | CG-OD2 | 12.11 | 1.53 | 1.25 |
| 2 | D | 44 | SER | CA-CB | -12.10 | 1.34 | 1.52 |
| 2 | D | 117 | HIS | ND1-CE1 | 12.09 | 1.65 | 1.34 |
| 2 | B | 74 | GLY | CA-C | -12.06 | 1.32 | 1.51 |
| 2 | D | 63 | HIS | CA-CB | -12.05 | 1.27 | 1.53 |
| 1 | A | 27 | GLU | CG-CD | 12.04 | 1.70 | 1.51 |
| 2 | B | 65 | LYS | CA-CB | 12.03 | 1.80 | 1.53 |
| 2 | D | 18 | VAL | N-CA | 12.03 | 1.70 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 61 | LYS | CG-CD | 12.01 | 1.93 | 1.52 |
| 1 | A | 52 | SER | CA-C | -12.00 | 1.21 | 1.52 |
| 1 | C | 61 | LYS | CD-CE | 11.97 | 1.81 | 1.51 |
| 2 | B | 94 | ASP | CG-OD2 | -11.95 | 0.97 | 1.25 |
| 1 | C | 115 | ALA | CA-C | -11.94 | 1.21 | 1.52 |
| 1 | C | 8 | THR | CA-CB | 11.94 | 1.84 | 1.53 |
| 2 | D | 146 | HIS | CE1-NE2 | 11.93 | 1.60 | 1.32 |
| 2 | D | 104 | ARG | CZ-NH1 | 11.92 | 1.48 | 1.33 |
| 2 | B | 63 | HIS | CG-ND1 | 11.89 | 1.65 | 1.38 |
| 2 | D | 7 | GLU | CD-OE2 | 11.86 | 1.38 | 1.25 |
| 1 | C | 7 | LYS | CD-CE | -11.86 | 1.21 | 1.51 |
| 1 | C | 20 | HIS | CG-ND1 | 11.84 | 1.64 | 1.38 |
| 1 | A | 12 | ALA | C-O | 11.82 | 1.45 | 1.23 |
| 2 | D | 145 | TYR | CE2-CZ | -11.82 | 1.23 | 1.38 |
| 1 | C | 1 | VAL | CA-C | 11.80 | 1.83 | 1.52 |
| 2 | D | 79 | ASP | CA-C | 11.80 | 1.83 | 1.52 |
| 1 | C | 18 | GLY | C-O | 11.79 | 1.42 | 1.23 |
| 2 | B | 45 | PHE | CD1-CE1 | 11.78 | 1.62 | 1.39 |
| 1 | A | 137 | THR | CB-OG1 | 11.78 | 1.66 | 1.43 |
| 1 | C | 72 | HIS | C-O | 11.76 | 1.45 | 1.23 |
| 2 | D | 35 | TYR | CG-CD2 | -11.76 | 1.23 | 1.39 |
| 1 | A | 5 | ALA | CA-CB | 11.74 | 1.77 | 1.52 |
| 2 | D | 17 | LYS | C-N | 11.73 | 1.61 | 1.34 |
| 1 | C | 20 | HIS | CB-CG | 11.70 | 1.71 | 1.50 |
| 2 | D | 121 | GLU | CA-CB | 11.69 | 1.79 | 1.53 |
| 1 | C | 7 | LYS | CE-NZ | -11.69 | 1.19 | 1.49 |
| 2 | D | 11 | VAL | CB-CG1 | -11.68 | 1.28 | 1.52 |
| 1 | C | 74 | ASP | CG-OD1 | 11.64 | 1.52 | 1.25 |
| 2 | D | 22 | GLU | CA-C | 11.58 | 1.83 | 1.52 |
| 2 | D | 47 | ASP | CB-CG | 11.55 | 1.76 | 1.51 |
| 2 | D | 63 | HIS | ND1-CE1 | 11.54 | 1.63 | 1.34 |
| 2 | D | 40 | ARG | CB-CG | -11.50 | 1.21 | 1.52 |
| 2 | D | 82 | LYS | C-N | 11.45 | 1.53 | 1.33 |
| 1 | A | 14 | TRP | CZ2-CH2 | -11.43 | 1.15 | 1.37 |
| 1 | C | 133 | SER | C-O | 11.43 | 1.45 | 1.23 |
| 2 | B | 118 | PHE | CD2-CE2 | -11.43 | 1.16 | 1.39 |
| 2 | B | 104 | ARG | CD-NE | 11.41 | 1.65 | 1.46 |
| 2 | D | 131 | GLN | CG-CD | 11.41 | 1.77 | 1.51 |
| 2 | D | 52 | ASP | CB-CG | 11.40 | 1.75 | 1.51 |
| 2 | B | 142 | ALA | CA-C | 11.39 | 1.82 | 1.52 |
| 2 | B | 46 | GLY | C-N | -11.37 | 1.07 | 1.34 |
| 2 | B | 90 | GLU | CB-CG | -11.35 | 1.30 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 15 | GLY | CA-C | 11.35 | 1.70 | 1.51 |
| 1 | A | 64 | ASP | CG-OD1 | 11.35 | 1.51 | 1.25 |
| 1 | C | 71 | ALA | CA-CB | -11.34 | 1.28 | 1.52 |
| 1 | C | 116 | GLU | CD-OE1 | -11.32 | 1.13 | 1.25 |
| 2 | B | 1 | VAL | N-CA | 11.31 | 1.69 | 1.46 |
| 1 | C | 87 | HIS | CA-C | 11.31 | 1.82 | 1.52 |
| 1 | C | 119 | PRO | N-CD | 11.31 | 1.63 | 1.47 |
| 1 | A | 71 | ALA | C-O | 11.28 | 1.44 | 1.23 |
| 2 | D | 130 | TYR | CD1-CE1 | 11.28 | 1.56 | 1.39 |
| 2 | D | 78 | LEU | CA-CB | 11.27 | 1.79 | 1.53 |
| 2 | B | 145 | TYR | CA-CB | -11.27 | 1.29 | 1.53 |
| 2 | D | 78 | LEU | C-O | -11.26 | 1.01 | 1.23 |
| 1 | C | 78 | ASN | CB-CG | 11.25 | 1.76 | 1.51 |
| 1 | C | 16 | LYS | CA-C | 11.23 | 1.82 | 1.52 |
| 1 | A | 7 | LYS | C-N | 11.23 | 1.59 | 1.34 |
| 2 | B | 69 | GLY | N-CA | -11.22 | 1.29 | 1.46 |
| 2 | D | 12 | THR | N-CA | 11.22 | 1.68 | 1.46 |
| 1 | C | 72 | HIS | ND1-CE1 | -11.22 | 1.06 | 1.34 |
| 1 | C | 24 | TYR | CD2-CE2 | 11.18 | 1.56 | 1.39 |
| 1 | A | 4 | PRO | C-N | 11.18 | 1.59 | 1.34 |
| 1 | A | 29 | LEU | CA-CB | 11.18 | 1.79 | 1.53 |
| 1 | C | 24 | TYR | CG-CD1 | 11.17 | 1.53 | 1.39 |
| 2 | D | 19 | ASN | C-O | 11.15 | 1.44 | 1.23 |
| 2 | B | 81 | LEU | N-CA | 11.14 | 1.68 | 1.46 |
| 2 | B | 121 | GLU | CD-OE2 | -11.14 | 1.13 | 1.25 |
| 1 | C | 11 | LYS | CA-C | -11.13 | 1.24 | 1.52 |
| 2 | D | 4 | THR | CA-CB | 11.10 | 1.82 | 1.53 |
| 2 | B | 79 | ASP | C-O | -11.10 | 1.02 | 1.23 |
| 1 | A | 72 | HIS | CA-CB | 11.10 | 1.78 | 1.53 |
| 2 | D | 143 | HIS | ND1-CE1 | 11.08 | 1.62 | 1.34 |
| 1 | C | 90 | LYS | CG-CD | 11.07 | 1.90 | 1.52 |
| 2 | D | 6 | GLU | C-O | -11.07 | 1.02 | 1.23 |
| 2 | D | 7 | GLU | CG-CD | -11.07 | 1.35 | 1.51 |
| 1 | C | 10 | VAL | CA-C | 11.05 | 1.81 | 1.52 |
| 2 | D | 102 | ASN | C-O | 11.03 | 1.44 | 1.23 |
| 2 | D | 8 | LYS | N-CA | 11.02 | 1.68 | 1.46 |
| 1 | A | 128 | PHE | CG-CD2 | -11.01 | 1.22 | 1.38 |
| 2 | D | 73 | ASP | CB-CG | -10.99 | 1.28 | 1.51 |
| 2 | B | 118 | PHE | CG-CD2 | 10.98 | 1.55 | 1.38 |
| 1 | C | 128 | PHE | CG-CD2 | -10.98 | 1.22 | 1.38 |
| 1 | C | 75 | ASP | C-N | 10.96 | 1.59 | 1.34 |
| 1 | C | 19 | ALA | C-O | 10.96 | 1.44 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 26 | GLU | CB-CG | 10.96 | 1.73 | 1.52 |
| 2 | D | 18 | VAL | CB-CG1 | -10.95 | 1.29 | 1.52 |
| 1 | A | 33 | PHE | CG-CD2 | 10.92 | 1.55 | 1.38 |
| 1 | C | 70 | VAL | N-CA | 10.89 | 1.68 | 1.46 |
| 2 | D | 94 | ASP | N-CA | 10.89 | 1.68 | 1.46 |
| 2 | D | 82 | LYS | CG-CD | 10.85 | 1.89 | 1.52 |
| 2 | D | 45 | PHE | CD1-CE1 | 10.83 | 1.60 | 1.39 |
| 2 | D | 4 | THR | N-CA | -10.82 | 1.24 | 1.46 |
| 2 | D | 53 | ALA | CA-CB | -10.82 | 1.29 | 1.52 |
| 2 | B | 49 | SER | N-CA | 10.79 | 1.68 | 1.46 |
| 1 | A | 141 | ARG | NE-CZ | 10.78 | 1.47 | 1.33 |
| 1 | A | 112 | HIS | ND1-CE1 | 10.77 | 1.61 | 1.34 |
| 2 | D | 40 | ARG | NE-CZ | 10.77 | 1.47 | 1.33 |
| 1 | C | 20 | HIS | CE1-NE2 | 10.73 | 1.57 | 1.32 |
| 1 | C | 49 | SER | C-N | 10.72 | 1.58 | 1.34 |
| 2 | B | 2 | HIS | C-O | 10.71 | 1.43 | 1.23 |
| 1 | A | 58 | HIS | CB-CG | 10.69 | 1.69 | 1.50 |
| 2 | D | 144 | LYS | CA-CB | -10.69 | 1.30 | 1.53 |
| 2 | B | 7 | GLU | CD-OE2 | 10.68 | 1.37 | 1.25 |
| 1 | C | 15 | GLY | C-N | -10.68 | 1.09 | 1.34 |
| 1 | A | 49 | SER | C-N | 10.66 | 1.58 | 1.34 |
| 1 | C | 38 | THR | CA-CB | 10.65 | 1.81 | 1.53 |
| 2 | B | 80 | ASN | CB-CG | 10.65 | 1.75 | 1.51 |
| 2 | B | 22 | GLU | CB-CG | -10.61 | 1.31 | 1.52 |
| 2 | D | 101 | GLU | CB-CG | 10.61 | 1.72 | 1.52 |
| 2 | D | 93 | CYS | CB-SG | 10.60 | 2.00 | 1.82 |
| 1 | C | 24 | TYR | CE1-CZ | -10.59 | 1.24 | 1.38 |
| 1 | C | 114 | PRO | CA-CB | -10.58 | 1.32 | 1.53 |
| 2 | B | 47 | ASP | N-CA | 10.56 | 1.67 | 1.46 |
| 2 | D | 46 | GLY | C-O | 10.56 | 1.40 | 1.23 |
| 2 | D | 80 | ASN | CB-CG | -10.55 | 1.26 | 1.51 |
| 1 | C | 117 | PHE | CD1-CE1 | 10.54 | 1.60 | 1.39 |
| 2 | D | 40 | ARG | CZ-NH2 | 10.54 | 1.46 | 1.33 |
| 2 | B | 143 | HIS | CG-CD2 | -10.53 | 1.17 | 1.35 |
| 2 | D | 40 | ARG | CD-NE | -10.53 | 1.28 | 1.46 |
| 1 | A | 89 | HIS | CG-CD2 | 10.52 | 1.53 | 1.35 |
| 2 | D | 45 | PHE | CG-CD2 | -10.49 | 1.23 | 1.38 |
| 1 | A | 49 | SER | CA-CB | -10.49 | 1.37 | 1.52 |
| 2 | B | 61 | LYS | CB-CG | -10.49 | 1.24 | 1.52 |
| 1 | C | 137 | THR | CB-OG1 | -10.47 | 1.22 | 1.43 |
| 2 | B | 73 | ASP | CG-OD2 | -10.47 | 1.01 | 1.25 |
| 1 | C | 46 | PHE | CE2-CZ | 10.46 | 1.57 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | B | 80 | ASN | CA-C | 10.46 | 1.80 | 1.52 |
| 2 | D | 63 | HIS | CB-CG | 10.45 | 1.68 | 1.50 |
| 2 | B | 61 | LYS | CE-NZ | 10.41 | 1.75 | 1.49 |
| 2 | B | 143 | HIS | CE1-NE2 | 10.41 | 1.56 | 1.32 |
| 1 | C | 71 | ALA | N-CA | 10.41 | 1.67 | 1.46 |
| 2 | D | 113 | VAL | CB-CG2 | 10.38 | 1.74 | 1.52 |
| 1 | A | 20 | HIS | CG-CD2 | 10.36 | 1.53 | 1.35 |
| 1 | C | 50 | HIS | CB-CG | -10.33 | 1.31 | 1.50 |
| 2 | D | 60 | VAL | N-CA | 10.32 | 1.67 | 1.46 |
| 2 | D | 136 | GLY | N-CA | -10.31 | 1.30 | 1.46 |
| 2 | D | 67 | VAL | CA-CB | 10.31 | 1.76 | 1.54 |
| 1 | C | 112 | HIS | CB-CG | -10.31 | 1.31 | 1.50 |
| 2 | B | 3 | LEU | CA-CB | 10.30 | 1.77 | 1.53 |
| 1 | A | 83 | LEU | CB-CG | -10.30 | 1.22 | 1.52 |
| 2 | D | 78 | LEU | N-CA | -10.26 | 1.25 | 1.46 |
| 1 | A | 36 | PHE | CG-CD2 | 10.25 | 1.54 | 1.38 |
| 2 | B | 12 | THR | CB-OG1 | -10.25 | 1.22 | 1.43 |
| 2 | D | 19 | ASN | CA-C | -10.25 | 1.26 | 1.52 |
| 1 | A | 61 | LYS | CE-NZ | 10.23 | 1.74 | 1.49 |
| 1 | C | 2 | LEU | CA-C | 10.23 | 1.79 | 1.52 |
| 1 | A | 77 | PRO | C-O | 10.21 | 1.43 | 1.23 |
| 1 | C | 24 | TYR | CZ-OH | 10.20 | 1.55 | 1.37 |
| 2 | D | 58 | PRO | C-O | 10.19 | 1.43 | 1.23 |
| 2 | B | 46 | GLY | CA-C | 10.19 | 1.68 | 1.51 |
| 2 | B | 41 | PHE | CG-CD2 | 10.18 | 1.54 | 1.38 |
| 1 | A | 3 | SER | CB-OG | -10.17 | 1.29 | 1.42 |
| 1 | C | 92 | ARG | C-O | -10.15 | 1.04 | 1.23 |
| 2 | B | 51 | PRO | N-CD | 10.15 | 1.62 | 1.47 |
| 2 | D | 84 | THR | CB-OG1 | -10.14 | 1.23 | 1.43 |
| 1 | A | 4 | PRO | CA-CB | 10.11 | 1.73 | 1.53 |
| 1 | C | 127 | LYS | C-O | 10.11 | 1.42 | 1.23 |
| 2 | D | 61 | LYS | CE-NZ | -10.09 | 1.23 | 1.49 |
| 2 | D | 58 | PRO | CB-CG | 10.08 | 2.00 | 1.50 |
| 1 | A | 72 | HIS | CD2-NE2 | 10.06 | 1.63 | 1.42 |
| 1 | C | 41 | THR | C-O | 10.04 | 1.42 | 1.23 |
| 1 | C | 14 | TRP | NE1-CE2 | -10.03 | 1.24 | 1.37 |
| 1 | A | 141 | ARG | CB-CG | 10.02 | 1.79 | 1.52 |
| 2 | B | 4 | THR | CA-C | -9.97 | 1.27 | 1.52 |
| 2 | D | 42 | PHE | CE2-CZ | 9.96 | 1.56 | 1.37 |
| 1 | C | 128 | PHE | CB-CG | 9.95 | 1.68 | 1.51 |
| 1 | C | 17 | VAL | CB-CG1 | -9.94 | 1.31 | 1.52 |
| 2 | B | 113 | VAL | C-O | 9.94 | 1.42 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 17 | VAL | C-N | 9.94 | 1.50 | 1.33 |
| 2 | D | 8 | LYS | CB-CG | 9.94 | 1.79 | 1.52 |
| 1 | A | 122 | HIS | N-CA | 9.93 | 1.66 | 1.46 |
| 2 | D | 77 | HIS | CA-CB | 9.92 | 1.75 | 1.53 |
| 2 | D | 37 | TRP | CE2-CZ2 | 9.92 | 1.56 | 1.39 |
| 1 | A | 33 | PHE | CG-CD1 | -9.90 | 1.24 | 1.38 |
| 1 | C | 47 | ASP | CB-CG | 9.88 | 1.72 | 1.51 |
| 1 | C | 50 | HIS | CE1-NE2 | 9.87 | 1.55 | 1.32 |
| 1 | A | 140 | TYR | CG-CD1 | 9.86 | 1.51 | 1.39 |
| 1 | A | 40 | LYS | CA-CB | 9.86 | 1.75 | 1.53 |
| 1 | C | 44 | PRO | C-N | -9.85 | 1.11 | 1.34 |
| 2 | B | 103 | PHE | CE1-CZ | -9.84 | 1.18 | 1.37 |
| 1 | A | 140 | TYR | CZ-OH | -9.84 | 1.21 | 1.37 |
| 1 | C | 51 | GLY | N-CA | -9.84 | 1.31 | 1.46 |
| 1 | A | 1 | VAL | CB-CG1 | -9.83 | 1.32 | 1.52 |
| 2 | B | 17 | LYS | C-O | 9.83 | 1.42 | 1.23 |
| 2 | B | 132 | LYS | CA-CB | -9.82 | 1.32 | 1.53 |
| 1 | C | 36 | PHE | CG-CD2 | 9.81 | 1.53 | 1.38 |
| 2 | B | 10 | ALA | CA-C | 9.79 | 1.78 | 1.52 |
| 1 | C | 46 | PHE | CE1-CZ | -9.78 | 1.18 | 1.37 |
| 2 | D | 1 | VAL | CB-CG1 | 9.76 | 1.73 | 1.52 |
| 1 | A | 90 | LYS | CG-CD | -9.75 | 1.19 | 1.52 |
| 2 | B | 126 | VAL | C-O | 9.74 | 1.41 | 1.23 |
| 2 | D | 139 | ASN | CG-ND2 | 9.72 | 1.57 | 1.32 |
| 1 | A | 44 | PRO | N-CD | -9.71 | 1.34 | 1.47 |
| 2 | B | 104 | ARG | CG-CD | 9.70 | 1.76 | 1.51 |
| 1 | C | 138 | SER | CB-OG | -9.69 | 1.29 | 1.42 |
| 2 | B | 50 | THR | CA-CB | -9.68 | 1.28 | 1.53 |
| 1 | A | 72 | HIS | CB-CG | -9.67 | 1.32 | 1.50 |
| 1 | A | 33 | PHE | CD2-CE2 | 9.64 | 1.58 | 1.39 |
| 2 | B | 73 | ASP | CB-CG | 9.64 | 1.72 | 1.51 |
| 2 | D | 4 | THR | C-O | 9.60 | 1.41 | 1.23 |
| 2 | B | 118 | PHE | CB-CG | -9.59 | 1.35 | 1.51 |
| 1 | C | 44 | PRO | CA-CB | 9.59 | 1.72 | 1.53 |
| 2 | D | 53 | ALA | C-N | 9.59 | 1.56 | 1.34 |
| 1 | C | 18 | GLY | CA-C | -9.59 | 1.36 | 1.51 |
| 1 | A | 2 | LEU | CA-C | 9.58 | 1.77 | 1.52 |
| 2 | B | 41 | PHE | CA-C | 9.57 | 1.77 | 1.52 |
| 1 | A | 17 | VAL | N-CA | -9.56 | 1.27 | 1.46 |
| 2 | B | 42 | PHE | CE1-CZ | -9.56 | 1.19 | 1.37 |
| 2 | B | 82 | LYS | CA-C | -9.55 | 1.28 | 1.52 |
| 1 | C | 56 | LYS | CE-NZ | 9.53 | 1.72 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 8 | LYS | CA-CB | 9.51 | 1.74 | 1.53 |
| 1 | C | 46 | PHE | CB-CG | -9.50 | 1.35 | 1.51 |
| 2 | B | 73 | ASP | CG-OD1 | 9.48 | 1.47 | 1.25 |
| 2 | D | 46 | GLY | N-CA | -9.48 | 1.31 | 1.46 |
| 1 | C | 20 | HIS | CD2-NE2 | -9.48 | 1.17 | 1.38 |
| 2 | B | 2 | HIS | C-N | -9.47 | 1.12 | 1.34 |
| 2 | B | 6 | GLU | CA-C | 9.46 | 1.77 | 1.52 |
| 2 | D | 72 | SER | CA-CB | 9.45 | 1.67 | 1.52 |
| 1 | A | 77 | PRO | CA-CB | 9.43 | 1.72 | 1.53 |
| 1 | C | 76 | MET | CG-SD | 9.40 | 2.05 | 1.81 |
| 2 | B | 44 | SER | C-N | 9.38 | 1.55 | 1.34 |
| 1 | C | 128 | PHE | CD2-CE2 | 9.38 | 1.58 | 1.39 |
| 1 | C | 52 | SER | CA-C | -9.38 | 1.28 | 1.52 |
| 1 | A | 137 | THR | N-CA | 9.38 | 1.65 | 1.46 |
| 2 | D | 83 | GLY | C-N | 9.37 | 1.55 | 1.34 |
| 1 | C | 132 | VAL | CB-CG2 | 9.35 | 1.72 | 1.52 |
| 2 | D | 15 | TRP | CZ3-CH2 | 9.33 | 1.54 | 1.40 |
| 2 | D | 36 | PRO | N-CA | 9.32 | 1.63 | 1.47 |
| 1 | A | 14 | TRP | CD1-NE1 | 9.30 | 1.53 | 1.38 |
| 1 | C | 71 | ALA | CA-C | -9.28 | 1.28 | 1.52 |
| 1 | A | 46 | PHE | CE1-CZ | 9.26 | 1.54 | 1.37 |
| 1 | C | 81 | SER | CB-OG | 9.26 | 1.54 | 1.42 |
| 2 | B | 83 | GLY | N-CA | 9.25 | 1.59 | 1.46 |
| 2 | D | 77 | HIS | C-N | 9.24 | 1.55 | 1.34 |
| 1 | C | 47 | ASP | CG-OD1 | -9.23 | 1.04 | 1.25 |
| 1 | A | 90 | LYS | N-CA | -9.23 | 1.27 | 1.46 |
| 2 | D | 19 | ASN | CB-CG | 9.23 | 1.72 | 1.51 |
| 2 | B | 146 | HIS | N-CA | 9.22 | 1.64 | 1.46 |
| 1 | C | 61 | LYS | CA-C | 9.22 | 1.76 | 1.52 |
| 2 | B | 143 | HIS | CA-C | 9.21 | 1.76 | 1.52 |
| 1 | A | 50 | HIS | CB-CG | -9.21 | 1.33 | 1.50 |
| 2 | D | 93 | CYS | C-O | -9.19 | 1.05 | 1.23 |
| 1 | C | 22 | GLY | C-O | 9.19 | 1.38 | 1.23 |
| 2 | B | 51 | PRO | C-O | 9.18 | 1.41 | 1.23 |
| 1 | A | 104 | CYS | N-CA | 9.17 | 1.64 | 1.46 |
| 2 | B | 63 | HIS | ND1-CE1 | 9.16 | 1.57 | 1.34 |
| 1 | C | 12 | ALA | C-N | 9.16 | 1.55 | 1.34 |
| 1 | C | 43 | PHE | CG-CD2 | 9.16 | 1.52 | 1.38 |
| 1 | C | 38 | THR | CB-OG1 | 9.16 | 1.61 | 1.43 |
| 1 | C | 103 | HIS | CG-ND1 | 9.14 | 1.58 | 1.38 |
| 2 | B | 21 | ASP | CG-OD2 | 9.12 | 1.46 | 1.25 |
| 2 | D | 42 | PHE | CE1-CZ | -9.12 | 1.20 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 81 | SER | CA-CB | 9.12 | 1.66 | 1.52 |
| 1 | A | 58 | HIS | CA-C | 9.11 | 1.76 | 1.52 |
| 1 | C | 69 | ALA | N-CA | 9.11 | 1.64 | 1.46 |
| 2 | D | 53 | ALA | CA-C | 9.11 | 1.76 | 1.52 |
| 2 | D | 15 | TRP | NE1-CE2 | 9.10 | 1.49 | 1.37 |
| 1 | C | 42 | TYR | CG-CD1 | 9.09 | 1.50 | 1.39 |
| 1 | A | 86 | LEU | CB-CG | -9.07 | 1.26 | 1.52 |
| 2 | B | 37 | TRP | NE1-CE2 | -9.05 | 1.25 | 1.37 |
| 2 | D | 137 | VAL | CA-CB | 9.04 | 1.73 | 1.54 |
| 1 | C | 95 | PRO | CA-C | -9.04 | 1.34 | 1.52 |
| 1 | A | 67 | THR | C-O | 9.02 | 1.40 | 1.23 |
| 2 | B | 40 | ARG | C-N | -9.02 | 1.13 | 1.34 |
| 2 | D | 49 | SER | C-O | 9.02 | 1.40 | 1.23 |
| 1 | A | 88 | ALA | C-O | -9.01 | 1.06 | 1.23 |
| 2 | B | 117 | HIS | CE1-NE2 | 9.01 | 1.53 | 1.32 |
| 2 | B | 7 | GLU | CG-CD | -8.99 | 1.38 | 1.51 |
| 1 | C | 72 | HIS | N-CA | -8.98 | 1.28 | 1.46 |
| 2 | B | 18 | VAL | CB-CG2 | 8.98 | 1.71 | 1.52 |
| 1 | C | 14 | TRP | CZ2-CH2 | -8.98 | 1.20 | 1.37 |
| 2 | D | 59 | LYS | CA-C | 8.97 | 1.76 | 1.52 |
| 2 | B | 77 | HIS | CB-CG | 8.97 | 1.66 | 1.50 |
| 2 | D | 79 | ASP | CA-CB | 8.96 | 1.73 | 1.53 |
| 1 | C | 48 | LEU | C-O | 8.93 | 1.40 | 1.23 |
| 1 | C | 16 | LYS | CE-NZ | 8.92 | 1.71 | 1.49 |
| 2 | D | 92 | HIS | CA-C | 8.91 | 1.76 | 1.52 |
| 2 | B | 26 | GLU | CG-CD | -8.90 | 1.38 | 1.51 |
| 1 | C | 131 | SER | CA-C | 8.90 | 1.76 | 1.52 |
| 1 | C | 56 | LYS | CA-C | -8.89 | 1.29 | 1.52 |
| 2 | D | 146 | HIS | C-OXT | 8.88 | 1.40 | 1.23 |
| 1 | C | 99 | LYS | CG-CD | 8.87 | 1.82 | 1.52 |
| 1 | C | 141 | ARG | CZ-NH2 | 8.86 | 1.44 | 1.33 |
| 2 | D | 5 | PRO | CB-CG | -8.86 | 1.05 | 1.50 |
| 1 | C | 21 | ALA | C-N | -8.85 | 1.17 | 1.33 |
| 2 | D | 97 | HIS | CB-CG | 8.85 | 1.66 | 1.50 |
| 1 | C | 77 | PRO | CA-C | -8.84 | 1.35 | 1.52 |
| 1 | C | 126 | ASP | CB-CG | 8.84 | 1.70 | 1.51 |
| 1 | C | 42 | TYR | CE2-CZ | 8.82 | 1.50 | 1.38 |
| 1 | C | 57 | GLY | C-O | 8.82 | 1.37 | 1.23 |
| 2 | B | 94 | ASP | CB-CG | 8.82 | 1.70 | 1.51 |
| 2 | D | 10 | ALA | CA-C | 8.82 | 1.75 | 1.52 |
| 1 | C | 113 | LEU | CA-CB | -8.82 | 1.33 | 1.53 |
| 1 | C | 115 | ALA | CA-CB | 8.81 | 1.71 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 87 | HIS | CA-C | 8.80 | 1.75 | 1.52 |
| 1 | A | 4 | PRO | N-CA | -8.79 | 1.32 | 1.47 |
| 1 | A | 85 | ASP | N-CA | 8.79 | 1.64 | 1.46 |
| 1 | A | 47 | ASP | C-N | -8.78 | 1.13 | 1.34 |
| 1 | A | 73 | VAL | CA-CB | -8.78 | 1.36 | 1.54 |
| 1 | A | 138 | SER | CB-OG | -8.74 | 1.30 | 1.42 |
| 1 | A | 33 | PHE | CA-C | -8.74 | 1.30 | 1.52 |
| 2 | D | 143 | HIS | CB-CG | -8.73 | 1.34 | 1.50 |
| 1 | A | 57 | GLY | CA-C | 8.73 | 1.65 | 1.51 |
| 1 | C | 68 | ASN | CG-ND2 | 8.73 | 1.54 | 1.32 |
| 2 | D | 71 | PHE | N-CA | 8.72 | 1.63 | 1.46 |
| 2 | D | 12 | THR | C-O | 8.71 | 1.40 | 1.23 |
| 1 | A | 78 | ASN | C-O | 8.71 | 1.39 | 1.23 |
| 2 | D | 61 | LYS | CD-CE | 8.71 | 1.73 | 1.51 |
| 1 | A | 68 | ASN | C-O | 8.70 | 1.39 | 1.23 |
| 2 | B | 50 | THR | N-CA | -8.69 | 1.28 | 1.46 |
| 2 | D | 4 | THR | CB-CG2 | -8.69 | 1.23 | 1.52 |
| 1 | A | 45 | HIS | CE1-NE2 | 8.69 | 1.52 | 1.32 |
| 1 | C | 46 | PHE | C-N | 8.68 | 1.54 | 1.34 |
| 2 | B | 73 | ASP | C-O | 8.68 | 1.39 | 1.23 |
| 2 | D | 20 | VAL | N-CA | 8.67 | 1.63 | 1.46 |
| 1 | C | 85 | ASP | CG-OD1 | -8.67 | 1.05 | 1.25 |
| 1 | C | 115 | ALA | N-CA | -8.67 | 1.29 | 1.46 |
| 2 | D | 8 | LYS | CG-CD | -8.66 | 1.23 | 1.52 |
| 2 | D | 82 | LYS | CB-CG | -8.66 | 1.29 | 1.52 |
| 1 | A | 27 | GLU | CD-OE1 | -8.66 | 1.16 | 1.25 |
| 1 | A | 105 | LEU | CG-CD2 | -8.65 | 1.19 | 1.51 |
| 2 | D | 121 | GLU | N-CA | -8.65 | 1.29 | 1.46 |
| 1 | A | 29 | LEU | N-CA | 8.64 | 1.63 | 1.46 |
| 1 | A | 8 | THR | CB-OG1 | -8.64 | 1.25 | 1.43 |
| 2 | B | 145 | TYR | CA-C | 8.61 | 1.75 | 1.52 |
| 2 | B | 44 | SER | CA-CB | -8.61 | 1.40 | 1.52 |
| 2 | D | 146 | HIS | CA-CB | 8.60 | 1.72 | 1.53 |
| 2 | D | 6 | GLU | CA-CB | 8.59 | 1.72 | 1.53 |
| 1 | A | 37 | PRO | N-CA | 8.58 | 1.61 | 1.47 |
| 2 | D | 80 | ASN | C-O | -8.58 | 1.07 | 1.23 |
| 2 | D | 85 | PHE | N-CA | 8.57 | 1.63 | 1.46 |
| 1 | C | 16 | LYS | CG-CD | 8.57 | 1.81 | 1.52 |
| 1 | C | 118 | THR | CA-CB | 8.57 | 1.75 | 1.53 |
| 2 | B | 69 | GLY | C-N | 8.56 | 1.53 | 1.34 |
| 2 | D | 23 | VAL | CB-CG1 | -8.55 | 1.34 | 1.52 |
| 1 | A | 42 | TYR | CE1-CZ | -8.53 | 1.27 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 20 | VAL | CA-C | -8.53 | 1.30 | 1.52 |
| 2 | B | 47 | ASP | CA-C | 8.52 | 1.75 | 1.52 |
| 1 | C | 54 | GLN | CA-C | 8.51 | 1.75 | 1.52 |
| 2 | D | 43 | GLU | C-O | -8.51 | 1.07 | 1.23 |
| 1 | A | 10 | VAL | CB-CG2 | -8.50 | 1.34 | 1.52 |
| 1 | C | 95 | PRO | N-CA | 8.50 | 1.61 | 1.47 |
| 2 | B | 10 | ALA | N-CA | -8.49 | 1.29 | 1.46 |
| 2 | D | 7 | GLU | CA-C | 8.49 | 1.75 | 1.52 |
| 1 | A | 62 | VAL | CA-C | 8.48 | 1.75 | 1.52 |
| 2 | D | 145 | TYR | CD2-CE2 | 8.47 | 1.52 | 1.39 |
| 1 | A | 46 | PHE | CD2-CE2 | 8.47 | 1.56 | 1.39 |
| 1 | A | 30 | GLU | CB-CG | -8.46 | 1.36 | 1.52 |
| 1 | C | 26 | ALA | C-N | 8.45 | 1.53 | 1.34 |
| 2 | B | 42 | PHE | CB-CG | -8.45 | 1.36 | 1.51 |
| 1 | C | 47 | ASP | CA-CB | 8.44 | 1.72 | 1.53 |
| 2 | B | 75 | LEU | CB-CG | -8.43 | 1.28 | 1.52 |
| 2 | D | 125 | PRO | N-CA | -8.43 | 1.32 | 1.47 |
| 2 | B | 95 | LYS | CA-CB | 8.41 | 1.72 | 1.53 |
| 2 | D | 123 | THR | CB-CG2 | 8.39 | 1.80 | 1.52 |
| 2 | B | 134 | VAL | N-CA | -8.38 | 1.29 | 1.46 |
| 1 | C | 137 | THR | CA-C | 8.38 | 1.74 | 1.52 |
| 1 | C | 59 | GLY | N-CA | -8.38 | 1.33 | 1.46 |
| 1 | C | 131 | SER | N-CA | 8.38 | 1.63 | 1.46 |
| 1 | A | 3 | SER | N-CA | 8.36 | 1.63 | 1.46 |
| 2 | D | 146 | HIS | N-CA | 8.36 | 1.63 | 1.46 |
| 1 | C | 70 | VAL | CA-C | 8.34 | 1.74 | 1.52 |
| 2 | B | 54 | VAL | CA-C | -8.33 | 1.31 | 1.52 |
| 1 | A | 141 | ARG | CA-CB | -8.32 | 1.35 | 1.53 |
| 1 | C | 140 | TYR | CG-CD2 | 8.30 | 1.50 | 1.39 |
| 2 | D | 70 | ALA | C-O | 8.30 | 1.39 | 1.23 |
| 2 | D | 30 | ARG | CZ-NH2 | 8.29 | 1.43 | 1.33 |
| 1 | A | 21 | ALA | C-O | -8.28 | 1.07 | 1.23 |
| 2 | B | 41 | PHE | C-O | -8.28 | 1.07 | 1.23 |
| 2 | B | 69 | GLY | CA-C | 8.27 | 1.65 | 1.51 |
| 1 | C | 114 | PRO | N-CD | 8.27 | 1.59 | 1.47 |
| 2 | D | 41 | PHE | CG-CD2 | -8.25 | 1.26 | 1.38 |
| 1 | C | 50 | HIS | CA-CB | 8.25 | 1.72 | 1.53 |
| 2 | B | 52 | ASP | CG-OD1 | -8.24 | 1.06 | 1.25 |
| 2 | B | 37 | TRP | CG-CD1 | 8.24 | 1.48 | 1.36 |
| 2 | B | 49 | SER | CA-C | -8.24 | 1.31 | 1.52 |
| 2 | B | 95 | LYS | CA-C | -8.24 | 1.31 | 1.52 |
| 1 | A | 47 | ASP | CA-C | 8.23 | 1.74 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 110 | LEU | C-N | 8.23 | 1.52 | 1.34 |
| 1 | A | 70 | VAL | CA-CB | -8.22 | 1.37 | 1.54 |
| 2 | D | 48 | LEU | CA-CB | -8.22 | 1.34 | 1.53 |
| 1 | C | 40 | LYS | CE-NZ | 8.22 | 1.69 | 1.49 |
| 2 | B | 94 | ASP | C-O | 8.21 | 1.39 | 1.23 |
| 1 | A | 134 | THR | CA-C | -8.20 | 1.31 | 1.52 |
| 2 | B | 93 | CYS | CB-SG | 8.20 | 1.96 | 1.82 |
| 2 | B | 20 | VAL | C-O | 8.20 | 1.39 | 1.23 |
| 2 | D | 14 | LEU | CA-CB | 8.19 | 1.72 | 1.53 |
| 2 | D | 94 | ASP | CG-OD1 | -8.18 | 1.06 | 1.25 |
| 2 | B | 84 | THR | CB-OG1 | 8.17 | 1.59 | 1.43 |
| 1 | C | 96 | VAL | CB-CG2 | -8.17 | 1.35 | 1.52 |
| 1 | C | 14 | TRP | C-O | 8.16 | 1.38 | 1.23 |
| 2 | B | 84 | THR | CB-CG2 | -8.15 | 1.25 | 1.52 |
| 2 | B | 77 | HIS | ND1-CE1 | -8.15 | 1.14 | 1.34 |
| 2 | D | 11 | VAL | CB-CG2 | 8.15 | 1.70 | 1.52 |
| 2 | D | 13 | ALA | C-N | 8.15 | 1.52 | 1.34 |
| 2 | B | 142 | ALA | C-N | -8.13 | 1.15 | 1.34 |
| 2 | B | 69 | GLY | C-O | -8.12 | 1.10 | 1.23 |
| 2 | D | 55 | MET | CB-CG | -8.10 | 1.25 | 1.51 |
| 1 | A | 78 | ASN | CG-ND2 | -8.10 | 1.12 | 1.32 |
| 2 | D | 51 | PRO | N-CD | 8.09 | 1.59 | 1.47 |
| 1 | A | 76 | MET | CG-SD | 8.09 | 2.02 | 1.81 |
| 2 | D | 19 | ASN | C-N | -8.08 | 1.15 | 1.34 |
| 2 | D | 58 | PRO | CA-C | 8.08 | 1.69 | 1.52 |
| 1 | C | 25 | GLY | N-CA | -8.07 | 1.33 | 1.46 |
| 1 | C | 113 | LEU | CG-CD2 | -8.07 | 1.22 | 1.51 |
| 2 | B | 59 | LYS | CA-CB | -8.06 | 1.36 | 1.53 |
| 2 | D | 80 | ASN | CA-C | 8.05 | 1.73 | 1.52 |
| 2 | B | 16 | GLY | N-CA | 8.04 | 1.58 | 1.46 |
| 2 | B | 7 | GLU | N-CA | 8.04 | 1.62 | 1.46 |
| 1 | A | 105 | LEU | CB-CG | -8.03 | 1.29 | 1.52 |
| 2 | B | 118 | PHE | CE1-CZ | 8.03 | 1.52 | 1.37 |
| 1 | C | 3 | SER | CA-CB | -8.03 | 1.41 | 1.52 |
| 2 | D | 104 | ARG | CZ-NH2 | -8.02 | 1.22 | 1.33 |
| 2 | D | 54 | VAL | C-O | 8.02 | 1.38 | 1.23 |
| 1 | A | 17 | VAL | CA-CB | -8.01 | 1.38 | 1.54 |
| 2 | D | 76 | ALA | CA-CB | -8.00 | 1.35 | 1.52 |
| 1 | C | 58 | HIS | CG-CD2 | -8.00 | 1.22 | 1.35 |
| 2 | D | 3 | LEU | C-N | 8.00 | 1.52 | 1.34 |
| 2 | D | 130 | TYR | CE2-CZ | -7.99 | 1.28 | 1.38 |
| 1 | A | 88 | ALA | CA-C | 7.99 | 1.73 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 101 | GLU | C-N | 7.98 | 1.52 | 1.34 |
| 1 | C | 17 | VAL | C-O | 7.98 | 1.38 | 1.23 |
| 1 | C | 45 | HIS | ND1-CE1 | -7.98 | 1.14 | 1.34 |
| 2 | D | 41 | PHE | CA-C | 7.97 | 1.73 | 1.52 |
| 1 | A | 114 | PRO | N-CA | 7.97 | 1.60 | 1.47 |
| 2 | D | 132 | LYS | CD-CE | 7.95 | 1.71 | 1.51 |
| 2 | D | 41 | PHE | CB-CG | 7.95 | 1.64 | 1.51 |
| 2 | B | 45 | PHE | CB-CG | 7.94 | 1.64 | 1.51 |
| 2 | D | 122 | PHE | CG-CD2 | 7.93 | 1.50 | 1.38 |
| 2 | D | 122 | PHE | CG-CD1 | -7.93 | 1.26 | 1.38 |
| 2 | B | 80 | ASN | C-O | -7.92 | 1.08 | 1.23 |
| 1 | A | 132 | VAL | C-O | 7.90 | 1.38 | 1.23 |
| 2 | B | 81 | LEU | CA-C | -7.90 | 1.32 | 1.52 |
| 1 | A | 141 | ARG | N-CA | 7.89 | 1.62 | 1.46 |
| 2 | D | 39 | GLN | CD-OE1 | 7.88 | 1.41 | 1.24 |
| 2 | B | 121 | GLU | N-CA | -7.86 | 1.30 | 1.46 |
| 2 | B | 143 | HIS | CA-CB | -7.86 | 1.36 | 1.53 |
| 1 | C | 48 | LEU | CA-C | -7.85 | 1.32 | 1.52 |
| 2 | D | 116 | HIS | CE1-NE2 | 7.85 | 1.50 | 1.32 |
| 1 | A | 7 | LYS | N-CA | 7.84 | 1.62 | 1.46 |
| 1 | A | 16 | LYS | C-O | -7.84 | 1.08 | 1.23 |
| 1 | C | 11 | LYS | CD-CE | -7.84 | 1.31 | 1.51 |
| 1 | A | 44 | PRO | CA-CB | -7.84 | 1.37 | 1.53 |
| 2 | B | 117 | HIS | CB-CG | -7.83 | 1.35 | 1.50 |
| 2 | D | 54 | VAL | N-CA | 7.82 | 1.61 | 1.46 |
| 2 | D | 135 | ALA | CA-C | 7.82 | 1.73 | 1.52 |
| 2 | B | 15 | TRP | CG-CD1 | -7.82 | 1.25 | 1.36 |
| 2 | D | 18 | VAL | CA-C | 7.82 | 1.73 | 1.52 |
| 1 | C | 74 | ASP | CB-CG | -7.81 | 1.35 | 1.51 |
| 1 | A | 16 | LYS | C-N | 7.81 | 1.52 | 1.34 |
| 1 | A | 8 | THR | C-N | 7.80 | 1.51 | 1.34 |
| 2 | B | 22 | GLU | N-CA | 7.79 | 1.61 | 1.46 |
| 2 | D | 146 | HIS | CD2-NE2 | 7.79 | 1.58 | 1.42 |
| 1 | C | 64 | ASP | CG-OD2 | -7.79 | 1.07 | 1.25 |
| 2 | D | 16 | GLY | CA-C | -7.76 | 1.39 | 1.51 |
| 2 | B | 19 | ASN | CG-OD1 | -7.76 | 1.06 | 1.24 |
| 1 | C | 128 | PHE | CA-C | 7.75 | 1.73 | 1.52 |
| 2 | B | 8 | LYS | CG-CD | 7.75 | 1.78 | 1.52 |
| 2 | D | 16 | GLY | C-O | 7.74 | 1.36 | 1.23 |
| 1 | A | 13 | ALA | CA-C | 7.74 | 1.73 | 1.52 |
| 2 | D | 8 | LYS | CA-C | -7.73 | 1.32 | 1.52 |
| 1 | A | 49 | SER | N-CA | 7.72 | 1.61 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 123 | THR | C-N | -7.72 | 1.19 | 1.34 |
| 2 | B | 95 | LYS | C-N | 7.71 | 1.51 | 1.34 |
| 2 | B | 35 | TYR | CE2-CZ | -7.70 | 1.28 | 1.38 |
| 1 | C | 31 | ARG | CD-NE | 7.69 | 1.59 | 1.46 |
| 1 | A | 43 | PHE | CG-CD2 | -7.69 | 1.27 | 1.38 |
| 2 | B | 42 | PHE | CE2-CZ | 7.69 | 1.51 | 1.37 |
| 1 | A | 132 | VAL | CA-CB | -7.68 | 1.38 | 1.54 |
| 2 | B | 64 | GLY | C-O | -7.67 | 1.11 | 1.23 |
| 1 | C | 23 | GLU | N-CA | -7.67 | 1.31 | 1.46 |
| 2 | D | 97 | HIS | ND1-CE1 | 7.67 | 1.53 | 1.34 |
| 1 | C | 8 | THR | CA-C | -7.67 | 1.33 | 1.52 |
| 1 | C | 49 | SER | CA-C | -7.67 | 1.33 | 1.52 |
| 1 | A | 53 | ALA | CA-CB | 7.66 | 1.68 | 1.52 |
| 1 | A | 20 | HIS | CA-CB | -7.65 | 1.37 | 1.53 |
| 1 | C | 52 | SER | N-CA | 7.65 | 1.61 | 1.46 |
| 2 | D | 45 | PHE | CA-C | 7.65 | 1.72 | 1.52 |
| 2 | D | 118 | PHE | CD2-CE2 | 7.65 | 1.54 | 1.39 |
| 1 | C | 114 | PRO | C-O | 7.64 | 1.38 | 1.23 |
| 2 | D | 92 | HIS | CG-ND1 | 7.63 | 1.55 | 1.38 |
| 2 | B | 15 | TRP | NE1-CE2 | 7.62 | 1.47 | 1.37 |
| 2 | B | 101 | GLU | CD-OE1 | -7.61 | 1.17 | 1.25 |
| 2 | D | 48 | LEU | C-N | 7.61 | 1.51 | 1.34 |
| 2 | D | 2 | HIS | CD2-NE2 | 7.61 | 1.57 | 1.42 |
| 1 | A | 99 | LYS | CA-C | -7.60 | 1.33 | 1.52 |
| 1 | A | 60 | LYS | C-N | 7.60 | 1.51 | 1.34 |
| 2 | B | 112 | CYS | CA-CB | -7.60 | 1.37 | 1.53 |
| 2 | D | 25 | GLY | CA-C | -7.59 | 1.39 | 1.51 |
| 2 | B | 66 | LYS | CA-C | 7.58 | 1.72 | 1.52 |
| 1 | C | 55 | VAL | N-CA | 7.58 | 1.61 | 1.46 |
| 2 | D | 58 | PRO | C-N | -7.58 | 1.16 | 1.34 |
| 1 | C | 18 | GLY | N-CA | 7.56 | 1.57 | 1.46 |
| 2 | D | 17 | LYS | CB-CG | -7.56 | 1.32 | 1.52 |
| 1 | A | 42 | TYR | CA-C | 7.55 | 1.72 | 1.52 |
| 2 | B | 97 | HIS | CB-CG | 7.55 | 1.63 | 1.50 |
| 2 | B | 61 | LYS | CD-CE | 7.54 | 1.70 | 1.51 |
| 1 | C | 76 | MET | CA-C | -7.53 | 1.33 | 1.52 |
| 1 | A | 127 | LYS | C-N | -7.53 | 1.16 | 1.34 |
| 2 | D | 60 | VAL | CA-C | -7.52 | 1.33 | 1.52 |
| 2 | B | 134 | VAL | C-O | 7.52 | 1.37 | 1.23 |
| 2 | B | 71 | PHE | CG-CD2 | 7.51 | 1.50 | 1.38 |
| 1 | C | 24 | TYR | CD1-CE1 | 7.51 | 1.50 | 1.39 |
| 1 | A | 122 | HIS | ND1-CE1 | 7.50 | 1.53 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 15 | TRP | CZ2-CH2 | -7.50 | 1.23 | 1.37 |
| 1 | C | 90 | LYS | N-CA | -7.49 | 1.31 | 1.46 |
| 2 | B | 120 | LYS | CB-CG | -7.49 | 1.32 | 1.52 |
| 1 | C | 94 | ASP | CG-OD1 | -7.48 | 1.08 | 1.25 |
| 1 | C | 83 | LEU | C-O | 7.48 | 1.37 | 1.23 |
| 2 | D | 45 | PHE | C-O | 7.47 | 1.37 | 1.23 |
| 1 | C | 7 | LYS | C-N | 7.47 | 1.51 | 1.34 |
| 2 | D | 104 | ARG | CG-CD | 7.46 | 1.70 | 1.51 |
| 2 | D | 75 | LEU | CG-CD2 | -7.45 | 1.24 | 1.51 |
| 2 | D | 68 | LEU | CG-CD1 | -7.45 | 1.24 | 1.51 |
| 1 | C | 105 | LEU | CG-CD1 | 7.44 | 1.79 | 1.51 |
| 1 | A | 106 | LEU | C-O | 7.43 | 1.37 | 1.23 |
| 1 | A | 8 | THR | CB-CG2 | -7.43 | 1.27 | 1.52 |
| 2 | B | 53 | ALA | CA-CB | -7.43 | 1.36 | 1.52 |
| 1 | A | 90 | LYS | CB-CG | 7.42 | 1.72 | 1.52 |
| 2 | B | 16 | GLY | CA-C | -7.41 | 1.40 | 1.51 |
| 1 | C | 106 | LEU | CA-C | -7.41 | 1.33 | 1.52 |
| 2 | D | 86 | ALA | CA-CB | 7.41 | 1.68 | 1.52 |
| 2 | B | 136 | GLY | N-CA | 7.40 | 1.57 | 1.46 |
| 2 | D | 5 | PRO | N-CD | 7.39 | 1.58 | 1.47 |
| 2 | D | 43 | GLU | N-CA | 7.39 | 1.61 | 1.46 |
| 1 | C | 12 | ALA | C-O | 7.38 | 1.37 | 1.23 |
| 1 | C | 2 | LEU | CG-CD2 | -7.37 | 1.24 | 1.51 |
| 2 | D | 130 | TYR | CD2-CE2 | 7.37 | 1.50 | 1.39 |
| 1 | C | 12 | ALA | N-CA | -7.37 | 1.31 | 1.46 |
| 1 | A | 72 | HIS | CG-CD2 | 7.35 | 1.48 | 1.35 |
| 2 | B | 13 | ALA | CA-CB | 7.35 | 1.67 | 1.52 |
| 1 | A | 76 | MET | N-CA | 7.34 | 1.61 | 1.46 |
| 2 | B | 17 | LYS | CD-CE | 7.34 | 1.69 | 1.51 |
| 1 | A | 131 | SER | CA-CB | 7.33 | 1.64 | 1.52 |
| 2 | B | 72 | SER | N-CA | 7.32 | 1.60 | 1.46 |
| 2 | B | 28 | LEU | CB-CG | 7.32 | 1.73 | 1.52 |
| 2 | D | 10 | ALA | N-CA | 7.32 | 1.60 | 1.46 |
| 2 | B | 124 | PRO | C-N | -7.32 | 1.20 | 1.34 |
| 1 | A | 106 | LEU | CA-C | -7.31 | 1.33 | 1.52 |
| 2 | B | 112 | CYS | CB-SG | 7.31 | 1.94 | 1.82 |
| 2 | B | 145 | TYR | CB-CG | 7.31 | 1.62 | 1.51 |
| 1 | C | 112 | HIS | C-N | -7.30 | 1.17 | 1.34 |
| 2 | B | 57 | ASN | CG-OD1 | -7.29 | 1.07 | 1.24 |
| 2 | D | 6 | GLU | N-CA | -7.29 | 1.31 | 1.46 |
| 2 | B | 144 | LYS | C-O | 7.29 | 1.37 | 1.23 |
| 2 | D | 61 | LYS | CG-CD | -7.29 | 1.27 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 120 | ALA | C-N | -7.28 | 1.17 | 1.34 |
| 1 | A | 24 | TYR | CG-CD1 | -7.28 | 1.29 | 1.39 |
| 2 | D | 1 | VAL | CA-CB | 7.27 | 1.70 | 1.54 |
| 2 | D | 119 | GLY | CA-C | 7.27 | 1.63 | 1.51 |
| 1 | A | 74 | ASP | N-CA | 7.26 | 1.60 | 1.46 |
| 1 | A | 11 | LYS | CB-CG | -7.25 | 1.32 | 1.52 |
| 1 | A | 48 | LEU | CA-CB | 7.25 | 1.70 | 1.53 |
| 2 | D | 50 | THR | CA-C | 7.24 | 1.71 | 1.52 |
| 1 | C | 59 | GLY | C-O | 7.24 | 1.35 | 1.23 |
| 2 | D | 81 | LEU | CG-CD1 | -7.24 | 1.25 | 1.51 |
| 2 | B | 72 | SER | CB-OG | -7.23 | 1.32 | 1.42 |
| 1 | C | 2 | LEU | CG-CD1 | -7.23 | 1.25 | 1.51 |
| 2 | D | 44 | SER | CA-C | -7.21 | 1.34 | 1.52 |
| 1 | C | 2 | LEU | CA-CB | -7.20 | 1.37 | 1.53 |
| 1 | A | 69 | ALA | C-O | -7.18 | 1.09 | 1.23 |
| 1 | A | 20 | HIS | CB-CG | -7.17 | 1.37 | 1.50 |
| 1 | C | 29 | LEU | CA-C | -7.17 | 1.34 | 1.52 |
| 2 | D | 67 | VAL | CA-C | -7.17 | 1.34 | 1.52 |
| 2 | B | 46 | GLY | N-CA | -7.16 | 1.35 | 1.46 |
| 1 | A | 43 | PHE | CG-CD1 | 7.16 | 1.49 | 1.38 |
| 1 | A | 64 | ASP | C-N | 7.16 | 1.50 | 1.34 |
| 2 | B | 73 | ASP | CA-CB | 7.14 | 1.69 | 1.53 |
| 1 | C | 78 | ASN | C-N | 7.14 | 1.50 | 1.34 |
| 2 | B | 85 | PHE | CB-CG | -7.13 | 1.39 | 1.51 |
| 1 | C | 122 | HIS | CG-CD2 | 7.13 | 1.47 | 1.35 |
| 1 | A | 109 | LEU | CG-CD2 | -7.13 | 1.25 | 1.51 |
| 2 | D | 51 | PRO | C-O | 7.13 | 1.37 | 1.23 |
| 2 | D | 126 | VAL | C-N | 7.12 | 1.50 | 1.34 |
| 2 | D | 145 | TYR | CE1-CZ | 7.11 | 1.47 | 1.38 |
| 1 | C | 50 | HIS | CA-C | 7.10 | 1.71 | 1.52 |
| 2 | B | 54 | VAL | CA-CB | 7.10 | 1.69 | 1.54 |
| 2 | B | 11 | VAL | CA-CB | -7.09 | 1.39 | 1.54 |
| 2 | D | 141 | LEU | CG-CD2 | 7.09 | 1.78 | 1.51 |
| 1 | A | 90 | LYS | CA-CB | 7.08 | 1.69 | 1.53 |
| 1 | A | 79 | ALA | CA-CB | -7.08 | 1.37 | 1.52 |
| 2 | B | 15 | TRP | CD2-CE2 | 7.08 | 1.49 | 1.41 |
| 1 | C | 117 | PHE | CG-CD1 | 7.08 | 1.49 | 1.38 |
| 1 | C | 20 | HIS | CA-CB | -7.06 | 1.38 | 1.53 |
| 2 | D | 99 | ASP | CB-CG | 7.06 | 1.66 | 1.51 |
| 2 | D | 72 | SER | CB-OG | -7.06 | 1.33 | 1.42 |
| 2 | D | 64 | GLY | C-N | 7.05 | 1.50 | 1.34 |
| 1 | A | 59 | GLY | N-CA | 7.05 | 1.56 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 37 | TRP | CZ3-CH2 | -7.04 | 1.28 | 1.40 |
| 2 | D | 26 | GLU | CA-C | 7.03 | 1.71 | 1.52 |
| 2 | D | 103 | PHE | CG-CD1 | 7.03 | 1.49 | 1.38 |
| 1 | A | 48 | LEU | CG-CD2 | -7.02 | 1.25 | 1.51 |
| 2 | B | 95 | LYS | C-O | -7.01 | 1.10 | 1.23 |
| 1 | C | 61 | LYS | CB-CG | -7.01 | 1.33 | 1.52 |
| 2 | D | 126 | VAL | C-O | -7.00 | 1.10 | 1.23 |
| 1 | A | 62 | VAL | N-CA | 7.00 | 1.60 | 1.46 |
| 1 | A | 71 | ALA | CA-CB | -7.00 | 1.37 | 1.52 |
| 1 | A | 96 | VAL | CA-CB | 7.00 | 1.69 | 1.54 |
| 2 | D | 146 | HIS | CG-CD2 | -7.00 | 1.23 | 1.35 |
| 1 | C | 64 | ASP | CB-CG | 7.00 | 1.66 | 1.51 |
| 1 | A | 98 | PHE | CD1-CE1 | -6.99 | 1.25 | 1.39 |
| 1 | C | 23 | GLU | CA-C | 6.98 | 1.71 | 1.52 |
| 2 | D | 98 | VAL | CB-CG2 | 6.98 | 1.67 | 1.52 |
| 2 | D | 78 | LEU | C-N | 6.97 | 1.50 | 1.34 |
| 1 | A | 77 | PRO | N-CA | -6.96 | 1.35 | 1.47 |
| 1 | A | 114 | PRO | CA-C | 6.96 | 1.66 | 1.52 |
| 2 | B | 50 | THR | CB-CG2 | 6.96 | 1.75 | 1.52 |
| 1 | C | 52 | SER | C-O | 6.96 | 1.36 | 1.23 |
| 1 | C | 74 | ASP | N-CA | 6.95 | 1.60 | 1.46 |
| 2 | D | 143 | HIS | CG-ND1 | -6.93 | 1.23 | 1.38 |
| 1 | A | 56 | LYS | CA-C | -6.93 | 1.34 | 1.52 |
| 1 | A | 92 | ARG | CD-NE | -6.92 | 1.34 | 1.46 |
| 2 | D | 10 | ALA | CA-CB | -6.92 | 1.38 | 1.52 |
| 1 | A | 60 | LYS | C-O | -6.92 | 1.10 | 1.23 |
| 2 | B | 145 | TYR | CD1-CE1 | -6.92 | 1.28 | 1.39 |
| 1 | C | 133 | SER | C-N | -6.91 | 1.18 | 1.34 |
| 2 | D | 105 | LEU | CA-CB | -6.89 | 1.37 | 1.53 |
| 2 | D | 122 | PHE | CD1-CE1 | 6.89 | 1.53 | 1.39 |
| 2 | B | 41 | PHE | CE1-CZ | -6.89 | 1.24 | 1.37 |
| 2 | B | 142 | ALA | C-O | 6.89 | 1.36 | 1.23 |
| 1 | C | 130 | ALA | C-O | 6.89 | 1.36 | 1.23 |
| 1 | A | 76 | MET | C-N | -6.87 | 1.21 | 1.34 |
| 1 | A | 26 | ALA | C-N | 6.86 | 1.49 | 1.34 |
| 1 | C | 65 | ALA | C-N | 6.86 | 1.49 | 1.34 |
| 1 | A | 8 | THR | CA-CB | 6.86 | 1.71 | 1.53 |
| 1 | A | 98 | PHE | CE2-CZ | -6.86 | 1.24 | 1.37 |
| 1 | A | 119 | PRO | CA-C | -6.86 | 1.39 | 1.52 |
| 1 | C | 110 | ALA | C-O | 6.86 | 1.36 | 1.23 |
| 1 | C | 87 | HIS | CE1-NE2 | -6.85 | 1.17 | 1.32 |
| 1 | C | 40 | LYS | N-CA | 6.84 | 1.60 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 75 | LEU | CA-CB | 6.84 | 1.69 | 1.53 |
| 1 | C | 131 | SER | CB-OG | 6.83 | 1.51 | 1.42 |
| 2 | D | 28 | LEU | C-N | 6.82 | 1.45 | 1.33 |
| 2 | D | 131 | GLN | C-O | -6.82 | 1.10 | 1.23 |
| 2 | B | 32 | LEU | CG-CD1 | -6.81 | 1.26 | 1.51 |
| 2 | B | 79 | ASP | N-CA | 6.81 | 1.59 | 1.46 |
| 2 | D | 7 | GLU | C-N | -6.81 | 1.18 | 1.34 |
| 2 | D | 77 | HIS | N-CA | -6.81 | 1.32 | 1.46 |
| 2 | D | 86 | ALA | N-CA | 6.81 | 1.59 | 1.46 |
| 2 | B | 34 | VAL | N-CA | 6.80 | 1.59 | 1.46 |
| 2 | D | 51 | PRO | CA-C | -6.80 | 1.39 | 1.52 |
| 1 | C | 132 | VAL | CA-CB | -6.79 | 1.40 | 1.54 |
| 2 | B | 54 | VAL | C-O | 6.79 | 1.36 | 1.23 |
| 1 | A | 41 | THR | CA-C | -6.78 | 1.35 | 1.52 |
| 1 | A | 80 | LEU | N-CA | 6.78 | 1.59 | 1.46 |
| 2 | B | 121 | GLU | CA-CB | 6.78 | 1.68 | 1.53 |
| 2 | B | 120 | LYS | CE-NZ | -6.77 | 1.32 | 1.49 |
| 2 | B | 123 | THR | CB-OG1 | -6.77 | 1.29 | 1.43 |
| 2 | D | 13 | ALA | C-O | -6.77 | 1.10 | 1.23 |
| 1 | A | 79 | ALA | CA-C | 6.77 | 1.70 | 1.52 |
| 2 | B | 67 | VAL | N-CA | 6.75 | 1.59 | 1.46 |
| 1 | C | 14 | TRP | C-N | -6.75 | 1.20 | 1.33 |
| 1 | C | 48 | LEU | N-CA | 6.75 | 1.59 | 1.46 |
| 2 | B | 13 | ALA | N-CA | -6.74 | 1.32 | 1.46 |
| 2 | D | 95 | LYS | N-CA | 6.74 | 1.59 | 1.46 |
| 1 | C | 98 | PHE | CG-CD2 | -6.73 | 1.28 | 1.38 |
| 2 | D | 18 | VAL | C-N | -6.73 | 1.18 | 1.34 |
| 1 | C | 124 | SER | CA-CB | 6.72 | 1.63 | 1.52 |
| 2 | D | 91 | LEU | C-N | 6.72 | 1.49 | 1.34 |
| 2 | D | 32 | LEU | C-O | 6.72 | 1.36 | 1.23 |
| 2 | B | 39 | GLN | N-CA | 6.72 | 1.59 | 1.46 |
| 2 | B | 12 | THR | CA-CB | 6.71 | 1.70 | 1.53 |
| 1 | C | 38 | THR | CA-C | -6.71 | 1.35 | 1.52 |
| 1 | A | 8 | THR | CA-C | -6.70 | 1.35 | 1.52 |
| 2 | B | 13 | ALA | C-N | 6.70 | 1.49 | 1.34 |
| 1 | C | 139 | LYS | CG-CD | -6.70 | 1.29 | 1.52 |
| 2 | D | 15 | TRP | CG-CD2 | 6.70 | 1.55 | 1.43 |
| 2 | B | 37 | TRP | CD2-CE2 | 6.69 | 1.49 | 1.41 |
| 1 | A | 117 | PHE | CD2-CE2 | 6.69 | 1.52 | 1.39 |
| 2 | B | 35 | TYR | CD2-CE2 | -6.69 | 1.29 | 1.39 |
| 2 | B | 73 | ASP | N-CA | 6.69 | 1.59 | 1.46 |
| 2 | D | 1 | VAL | C-N | -6.68 | 1.18 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 94 | ASP | CB-CG | 6.68 | 1.65 | 1.51 |
| 1 | A | 139 | LYS | N-CA | 6.67 | 1.59 | 1.46 |
| 2 | D | 110 | LEU | CA-CB | -6.67 | 1.38 | 1.53 |
| 1 | A | 12 | ALA | N-CA | -6.67 | 1.33 | 1.46 |
| 1 | A | 73 | VAL | CB-CG2 | -6.66 | 1.38 | 1.52 |
| 2 | B | 19 | ASN | CG-ND2 | 6.66 | 1.49 | 1.32 |
| 1 | A | 81 | SER | C-O | 6.66 | 1.35 | 1.23 |
| 2 | D | 84 | THR | N-CA | -6.66 | 1.33 | 1.46 |
| 1 | C | 60 | LYS | CD-CE | -6.65 | 1.34 | 1.51 |
| 2 | B | 119 | GLY | C-O | 6.64 | 1.34 | 1.23 |
| 2 | B | 124 | PRO | C-O | 6.63 | 1.36 | 1.23 |
| 2 | B | 83 | GLY | CA-C | -6.63 | 1.41 | 1.51 |
| 1 | A | 120 | ALA | N-CA | -6.62 | 1.33 | 1.46 |
| 1 | A | 33 | PHE | C-N | 6.62 | 1.49 | 1.34 |
| 2 | D | 68 | LEU | CB-CG | -6.62 | 1.33 | 1.52 |
| 1 | A | 22 | GLY | C-N | 6.62 | 1.49 | 1.34 |
| 2 | D | 44 | SER | C-N | 6.61 | 1.49 | 1.34 |
| 2 | B | 144 | LYS | CA-C | -6.61 | 1.35 | 1.52 |
| 1 | C | 109 | LEU | C-N | 6.60 | 1.49 | 1.34 |
| 2 | D | 93 | CYS | N-CA | 6.60 | 1.59 | 1.46 |
| 2 | B | 63 | HIS | C-N | -6.59 | 1.21 | 1.33 |
| 2 | D | 54 | VAL | CB-CG1 | 6.59 | 1.66 | 1.52 |
| 1 | C | 43 | PHE | N-CA | 6.59 | 1.59 | 1.46 |
| 1 | A | 41 | THR | C-O | 6.58 | 1.35 | 1.23 |
| 2 | B | 63 | HIS | CA-CB | -6.58 | 1.39 | 1.53 |
| 1 | C | 87 | HIS | CG-CD2 | 6.58 | 1.47 | 1.35 |
| 2 | B | 8 | LYS | N-CA | -6.58 | 1.33 | 1.46 |
| 1 | C | 52 | SER | CA-CB | -6.57 | 1.43 | 1.52 |
| 2 | B | 120 | LYS | CA-CB | 6.56 | 1.68 | 1.53 |
| 1 | A | 42 | TYR | CG-CD2 | 6.56 | 1.47 | 1.39 |
| 2 | B | 3 | LEU | N-CA | 6.56 | 1.59 | 1.46 |
| 1 | A | 11 | LYS | N-CA | 6.55 | 1.59 | 1.46 |
| 2 | B | 76 | ALA | N-CA | -6.55 | 1.33 | 1.46 |
| 1 | C | 78 | ASN | CA-CB | 6.55 | 1.70 | 1.53 |
| 1 | C | 68 | ASN | N-CA | -6.55 | 1.33 | 1.46 |
| 2 | B | 123 | THR | CA-C | 6.55 | 1.70 | 1.52 |
| 1 | A | 20 | HIS | CD2-NE2 | 6.55 | 1.55 | 1.42 |
| 1 | A | 113 | LEU | CB-CG | 6.54 | 1.71 | 1.52 |
| 2 | B | 58 | PRO | CB-CG | -6.54 | 1.17 | 1.50 |
| 1 | A | 18 | GLY | C-O | 6.54 | 1.34 | 1.23 |
| 2 | D | 117 | HIS | CD2-NE2 | -6.53 | 1.23 | 1.38 |
| 1 | A | 5 | ALA | N-CA | -6.52 | 1.33 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 68 | LEU | CG-CD2 | -6.52 | 1.27 | 1.51 |
| 1 | A | 40 | LYS | C-O | -6.51 | 1.10 | 1.23 |
| 2 | B | 47 | ASP | C-N | 6.51 | 1.49 | 1.34 |
| 2 | B | 77 | HIS | CA-CB | -6.51 | 1.39 | 1.53 |
| 2 | D | 14 | LEU | N-CA | -6.51 | 1.33 | 1.46 |
| 2 | D | 32 | LEU | CG-CD2 | -6.51 | 1.27 | 1.51 |
| 2 | B | 102 | ASN | CG-ND2 | 6.51 | 1.49 | 1.32 |
| 2 | B | 93 | CYS | C-O | -6.50 | 1.11 | 1.23 |
| 2 | B | 123 | THR | C-O | -6.50 | 1.11 | 1.23 |
| 1 | C | 27 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 2 | D | 47 | ASP | C-N | -6.49 | 1.19 | 1.34 |
| 1 | A | 92 | ARG | CB-CG | -6.49 | 1.35 | 1.52 |
| 2 | D | 126 | VAL | CB-CG1 | -6.49 | 1.39 | 1.52 |
| 1 | C | 36 | PHE | CD2-CE2 | -6.49 | 1.26 | 1.39 |
| 1 | C | 46 | PHE | CA-CB | 6.46 | 1.68 | 1.53 |
| 1 | A | 113 | LEU | CA-CB | -6.46 | 1.39 | 1.53 |
| 1 | C | 95 | PRO | C-O | 6.44 | 1.36 | 1.23 |
| 2 | B | 35 | TYR | CG-CD1 | 6.43 | 1.47 | 1.39 |
| 1 | C | 58 | HIS | CA-C | 6.43 | 1.69 | 1.52 |
| 2 | D | 48 | LEU | CG-CD1 | 6.42 | 1.75 | 1.51 |
| 2 | B | 48 | LEU | N-CA | 6.42 | 1.59 | 1.46 |
| 1 | A | 60 | LYS | CA-CB | 6.42 | 1.68 | 1.53 |
| 2 | B | 53 | ALA | C-N | 6.42 | 1.48 | 1.34 |
| 2 | D | 83 | GLY | CA-C | -6.42 | 1.41 | 1.51 |
| 2 | B | 8 | LYS | CD-CE | -6.41 | 1.35 | 1.51 |
| 2 | B | 90 | GLU | C-N | 6.41 | 1.48 | 1.34 |
| 1 | A | 68 | ASN | C-N | 6.40 | 1.48 | 1.34 |
| 1 | C | 113 | LEU | CG-CD1 | 6.39 | 1.75 | 1.51 |
| 1 | A | 74 | ASP | C-O | 6.39 | 1.35 | 1.23 |
| 1 | A | 35 | SER | N-CA | -6.39 | 1.33 | 1.46 |
| 2 | D | 66 | LYS | C-N | 6.38 | 1.48 | 1.34 |
| 1 | A | 72 | HIS | CA-C | -6.38 | 1.36 | 1.52 |
| 1 | A | 45 | HIS | CA-CB | -6.38 | 1.40 | 1.53 |
| 2 | D | 71 | PHE | CE1-CZ | -6.38 | 1.25 | 1.37 |
| 1 | C | 120 | ALA | C-O | 6.37 | 1.35 | 1.23 |
| 1 | A | 63 | ALA | CA-C | -6.37 | 1.36 | 1.52 |
| 2 | B | 104 | ARG | CA-CB | 6.36 | 1.68 | 1.53 |
| 1 | A | 95 | PRO | C-O | 6.35 | 1.35 | 1.23 |
| 1 | C | 45 | HIS | CB-CG | 6.34 | 1.61 | 1.50 |
| 2 | D | 55 | MET | CA-CB | 6.34 | 1.67 | 1.53 |
| 2 | B | 133 | VAL | CB-CG1 | -6.34 | 1.39 | 1.52 |
| 1 | A | 44 | PRO | C-N | -6.33 | 1.19 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 70 | VAL | N-CA | 6.33 | 1.59 | 1.46 |
| 1 | A | 94 | ASP | CA-C | 6.33 | 1.69 | 1.52 |
| 1 | C | 63 | ALA | CA-C | -6.33 | 1.36 | 1.52 |
| 2 | B | 145 | TYR | C-O | 6.33 | 1.35 | 1.23 |
| 2 | B | 140 | ALA | CA-CB | 6.32 | 1.65 | 1.52 |
| 1 | A | 61 | LYS | CA-C | 6.32 | 1.69 | 1.52 |
| 1 | C | 50 | HIS | CG-CD2 | -6.31 | 1.25 | 1.35 |
| 2 | B | 98 | VAL | CA-C | 6.31 | 1.69 | 1.52 |
| 2 | B | 120 | LYS | CD-CE | 6.31 | 1.67 | 1.51 |
| 1 | C | 130 | ALA | CA-CB | -6.31 | 1.39 | 1.52 |
| 1 | C | 128 | PHE | CE2-CZ | -6.31 | 1.25 | 1.37 |
| 1 | C | 122 | HIS | CA-CB | -6.30 | 1.40 | 1.53 |
| 2 | B | 109 | VAL | CB-CG2 | 6.29 | 1.66 | 1.52 |
| 2 | B | 15 | TRP | CB-CG | 6.29 | 1.61 | 1.50 |
| 1 | A | 60 | LYS | CA-C | -6.28 | 1.36 | 1.52 |
| 2 | B | 80 | ASN | CA-CB | -6.27 | 1.36 | 1.53 |
| 2 | B | 98 | VAL | CB-CG2 | 6.26 | 1.66 | 1.52 |
| 1 | C | 17 | VAL | CB-CG2 | 6.25 | 1.66 | 1.52 |
| 1 | C | 73 | VAL | CA-C | 6.25 | 1.69 | 1.52 |
| 1 | A | 108 | THR | CA-CB | 6.25 | 1.69 | 1.53 |
| 1 | A | 11 | LYS | CA-CB | -6.25 | 1.40 | 1.53 |
| 2 | B | 92 | HIS | CD2-NE2 | -6.24 | 1.24 | 1.38 |
| 2 | D | 30 | ARG | C-N | -6.24 | 1.19 | 1.34 |
| 1 | A | 128 | PHE | CD2-CE2 | 6.22 | 1.51 | 1.39 |
| 1 | C | 73 | VAL | N-CA | -6.22 | 1.33 | 1.46 |
| 2 | B | 106 | LEU | CG-CD2 | -6.21 | 1.28 | 1.51 |
| 1 | A | 60 | LYS | CB-CG | -6.21 | 1.35 | 1.52 |
| 1 | A | 25 | GLY | CA-C | -6.21 | 1.42 | 1.51 |
| 2 | D | 85 | PHE | CE1-CZ | 6.21 | 1.49 | 1.37 |
| 2 | D | 112 | CYS | C-O | -6.21 | 1.11 | 1.23 |
| 2 | D | 120 | LYS | CB-CG | -6.21 | 1.35 | 1.52 |
| 2 | B | 48 | LEU | CA-CB | -6.20 | 1.39 | 1.53 |
| 2 | B | 118 | PHE | CD1-CE1 | 6.20 | 1.51 | 1.39 |
| 1 | C | 99 | LYS | C-O | -6.20 | 1.11 | 1.23 |
| 1 | C | 10 | VAL | CB-CG1 | 6.20 | 1.65 | 1.52 |
| 1 | A | 128 | PHE | CG-CD1 | 6.17 | 1.48 | 1.38 |
| 2 | D | 118 | PHE | CG-CD2 | 6.17 | 1.48 | 1.38 |
| 1 | C | 128 | PHE | CE1-CZ | -6.17 | 1.25 | 1.37 |
| 2 | B | 103 | PHE | CG-CD2 | -6.17 | 1.29 | 1.38 |
| 2 | D | 48 | LEU | CA-C | 6.17 | 1.69 | 1.52 |
| 1 | C | 41 | THR | N-CA | 6.16 | 1.58 | 1.46 |
| 2 | D | 47 | ASP | C-O | 6.16 | 1.35 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 48 | LEU | CG-CD2 | 6.16 | 1.74 | 1.51 |
| 1 | C | 106 | LEU | N-CA | 6.16 | 1.58 | 1.46 |
| 2 | B | 130 | TYR | CE1-CZ | -6.15 | 1.30 | 1.38 |
| 1 | A | 97 | ASN | CG-ND2 | 6.15 | 1.48 | 1.32 |
| 1 | A | 10 | VAL | CA-C | 6.15 | 1.69 | 1.52 |
| 2 | D | 37 | TRP | CD2-CE2 | -6.15 | 1.33 | 1.41 |
| 2 | D | 116 | HIS | CG-ND1 | -6.14 | 1.25 | 1.38 |
| 2 | B | 91 | LEU | CG-CD2 | -6.13 | 1.29 | 1.51 |
| 1 | A | 30 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | A | 52 | SER | CB-OG | -6.13 | 1.34 | 1.42 |
| 2 | B | 35 | TYR | C-N | -6.13 | 1.22 | 1.34 |
| 2 | D | 95 | LYS | CA-C | -6.12 | 1.37 | 1.52 |
| 2 | D | 59 | LYS | N-CA | -6.12 | 1.34 | 1.46 |
| 2 | D | 118 | PHE | CE1-CZ | 6.12 | 1.49 | 1.37 |
| 2 | B | 90 | GLU | N-CA | -6.12 | 1.34 | 1.46 |
| 2 | B | 6 | GLU | C-N | -6.11 | 1.20 | 1.34 |
| 1 | C | 19 | ALA | N-CA | -6.11 | 1.34 | 1.46 |
| 2 | B | 44 | SER | N-CA | 6.11 | 1.58 | 1.46 |
| 2 | B | 132 | LYS | CD-CE | 6.11 | 1.66 | 1.51 |
| 2 | D | 140 | ALA | C-N | -6.10 | 1.20 | 1.34 |
| 1 | A | 16 | LYS | CB-CG | 6.09 | 1.69 | 1.52 |
| 1 | C | 4 | PRO | CA-C | 6.09 | 1.65 | 1.52 |
| 2 | D | 60 | VAL | C-N | 6.08 | 1.48 | 1.34 |
| 1 | C | 73 | VAL | CB-CG1 | -6.08 | 1.40 | 1.52 |
| 2 | D | 144 | LYS | CB-CG | 6.08 | 1.69 | 1.52 |
| 1 | C | 2 | LEU | C-N | -6.08 | 1.20 | 1.34 |
| 2 | D | 84 | THR | CA-C | 6.07 | 1.68 | 1.52 |
| 1 | A | 11 | LYS | CG-CD | -6.06 | 1.31 | 1.52 |
| 2 | D | 74 | GLY | N-CA | -6.06 | 1.36 | 1.46 |
| 1 | C | 50 | HIS | C-N | -6.05 | 1.22 | 1.33 |
| 2 | D | 23 | VAL | C-N | -6.05 | 1.22 | 1.33 |
| 1 | A | 87 | HIS | CB-CG | 6.04 | 1.60 | 1.50 |
| 1 | A | 92 | ARG | CA-C | -6.04 | 1.37 | 1.52 |
| 1 | A | 40 | LYS | CD-CE | -6.04 | 1.36 | 1.51 |
| 1 | C | 128 | PHE | C-O | 6.04 | 1.34 | 1.23 |
| 2 | D | 145 | TYR | N-CA | -6.03 | 1.34 | 1.46 |
| 1 | A | 46 | PHE | CG-CD1 | 6.03 | 1.47 | 1.38 |
| 2 | B | 145 | TYR | CE2-CZ | 6.02 | 1.46 | 1.38 |
| 2 | B | 82 | LYS | CG-CD | 6.02 | 1.73 | 1.52 |
| 2 | D | 12 | THR | CA-C | -6.01 | 1.37 | 1.52 |
| 1 | C | 88 | ALA | CA-C | 6.00 | 1.68 | 1.52 |
| 2 | D | 51 | PRO | C-N | 5.99 | 1.47 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 64 | ASP | C-O | -5.99 | 1.11 | 1.23 |
| 1 | A | 76 | MET | SD-CE | -5.99 | 1.44 | 1.77 |
| 2 | B | 118 | PHE | CA-CB | -5.98 | 1.40 | 1.53 |
| 2 | B | 23 | VAL | C-O | 5.97 | 1.34 | 1.23 |
| 2 | B | 40 | ARG | CG-CD | 5.96 | 1.66 | 1.51 |
| 2 | D | 78 | LEU | CA-C | -5.96 | 1.37 | 1.52 |
| 1 | A | 86 | LEU | C-N | 5.96 | 1.47 | 1.34 |
| 1 | C | 17 | VAL | CA-CB | 5.96 | 1.67 | 1.54 |
| 2 | B | 52 | ASP | CG-OD2 | 5.96 | 1.39 | 1.25 |
| 1 | C | 3 | SER | C-N | 5.95 | 1.45 | 1.34 |
| 2 | B | 129 | ALA | C-O | 5.95 | 1.34 | 1.23 |
| 1 | A | 12 | ALA | CA-CB | 5.95 | 1.65 | 1.52 |
| 1 | A | 34 | LEU | CB-CG | -5.94 | 1.35 | 1.52 |
| 2 | B | 117 | HIS | CA-CB | 5.93 | 1.67 | 1.53 |
| 2 | D | 125 | PRO | CG-CD | -5.93 | 1.31 | 1.50 |
| 2 | B | 94 | ASP | CG-OD1 | -5.93 | 1.11 | 1.25 |
| 1 | C | 2 | LEU | C-O | 5.92 | 1.34 | 1.23 |
| 1 | A | 26 | ALA | CA-C | 5.92 | 1.68 | 1.52 |
| 1 | A | 58 | HIS | CE1-NE2 | -5.92 | 1.19 | 1.32 |
| 1 | C | 25 | GLY | CA-C | -5.91 | 1.42 | 1.51 |
| 2 | B | 34 | VAL | CB-CG2 | -5.91 | 1.40 | 1.52 |
| 2 | B | 7 | GLU | CD-OE1 | 5.91 | 1.32 | 1.25 |
| 2 | B | 146 | HIS | CA-C | -5.91 | 1.37 | 1.52 |
| 1 | C | 6 | ASP | CG-OD1 | 5.90 | 1.39 | 1.25 |
| 1 | A | 140 | TYR | N-CA | -5.90 | 1.34 | 1.46 |
| 2 | D | 121 | GLU | CA-C | 5.90 | 1.68 | 1.52 |
| 2 | D | 68 | LEU | C-N | 5.90 | 1.43 | 1.33 |
| 2 | B | 58 | PRO | CA-CB | 5.89 | 1.65 | 1.53 |
| 2 | D | 11 | VAL | N-CA | 5.89 | 1.58 | 1.46 |
| 1 | A | 114 | PRO | N-CD | -5.89 | 1.39 | 1.47 |
| 2 | D | 58 | PRO | CA-CB | 5.88 | 1.65 | 1.53 |
| 1 | C | 24 | TYR | C-O | -5.88 | 1.12 | 1.23 |
| 2 | D | 85 | PHE | CD2-CE2 | 5.87 | 1.50 | 1.39 |
| 1 | C | 14 | TRP | CD1-NE1 | 5.87 | 1.48 | 1.38 |
| 2 | D | 72 | SER | C-O | 5.87 | 1.34 | 1.23 |
| 1 | C | 51 | GLY | CA-C | -5.86 | 1.42 | 1.51 |
| 2 | D | 71 | PHE | CD2-CE2 | 5.86 | 1.50 | 1.39 |
| 1 | A | 71 | ALA | N-CA | 5.86 | 1.58 | 1.46 |
| 2 | B | 116 | HIS | CG-ND1 | 5.85 | 1.51 | 1.38 |
| 2 | B | 92 | HIS | CA-C | 5.85 | 1.68 | 1.52 |
| 2 | D | 126 | VAL | CA-C | 5.85 | 1.68 | 1.52 |
| 1 | A | 64 | ASP | N-CA | -5.84 | 1.34 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 66 | LYS | CA-CB | 5.84 | 1.66 | 1.53 |
| 1 | C | 26 | ALA | C-O | -5.84 | 1.12 | 1.23 |
| 2 | B | 29 | GLY | N-CA | -5.82 | 1.37 | 1.46 |
| 1 | C | 57 | GLY | N-CA | -5.82 | 1.37 | 1.46 |
| 1 | C | 89 | HIS | CE1-NE2 | -5.81 | 1.19 | 1.32 |
| 2 | B | 84 | THR | C-N | 5.81 | 1.47 | 1.34 |
| 2 | D | 37 | TRP | N-CA | -5.81 | 1.34 | 1.46 |
| 2 | B | 63 | HIS | CG-CD2 | 5.81 | 1.45 | 1.35 |
| 2 | D | 63 | HIS | CE1-NE2 | -5.81 | 1.19 | 1.32 |
| 1 | C | 105 | LEU | N-CA | -5.81 | 1.34 | 1.46 |
| 1 | A | 43 | PHE | CE1-CZ | -5.80 | 1.26 | 1.37 |
| 2 | D | 92 | HIS | CB-CG | 5.80 | 1.60 | 1.50 |
| 2 | B | 84 | THR | C-O | -5.80 | 1.12 | 1.23 |
| 1 | A | 20 | HIS | C-N | -5.79 | 1.20 | 1.34 |
| 1 | A | 51 | GLY | C-O | -5.79 | 1.14 | 1.23 |
| 2 | B | 35 | TYR | CZ-OH | 5.79 | 1.47 | 1.37 |
| 2 | B | 14 | LEU | CG-CD1 | -5.79 | 1.30 | 1.51 |
| 2 | B | 26 | GLU | CA-CB | -5.79 | 1.41 | 1.53 |
| 2 | B | 92 | HIS | CG-ND1 | 5.79 | 1.51 | 1.38 |
| 2 | D | 118 | PHE | C-O | 5.78 | 1.34 | 1.23 |
| 1 | C | 33 | PHE | CA-C | -5.78 | 1.38 | 1.52 |
| 1 | A | 6 | ASP | CA-CB | -5.78 | 1.41 | 1.53 |
| 2 | D | 139 | ASN | CB-CG | -5.78 | 1.37 | 1.51 |
| 1 | A | 24 | TYR | CD1-CE1 | 5.77 | 1.48 | 1.39 |
| 1 | C | 47 | ASP | CA-C | 5.77 | 1.68 | 1.52 |
| 1 | C | 29 | LEU | CA-CB | 5.76 | 1.67 | 1.53 |
| 1 | C | 61 | LYS | C-N | 5.76 | 1.47 | 1.34 |
| 2 | D | 60 | VAL | CB-CG1 | 5.76 | 1.65 | 1.52 |
| 1 | C | 121 | VAL | CA-CB | -5.75 | 1.42 | 1.54 |
| 1 | A | 28 | ALA | C-O | -5.75 | 1.12 | 1.23 |
| 2 | D | 103 | PHE | CB-CG | 5.75 | 1.61 | 1.51 |
| 1 | A | 47 | ASP | CA-CB | 5.74 | 1.66 | 1.53 |
| 2 | B | 72 | SER | C-O | 5.74 | 1.34 | 1.23 |
| 2 | D | 97 | HIS | C-N | 5.74 | 1.47 | 1.34 |
| 2 | D | 115 | ALA | C-O | -5.74 | 1.12 | 1.23 |
| 2 | D | 51 | PRO | CG-CD | 5.74 | 1.69 | 1.50 |
| 2 | D | 21 | ASP | N-CA | 5.73 | 1.57 | 1.46 |
| 2 | B | 33 | VAL | CB-CG2 | -5.72 | 1.40 | 1.52 |
| 1 | A | 112 | HIS | CA-CB | 5.72 | 1.66 | 1.53 |
| 1 | A | 33 | PHE | CD1-CE1 | 5.72 | 1.50 | 1.39 |
| 2 | B | 71 | PHE | CE1-CZ | -5.71 | 1.26 | 1.37 |
| 1 | C | 124 | SER | CB-OG | 5.71 | 1.49 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | C | 9 | ASN | CG-ND2 | -5.70 | 1.18 | 1.32 |
| 1 | A | 92 | ARG | N-CA | 5.70 | 1.57 | 1.46 |
| 2 | B | 87 | THR | CB-OG1 | -5.70 | 1.31 | 1.43 |
| 1 | A | 21 | ALA | CA-CB | -5.70 | 1.40 | 1.52 |
| 1 | A | 37 | PRO | CA-C | -5.69 | 1.41 | 1.52 |
| 2 | D | 90 | GLU | C-O | -5.69 | 1.12 | 1.23 |
| 2 | D | 145 | TYR | CG-CD2 | 5.69 | 1.46 | 1.39 |
| 1 | A | 36 | PHE | C-O | 5.69 | 1.34 | 1.23 |
| 1 | A | 59 | GLY | C-O | 5.69 | 1.32 | 1.23 |
| 1 | A | 5 | ALA | CA-C | 5.68 | 1.67 | 1.52 |
| 1 | A | 34 | LEU | CA-CB | -5.68 | 1.40 | 1.53 |
| 1 | C | 141 | ARG | CA-C | 5.68 | 1.67 | 1.52 |
| 1 | C | 141 | ARG | CZ-NH1 | -5.67 | 1.25 | 1.33 |
| 1 | C | 136 | LEU | C-O | 5.67 | 1.34 | 1.23 |
| 2 | B | 126 | VAL | C-N | -5.66 | 1.21 | 1.34 |
| 1 | C | 31 | ARG | CZ-NH2 | -5.66 | 1.25 | 1.33 |
| 1 | C | 33 | PHE | CE1-CZ | -5.66 | 1.26 | 1.37 |
| 1 | A | 78 | ASN | N-CA | -5.66 | 1.35 | 1.46 |
| 2 | B | 140 | ALA | C-O | 5.66 | 1.34 | 1.23 |
| 1 | C | 134 | THR | CB-OG1 | -5.65 | 1.31 | 1.43 |
| 2 | D | 85 | PHE | CG-CD1 | 5.65 | 1.47 | 1.38 |
| 1 | C | 46 | PHE | CA-C | -5.65 | 1.38 | 1.52 |
| 1 | C | 84 | SER | C-N | 5.65 | 1.47 | 1.34 |
| 1 | C | 54 | GLN | CA-CB | -5.64 | 1.41 | 1.53 |
| 2 | B | 62 | ALA | C-O | -5.64 | 1.12 | 1.23 |
| 1 | A | 109 | LEU | CG-CD1 | -5.64 | 1.30 | 1.51 |
| 1 | A | 75 | ASP | N-CA | 5.63 | 1.57 | 1.46 |
| 1 | C | 141 | ARG | CG-CD | 5.63 | 1.66 | 1.51 |
| 1 | A | 46 | PHE | N-CA | -5.62 | 1.35 | 1.46 |
| 2 | D | 30 | ARG | CG-CD | -5.62 | 1.38 | 1.51 |
| 1 | C | 129 | LEU | CA-CB | -5.62 | 1.40 | 1.53 |
| 1 | C | 28 | ALA | N-CA | 5.61 | 1.57 | 1.46 |
| 1 | C | 113 | LEU | C-N | -5.61 | 1.23 | 1.34 |
| 2 | D | 14 | LEU | CG-CD2 | -5.61 | 1.31 | 1.51 |
| 2 | B | 17 | LYS | CB-CG | 5.59 | 1.67 | 1.52 |
| 1 | C | 8 | THR | CB-CG2 | -5.59 | 1.33 | 1.52 |
| 1 | C | 134 | THR | C-O | 5.59 | 1.33 | 1.23 |
| 2 | B | 9 | SER | CB-OG | 5.58 | 1.49 | 1.42 |
| 2 | D | 49 | SER | CA-CB | 5.58 | 1.61 | 1.52 |
| 1 | A | 63 | ALA | CA-CB | 5.57 | 1.64 | 1.52 |
| 1 | A | 2 | LEU | N-CA | 5.57 | 1.57 | 1.46 |
| 1 | A | 115 | ALA | C-O | -5.57 | 1.12 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 71 | PHE | CD1-CE1 | 5.57 | 1.50 | 1.39 |
| 1 | C | 92 | ARG | C-N | 5.57 | 1.46 | 1.34 |
| 2 | B | 37 | TRP | CB-CG | -5.56 | 1.40 | 1.50 |
| 2 | B | 114 | LEU | CA-CB | -5.56 | 1.41 | 1.53 |
| 2 | D | 102 | ASN | CG-OD1 | -5.55 | 1.11 | 1.24 |
| 2 | B | 47 | ASP | CB-CG | -5.55 | 1.40 | 1.51 |
| 1 | C | 53 | ALA | CA-CB | -5.55 | 1.40 | 1.52 |
| 2 | D | 51 | PRO | N-CA | -5.54 | 1.37 | 1.47 |
| 2 | B | 92 | HIS | ND1-CE1 | 5.54 | 1.48 | 1.34 |
| 1 | C | 19 | ALA | CA-CB | -5.54 | 1.40 | 1.52 |
| 1 | C | 14 | TRP | CE3-CZ3 | 5.54 | 1.47 | 1.38 |
| 1 | A | 105 | LEU | CA-CB | 5.54 | 1.66 | 1.53 |
| 1 | A | 54 | GLN | CA-C | 5.54 | 1.67 | 1.52 |
| 1 | C | 13 | ALA | C-O | 5.54 | 1.33 | 1.23 |
| 1 | C | 30 | GLU | N-CA | -5.53 | 1.35 | 1.46 |
| 1 | C | 140 | TYR | C-O | 5.53 | 1.33 | 1.23 |
| 1 | A | 93 | VAL | CA-C | -5.53 | 1.38 | 1.52 |
| 2 | B | 43 | GLU | C-N | 5.53 | 1.46 | 1.34 |
| 2 | B | 120 | LYS | C-N | -5.53 | 1.21 | 1.34 |
| 1 | A | 9 | ASN | C-O | -5.52 | 1.12 | 1.23 |
| 1 | A | 48 | LEU | CG-CD1 | 5.52 | 1.72 | 1.51 |
| 2 | D | 99 | ASP | C-N | -5.51 | 1.23 | 1.34 |
| 2 | B | 119 | GLY | CA-C | -5.51 | 1.43 | 1.51 |
| 1 | C | 141 | ARG | NE-CZ | 5.50 | 1.40 | 1.33 |
| 2 | B | 28 | LEU | C-N | 5.50 | 1.43 | 1.33 |
| 2 | B | 116 | HIS | ND1-CE1 | 5.49 | 1.48 | 1.34 |
| 2 | B | 57 | ASN | N-CA | -5.49 | 1.35 | 1.46 |
| 1 | A | 123 | ALA | C-O | 5.49 | 1.33 | 1.23 |
| 1 | C | 97 | ASN | CA-CB | -5.49 | 1.38 | 1.53 |
| 2 | D | 71 | PHE | CG-CD2 | 5.48 | 1.47 | 1.38 |
| 2 | B | 30 | ARG | NE-CZ | -5.48 | 1.25 | 1.33 |
| 2 | D | 31 | LEU | C-N | 5.48 | 1.46 | 1.34 |
| 1 | A | 112 | HIS | C-O | 5.47 | 1.33 | 1.23 |
| 2 | D | 50 | THR | CB-OG1 | 5.47 | 1.54 | 1.43 |
| 1 | A | 72 | HIS | N-CA | -5.47 | 1.35 | 1.46 |
| 2 | B | 23 | VAL | C-N | -5.46 | 1.23 | 1.33 |
| 1 | A | 3 | SER | CA-C | -5.46 | 1.38 | 1.52 |
| 1 | C | 12 | ALA | CA-C | -5.46 | 1.38 | 1.52 |
| 1 | C | 135 | VAL | C-N | 5.46 | 1.46 | 1.34 |
| 1 | A | 43 | PHE | CB-CG | 5.46 | 1.60 | 1.51 |
| 2 | D | 59 | LYS | CE-NZ | 5.45 | 1.62 | 1.49 |
| 2 | B | 70 | ALA | N-CA | -5.45 | 1.35 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 74 | GLY | C-N | 5.45 | 1.46 | 1.34 |
| 2 | D | 17 | LYS | N-CA | -5.43 | 1.35 | 1.46 |
| 1 | A | 139 | LYS | CD-CE | -5.43 | 1.37 | 1.51 |
| 2 | B | 17 | LYS | CG-CD | -5.43 | 1.34 | 1.52 |
| 2 | B | 41 | PHE | C-N | -5.42 | 1.21 | 1.34 |
| 1 | A | 140 | TYR | C-N | -5.42 | 1.21 | 1.34 |
| 1 | A | 87 | HIS | CG-ND1 | 5.42 | 1.50 | 1.38 |
| 2 | B | 68 | LEU | C-O | 5.42 | 1.33 | 1.23 |
| 1 | C | 46 | PHE | C-O | 5.42 | 1.33 | 1.23 |
| 1 | A | 129 | LEU | CA-C | -5.41 | 1.38 | 1.52 |
| 2 | D | 92 | HIS | N-CA | 5.41 | 1.57 | 1.46 |
| 2 | D | 60 | VAL | CB-CG2 | -5.41 | 1.41 | 1.52 |
| 2 | B | 109 | VAL | C-O | 5.39 | 1.33 | 1.23 |
| 2 | B | 23 | VAL | CA-C | 5.39 | 1.67 | 1.52 |
| 2 | B | 144 | LYS | CB-CG | 5.39 | 1.67 | 1.52 |
| 1 | A | 61 | LYS | CB-CG | 5.39 | 1.67 | 1.52 |
| 1 | A | 141 | ARG | CZ-NH2 | 5.38 | 1.40 | 1.33 |
| 1 | C | 37 | PRO | CA-C | 5.38 | 1.63 | 1.52 |
| 2 | D | 42 | PHE | CD1-CE1 | 5.38 | 1.50 | 1.39 |
| 1 | A | 39 | THR | C-N | -5.38 | 1.21 | 1.34 |
| 2 | B | 100 | PRO | C-O | 5.38 | 1.34 | 1.23 |
| 1 | C | 139 | LYS | CB-CG | 5.38 | 1.67 | 1.52 |
| 2 | D | 104 | ARG | CB-CG | -5.38 | 1.38 | 1.52 |
| 1 | C | 109 | LEU | CG-CD2 | -5.38 | 1.31 | 1.51 |
| 2 | B | 6 | GLU | CA-CB | 5.37 | 1.65 | 1.53 |
| 2 | B | 33 | VAL | CA-C | 5.37 | 1.66 | 1.52 |
| 1 | C | 38 | THR | N-CA | 5.37 | 1.57 | 1.46 |
| 1 | A | 91 | LEU | CG-CD1 | -5.36 | 1.32 | 1.51 |
| 1 | C | 89 | HIS | C-N | -5.36 | 1.21 | 1.34 |
| 1 | A | 85 | ASP | C-O | -5.36 | 1.13 | 1.23 |
| 1 | C | 4 | PRO | CA-CB | 5.36 | 1.64 | 1.53 |
| 1 | A | 91 | LEU | CA-CB | 5.36 | 1.66 | 1.53 |
| 1 | C | 46 | PHE | N-CA | -5.36 | 1.35 | 1.46 |
| 1 | C | 35 | SER | C-N | 5.35 | 1.46 | 1.34 |
| 2 | B | 17 | LYS | CA-C | -5.35 | 1.39 | 1.52 |
| 2 | D | 49 | SER | N-CA | 5.34 | 1.57 | 1.46 |
| 2 | B | 48 | LEU | CG-CD2 | -5.34 | 1.32 | 1.51 |
| 2 | B | 15 | TRP | CA-CB | -5.34 | 1.42 | 1.53 |
| 2 | B | 57 | ASN | C-O | 5.34 | 1.33 | 1.23 |
| 2 | B | 112 | CYS | C-N | -5.33 | 1.21 | 1.34 |
| 2 | D | 35 | TYR | CD1-CE1 | 5.33 | 1.47 | 1.39 |
| 2 | D | 102 | ASN | CG-ND2 | 5.32 | 1.46 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 52 | SER | C-N | 5.32 | 1.46 | 1.34 |
| 2 | B | 13 | ALA | CA-C | -5.32 | 1.39 | 1.52 |
| 1 | C | 85 | ASP | CG-OD2 | 5.32 | 1.37 | 1.25 |
| 2 | B | 43 | GLU | N-CA | 5.31 | 1.56 | 1.46 |
| 1 | C | 115 | ALA | C-O | 5.31 | 1.33 | 1.23 |
| 1 | C | 12 | ALA | CA-CB | -5.31 | 1.41 | 1.52 |
| 1 | A | 21 | ALA | N-CA | 5.30 | 1.56 | 1.46 |
| 2 | B | 86 | ALA | CA-C | -5.29 | 1.39 | 1.52 |
| 1 | C | 54 | GLN | N-CA | 5.29 | 1.56 | 1.46 |
| 1 | A | 107 | VAL | CB-CG2 | 5.29 | 1.64 | 1.52 |
| 2 | B | 108 | ASN | CG-OD1 | 5.28 | 1.35 | 1.24 |
| 2 | D | 12 | THR | CB-OG1 | 5.28 | 1.53 | 1.43 |
| 1 | A | 84 | SER | C-O | -5.28 | 1.13 | 1.23 |
| 1 | C | 94 | ASP | N-CA | -5.27 | 1.35 | 1.46 |
| 2 | B | 101 | GLU | CA-CB | -5.27 | 1.42 | 1.53 |
| 1 | C | 5 | ALA | CA-C | 5.26 | 1.66 | 1.52 |
| 1 | A | 27 | GLU | CD-OE2 | -5.26 | 1.19 | 1.25 |
| 2 | B | 28 | LEU | CA-C | -5.26 | 1.39 | 1.52 |
| 2 | B | 63 | HIS | CE1-NE2 | -5.26 | 1.20 | 1.32 |
| 2 | D | 102 | ASN | N-CA | 5.26 | 1.56 | 1.46 |
| 1 | A | 14 | TRP | CA-C | 5.25 | 1.66 | 1.52 |
| 2 | B | 3 | LEU | CG-CD1 | -5.25 | 1.32 | 1.51 |
| 2 | B | 79 | ASP | C-N | 5.25 | 1.46 | 1.34 |
| 1 | A | 114 | PRO | C-O | -5.25 | 1.12 | 1.23 |
| 1 | C | 54 | GLN | CB-CG | -5.25 | 1.38 | 1.52 |
| 1 | C | 56 | LYS | C-N | 5.24 | 1.42 | 1.33 |
| 2 | D | 68 | LEU | CG-CD2 | -5.24 | 1.32 | 1.51 |
| 1 | C | 27 | GLU | C-N | 5.23 | 1.46 | 1.34 |
| 1 | C | 45 | HIS | CG-ND1 | 5.23 | 1.50 | 1.38 |
| 2 | B | 85 | PHE | CD2-CE2 | 5.22 | 1.49 | 1.39 |
| 1 | C | 29 | LEU | N-CA | 5.22 | 1.56 | 1.46 |
| 2 | B | 42 | PHE | C-N | -5.22 | 1.22 | 1.34 |
| 2 | B | 119 | GLY | C-N | -5.22 | 1.22 | 1.34 |
| 2 | B | 24 | GLY | N-CA | -5.22 | 1.38 | 1.46 |
| 1 | C | 82 | ALA | CA-C | -5.22 | 1.39 | 1.52 |
| 2 | B | 71 | PHE | CG-CD1 | -5.22 | 1.30 | 1.38 |
| 2 | B | 78 | LEU | CB-CG | 5.21 | 1.67 | 1.52 |
| 1 | C | 116 | GLU | C-N | -5.21 | 1.22 | 1.34 |
| 2 | D | 42 | PHE | CB-CG | 5.21 | 1.60 | 1.51 |
| 2 | D | 131 | GLN | CB-CG | -5.21 | 1.38 | 1.52 |
| 1 | A | 46 | PHE | C-N | 5.20 | 1.46 | 1.34 |
| 2 | D | 145 | TYR | CD1-CE1 | -5.19 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 116 | HIS | CB-CG | -5.19 | 1.40 | 1.50 |
| 2 | D | 91 | LEU | CG-CD1 | 5.19 | 1.71 | 1.51 |
| 2 | B | 122 | PHE | CE2-CZ | 5.18 | 1.47 | 1.37 |
| 1 | A | 107 | VAL | CB-CG1 | -5.18 | 1.42 | 1.52 |
| 2 | D | 112 | CYS | CA-C | 5.18 | 1.66 | 1.52 |
| 2 | D | 119 | GLY | C-N | 5.18 | 1.46 | 1.34 |
| 1 | C | 86 | LEU | N-CA | -5.17 | 1.36 | 1.46 |
| 1 | A | 88 | ALA | N-CA | 5.16 | 1.56 | 1.46 |
| 1 | C | 124 | SER | C-N | -5.16 | 1.22 | 1.34 |
| 2 | D | 31 | LEU | C-O | -5.16 | 1.13 | 1.23 |
| 2 | D | 102 | ASN | CA-CB | -5.16 | 1.39 | 1.53 |
| 1 | C | 114 | PRO | CG-CD | 5.15 | 1.67 | 1.50 |
| 1 | A | 79 | ALA | C-N | -5.14 | 1.22 | 1.34 |
| 2 | D | 77 | HIS | CA-C | 5.14 | 1.66 | 1.52 |
| 1 | A | 35 | SER | CA-CB | 5.14 | 1.60 | 1.52 |
| 1 | C | 55 | VAL | CB-CG2 | -5.14 | 1.42 | 1.52 |
| 2 | D | 16 | GLY | N-CA | 5.14 | 1.53 | 1.46 |
| 2 | D | 118 | PHE | CB-CG | 5.14 | 1.60 | 1.51 |
| 1 | A | 93 | VAL | C-O | 5.12 | 1.33 | 1.23 |
| 1 | A | 117 | PHE | CB-CG | 5.12 | 1.60 | 1.51 |
| 1 | A | 9 | ASN | CA-C | 5.12 | 1.66 | 1.52 |
| 1 | A | 135 | VAL | C-O | 5.12 | 1.33 | 1.23 |
| 2 | B | 67 | VAL | C-O | 5.12 | 1.33 | 1.23 |
| 1 | A | 75 | ASP | C-O | 5.11 | 1.33 | 1.23 |
| 2 | B | 30 | ARG | CZ-NH1 | 5.11 | 1.39 | 1.33 |
| 1 | A | 115 | ALA | N-CA | 5.11 | 1.56 | 1.46 |
| 2 | D | 144 | LYS | CA-C | -5.11 | 1.39 | 1.52 |
| 2 | B | 68 | LEU | CA-CB | -5.10 | 1.42 | 1.53 |
| 2 | D | 111 | VAL | C-N | 5.10 | 1.45 | 1.34 |
| 2 | B | 105 | LEU | CA-CB | -5.10 | 1.42 | 1.53 |
| 2 | D | 125 | PRO | C-N | 5.10 | 1.45 | 1.34 |
| 1 | C | 43 | PHE | CE1-CZ | 5.09 | 1.47 | 1.37 |
| 1 | C | 4 | PRO | C-N | -5.09 | 1.22 | 1.34 |
| 1 | A | 19 | ALA | CA-C | 5.09 | 1.66 | 1.52 |
| 1 | C | 73 | VAL | CB-CG2 | -5.09 | 1.42 | 1.52 |
| 1 | A | 121 | VAL | CB-CG1 | 5.09 | 1.63 | 1.52 |
| 1 | C | 58 | HIS | CA-CB | -5.09 | 1.42 | 1.53 |
| 1 | C | 85 | ASP | C-N | 5.08 | 1.45 | 1.34 |
| 1 | A | 63 | ALA | C-O | 5.08 | 1.33 | 1.23 |
| 1 | C | 66 | LEU | CG-CD1 | -5.07 | 1.33 | 1.51 |
| 2 | B | 64 | GLY | CA-C | -5.07 | 1.43 | 1.51 |
| 2 | D | 63 | HIS | CG-CD2 | 5.06 | 1.44 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 52 | ASP | CG-OD1 | -5.06 | 1.13 | 1.25 |
| 2 | B | 85 | PHE | N-CA | 5.05 | 1.56 | 1.46 |
| 2 | D | 57 | ASN | CG-ND2 | -5.05 | 1.20 | 1.32 |
| 1 | C | 86 | LEU | C-O | -5.05 | 1.13 | 1.23 |
| 1 | A | 69 | ALA | C-N | 5.04 | 1.45 | 1.34 |
| 1 | A | 112 | HIS | C-N | -5.04 | 1.22 | 1.34 |
| 1 | A | 137 | THR | C-N | -5.03 | 1.22 | 1.34 |
| 2 | B | 107 | GLY | C-O | 5.03 | 1.31 | 1.23 |
| 2 | B | 132 | LYS | C-N | 5.03 | 1.45 | 1.34 |
| 1 | A | 129 | LEU | CG-CD2 | 5.02 | 1.70 | 1.51 |
| 1 | A | 85 | ASP | C-N | 5.02 | 1.45 | 1.34 |
| 1 | A | 68 | ASN | CG-OD1 | -5.02 | 1.12 | 1.24 |
| 1 | C | 113 | LEU | CA-C | 5.02 | 1.66 | 1.52 |
| 1 | C | 43 | PHE | CG-CD1 | 5.01 | 1.46 | 1.38 |
| 1 | A | 54 | GLN | CD-NE2 | 5.01 | 1.45 | 1.32 |
| 2 | B | 103 | PHE | CD2-CE2 | 5.00 | 1.49 | 1.39 |
| 2 | D | 116 | HIS | C-O | 5.00 | 1.32 | 1.23 |

All (1823) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|---------|-------------|----------|
| 1 | C | 92 | ARG | NE-CZ-NH2 | -165.65 | 37.48 | 120.30 |
| 2 | D | 104 | ARG | NE-CZ-NH2 | -86.93 | 76.83 | 120.30 |
| 2 | D | 6 | GLU | OE1-CD-OE2 | -66.27 | 43.78 | 123.30 |
| 2 | D | 20 | VAL | CG1-CB-CG2 | -63.99 | 8.52 | 110.90 |
| 2 | D | 104 | ARG | NE-CZ-NH1 | -58.44 | 91.08 | 120.30 |
| 1 | A | 92 | ARG | NE-CZ-NH2 | -57.11 | 91.75 | 120.30 |
| 1 | C | 92 | ARG | NE-CZ-NH1 | -56.22 | 92.19 | 120.30 |
| 1 | A | 92 | ARG | CD-NE-CZ | -51.91 | 50.92 | 123.60 |
| 2 | B | 26 | GLU | OE1-CD-OE2 | -50.93 | 62.19 | 123.30 |
| 2 | B | 101 | GLU | OE1-CD-OE2 | 46.02 | 178.53 | 123.30 |
| 1 | A | 75 | ASP | CB-CG-OD2 | -43.83 | 78.85 | 118.30 |
| 2 | B | 22 | GLU | OE1-CD-OE2 | -43.42 | 71.19 | 123.30 |
| 2 | D | 73 | ASP | CB-CG-OD1 | 43.24 | 157.21 | 118.30 |
| 1 | A | 92 | ARG | NE-CZ-NH1 | -40.84 | 99.88 | 120.30 |
| 2 | D | 40 | ARG | NE-CZ-NH2 | -38.42 | 101.09 | 120.30 |
| 1 | A | 75 | ASP | CB-CG-OD1 | 38.31 | 152.78 | 118.30 |
| 2 | B | 104 | ARG | CD-NE-CZ | -37.22 | 71.50 | 123.60 |
| 1 | C | 1 | VAL | CG1-CB-CG2 | -35.84 | 53.56 | 110.90 |
| 2 | B | 40 | ARG | NE-CZ-NH2 | -35.62 | 102.49 | 120.30 |
| 2 | B | 104 | ARG | NE-CZ-NH2 | -34.69 | 102.95 | 120.30 |
| 2 | B | 143 | HIS | CG-ND1-CE1 | -34.66 | 59.68 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | C | 141 | ARG | NE-CZ-NH2 | -34.61 | 103.00 | 120.30 |
| 1 | C | 92 | ARG | CD-NE-CZ | -34.45 | 75.38 | 123.60 |
| 2 | D | 26 | GLU | OE1-CD-OE2 | -34.40 | 82.02 | 123.30 |
| 2 | B | 143 | HIS | ND1-CG-CD2 | 32.83 | 154.76 | 108.80 |
| 2 | B | 26 | GLU | CG-CD-OE2 | -32.52 | 53.26 | 118.30 |
| 1 | C | 75 | ASP | CB-CG-OD2 | -32.33 | 89.20 | 118.30 |
| 1 | C | 30 | GLU | OE1-CD-OE2 | 32.31 | 162.07 | 123.30 |
| 2 | D | 73 | ASP | CB-CG-OD2 | -31.97 | 89.53 | 118.30 |
| 2 | B | 30 | ARG | NE-CZ-NH2 | 31.85 | 136.23 | 120.30 |
| 2 | D | 52 | ASP | CB-CG-OD2 | -31.76 | 89.72 | 118.30 |
| 2 | B | 43 | GLU | OE1-CD-OE2 | 31.63 | 161.26 | 123.30 |
| 1 | A | 92 | ARG | CG-CD-NE | -31.16 | 46.35 | 111.80 |
| 2 | D | 58 | PRO | N-CD-CG | -30.97 | 56.75 | 103.20 |
| 2 | D | 30 | ARG | NE-CZ-NH1 | 29.94 | 135.27 | 120.30 |
| 2 | B | 5 | PRO | N-CA-CB | 29.91 | 139.19 | 103.30 |
| 1 | A | 92 | ARG | NH1-CZ-NH2 | 29.46 | 151.81 | 119.40 |
| 2 | D | 43 | GLU | OE1-CD-OE2 | -29.30 | 88.14 | 123.30 |
| 2 | D | 3 | LEU | O-C-N | -29.20 | 75.98 | 122.70 |
| 2 | D | 79 | ASP | CB-CG-OD2 | -29.16 | 92.06 | 118.30 |
| 1 | C | 23 | GLU | OE1-CD-OE2 | -28.52 | 89.08 | 123.30 |
| 2 | D | 20 | VAL | CA-CB-CG2 | -28.51 | 68.13 | 110.90 |
| 2 | D | 80 | ASN | CA-CB-CG | 28.39 | 175.86 | 113.40 |
| 2 | D | 101 | GLU | OE1-CD-OE2 | 28.06 | 156.98 | 123.30 |
| 2 | B | 42 | PHE | CB-CG-CD2 | 27.91 | 140.34 | 120.80 |
| 2 | D | 73 | ASP | OD1-CG-OD2 | -27.45 | 71.14 | 123.30 |
| 2 | B | 45 | PHE | CG-CD2-CE2 | 27.02 | 150.52 | 120.80 |
| 2 | D | 104 | ARG | CD-NE-CZ | -26.61 | 86.35 | 123.60 |
| 1 | C | 74 | ASP | CB-CG-OD2 | 25.98 | 141.69 | 118.30 |
| 1 | A | 75 | ASP | OD1-CG-OD2 | -25.96 | 73.98 | 123.30 |
| 1 | C | 1 | VAL | CA-CB-CG1 | -25.93 | 72.00 | 110.90 |
| 2 | B | 44 | SER | O-C-N | -25.83 | 81.38 | 122.70 |
| 2 | D | 52 | ASP | CB-CG-OD1 | -25.80 | 95.08 | 118.30 |
| 2 | D | 47 | ASP | O-C-N | 25.76 | 163.91 | 122.70 |
| 2 | B | 139 | ASN | OD1-CG-ND2 | -25.63 | 62.94 | 121.90 |
| 2 | D | 26 | GLU | CG-CD-OE1 | -25.55 | 67.20 | 118.30 |
| 1 | A | 31 | ARG | NE-CZ-NH2 | -25.32 | 107.64 | 120.30 |
| 2 | D | 26 | GLU | CB-CG-CD | -25.23 | 46.06 | 114.20 |
| 1 | A | 141 | ARG | NE-CZ-NH1 | 25.18 | 132.89 | 120.30 |
| 1 | C | 46 | PHE | CB-CG-CD2 | 25.10 | 138.37 | 120.80 |
| 2 | B | 43 | GLU | CG-CD-OE2 | -24.55 | 69.20 | 118.30 |
| 1 | A | 47 | ASP | CB-CG-OD2 | -24.55 | 96.21 | 118.30 |
| 2 | D | 94 | ASP | CB-CG-OD1 | -24.43 | 96.31 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | A | 72 | HIS | ND1-CG-CD2 | -24.25 | 72.06 | 106.00 |
| 2 | D | 43 | GLU | CA-CB-CG | 23.84 | 165.85 | 113.40 |
| 2 | D | 82 | LYS | CD-CE-NZ | -23.77 | 57.02 | 111.70 |
| 2 | D | 47 | ASP | N-CA-CB | -23.76 | 67.83 | 110.60 |
| 2 | D | 20 | VAL | CA-CB-CG1 | -23.54 | 75.59 | 110.90 |
| 2 | B | 45 | PHE | CZ-CE2-CD2 | -23.48 | 91.93 | 120.10 |
| 1 | A | 141 | ARG | NE-CZ-NH2 | -23.44 | 108.58 | 120.30 |
| 1 | C | 38 | THR | OG1-CB-CG2 | -23.39 | 56.20 | 110.00 |
| 2 | B | 12 | THR | OG1-CB-CG2 | 23.36 | 163.74 | 110.00 |
| 2 | B | 94 | ASP | CB-CG-OD1 | -23.18 | 97.44 | 118.30 |
| 1 | A | 64 | ASP | CB-CG-OD1 | -23.16 | 97.46 | 118.30 |
| 2 | D | 146 | HIS | ND1-CG-CD2 | -23.13 | 73.62 | 106.00 |
| 2 | D | 145 | TYR | CB-CG-CD1 | 23.04 | 134.83 | 121.00 |
| 2 | D | 47 | ASP | CB-CG-OD1 | -22.89 | 97.70 | 118.30 |
| 1 | C | 46 | PHE | CZ-CE2-CD2 | 22.88 | 147.55 | 120.10 |
| 1 | C | 1 | VAL | CA-CB-CG2 | -22.79 | 76.72 | 110.90 |
| 2 | B | 145 | TYR | CB-CG-CD2 | -22.52 | 107.48 | 121.00 |
| 2 | D | 6 | GLU | O-C-N | 22.45 | 158.63 | 122.70 |
| 1 | A | 46 | PHE | CB-CG-CD2 | 22.39 | 136.47 | 120.80 |
| 2 | D | 5 | PRO | N-CA-CB | -22.35 | 76.48 | 103.30 |
| 1 | C | 24 | TYR | CG-CD1-CE1 | -22.27 | 103.48 | 121.30 |
| 2 | B | 40 | ARG | NH1-CZ-NH2 | 22.23 | 143.86 | 119.40 |
| 2 | D | 90 | GLU | CG-CD-OE1 | -22.02 | 74.26 | 118.30 |
| 2 | D | 71 | PHE | CG-CD2-CE2 | -22.01 | 96.59 | 120.80 |
| 1 | A | 14 | TRP | CD1-NE1-CE2 | 21.98 | 128.78 | 109.00 |
| 2 | D | 42 | PHE | CB-CG-CD1 | -21.92 | 105.46 | 120.80 |
| 2 | B | 40 | ARG | NE-CZ-NH1 | -21.87 | 109.36 | 120.30 |
| 2 | D | 55 | MET | O-C-N | 21.86 | 160.37 | 123.20 |
| 2 | D | 26 | GLU | CG-CD-OE2 | -21.76 | 74.78 | 118.30 |
| 2 | B | 52 | ASP | CB-CG-OD2 | -21.74 | 98.73 | 118.30 |
| 2 | D | 17 | LYS | O-C-N | -21.70 | 87.99 | 122.70 |
| 1 | A | 138 | SER | CA-CB-OG | -21.69 | 52.63 | 111.20 |
| 2 | D | 79 | ASP | OD1-CG-OD2 | -21.68 | 82.10 | 123.30 |
| 1 | C | 73 | VAL | CG1-CB-CG2 | 21.66 | 145.56 | 110.90 |
| 2 | B | 1 | VAL | CG1-CB-CG2 | 21.62 | 145.49 | 110.90 |
| 2 | B | 49 | SER | O-C-N | -21.42 | 88.43 | 122.70 |
| 2 | D | 76 | ALA | N-CA-CB | -21.36 | 80.19 | 110.10 |
| 1 | C | 138 | SER | CA-CB-OG | -21.29 | 53.73 | 111.20 |
| 2 | B | 101 | GLU | CG-CD-OE2 | -21.23 | 75.83 | 118.30 |
| 1 | C | 14 | TRP | CD1-NE1-CE2 | 21.02 | 127.91 | 109.00 |
| 2 | D | 45 | PHE | CB-CG-CD2 | 20.98 | 135.49 | 120.80 |
| 2 | D | 55 | MET | C-N-CA | -20.95 | 78.31 | 122.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 64 | ASP | CB-CG-OD2 | -20.92 | 99.47 | 118.30 |
| 2 | B | 26 | GLU | CB-CG-CD | 20.80 | 170.36 | 114.20 |
| 2 | B | 42 | PHE | CD1-CE1-CZ | 20.70 | 144.95 | 120.10 |
| 2 | D | 41 | PHE | CG-CD1-CE1 | -20.56 | 98.18 | 120.80 |
| 2 | D | 118 | PHE | CB-CG-CD1 | 20.55 | 135.19 | 120.80 |
| 1 | C | 128 | PHE | CB-CG-CD2 | -20.23 | 106.64 | 120.80 |
| 1 | C | 14 | TRP | CG-CD1-NE1 | -20.13 | 89.97 | 110.10 |
| 1 | C | 23 | GLU | CG-CD-OE1 | -20.04 | 78.22 | 118.30 |
| 2 | D | 72 | SER | N-CA-CB | 19.95 | 140.43 | 110.50 |
| 1 | A | 12 | ALA | CB-CA-C | -19.65 | 80.62 | 110.10 |
| 1 | C | 47 | ASP | CB-CG-OD2 | -19.45 | 100.79 | 118.30 |
| 1 | C | 1 | VAL | N-CA-CB | -19.31 | 69.02 | 111.50 |
| 1 | C | 24 | TYR | CZ-CE2-CD2 | -19.11 | 102.60 | 119.80 |
| 2 | B | 21 | ASP | CB-CG-OD2 | -18.95 | 101.24 | 118.30 |
| 1 | A | 90 | LYS | CD-CE-NZ | -18.86 | 68.32 | 111.70 |
| 1 | A | 2 | LEU | O-C-N | 18.85 | 152.86 | 122.70 |
| 2 | D | 118 | PHE | CG-CD1-CE1 | 18.84 | 141.52 | 120.80 |
| 1 | C | 128 | PHE | CD1-CG-CD2 | 18.79 | 142.72 | 118.30 |
| 2 | D | 19 | ASN | OD1-CG-ND2 | -18.78 | 78.71 | 121.90 |
| 2 | D | 101 | GLU | CG-CD-OE2 | -18.71 | 80.88 | 118.30 |
| 2 | D | 94 | ASP | CB-CG-OD2 | -18.70 | 101.47 | 118.30 |
| 1 | A | 75 | ASP | CA-CB-CG | -18.58 | 72.52 | 113.40 |
| 2 | D | 78 | LEU | CB-CG-CD2 | 18.57 | 142.56 | 111.00 |
| 2 | D | 42 | PHE | CG-CD1-CE1 | -18.55 | 100.40 | 120.80 |
| 2 | D | 41 | PHE | CD1-CE1-CZ | 18.47 | 142.26 | 120.10 |
| 2 | D | 145 | TYR | CB-CG-CD2 | -18.45 | 109.93 | 121.00 |
| 2 | B | 108 | ASN | OD1-CG-ND2 | 18.43 | 164.28 | 121.90 |
| 2 | D | 56 | GLY | O-C-N | -18.39 | 93.28 | 122.70 |
| 1 | C | 128 | PHE | CG-CD1-CE1 | -18.19 | 100.80 | 120.80 |
| 2 | B | 22 | GLU | CG-CD-OE2 | -18.14 | 82.02 | 118.30 |
| 1 | C | 47 | ASP | CB-CG-OD1 | -18.10 | 102.01 | 118.30 |
| 2 | D | 46 | GLY | C-N-CA | -18.04 | 76.60 | 121.70 |
| 1 | A | 85 | ASP | CB-CG-OD1 | 17.99 | 134.49 | 118.30 |
| 1 | A | 17 | VAL | O-C-N | 17.92 | 153.67 | 123.20 |
| 2 | B | 144 | LYS | CG-CD-CE | 17.88 | 165.54 | 111.90 |
| 2 | B | 45 | PHE | CB-CG-CD2 | 17.87 | 133.31 | 120.80 |
| 1 | A | 49 | SER | CB-CA-C | 17.80 | 143.92 | 110.10 |
| 1 | C | 74 | ASP | OD1-CG-OD2 | -17.77 | 89.54 | 123.30 |
| 1 | C | 116 | GLU | CG-CD-OE2 | -17.75 | 82.79 | 118.30 |
| 1 | C | 16 | LYS | N-CA-CB | 17.66 | 142.39 | 110.60 |
| 2 | B | 65 | LYS | CD-CE-NZ | -17.59 | 71.24 | 111.70 |
| 2 | B | 50 | THR | CA-CB-CG2 | 17.58 | 137.02 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 6 | GLU | OE1-CD-OE2 | -17.57 | 102.21 | 123.30 |
| 1 | A | 22 | GLY | O-C-N | -17.57 | 94.58 | 122.70 |
| 2 | D | 44 | SER | O-C-N | -17.49 | 94.72 | 122.70 |
| 1 | A | 30 | GLU | OE1-CD-OE2 | 17.45 | 144.24 | 123.30 |
| 2 | B | 59 | LYS | CD-CE-NZ | -17.45 | 71.57 | 111.70 |
| 2 | D | 132 | LYS | CD-CE-NZ | -17.44 | 71.58 | 111.70 |
| 1 | A | 128 | PHE | CZ-CE2-CD2 | -17.39 | 99.23 | 120.10 |
| 1 | A | 31 | ARG | NE-CZ-NH1 | 17.39 | 129.00 | 120.30 |
| 2 | D | 17 | LYS | CA-C-O | 17.32 | 156.46 | 120.10 |
| 1 | A | 1 | VAL | CA-CB-CG2 | -17.30 | 84.96 | 110.90 |
| 2 | B | 21 | ASP | CB-CG-OD1 | -17.20 | 102.82 | 118.30 |
| 1 | A | 1 | VAL | CG1-CB-CG2 | 17.16 | 138.36 | 110.90 |
| 2 | D | 130 | TYR | CG-CD1-CE1 | 17.12 | 135.00 | 121.30 |
| 1 | A | 33 | PHE | CB-CG-CD1 | 17.08 | 132.76 | 120.80 |
| 1 | A | 23 | GLU | CG-CD-OE1 | -17.05 | 84.20 | 118.30 |
| 2 | D | 58 | PRO | CA-CB-CG | -16.98 | 71.73 | 104.00 |
| 2 | B | 139 | ASN | CB-CG-OD1 | 16.96 | 155.53 | 121.60 |
| 2 | B | 2 | HIS | CB-CA-C | -16.86 | 76.68 | 110.40 |
| 1 | A | 72 | HIS | CA-CB-CG | -16.82 | 85.01 | 113.60 |
| 2 | D | 18 | VAL | O-C-N | 16.82 | 149.60 | 122.70 |
| 2 | B | 4 | THR | CA-CB-CG2 | 16.73 | 135.82 | 112.40 |
| 1 | C | 22 | GLY | O-C-N | -16.72 | 95.94 | 122.70 |
| 2 | D | 130 | TYR | CD1-CE1-CZ | -16.62 | 104.84 | 119.80 |
| 2 | B | 74 | GLY | CA-C-O | 16.59 | 150.46 | 120.60 |
| 1 | C | 14 | TRP | CE3-CZ3-CH2 | -16.59 | 102.95 | 121.20 |
| 2 | B | 94 | ASP | OD1-CG-OD2 | 16.57 | 154.79 | 123.30 |
| 1 | C | 139 | LYS | CD-CE-NZ | -16.57 | 73.59 | 111.70 |
| 2 | B | 121 | GLU | CG-CD-OE2 | -16.55 | 85.20 | 118.30 |
| 1 | A | 60 | LYS | CD-CE-NZ | -16.50 | 73.75 | 111.70 |
| 1 | C | 64 | ASP | CB-CG-OD2 | -16.48 | 103.47 | 118.30 |
| 2 | B | 20 | VAL | O-C-N | -16.43 | 96.41 | 122.70 |
| 1 | C | 14 | TRP | C-N-CA | 16.34 | 156.60 | 122.30 |
| 1 | C | 61 | LYS | CD-CE-NZ | -16.32 | 74.17 | 111.70 |
| 1 | C | 46 | PHE | CE1-CZ-CE2 | -16.29 | 90.68 | 120.00 |
| 1 | A | 17 | VAL | CA-C-N | -16.28 | 83.64 | 116.20 |
| 1 | A | 16 | LYS | CG-CD-CE | -16.18 | 63.34 | 111.90 |
| 1 | A | 12 | ALA | O-C-N | -16.17 | 96.83 | 122.70 |
| 2 | B | 118 | PHE | CB-CG-CD2 | 16.17 | 132.12 | 120.80 |
| 2 | D | 8 | LYS | CA-CB-CG | -16.15 | 77.88 | 113.40 |
| 1 | C | 128 | PHE | CG-CD2-CE2 | -16.07 | 103.12 | 120.80 |
| 1 | C | 14 | TRP | O-C-N | -16.05 | 95.92 | 123.20 |
| 1 | A | 78 | ASN | OD1-CG-ND2 | -16.05 | 84.99 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | C | 56 | LYS | CD-CE-NZ | -16.03 | 74.83 | 111.70 |
| 2 | B | 1 | VAL | C-N-CA | -16.02 | 81.66 | 121.70 |
| 2 | D | 78 | LEU | CA-C-O | 16.02 | 153.73 | 120.10 |
| 2 | B | 85 | PHE | CZ-CE2-CD2 | 16.01 | 139.31 | 120.10 |
| 2 | D | 47 | ASP | CA-C-N | -16.00 | 82.00 | 117.20 |
| 2 | D | 46 | GLY | CA-C-O | -15.99 | 91.81 | 120.60 |
| 2 | D | 13 | ALA | N-CA-CB | 15.97 | 132.46 | 110.10 |
| 2 | D | 94 | ASP | OD1-CG-OD2 | 15.88 | 153.46 | 123.30 |
| 2 | B | 65 | LYS | CG-CD-CE | -15.84 | 64.38 | 111.90 |
| 2 | D | 12 | THR | CA-CB-CG2 | -15.73 | 90.38 | 112.40 |
| 1 | C | 24 | TYR | CE1-CZ-CE2 | 15.68 | 144.88 | 119.80 |
| 1 | A | 18 | GLY | O-C-N | 15.67 | 147.77 | 122.70 |
| 1 | A | 43 | PHE | CB-CG-CD2 | 15.66 | 131.76 | 120.80 |
| 2 | B | 32 | LEU | CB-CG-CD1 | 15.64 | 137.60 | 111.00 |
| 2 | D | 76 | ALA | CA-C-N | 15.57 | 151.46 | 117.20 |
| 2 | D | 76 | ALA | O-C-N | -15.56 | 97.80 | 122.70 |
| 1 | C | 23 | GLU | CG-CD-OE2 | -15.53 | 87.24 | 118.30 |
| 2 | B | 73 | ASP | O-C-N | -15.52 | 96.82 | 123.20 |
| 1 | C | 71 | ALA | CB-CA-C | 15.47 | 133.31 | 110.10 |
| 2 | D | 71 | PHE | CD1-CG-CD2 | 15.47 | 138.41 | 118.30 |
| 2 | B | 117 | HIS | CG-CD2-NE2 | -15.46 | 79.82 | 109.20 |
| 2 | D | 71 | PHE | CB-CG-CD2 | -15.45 | 109.98 | 120.80 |
| 2 | D | 2 | HIS | CE1-NE2-CD2 | 15.45 | 145.22 | 106.60 |
| 2 | D | 77 | HIS | CG-CD2-NE2 | -15.44 | 79.87 | 109.20 |
| 2 | B | 74 | GLY | O-C-N | -15.42 | 98.03 | 122.70 |
| 1 | C | 7 | LYS | CD-CE-NZ | 15.42 | 147.16 | 111.70 |
| 1 | C | 75 | ASP | OD1-CG-OD2 | 15.41 | 152.58 | 123.30 |
| 2 | D | 43 | GLU | O-C-N | 15.41 | 147.35 | 122.70 |
| 2 | D | 6 | GLU | CG-CD-OE2 | -15.40 | 87.49 | 118.30 |
| 1 | C | 85 | ASP | CB-CG-OD1 | 15.40 | 132.16 | 118.30 |
| 1 | A | 98 | PHE | CB-CG-CD1 | -15.40 | 110.02 | 120.80 |
| 1 | A | 33 | PHE | CB-CG-CD2 | -15.32 | 110.08 | 120.80 |
| 2 | D | 146 | HIS | CG-CD2-NE2 | 15.29 | 138.24 | 109.20 |
| 2 | D | 47 | ASP | N-CA-C | -15.28 | 69.75 | 111.00 |
| 2 | B | 2 | HIS | CG-ND1-CE1 | -15.25 | 85.88 | 105.70 |
| 2 | D | 139 | ASN | CB-CG-OD1 | -15.19 | 91.22 | 121.60 |
| 1 | C | 56 | LYS | CG-CD-CE | -15.18 | 66.36 | 111.90 |
| 1 | A | 81 | SER | N-CA-CB | -15.14 | 87.78 | 110.50 |
| 1 | C | 45 | HIS | CG-ND1-CE1 | -15.08 | 86.09 | 105.70 |
| 2 | D | 47 | ASP | CB-CA-C | -15.08 | 80.24 | 110.40 |
| 2 | D | 1 | VAL | CA-C-N | -15.07 | 84.04 | 117.20 |
| 2 | B | 37 | TRP | CD1-NE1-CE2 | 15.07 | 122.56 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | D | 1 | VAL | O-C-N | 14.88 | 146.51 | 122.70 |
| 2 | D | 121 | GLU | OE1-CD-OE2 | -14.85 | 105.48 | 123.30 |
| 2 | D | 41 | PHE | O-C-N | 14.82 | 146.41 | 122.70 |
| 1 | A | 137 | THR | CA-CB-OG1 | -14.81 | 77.90 | 109.00 |
| 2 | D | 79 | ASP | CB-CA-C | -14.74 | 80.92 | 110.40 |
| 2 | B | 56 | GLY | O-C-N | -14.70 | 99.19 | 122.70 |
| 2 | D | 90 | GLU | OE1-CD-OE2 | -14.68 | 105.68 | 123.30 |
| 2 | D | 50 | THR | N-CA-CB | -14.67 | 82.42 | 110.30 |
| 1 | C | 73 | VAL | CA-CB-CG1 | -14.66 | 88.90 | 110.90 |
| 2 | B | 58 | PRO | N-CD-CG | -14.64 | 81.24 | 103.20 |
| 1 | C | 128 | PHE | CB-CG-CD1 | -14.64 | 110.55 | 120.80 |
| 1 | C | 98 | PHE | CZ-CE2-CD2 | 14.63 | 137.65 | 120.10 |
| 1 | C | 72 | HIS | ND1-CG-CD2 | -14.60 | 85.56 | 106.00 |
| 2 | D | 59 | LYS | O-C-N | 14.53 | 145.94 | 122.70 |
| 1 | C | 12 | ALA | CA-C-O | 14.50 | 150.54 | 120.10 |
| 2 | B | 145 | TYR | CG-CD2-CE2 | -14.45 | 109.74 | 121.30 |
| 2 | D | 30 | ARG | NH1-CZ-NH2 | -14.43 | 103.53 | 119.40 |
| 1 | A | 46 | PHE | CG-CD2-CE2 | 14.40 | 136.64 | 120.80 |
| 2 | D | 101 | GLU | CG-CD-OE1 | -14.37 | 89.56 | 118.30 |
| 2 | D | 71 | PHE | CB-CG-CD1 | -14.35 | 110.75 | 120.80 |
| 1 | A | 116 | GLU | OE1-CD-OE2 | -14.33 | 106.10 | 123.30 |
| 1 | C | 71 | ALA | O-C-N | -14.28 | 99.85 | 122.70 |
| 1 | A | 85 | ASP | CB-CG-OD2 | -14.27 | 105.46 | 118.30 |
| 2 | B | 132 | LYS | CD-CE-NZ | -14.19 | 79.06 | 111.70 |
| 2 | B | 49 | SER | C-N-CA | 14.17 | 157.13 | 121.70 |
| 2 | D | 77 | HIS | ND1-CG-CD2 | 14.17 | 128.64 | 108.80 |
| 2 | D | 80 | ASN | OD1-CG-ND2 | 14.13 | 154.40 | 121.90 |
| 2 | B | 87 | THR | OG1-CB-CG2 | -14.12 | 77.53 | 110.00 |
| 1 | A | 47 | ASP | CB-CG-OD1 | 14.09 | 130.98 | 118.30 |
| 2 | B | 26 | GLU | CG-CD-OE1 | -14.09 | 90.13 | 118.30 |
| 1 | A | 50 | HIS | N-CA-CB | -14.07 | 85.28 | 110.60 |
| 1 | C | 43 | PHE | CG-CD2-CE2 | -14.04 | 105.36 | 120.80 |
| 2 | B | 146 | HIS | CG-CD2-NE2 | -14.03 | 82.54 | 109.20 |
| 1 | A | 62 | VAL | O-C-N | 14.02 | 145.12 | 122.70 |
| 2 | B | 146 | HIS | ND1-CE1-NE2 | -14.00 | 79.09 | 109.90 |
| 2 | D | 73 | ASP | O-C-N | -13.94 | 99.50 | 123.20 |
| 2 | B | 94 | ASP | CB-CG-OD2 | -13.93 | 105.76 | 118.30 |
| 1 | A | 21 | ALA | CA-C-N | -13.89 | 88.42 | 116.20 |
| 1 | C | 43 | PHE | CZ-CE2-CD2 | 13.85 | 136.72 | 120.10 |
| 2 | B | 77 | HIS | CG-CD2-NE2 | -13.84 | 82.91 | 109.20 |
| 2 | D | 20 | VAL | CA-C-O | 13.76 | 148.99 | 120.10 |
| 2 | B | 145 | TYR | CD1-CG-CD2 | 13.75 | 133.03 | 117.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | D | 43 | GLU | CG-CD-OE2 | 13.75 | 145.79 | 118.30 |
| 1 | C | 14 | TRP | NE1-CE2-CZ2 | 13.74 | 145.51 | 130.40 |
| 1 | C | 78 | ASN | CA-C-O | 13.74 | 148.95 | 120.10 |
| 1 | A | 21 | ALA | C-N-CA | -13.72 | 93.49 | 122.30 |
| 2 | D | 66 | LYS | CA-CB-CG | 13.70 | 143.54 | 113.40 |
| 1 | C | 25 | GLY | O-C-N | -13.69 | 100.80 | 122.70 |
| 2 | B | 28 | LEU | CB-CG-CD2 | -13.69 | 87.73 | 111.00 |
| 1 | A | 33 | PHE | CG-CD2-CE2 | -13.68 | 105.75 | 120.80 |
| 2 | B | 121 | GLU | CG-CD-OE1 | -13.68 | 90.95 | 118.30 |
| 1 | A | 58 | HIS | O-C-N | 13.68 | 146.45 | 123.20 |
| 2 | D | 73 | ASP | CA-CB-CG | -13.58 | 83.52 | 113.40 |
| 1 | C | 48 | LEU | O-C-N | -13.57 | 100.99 | 122.70 |
| 1 | A | 14 | TRP | CG-CD1-NE1 | -13.54 | 96.56 | 110.10 |
| 2 | B | 22 | GLU | CG-CD-OE1 | -13.54 | 91.22 | 118.30 |
| 1 | C | 33 | PHE | CB-CG-CD1 | -13.54 | 111.32 | 120.80 |
| 2 | B | 41 | PHE | O-C-N | 13.51 | 144.31 | 122.70 |
| 1 | A | 50 | HIS | C-N-CA | 13.46 | 150.57 | 122.30 |
| 2 | B | 44 | SER | CA-CB-OG | 13.45 | 147.52 | 111.20 |
| 2 | B | 45 | PHE | CB-CG-CD1 | -13.44 | 111.39 | 120.80 |
| 2 | D | 32 | LEU | CB-CG-CD2 | 13.44 | 133.84 | 111.00 |
| 2 | B | 108 | ASN | CB-CG-ND2 | -13.42 | 84.50 | 116.70 |
| 2 | D | 146 | HIS | CE1-NE2-CD2 | -13.41 | 73.07 | 106.60 |
| 2 | D | 46 | GLY | O-C-N | 13.41 | 144.15 | 122.70 |
| 2 | B | 143 | HIS | CB-CG-ND1 | -13.41 | 89.68 | 123.20 |
| 2 | D | 118 | PHE | CD1-CE1-CZ | -13.40 | 104.02 | 120.10 |
| 2 | D | 2 | HIS | O-C-N | 13.40 | 144.13 | 122.70 |
| 2 | D | 8 | LYS | O-C-N | -13.39 | 101.28 | 122.70 |
| 1 | C | 16 | LYS | CB-CG-CD | -13.38 | 76.81 | 111.60 |
| 2 | B | 49 | SER | CA-C-O | -13.37 | 92.03 | 120.10 |
| 1 | A | 21 | ALA | CB-CA-C | 13.36 | 130.14 | 110.10 |
| 1 | C | 46 | PHE | CD1-CG-CD2 | -13.35 | 100.94 | 118.30 |
| 1 | C | 24 | TYR | CD1-CG-CD2 | 13.34 | 132.57 | 117.90 |
| 2 | D | 67 | VAL | CG1-CB-CG2 | 13.34 | 132.24 | 110.90 |
| 2 | B | 49 | SER | CB-CA-C | -13.33 | 84.78 | 110.10 |
| 2 | D | 10 | ALA | CB-CA-C | -13.31 | 90.14 | 110.10 |
| 2 | D | 22 | GLU | CG-CD-OE2 | -13.28 | 91.74 | 118.30 |
| 2 | B | 117 | HIS | CB-CG-ND1 | -13.23 | 90.12 | 123.20 |
| 1 | A | 140 | TYR | CB-CG-CD2 | 13.23 | 128.94 | 121.00 |
| 1 | A | 14 | TRP | CH2-CZ2-CE2 | 13.21 | 130.61 | 117.40 |
| 1 | A | 110 | ALA | O-C-N | -13.19 | 101.60 | 122.70 |
| 2 | D | 37 | TRP | CZ3-CH2-CZ2 | 13.11 | 137.34 | 121.60 |
| 2 | B | 5 | PRO | CA-N-CD | -13.09 | 93.17 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 125 | PRO | N-CA-CB | 13.08 | 119.00 | 103.30 |
| 2 | D | 121 | GLU | CG-CD-OE2 | -13.07 | 92.16 | 118.30 |
| 2 | D | 76 | ALA | CB-CA-C | 13.05 | 129.67 | 110.10 |
| 2 | D | 77 | HIS | CB-CA-C | -13.01 | 84.38 | 110.40 |
| 2 | D | 73 | ASP | CA-C-O | 12.96 | 147.31 | 120.10 |
| 1 | C | 140 | TYR | CB-CG-CD1 | 12.93 | 128.76 | 121.00 |
| 2 | B | 146 | HIS | ND1-CG-CD2 | -12.92 | 87.91 | 106.00 |
| 2 | D | 45 | PHE | CG-CD2-CE2 | 12.91 | 135.00 | 120.80 |
| 2 | B | 8 | LYS | O-C-N | -12.88 | 102.09 | 122.70 |
| 2 | D | 79 | ASP | N-CA-CB | -12.88 | 87.41 | 110.60 |
| 1 | C | 46 | PHE | O-C-N | -12.88 | 102.10 | 122.70 |
| 1 | C | 85 | ASP | CB-CG-OD2 | -12.87 | 106.71 | 118.30 |
| 1 | C | 19 | ALA | O-C-N | -12.85 | 102.14 | 122.70 |
| 2 | D | 99 | ASP | CB-CG-OD1 | -12.84 | 106.74 | 118.30 |
| 1 | C | 15 | GLY | C-N-CA | 12.82 | 153.75 | 121.70 |
| 2 | B | 37 | TRP | CH2-CZ2-CE2 | -12.79 | 104.61 | 117.40 |
| 1 | C | 31 | ARG | NE-CZ-NH2 | -12.79 | 113.90 | 120.30 |
| 1 | A | 61 | LYS | O-C-N | 12.79 | 143.17 | 122.70 |
| 2 | B | 76 | ALA | CB-CA-C | -12.78 | 90.93 | 110.10 |
| 1 | A | 48 | LEU | CB-CG-CD2 | 12.72 | 132.62 | 111.00 |
| 1 | A | 74 | ASP | CA-C-N | 12.70 | 145.14 | 117.20 |
| 2 | B | 87 | THR | CA-CB-CG2 | -12.70 | 94.63 | 112.40 |
| 1 | C | 30 | GLU | CG-CD-OE1 | -12.70 | 92.91 | 118.30 |
| 1 | C | 113 | LEU | CB-CG-CD1 | -12.69 | 89.42 | 111.00 |
| 2 | D | 7 | GLU | CG-CD-OE1 | -12.69 | 92.93 | 118.30 |
| 1 | C | 70 | VAL | O-C-N | 12.67 | 142.98 | 122.70 |
| 1 | C | 64 | ASP | CB-CG-OD1 | -12.67 | 106.89 | 118.30 |
| 2 | D | 20 | VAL | O-C-N | -12.63 | 102.50 | 122.70 |
| 2 | D | 118 | PHE | CB-CG-CD2 | -12.62 | 111.97 | 120.80 |
| 1 | A | 46 | PHE | CD1-CG-CD2 | -12.60 | 101.92 | 118.30 |
| 1 | C | 50 | HIS | CG-CD2-NE2 | 12.60 | 133.14 | 109.20 |
| 2 | D | 49 | SER | C-N-CA | -12.58 | 90.26 | 121.70 |
| 2 | D | 71 | PHE | CG-CD1-CE1 | -12.54 | 107.00 | 120.80 |
| 2 | D | 37 | TRP | CH2-CZ2-CE2 | -12.54 | 104.86 | 117.40 |
| 2 | D | 145 | TYR | CG-CD1-CE1 | 12.54 | 131.33 | 121.30 |
| 1 | A | 24 | TYR | CZ-CE2-CD2 | -12.53 | 108.52 | 119.80 |
| 2 | D | 7 | GLU | CG-CD-OE2 | 12.52 | 143.34 | 118.30 |
| 1 | C | 14 | TRP | CB-CG-CD1 | -12.52 | 110.73 | 127.00 |
| 1 | C | 84 | SER | N-CA-CB | 12.51 | 129.27 | 110.50 |
| 2 | B | 1 | VAL | CA-C-N | -12.51 | 89.69 | 117.20 |
| 2 | D | 63 | HIS | CG-CD2-NE2 | -12.49 | 85.46 | 109.20 |
| 2 | B | 146 | HIS | CB-CG-CD2 | -12.49 | 92.09 | 130.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | C | 33 | PHE | CG-CD2-CE2 | -12.49 | 107.06 | 120.80 |
| 1 | C | 14 | TRP | CD1-CG-CD2 | 12.46 | 116.27 | 106.30 |
| 2 | D | 97 | HIS | CG-CD2-NE2 | -12.46 | 85.54 | 109.20 |
| 2 | B | 68 | LEU | CB-CG-CD1 | -12.42 | 89.88 | 111.00 |
| 1 | A | 4 | PRO | CB-CA-C | -12.41 | 80.97 | 112.00 |
| 1 | C | 126 | ASP | CB-CG-OD1 | -12.41 | 107.13 | 118.30 |
| 1 | A | 36 | PHE | CB-CG-CD2 | -12.41 | 112.11 | 120.80 |
| 2 | D | 65 | LYS | CB-CG-CD | -12.41 | 79.34 | 111.60 |
| 2 | D | 45 | PHE | O-C-N | 12.40 | 144.28 | 123.20 |
| 1 | A | 111 | ALA | N-CA-CB | 12.39 | 127.45 | 110.10 |
| 1 | C | 20 | HIS | CG-ND1-CE1 | -12.36 | 89.63 | 105.70 |
| 1 | A | 65 | ALA | O-C-N | 12.34 | 142.45 | 122.70 |
| 1 | C | 24 | TYR | CB-CG-CD1 | -12.32 | 113.61 | 121.00 |
| 1 | C | 24 | TYR | CB-CG-CD2 | -12.32 | 113.61 | 121.00 |
| 2 | B | 64 | GLY | CA-C-O | 12.32 | 142.77 | 120.60 |
| 2 | D | 24 | GLY | O-C-N | -12.30 | 102.29 | 123.20 |
| 2 | D | 75 | LEU | CB-CG-CD2 | 12.30 | 131.91 | 111.00 |
| 1 | A | 89 | HIS | CE1-NE2-CD2 | 12.29 | 137.32 | 106.60 |
| 2 | D | 53 | ALA | N-CA-CB | 12.29 | 127.30 | 110.10 |
| 1 | A | 89 | HIS | ND1-CE1-NE2 | -12.28 | 82.88 | 109.90 |
| 1 | C | 105 | LEU | CB-CG-CD2 | -12.28 | 90.12 | 111.00 |
| 1 | A | 75 | ASP | CB-CA-C | -12.25 | 85.89 | 110.40 |
| 1 | A | 34 | LEU | CB-CG-CD1 | 12.25 | 131.82 | 111.00 |
| 1 | C | 52 | SER | O-C-N | -12.24 | 103.12 | 122.70 |
| 2 | D | 77 | HIS | CA-C-O | 12.23 | 145.78 | 120.10 |
| 2 | D | 42 | PHE | CB-CG-CD2 | 12.22 | 129.35 | 120.80 |
| 2 | D | 130 | TYR | CB-CG-CD2 | 12.19 | 128.31 | 121.00 |
| 1 | C | 113 | LEU | CB-CG-CD2 | 12.17 | 131.68 | 111.00 |
| 2 | B | 53 | ALA | CA-C-O | 12.15 | 145.62 | 120.10 |
| 2 | D | 93 | CYS | O-C-N | 12.15 | 142.14 | 122.70 |
| 2 | B | 4 | THR | N-CA-CB | -12.15 | 87.22 | 110.30 |
| 2 | B | 22 | GLU | CB-CG-CD | 12.14 | 146.99 | 114.20 |
| 1 | A | 141 | ARG | CD-NE-CZ | -12.09 | 106.67 | 123.60 |
| 2 | D | 65 | LYS | CD-CE-NZ | -12.07 | 83.95 | 111.70 |
| 2 | D | 121 | GLU | CG-CD-OE1 | -12.07 | 94.17 | 118.30 |
| 2 | B | 85 | PHE | CG-CD2-CE2 | -12.06 | 107.53 | 120.80 |
| 1 | C | 14 | TRP | CH2-CZ2-CE2 | 12.06 | 129.46 | 117.40 |
| 2 | D | 79 | ASP | CA-C-N | -12.05 | 90.69 | 117.20 |
| 2 | D | 52 | ASP | OD1-CG-OD2 | -12.05 | 100.41 | 123.30 |
| 1 | A | 42 | TYR | CD1-CE1-CZ | 12.01 | 130.60 | 119.80 |
| 2 | D | 78 | LEU | N-CA-C | 11.99 | 143.39 | 111.00 |
| 1 | C | 116 | GLU | CB-CG-CD | -11.99 | 81.84 | 114.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | B | 43 | GLU | O-C-N | -11.98 | 103.53 | 122.70 |
| 1 | A | 15 | GLY | CA-C-O | -11.98 | 99.04 | 120.60 |
| 2 | D | 2 | HIS | CB-CG-CD2 | 11.98 | 167.93 | 130.80 |
| 1 | A | 20 | HIS | CG-ND1-CE1 | -11.97 | 90.13 | 105.70 |
| 2 | B | 18 | VAL | CA-CB-CG2 | -11.97 | 92.95 | 110.90 |
| 1 | C | 48 | LEU | CB-CG-CD1 | 11.96 | 131.34 | 111.00 |
| 1 | C | 53 | ALA | CB-CA-C | 11.96 | 128.03 | 110.10 |
| 2 | D | 80 | ASN | CA-C-N | -11.96 | 90.90 | 117.20 |
| 1 | A | 7 | LYS | CD-CE-NZ | -11.93 | 84.27 | 111.70 |
| 1 | A | 24 | TYR | CD1-CE1-CZ | 11.93 | 130.53 | 119.80 |
| 2 | D | 83 | GLY | O-C-N | -11.91 | 103.64 | 122.70 |
| 2 | B | 82 | LYS | N-CA-CB | -11.89 | 89.19 | 110.60 |
| 1 | C | 116 | GLU | CG-CD-OE1 | 11.89 | 142.09 | 118.30 |
| 2 | D | 52 | ASP | N-CA-CB | -11.88 | 89.21 | 110.60 |
| 2 | B | 44 | SER | CB-CA-C | 11.86 | 132.63 | 110.10 |
| 1 | A | 26 | ALA | N-CA-CB | 11.84 | 126.68 | 110.10 |
| 1 | C | 114 | PRO | O-C-N | -11.83 | 103.78 | 122.70 |
| 2 | D | 42 | PHE | CD1-CE1-CZ | 11.82 | 134.28 | 120.10 |
| 2 | D | 65 | LYS | CG-CD-CE | -11.82 | 76.44 | 111.90 |
| 2 | B | 1 | VAL | CA-C-O | -11.81 | 95.30 | 120.10 |
| 2 | D | 21 | ASP | N-CA-C | 11.79 | 142.84 | 111.00 |
| 2 | D | 120 | LYS | O-C-N | -11.78 | 103.85 | 122.70 |
| 1 | A | 14 | TRP | CA-CB-CG | -11.77 | 91.34 | 113.70 |
| 2 | D | 58 | PRO | CB-CG-CD | 11.77 | 152.38 | 106.50 |
| 2 | D | 41 | PHE | CZ-CE2-CD2 | -11.76 | 105.99 | 120.10 |
| 1 | A | 47 | ASP | O-C-N | 11.75 | 141.50 | 122.70 |
| 1 | C | 41 | THR | O-C-N | -11.75 | 103.90 | 122.70 |
| 2 | D | 2 | HIS | CA-C-O | -11.74 | 95.44 | 120.10 |
| 2 | B | 79 | ASP | O-C-N | -11.74 | 103.92 | 122.70 |
| 1 | C | 12 | ALA | O-C-N | -11.74 | 103.92 | 122.70 |
| 2 | D | 4 | THR | CA-C-O | -11.74 | 95.44 | 120.10 |
| 1 | A | 21 | ALA | CA-C-O | -11.72 | 95.49 | 120.10 |
| 1 | C | 112 | HIS | ND1-CG-CD2 | -11.71 | 89.61 | 106.00 |
| 2 | D | 63 | HIS | CA-CB-CG | 11.69 | 133.48 | 113.60 |
| 1 | A | 19 | ALA | N-CA-CB | 11.69 | 126.46 | 110.10 |
| 2 | D | 21 | ASP | CB-CG-OD2 | -11.69 | 107.78 | 118.30 |
| 2 | D | 78 | LEU | CA-C-N | -11.68 | 91.50 | 117.20 |
| 1 | A | 141 | ARG | CG-CD-NE | -11.68 | 87.28 | 111.80 |
| 1 | C | 98 | PHE | CG-CD2-CE2 | -11.68 | 107.95 | 120.80 |
| 1 | A | 112 | HIS | CG-ND1-CE1 | -11.67 | 90.52 | 105.70 |
| 2 | B | 42 | PHE | CG-CD2-CE2 | 11.67 | 133.63 | 120.80 |
| 1 | C | 89 | HIS | CG-ND1-CE1 | -11.65 | 90.55 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | A | 15 | GLY | CA-C-N | 11.64 | 142.80 | 117.20 |
| 1 | C | 16 | LYS | CD-CE-NZ | -11.64 | 84.94 | 111.70 |
| 2 | B | 2 | HIS | CA-CB-CG | 11.63 | 133.37 | 113.60 |
| 2 | D | 47 | ASP | OD1-CG-OD2 | 11.62 | 145.39 | 123.30 |
| 1 | A | 73 | VAL | O-C-N | -11.62 | 104.11 | 122.70 |
| 1 | A | 89 | HIS | CG-ND1-CE1 | 11.57 | 124.40 | 108.20 |
| 2 | B | 78 | LEU | CB-CG-CD2 | 11.55 | 130.64 | 111.00 |
| 2 | D | 6 | GLU | CB-CA-C | -11.55 | 87.31 | 110.40 |
| 1 | A | 140 | TYR | CD1-CE1-CZ | 11.54 | 130.18 | 119.80 |
| 2 | D | 2 | HIS | CB-CG-ND1 | -11.53 | 94.37 | 123.20 |
| 1 | C | 53 | ALA | O-C-N | 11.52 | 141.14 | 122.70 |
| 2 | D | 45 | PHE | CA-C-O | -11.46 | 96.03 | 120.10 |
| 2 | B | 43 | GLU | N-CA-CB | -11.43 | 90.02 | 110.60 |
| 1 | A | 64 | ASP | OD1-CG-OD2 | 11.43 | 145.01 | 123.30 |
| 2 | B | 42 | PHE | CG-CD1-CE1 | -11.41 | 108.25 | 120.80 |
| 2 | D | 40 | ARG | NE-CZ-NH1 | -11.41 | 114.59 | 120.30 |
| 1 | C | 114 | PRO | CB-CA-C | 11.39 | 140.48 | 112.00 |
| 2 | B | 145 | TYR | N-CA-CB | 11.38 | 131.08 | 110.60 |
| 2 | D | 82 | LYS | CG-CD-CE | -11.37 | 77.78 | 111.90 |
| 2 | B | 73 | ASP | CB-CG-OD2 | -11.37 | 108.07 | 118.30 |
| 1 | C | 72 | HIS | ND1-CE1-NE2 | 11.35 | 134.88 | 109.90 |
| 2 | B | 9 | SER | CA-CB-OG | -11.35 | 80.55 | 111.20 |
| 2 | D | 58 | PRO | CA-N-CD | -11.34 | 95.62 | 111.50 |
| 2 | D | 2 | HIS | ND1-CE1-NE2 | -11.30 | 85.04 | 109.90 |
| 2 | D | 43 | GLU | CB-CA-C | -11.30 | 87.80 | 110.40 |
| 2 | B | 96 | LEU | CB-CG-CD2 | -11.28 | 91.83 | 111.00 |
| 2 | B | 117 | HIS | ND1-CG-CD2 | 11.27 | 124.57 | 108.80 |
| 2 | D | 50 | THR | CB-CA-C | -11.26 | 81.21 | 111.60 |
| 1 | C | 45 | HIS | ND1-CE1-NE2 | 11.23 | 134.61 | 109.90 |
| 2 | D | 97 | HIS | CE1-NE2-CD2 | 11.23 | 134.69 | 106.60 |
| 1 | A | 74 | ASP | CA-C-O | -11.23 | 96.52 | 120.10 |
| 1 | C | 118 | THR | CA-CB-CG2 | 11.22 | 128.10 | 112.40 |
| 2 | D | 57 | ASN | CA-C-O | 11.18 | 143.58 | 120.10 |
| 1 | C | 49 | SER | CB-CA-C | 11.16 | 131.31 | 110.10 |
| 1 | A | 25 | GLY | O-C-N | -11.16 | 104.84 | 122.70 |
| 1 | C | 90 | LYS | CD-CE-NZ | -11.15 | 86.05 | 111.70 |
| 2 | D | 63 | HIS | CG-ND1-CE1 | -11.15 | 91.20 | 105.70 |
| 1 | A | 57 | GLY | O-C-N | 11.13 | 140.51 | 122.70 |
| 2 | B | 43 | GLU | CA-CB-CG | 11.13 | 137.88 | 113.40 |
| 1 | C | 81 | SER | N-CA-CB | -11.13 | 93.80 | 110.50 |
| 2 | B | 17 | LYS | CD-CE-NZ | -11.12 | 86.12 | 111.70 |
| 1 | A | 120 | ALA | N-CA-CB | 11.11 | 125.66 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | C | 2 | LEU | CA-C-O | -11.11 | 96.76 | 120.10 |
| 1 | A | 73 | VAL | CA-C-O | 11.10 | 143.41 | 120.10 |
| 2 | D | 49 | SER | CB-CA-C | -11.08 | 89.04 | 110.10 |
| 1 | C | 20 | HIS | CB-CG-ND1 | -11.08 | 95.50 | 123.20 |
| 2 | B | 144 | LYS | O-C-N | -11.07 | 104.99 | 122.70 |
| 2 | D | 117 | HIS | ND1-CG-CD2 | -11.07 | 90.50 | 106.00 |
| 2 | D | 122 | PHE | CZ-CE2-CD2 | -11.06 | 106.83 | 120.10 |
| 2 | D | 105 | LEU | CB-CG-CD1 | 11.04 | 129.78 | 111.00 |
| 1 | A | 71 | ALA | CA-C-N | 11.04 | 141.49 | 117.20 |
| 1 | A | 46 | PHE | CE1-CZ-CE2 | -11.04 | 100.14 | 120.00 |
| 2 | B | 5 | PRO | CA-CB-CG | -11.02 | 83.06 | 104.00 |
| 2 | D | 18 | VAL | CA-CB-CG1 | 11.02 | 127.43 | 110.90 |
| 2 | B | 17 | LYS | O-C-N | -11.01 | 105.09 | 122.70 |
| 2 | D | 55 | MET | CA-C-N | -11.01 | 94.19 | 116.20 |
| 2 | D | 85 | PHE | CB-CG-CD1 | -11.00 | 113.10 | 120.80 |
| 1 | C | 41 | THR | CA-C-N | 10.98 | 141.37 | 117.20 |
| 2 | B | 85 | PHE | CB-CG-CD2 | -10.98 | 113.11 | 120.80 |
| 1 | A | 128 | PHE | CG-CD2-CE2 | 10.98 | 132.88 | 120.80 |
| 2 | D | 21 | ASP | OD1-CG-OD2 | -10.96 | 102.47 | 123.30 |
| 1 | C | 29 | LEU | O-C-N | -10.96 | 105.17 | 122.70 |
| 2 | D | 12 | THR | O-C-N | -10.96 | 105.17 | 122.70 |
| 1 | A | 45 | HIS | CA-CB-CG | 10.95 | 132.22 | 113.60 |
| 2 | B | 104 | ARG | NH1-CZ-NH2 | 10.95 | 131.45 | 119.40 |
| 2 | B | 6 | GLU | CA-CB-CG | 10.94 | 137.46 | 113.40 |
| 1 | C | 89 | HIS | ND1-CE1-NE2 | 10.93 | 133.94 | 109.90 |
| 2 | D | 126 | VAL | CA-CB-CG2 | -10.92 | 94.52 | 110.90 |
| 2 | D | 45 | PHE | CB-CG-CD1 | -10.89 | 113.17 | 120.80 |
| 1 | A | 26 | ALA | CB-CA-C | -10.89 | 93.77 | 110.10 |
| 2 | B | 80 | ASN | CB-CG-OD1 | -10.88 | 99.84 | 121.60 |
| 1 | C | 115 | ALA | O-C-N | -10.88 | 105.29 | 122.70 |
| 2 | B | 60 | VAL | O-C-N | -10.84 | 105.35 | 122.70 |
| 2 | B | 49 | SER | N-CA-CB | -10.84 | 94.24 | 110.50 |
| 2 | D | 67 | VAL | CA-CB-CG1 | -10.84 | 94.64 | 110.90 |
| 2 | B | 23 | VAL | CA-CB-CG2 | -10.83 | 94.66 | 110.90 |
| 1 | C | 45 | HIS | CA-CB-CG | 10.80 | 131.96 | 113.60 |
| 2 | B | 43 | GLU | CG-CD-OE1 | -10.79 | 96.71 | 118.30 |
| 1 | C | 30 | GLU | CG-CD-OE2 | -10.79 | 96.71 | 118.30 |
| 1 | A | 122 | HIS | CB-CA-C | 10.77 | 131.94 | 110.40 |
| 1 | C | 14 | TRP | CA-C-N | 10.77 | 137.74 | 116.20 |
| 2 | D | 90 | GLU | CG-CD-OE2 | -10.77 | 96.76 | 118.30 |
| 1 | C | 44 | PRO | N-CA-CB | -10.77 | 90.38 | 103.30 |
| 1 | A | 49 | SER | C-N-CA | -10.76 | 94.79 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | B | 134 | VAL | N-CA-CB | 10.76 | 135.18 | 111.50 |
| 1 | C | 63 | ALA | O-C-N | -10.74 | 105.52 | 122.70 |
| 1 | C | 10 | VAL | O-C-N | 10.73 | 139.87 | 122.70 |
| 1 | C | 78 | ASN | O-C-N | -10.73 | 105.52 | 122.70 |
| 1 | A | 42 | TYR | CB-CG-CD1 | 10.72 | 127.43 | 121.00 |
| 1 | A | 116 | GLU | CG-CD-OE1 | 10.71 | 139.71 | 118.30 |
| 2 | D | 104 | ARG | CG-CD-NE | -10.71 | 89.32 | 111.80 |
| 2 | B | 48 | LEU | CB-CG-CD2 | 10.68 | 129.16 | 111.00 |
| 2 | D | 9 | SER | O-C-N | 10.67 | 139.78 | 122.70 |
| 2 | D | 79 | ASP | C-N-CA | -10.66 | 95.05 | 121.70 |
| 2 | B | 3 | LEU | C-N-CA | -10.63 | 95.12 | 121.70 |
| 2 | B | 45 | PHE | CG-CD1-CE1 | -10.63 | 109.11 | 120.80 |
| 2 | B | 45 | PHE | CA-C-N | 10.62 | 137.45 | 116.20 |
| 2 | D | 7 | GLU | O-C-N | 10.62 | 139.70 | 122.70 |
| 2 | B | 78 | LEU | CB-CA-C | -10.61 | 90.04 | 110.20 |
| 2 | B | 81 | LEU | CB-CA-C | 10.60 | 130.35 | 110.20 |
| 1 | C | 72 | HIS | N-CA-C | 10.56 | 139.53 | 111.00 |
| 1 | C | 73 | VAL | O-C-N | 10.56 | 139.60 | 122.70 |
| 1 | C | 17 | VAL | CG1-CB-CG2 | 10.55 | 127.79 | 110.90 |
| 1 | A | 20 | HIS | ND1-CE1-NE2 | 10.53 | 133.06 | 109.90 |
| 2 | D | 77 | HIS | CE1-NE2-CD2 | 10.52 | 132.91 | 106.60 |
| 2 | D | 80 | ASN | CB-CG-ND2 | -10.51 | 91.49 | 116.70 |
| 2 | D | 3 | LEU | CA-C-O | -10.50 | 98.04 | 120.10 |
| 1 | A | 41 | THR | O-C-N | -10.50 | 105.90 | 122.70 |
| 1 | C | 113 | LEU | CA-C-O | -10.50 | 98.06 | 120.10 |
| 2 | D | 3 | LEU | N-CA-C | -10.47 | 82.74 | 111.00 |
| 2 | D | 54 | VAL | CA-CB-CG1 | -10.46 | 95.21 | 110.90 |
| 2 | B | 72 | SER | CB-CA-C | 10.46 | 129.97 | 110.10 |
| 1 | C | 116 | GLU | CB-CA-C | -10.43 | 89.54 | 110.40 |
| 2 | D | 72 | SER | CA-C-O | 10.43 | 142.00 | 120.10 |
| 2 | D | 12 | THR | CA-CB-OG1 | -10.42 | 87.12 | 109.00 |
| 1 | A | 22 | GLY | CA-C-O | 10.42 | 139.35 | 120.60 |
| 1 | A | 131 | SER | O-C-N | 10.42 | 139.37 | 122.70 |
| 2 | D | 3 | LEU | N-CA-CB | 10.40 | 131.20 | 110.40 |
| 2 | B | 85 | PHE | CD1-CE1-CZ | 10.40 | 132.58 | 120.10 |
| 1 | A | 43 | PHE | CG-CD2-CE2 | 10.40 | 132.24 | 120.80 |
| 2 | D | 63 | HIS | ND1-CG-CD2 | 10.40 | 123.36 | 108.80 |
| 1 | C | 22 | GLY | CA-C-N | 10.38 | 140.04 | 117.20 |
| 1 | A | 2 | LEU | CA-C-O | -10.37 | 98.33 | 120.10 |
| 2 | D | 21 | ASP | CB-CG-OD1 | 10.35 | 127.62 | 118.30 |
| 1 | A | 12 | ALA | N-CA-CB | -10.35 | 95.61 | 110.10 |
| 1 | C | 56 | LYS | O-C-N | -10.34 | 105.62 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 1 | A | 26 | ALA | CA-C-O | 10.34 | 141.81 | 120.10 |
| 1 | A | 72 | HIS | CG-CD2-NE2 | 10.34 | 128.84 | 109.20 |
| 2 | B | 1 | VAL | CA-CB-CG1 | -10.31 | 95.43 | 110.90 |
| 2 | B | 35 | TYR | CB-CG-CD2 | 10.31 | 127.19 | 121.00 |
| 1 | A | 43 | PHE | CZ-CE2-CD2 | -10.31 | 107.73 | 120.10 |
| 1 | A | 81 | SER | CA-CB-OG | -10.29 | 83.41 | 111.20 |
| 1 | A | 141 | ARG | CB-CA-C | 10.29 | 130.97 | 110.40 |
| 2 | D | 60 | VAL | CG1-CB-CG2 | 10.25 | 127.30 | 110.90 |
| 2 | B | 2 | HIS | ND1-CE1-NE2 | 10.25 | 132.44 | 109.90 |
| 1 | C | 7 | LYS | CA-C-O | 10.23 | 141.58 | 120.10 |
| 2 | B | 85 | PHE | CE1-CZ-CE2 | -10.23 | 101.59 | 120.00 |
| 2 | B | 90 | GLU | N-CA-C | 10.20 | 138.54 | 111.00 |
| 2 | D | 35 | TYR | CD1-CE1-CZ | -10.19 | 110.63 | 119.80 |
| 1 | C | 84 | SER | CA-CB-OG | -10.19 | 83.70 | 111.20 |
| 2 | D | 73 | ASP | N-CA-C | 10.17 | 138.46 | 111.00 |
| 1 | A | 106 | LEU | CA-CB-CG | 10.15 | 138.65 | 115.30 |
| 1 | A | 14 | TRP | NE1-CE2-CZ2 | 10.15 | 141.56 | 130.40 |
| 1 | A | 8 | THR | CA-C-O | 10.14 | 141.41 | 120.10 |
| 2 | B | 47 | ASP | OD1-CG-OD2 | -10.14 | 104.03 | 123.30 |
| 2 | D | 19 | ASN | CA-C-N | 10.14 | 139.51 | 117.20 |
| 2 | B | 68 | LEU | CD1-CG-CD2 | 10.12 | 140.87 | 110.50 |
| 2 | D | 3 | LEU | CA-CB-CG | -10.11 | 92.04 | 115.30 |
| 1 | C | 2 | LEU | O-C-N | 10.10 | 138.86 | 122.70 |
| 1 | A | 74 | ASP | CB-CG-OD1 | 10.10 | 127.39 | 118.30 |
| 2 | D | 8 | LYS | N-CA-CB | -10.09 | 92.43 | 110.60 |
| 2 | D | 5 | PRO | CB-CA-C | -10.08 | 86.80 | 112.00 |
| 2 | D | 146 | HIS | ND1-CE1-NE2 | 10.07 | 132.06 | 109.90 |
| 2 | D | 117 | HIS | CG-ND1-CE1 | -10.07 | 92.61 | 105.70 |
| 1 | A | 87 | HIS | O-C-N | 10.05 | 138.79 | 122.70 |
| 2 | B | 42 | PHE | CD1-CG-CD2 | -10.05 | 105.23 | 118.30 |
| 2 | D | 84 | THR | CA-CB-CG2 | 10.05 | 126.47 | 112.40 |
| 1 | C | 131 | SER | O-C-N | 10.03 | 138.74 | 122.70 |
| 2 | B | 30 | ARG | NH1-CZ-NH2 | -10.02 | 108.38 | 119.40 |
| 2 | B | 30 | ARG | NE-CZ-NH1 | -10.01 | 115.29 | 120.30 |
| 2 | D | 82 | LYS | O-C-N | -10.01 | 106.18 | 123.20 |
| 2 | D | 14 | LEU | CB-CG-CD1 | -10.01 | 93.98 | 111.00 |
| 1 | A | 53 | ALA | CB-CA-C | -10.00 | 95.10 | 110.10 |
| 2 | B | 94 | ASP | O-C-N | -9.99 | 106.72 | 122.70 |
| 1 | C | 43 | PHE | CB-CG-CD2 | -9.98 | 113.81 | 120.80 |
| 1 | A | 126 | ASP | O-C-N | -9.95 | 106.78 | 122.70 |
| 2 | B | 58 | PRO | CB-CG-CD | 9.94 | 145.28 | 106.50 |
| 2 | D | 133 | VAL | CG1-CB-CG2 | 9.92 | 126.77 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 6 | GLU | CA-C-O | -9.91 | 99.29 | 120.10 |
| 2 | B | 142 | ALA | O-C-N | 9.91 | 138.55 | 122.70 |
| 2 | D | 11 | VAL | O-C-N | 9.90 | 138.55 | 122.70 |
| 1 | C | 79 | ALA | CB-CA-C | -9.90 | 95.25 | 110.10 |
| 1 | A | 76 | MET | CG-SD-CE | 9.89 | 116.03 | 100.20 |
| 1 | A | 50 | HIS | CB-CA-C | -9.87 | 90.66 | 110.40 |
| 1 | A | 105 | LEU | CB-CG-CD2 | 9.87 | 127.78 | 111.00 |
| 2 | B | 81 | LEU | N-CA-CB | -9.85 | 90.70 | 110.40 |
| 2 | D | 60 | VAL | CB-CA-C | 9.84 | 130.10 | 111.40 |
| 2 | D | 95 | LYS | O-C-N | -9.84 | 106.95 | 122.70 |
| 2 | B | 90 | GLU | CG-CD-OE1 | -9.82 | 98.66 | 118.30 |
| 1 | A | 88 | ALA | O-C-N | 9.82 | 138.41 | 122.70 |
| 2 | B | 42 | PHE | CB-CG-CD1 | -9.82 | 113.93 | 120.80 |
| 2 | B | 125 | PRO | CA-N-CD | -9.81 | 97.76 | 111.50 |
| 1 | C | 4 | PRO | O-C-N | 9.81 | 138.40 | 122.70 |
| 2 | B | 61 | LYS | CD-CE-NZ | -9.80 | 89.16 | 111.70 |
| 1 | A | 43 | PHE | CB-CG-CD1 | -9.79 | 113.95 | 120.80 |
| 2 | B | 87 | THR | CA-CB-OG1 | -9.78 | 88.45 | 109.00 |
| 1 | A | 82 | ALA | N-CA-CB | 9.78 | 123.79 | 110.10 |
| 2 | D | 97 | HIS | ND1-CE1-NE2 | -9.78 | 88.39 | 109.90 |
| 1 | A | 6 | ASP | CB-CG-OD2 | -9.77 | 109.51 | 118.30 |
| 1 | C | 71 | ALA | C-N-CA | 9.76 | 146.09 | 121.70 |
| 2 | B | 8 | LYS | CB-CG-CD | 9.74 | 136.94 | 111.60 |
| 2 | B | 45 | PHE | CE1-CZ-CE2 | 9.74 | 137.54 | 120.00 |
| 2 | D | 30 | ARG | CD-NE-CZ | 9.73 | 137.23 | 123.60 |
| 1 | A | 15 | GLY | N-CA-C | -9.72 | 88.80 | 113.10 |
| 1 | C | 90 | LYS | N-CA-CB | 9.69 | 128.04 | 110.60 |
| 2 | B | 145 | TYR | CA-C-O | -9.69 | 99.76 | 120.10 |
| 1 | C | 90 | LYS | CB-CG-CD | -9.68 | 86.44 | 111.60 |
| 1 | C | 58 | HIS | CG-ND1-CE1 | -9.67 | 93.12 | 105.70 |
| 2 | B | 60 | VAL | CA-C-O | 9.67 | 140.40 | 120.10 |
| 2 | D | 78 | LEU | CB-CG-CD1 | -9.66 | 94.58 | 111.00 |
| 1 | A | 33 | PHE | CZ-CE2-CD2 | 9.65 | 131.68 | 120.10 |
| 1 | C | 60 | LYS | CD-CE-NZ | -9.65 | 89.51 | 111.70 |
| 1 | A | 78 | ASN | N-CA-CB | 9.64 | 127.95 | 110.60 |
| 1 | C | 49 | SER | CA-C-O | 9.64 | 140.34 | 120.10 |
| 1 | C | 82 | ALA | O-C-N | -9.63 | 107.29 | 122.70 |
| 2 | D | 137 | VAL | O-C-N | -9.63 | 107.30 | 122.70 |
| 2 | D | 144 | LYS | CD-CE-NZ | 9.62 | 133.84 | 111.70 |
| 1 | C | 14 | TRP | CD2-CE2-CZ2 | -9.62 | 110.76 | 122.30 |
| 1 | C | 56 | LYS | CB-CG-CD | -9.61 | 86.61 | 111.60 |
| 2 | B | 47 | ASP | CA-C-N | -9.60 | 96.08 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 64 | ASP | OD1-CG-OD2 | 9.60 | 141.54 | 123.30 |
| 2 | D | 54 | VAL | O-C-N | -9.60 | 107.35 | 122.70 |
| 1 | C | 70 | VAL | CA-C-O | -9.58 | 99.97 | 120.10 |
| 2 | D | 65 | LYS | CA-CB-CG | -9.58 | 92.33 | 113.40 |
| 2 | B | 53 | ALA | O-C-N | -9.57 | 107.39 | 122.70 |
| 1 | A | 76 | MET | CA-CB-CG | -9.55 | 97.06 | 113.30 |
| 1 | A | 89 | HIS | O-C-N | -9.55 | 107.42 | 122.70 |
| 2 | B | 122 | PHE | CB-CG-CD2 | -9.54 | 114.12 | 120.80 |
| 1 | C | 138 | SER | N-CA-CB | -9.52 | 96.22 | 110.50 |
| 2 | D | 18 | VAL | CA-C-O | -9.52 | 100.11 | 120.10 |
| 2 | D | 85 | PHE | CZ-CE2-CD2 | 9.52 | 131.52 | 120.10 |
| 2 | D | 143 | HIS | CG-ND1-CE1 | -9.52 | 93.33 | 105.70 |
| 2 | B | 139 | ASN | CB-CA-C | -9.52 | 91.37 | 110.40 |
| 1 | C | 38 | THR | CA-CB-CG2 | -9.50 | 99.09 | 112.40 |
| 1 | C | 109 | LEU | CB-CA-C | 9.50 | 128.25 | 110.20 |
| 1 | A | 42 | TYR | CG-CD1-CE1 | -9.48 | 113.71 | 121.30 |
| 1 | C | 138 | SER | O-C-N | 9.48 | 137.87 | 122.70 |
| 2 | D | 20 | VAL | N-CA-CB | 9.48 | 132.35 | 111.50 |
| 2 | D | 19 | ASN | CB-CG-OD1 | -9.47 | 102.66 | 121.60 |
| 1 | A | 96 | VAL | CA-CB-CG2 | -9.45 | 96.72 | 110.90 |
| 2 | B | 126 | VAL | CG1-CB-CG2 | -9.45 | 95.78 | 110.90 |
| 2 | B | 73 | ASP | CB-CG-OD1 | 9.45 | 126.80 | 118.30 |
| 2 | B | 134 | VAL | CA-CB-CG1 | -9.45 | 96.72 | 110.90 |
| 2 | D | 79 | ASP | CB-CG-OD1 | -9.45 | 109.80 | 118.30 |
| 2 | B | 130 | TYR | CB-CG-CD1 | 9.43 | 126.66 | 121.00 |
| 2 | B | 144 | LYS | CA-C-N | 9.42 | 137.92 | 117.20 |
| 1 | A | 127 | LYS | CB-CA-C | 9.41 | 129.22 | 110.40 |
| 1 | C | 96 | VAL | CA-CB-CG2 | 9.40 | 125.01 | 110.90 |
| 1 | C | 105 | LEU | CD1-CG-CD2 | -9.39 | 82.32 | 110.50 |
| 1 | A | 24 | TYR | CG-CD2-CE2 | 9.37 | 128.79 | 121.30 |
| 2 | D | 48 | LEU | CB-CG-CD2 | 9.37 | 126.92 | 111.00 |
| 2 | D | 99 | ASP | OD1-CG-OD2 | 9.36 | 141.09 | 123.30 |
| 2 | B | 49 | SER | CA-C-N | 9.35 | 137.78 | 117.20 |
| 2 | D | 89 | SER | CA-C-O | 9.35 | 139.74 | 120.10 |
| 2 | B | 127 | GLN | O-C-N | -9.34 | 107.75 | 122.70 |
| 1 | A | 19 | ALA | CB-CA-C | -9.33 | 96.10 | 110.10 |
| 1 | C | 103 | HIS | CG-ND1-CE1 | -9.33 | 93.57 | 105.70 |
| 2 | D | 35 | TYR | CB-CG-CD2 | 9.33 | 126.60 | 121.00 |
| 1 | C | 94 | ASP | CB-CG-OD2 | -9.32 | 109.91 | 118.30 |
| 2 | D | 40 | ARG | CA-CB-CG | 9.32 | 133.91 | 113.40 |
| 2 | D | 145 | TYR | CG-CD2-CE2 | -9.32 | 113.84 | 121.30 |
| 1 | C | 5 | ALA | N-CA-CB | 9.32 | 123.14 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 56 | LYS | CB-CG-CD | -9.32 | 87.38 | 111.60 |
| 2 | B | 3 | LEU | N-CA-CB | -9.31 | 91.78 | 110.40 |
| 2 | D | 1 | VAL | CA-C-O | -9.31 | 100.55 | 120.10 |
| 1 | A | 52 | SER | O-C-N | -9.31 | 107.81 | 122.70 |
| 1 | C | 48 | LEU | C-N-CA | 9.29 | 144.94 | 121.70 |
| 2 | D | 67 | VAL | N-CA-CB | -9.28 | 91.08 | 111.50 |
| 2 | D | 122 | PHE | CD1-CE1-CZ | -9.28 | 108.96 | 120.10 |
| 2 | D | 16 | GLY | C-N-CA | 9.28 | 144.90 | 121.70 |
| 2 | D | 116 | HIS | ND1-CG-CD2 | 9.27 | 121.78 | 108.80 |
| 2 | B | 81 | LEU | CA-CB-CG | 9.26 | 136.59 | 115.30 |
| 1 | A | 6 | ASP | O-C-N | 9.25 | 137.50 | 122.70 |
| 1 | C | 112 | HIS | O-C-N | -9.25 | 107.91 | 122.70 |
| 2 | D | 23 | VAL | CA-CB-CG2 | -9.24 | 97.03 | 110.90 |
| 2 | B | 10 | ALA | CB-CA-C | -9.22 | 96.27 | 110.10 |
| 2 | D | 122 | PHE | CG-CD2-CE2 | 9.20 | 130.92 | 120.80 |
| 1 | A | 11 | LYS | C-N-CA | -9.17 | 98.78 | 121.70 |
| 2 | D | 51 | PRO | N-CD-CG | -9.15 | 89.47 | 103.20 |
| 1 | C | 72 | HIS | O-C-N | -9.15 | 108.06 | 122.70 |
| 2 | D | 90 | GLU | CB-CG-CD | -9.15 | 89.49 | 114.20 |
| 1 | A | 43 | PHE | CD1-CE1-CZ | 9.15 | 131.08 | 120.10 |
| 1 | A | 19 | ALA | O-C-N | -9.14 | 108.07 | 122.70 |
| 2 | D | 53 | ALA | CA-C-O | 9.14 | 139.29 | 120.10 |
| 2 | D | 41 | PHE | CA-C-O | -9.13 | 100.93 | 120.10 |
| 1 | A | 7 | LYS | CA-C-N | -9.12 | 97.13 | 117.20 |
| 2 | B | 118 | PHE | CE1-CZ-CE2 | -9.12 | 103.58 | 120.00 |
| 1 | C | 131 | SER | CA-C-O | -9.12 | 100.95 | 120.10 |
| 1 | C | 45 | HIS | O-C-N | 9.11 | 137.28 | 122.70 |
| 2 | B | 146 | HIS | CB-CG-ND1 | -9.10 | 100.45 | 123.20 |
| 2 | D | 10 | ALA | N-CA-CB | -9.08 | 97.38 | 110.10 |
| 2 | D | 95 | LYS | CA-C-O | 9.07 | 139.16 | 120.10 |
| 1 | A | 29 | LEU | CB-CG-CD1 | -9.07 | 95.58 | 111.00 |
| 1 | A | 86 | LEU | CB-CG-CD2 | 9.07 | 126.42 | 111.00 |
| 2 | B | 66 | LYS | CD-CE-NZ | -9.06 | 90.85 | 111.70 |
| 1 | C | 86 | LEU | CA-C-O | 9.06 | 139.13 | 120.10 |
| 1 | A | 14 | TRP | C-N-CA | -9.06 | 103.27 | 122.30 |
| 1 | C | 38 | THR | CA-CB-OG1 | -9.05 | 89.99 | 109.00 |
| 1 | C | 112 | HIS | C-N-CA | 9.03 | 144.28 | 121.70 |
| 1 | C | 12 | ALA | N-CA-C | 9.03 | 135.38 | 111.00 |
| 1 | A | 118 | THR | CA-CB-OG1 | 9.03 | 127.95 | 109.00 |
| 2 | B | 15 | TRP | O-C-N | 9.00 | 138.51 | 123.20 |
| 1 | C | 44 | PRO | CA-N-CD | 9.00 | 124.30 | 111.70 |
| 2 | B | 41 | PHE | CG-CD2-CE2 | -8.99 | 110.91 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | C | 117 | PHE | CB-CG-CD2 | 8.98 | 127.09 | 120.80 |
| 2 | D | 77 | HIS | CA-C-N | -8.98 | 97.44 | 117.20 |
| 2 | B | 90 | GLU | CA-C-N | -8.98 | 97.45 | 117.20 |
| 1 | A | 38 | THR | CA-CB-CG2 | -8.97 | 99.84 | 112.40 |
| 2 | B | 144 | LYS | C-N-CA | 8.97 | 144.13 | 121.70 |
| 1 | A | 134 | THR | O-C-N | -8.97 | 108.35 | 122.70 |
| 2 | D | 17 | LYS | CD-CE-NZ | -8.97 | 91.08 | 111.70 |
| 2 | B | 37 | TRP | CZ3-CH2-CZ2 | 8.96 | 132.35 | 121.60 |
| 1 | A | 62 | VAL | CG1-CB-CG2 | -8.95 | 96.58 | 110.90 |
| 2 | D | 53 | ALA | CB-CA-C | -8.95 | 96.68 | 110.10 |
| 1 | A | 78 | ASN | CB-CG-ND2 | 8.94 | 138.16 | 116.70 |
| 1 | A | 2 | LEU | N-CA-CB | -8.94 | 92.52 | 110.40 |
| 2 | D | 52 | ASP | CA-C-O | -8.94 | 101.33 | 120.10 |
| 2 | B | 2 | HIS | CA-C-N | -8.92 | 97.57 | 117.20 |
| 1 | A | 112 | HIS | CA-C-O | -8.92 | 101.37 | 120.10 |
| 2 | B | 5 | PRO | O-C-N | 8.92 | 136.97 | 122.70 |
| 2 | D | 21 | ASP | O-C-N | -8.91 | 108.45 | 122.70 |
| 2 | D | 120 | LYS | CB-CG-CD | 8.90 | 134.75 | 111.60 |
| 1 | C | 87 | HIS | O-C-N | 8.90 | 136.94 | 122.70 |
| 1 | A | 56 | LYS | CA-C-O | 8.88 | 138.74 | 120.10 |
| 1 | A | 98 | PHE | CB-CG-CD2 | 8.87 | 127.01 | 120.80 |
| 1 | C | 77 | PRO | O-C-N | -8.88 | 108.50 | 122.70 |
| 2 | B | 42 | PHE | CE1-CZ-CE2 | -8.87 | 104.04 | 120.00 |
| 2 | D | 44 | SER | CA-C-N | 8.87 | 136.71 | 117.20 |
| 2 | D | 77 | HIS | ND1-CE1-NE2 | -8.85 | 90.44 | 109.90 |
| 2 | B | 7 | GLU | CB-CA-C | 8.84 | 128.08 | 110.40 |
| 2 | D | 2 | HIS | C-N-CA | -8.84 | 99.60 | 121.70 |
| 2 | B | 47 | ASP | N-CA-CB | -8.84 | 94.69 | 110.60 |
| 2 | D | 3 | LEU | C-N-CA | 8.83 | 143.78 | 121.70 |
| 1 | C | 77 | PRO | N-CA-C | 8.82 | 135.03 | 112.10 |
| 1 | C | 128 | PHE | CD1-CE1-CZ | 8.82 | 130.68 | 120.10 |
| 2 | B | 12 | THR | CA-CB-CG2 | -8.81 | 100.06 | 112.40 |
| 1 | A | 62 | VAL | CA-C-N | -8.81 | 97.83 | 117.20 |
| 1 | C | 82 | ALA | CA-C-O | 8.79 | 138.56 | 120.10 |
| 1 | C | 50 | HIS | O-C-N | 8.78 | 138.13 | 123.20 |
| 2 | D | 20 | VAL | CB-CA-C | -8.78 | 94.72 | 111.40 |
| 1 | C | 53 | ALA | CA-C-N | -8.76 | 97.93 | 117.20 |
| 1 | C | 112 | HIS | CA-C-N | 8.76 | 136.47 | 117.20 |
| 2 | D | 57 | ASN | O-C-N | -8.76 | 104.46 | 121.10 |
| 2 | B | 47 | ASP | CB-CA-C | -8.73 | 92.94 | 110.40 |
| 2 | B | 130 | TYR | CZ-CE2-CD2 | -8.73 | 111.94 | 119.80 |
| 2 | D | 35 | TYR | CB-CG-CD1 | -8.73 | 115.76 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 108 | ASN | OD1-CG-ND2 | 8.72 | 141.97 | 121.90 |
| 2 | B | 111 | VAL | O-C-N | -8.72 | 108.75 | 122.70 |
| 1 | C | 1 | VAL | N-CA-C | -8.72 | 87.46 | 111.00 |
| 2 | B | 6 | GLU | CG-CD-OE1 | -8.71 | 100.87 | 118.30 |
| 1 | A | 50 | HIS | CG-CD2-NE2 | -8.71 | 92.64 | 109.20 |
| 1 | C | 84 | SER | CB-CA-C | -8.70 | 93.57 | 110.10 |
| 2 | D | 122 | PHE | CE1-CZ-CE2 | 8.70 | 135.66 | 120.00 |
| 1 | C | 11 | LYS | CA-CB-CG | 8.70 | 132.53 | 113.40 |
| 2 | D | 93 | CYS | CA-CB-SG | -8.68 | 98.37 | 114.00 |
| 1 | C | 74 | ASP | O-C-N | 8.68 | 136.58 | 122.70 |
| 2 | D | 16 | GLY | CA-C-N | 8.67 | 136.28 | 117.20 |
| 1 | A | 50 | HIS | CA-C-N | 8.67 | 133.53 | 116.20 |
| 1 | A | 106 | LEU | CB-CG-CD1 | 8.66 | 125.72 | 111.00 |
| 2 | B | 5 | PRO | CA-C-N | -8.64 | 98.20 | 117.20 |
| 1 | A | 56 | LYS | O-C-N | -8.63 | 108.52 | 123.20 |
| 2 | B | 60 | VAL | CG1-CB-CG2 | 8.63 | 124.71 | 110.90 |
| 2 | B | 3 | LEU | CA-C-N | -8.63 | 98.22 | 117.20 |
| 1 | C | 137 | THR | OG1-CB-CG2 | 8.63 | 129.84 | 110.00 |
| 1 | C | 18 | GLY | CA-C-N | -8.61 | 98.25 | 117.20 |
| 2 | B | 48 | LEU | C-N-CA | -8.61 | 100.17 | 121.70 |
| 1 | A | 128 | PHE | CE1-CZ-CE2 | 8.59 | 135.46 | 120.00 |
| 2 | D | 43 | GLU | CA-C-N | -8.59 | 98.31 | 117.20 |
| 2 | B | 40 | ARG | CA-C-N | 8.58 | 136.08 | 117.20 |
| 2 | D | 55 | MET | CA-C-O | -8.57 | 102.11 | 120.10 |
| 2 | D | 40 | ARG | O-C-N | -8.56 | 109.00 | 122.70 |
| 2 | B | 51 | PRO | O-C-N | -8.54 | 109.04 | 122.70 |
| 1 | C | 36 | PHE | CG-CD2-CE2 | -8.52 | 111.42 | 120.80 |
| 2 | D | 143 | HIS | CG-CD2-NE2 | -8.52 | 93.01 | 109.20 |
| 1 | A | 13 | ALA | O-C-N | 8.51 | 136.32 | 122.70 |
| 1 | C | 114 | PRO | N-CD-CG | -8.50 | 90.45 | 103.20 |
| 1 | C | 62 | VAL | CA-C-N | -8.49 | 98.51 | 117.20 |
| 2 | D | 95 | LYS | CB-CG-CD | -8.49 | 89.52 | 111.60 |
| 2 | B | 80 | ASN | CB-CG-ND2 | -8.46 | 96.39 | 116.70 |
| 2 | D | 119 | GLY | CA-C-O | 8.46 | 135.83 | 120.60 |
| 1 | C | 46 | PHE | CD1-CE1-CZ | 8.46 | 130.25 | 120.10 |
| 2 | D | 122 | PHE | CB-CG-CD1 | 8.46 | 126.72 | 120.80 |
| 1 | A | 63 | ALA | O-C-N | -8.45 | 109.18 | 122.70 |
| 2 | B | 71 | PHE | CZ-CE2-CD2 | 8.45 | 130.24 | 120.10 |
| 2 | D | 71 | PHE | CZ-CE2-CD2 | 8.45 | 130.24 | 120.10 |
| 1 | C | 124 | SER | O-C-N | 8.44 | 136.21 | 122.70 |
| 1 | C | 50 | HIS | CB-CG-CD2 | 8.44 | 156.96 | 130.80 |
| 2 | D | 146 | HIS | N-CA-CB | -8.44 | 95.41 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 36 | PRO | N-CD-CG | 8.43 | 115.84 | 103.20 |
| 1 | A | 60 | LYS | CA-C-O | 8.43 | 137.79 | 120.10 |
| 1 | A | 62 | VAL | C-N-CA | -8.41 | 100.67 | 121.70 |
| 2 | B | 88 | LEU | CB-CG-CD2 | -8.41 | 96.71 | 111.00 |
| 2 | B | 9 | SER | N-CA-CB | 8.40 | 123.10 | 110.50 |
| 1 | C | 69 | ALA | O-C-N | 8.40 | 136.14 | 122.70 |
| 2 | B | 115 | ALA | N-CA-CB | -8.38 | 98.36 | 110.10 |
| 1 | A | 71 | ALA | O-C-N | -8.38 | 109.29 | 122.70 |
| 2 | B | 50 | THR | N-CA-CB | -8.38 | 94.38 | 110.30 |
| 1 | A | 77 | PRO | CA-CB-CG | -8.37 | 88.10 | 104.00 |
| 2 | D | 2 | HIS | ND1-CG-CD2 | -8.35 | 94.31 | 106.00 |
| 2 | D | 59 | LYS | CA-C-N | -8.35 | 98.83 | 117.20 |
| 2 | B | 114 | LEU | CB-CA-C | 8.34 | 126.05 | 110.20 |
| 2 | D | 7 | GLU | OE1-CD-OE2 | -8.34 | 113.30 | 123.30 |
| 2 | B | 35 | TYR | CD1-CG-CD2 | -8.33 | 108.73 | 117.90 |
| 1 | A | 54 | GLN | O-C-N | 8.33 | 136.03 | 122.70 |
| 2 | B | 85 | PHE | CB-CG-CD1 | 8.32 | 126.63 | 120.80 |
| 2 | B | 103 | PHE | CB-CG-CD1 | -8.31 | 114.98 | 120.80 |
| 1 | A | 75 | ASP | N-CA-CB | -8.30 | 95.65 | 110.60 |
| 1 | C | 81 | SER | CA-CB-OG | -8.30 | 88.78 | 111.20 |
| 1 | A | 90 | LYS | N-CA-C | 8.30 | 133.42 | 111.00 |
| 2 | D | 60 | VAL | CA-CB-CG1 | -8.30 | 98.45 | 110.90 |
| 2 | B | 73 | ASP | CA-C-N | 8.30 | 132.79 | 116.20 |
| 1 | C | 95 | PRO | CA-C-N | 8.30 | 135.45 | 117.20 |
| 2 | D | 90 | GLU | CA-CB-CG | -8.29 | 95.16 | 113.40 |
| 1 | C | 50 | HIS | ND1-CG-CD2 | -8.28 | 94.40 | 106.00 |
| 2 | B | 146 | HIS | CA-CB-CG | -8.28 | 99.52 | 113.60 |
| 2 | D | 55 | MET | CB-CG-SD | 8.28 | 137.24 | 112.40 |
| 1 | A | 126 | ASP | CB-CG-OD1 | -8.28 | 110.85 | 118.30 |
| 1 | A | 58 | HIS | C-N-CA | -8.27 | 104.94 | 122.30 |
| 2 | D | 52 | ASP | O-C-N | 8.26 | 135.91 | 122.70 |
| 1 | A | 1 | VAL | C-N-CA | -8.25 | 101.07 | 121.70 |
| 2 | B | 48 | LEU | CB-CA-C | 8.25 | 125.87 | 110.20 |
| 2 | B | 99 | ASP | CB-CG-OD2 | -8.25 | 110.88 | 118.30 |
| 1 | A | 4 | PRO | N-CD-CG | -8.24 | 90.84 | 103.20 |
| 2 | D | 118 | PHE | CG-CD2-CE2 | -8.23 | 111.74 | 120.80 |
| 2 | D | 6 | GLU | CA-C-N | -8.23 | 99.09 | 117.20 |
| 2 | B | 41 | PHE | CB-CG-CD1 | -8.23 | 115.04 | 120.80 |
| 2 | B | 89 | SER | N-CA-CB | -8.23 | 98.16 | 110.50 |
| 1 | C | 83 | LEU | CB-CA-C | -8.22 | 94.58 | 110.20 |
| 1 | C | 22 | GLY | C-N-CA | 8.22 | 142.25 | 121.70 |
| 1 | A | 16 | LYS | N-CA-CB | 8.21 | 125.38 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | A | 117 | PHE | CD1-CG-CD2 | 8.21 | 128.98 | 118.30 |
| 1 | C | 7 | LYS | CB-CA-C | 8.21 | 126.82 | 110.40 |
| 1 | C | 25 | GLY | CA-C-N | 8.21 | 135.26 | 117.20 |
| 2 | B | 2 | HIS | N-CA-CB | -8.20 | 95.83 | 110.60 |
| 1 | C | 117 | PHE | CG-CD2-CE2 | 8.21 | 129.82 | 120.80 |
| 2 | D | 93 | CYS | CB-CA-C | 8.19 | 126.78 | 110.40 |
| 2 | B | 127 | GLN | CA-C-O | 8.18 | 137.27 | 120.10 |
| 1 | A | 117 | PHE | CB-CG-CD2 | -8.17 | 115.08 | 120.80 |
| 1 | A | 7 | LYS | N-CA-C | 8.17 | 133.06 | 111.00 |
| 2 | B | 94 | ASP | CA-C-N | 8.16 | 135.16 | 117.20 |
| 1 | A | 72 | HIS | O-C-N | -8.16 | 109.64 | 122.70 |
| 2 | D | 9 | SER | CA-CB-OG | 8.15 | 133.21 | 111.20 |
| 1 | A | 114 | PRO | N-CA-CB | -8.15 | 93.52 | 103.30 |
| 2 | D | 92 | HIS | ND1-CE1-NE2 | 8.15 | 127.83 | 109.90 |
| 2 | B | 40 | ARG | CA-C-O | -8.15 | 102.99 | 120.10 |
| 1 | C | 141 | ARG | CA-C-O | -8.15 | 102.99 | 120.10 |
| 1 | A | 70 | VAL | CG1-CB-CG2 | -8.14 | 97.87 | 110.90 |
| 2 | B | 23 | VAL | CG1-CB-CG2 | 8.14 | 123.93 | 110.90 |
| 2 | D | 37 | TRP | CE3-CZ3-CH2 | -8.14 | 112.24 | 121.20 |
| 2 | D | 2 | HIS | CB-CA-C | 8.14 | 126.68 | 110.40 |
| 2 | D | 143 | HIS | O-C-N | 8.14 | 135.72 | 122.70 |
| 2 | D | 85 | PHE | O-C-N | -8.13 | 109.69 | 122.70 |
| 2 | B | 67 | VAL | CG1-CB-CG2 | 8.12 | 123.89 | 110.90 |
| 1 | C | 50 | HIS | CE1-NE2-CD2 | -8.12 | 86.30 | 106.60 |
| 1 | A | 114 | PRO | CA-CB-CG | 8.11 | 120.21 | 104.80 |
| 1 | C | 54 | GLN | O-C-N | 8.11 | 135.68 | 122.70 |
| 2 | D | 93 | CYS | N-CA-CB | -8.11 | 96.00 | 110.60 |
| 1 | A | 33 | PHE | CG-CD1-CE1 | 8.11 | 129.72 | 120.80 |
| 1 | C | 138 | SER | CA-C-O | -8.11 | 103.07 | 120.10 |
| 2 | D | 86 | ALA | CB-CA-C | -8.11 | 97.94 | 110.10 |
| 1 | C | 90 | LYS | CG-CD-CE | -8.10 | 87.59 | 111.90 |
| 1 | A | 6 | ASP | C-N-CA | -8.10 | 101.45 | 121.70 |
| 2 | D | 92 | HIS | CB-CA-C | -8.10 | 94.21 | 110.40 |
| 1 | A | 117 | PHE | CG-CD1-CE1 | -8.09 | 111.90 | 120.80 |
| 2 | D | 146 | HIS | CB-CG-CD2 | 8.09 | 155.89 | 130.80 |
| 2 | D | 68 | LEU | CB-CG-CD1 | 8.09 | 124.75 | 111.00 |
| 2 | D | 47 | ASP | CA-CB-CG | -8.07 | 95.64 | 113.40 |
| 2 | B | 118 | PHE | CD1-CG-CD2 | -8.06 | 107.82 | 118.30 |
| 2 | D | 16 | GLY | O-C-N | -8.06 | 109.81 | 122.70 |
| 2 | B | 19 | ASN | CB-CG-ND2 | -8.05 | 97.37 | 116.70 |
| 2 | D | 110 | LEU | CA-C-O | 8.05 | 137.01 | 120.10 |
| 1 | C | 74 | ASP | CA-CB-CG | 8.05 | 131.11 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | C | 117 | PHE | CZ-CE2-CD2 | -8.05 | 110.44 | 120.10 |
| 1 | A | 52 | SER | CA-C-O | 8.04 | 136.98 | 120.10 |
| 1 | C | 17 | VAL | C-N-CA | -8.04 | 105.42 | 122.30 |
| 2 | D | 121 | GLU | O-C-N | 8.02 | 135.54 | 122.70 |
| 1 | A | 70 | VAL | CA-CB-CG1 | 8.02 | 122.92 | 110.90 |
| 2 | B | 134 | VAL | O-C-N | -8.00 | 109.90 | 122.70 |
| 2 | B | 54 | VAL | CG1-CB-CG2 | 8.00 | 123.69 | 110.90 |
| 2 | D | 92 | HIS | CG-CD2-NE2 | 8.00 | 124.39 | 109.20 |
| 2 | D | 63 | HIS | O-C-N | 7.97 | 136.76 | 123.20 |
| 1 | A | 52 | SER | CB-CA-C | 7.97 | 125.24 | 110.10 |
| 1 | A | 59 | GLY | O-C-N | -7.97 | 109.95 | 122.70 |
| 2 | D | 108 | ASN | CB-CG-ND2 | -7.97 | 97.57 | 116.70 |
| 1 | A | 42 | TYR | CB-CG-CD2 | -7.97 | 116.22 | 121.00 |
| 1 | C | 26 | ALA | CA-C-O | 7.96 | 136.83 | 120.10 |
| 2 | D | 6 | GLU | N-CA-CB | 7.96 | 124.93 | 110.60 |
| 1 | C | 43 | PHE | CD1-CE1-CZ | 7.96 | 129.65 | 120.10 |
| 2 | D | 144 | LYS | CG-CD-CE | 7.96 | 135.78 | 111.90 |
| 2 | B | 64 | GLY | O-C-N | -7.96 | 109.97 | 122.70 |
| 1 | C | 49 | SER | N-CA-CB | 7.95 | 122.42 | 110.50 |
| 2 | B | 38 | THR | N-CA-CB | 7.94 | 125.38 | 110.30 |
| 1 | A | 1 | VAL | O-C-N | 7.93 | 135.39 | 122.70 |
| 1 | A | 24 | TYR | CG-CD1-CE1 | -7.92 | 114.96 | 121.30 |
| 1 | A | 110 | ALA | CA-C-O | 7.92 | 136.73 | 120.10 |
| 1 | A | 81 | SER | O-C-N | -7.91 | 110.04 | 122.70 |
| 2 | B | 12 | THR | O-C-N | -7.91 | 110.04 | 122.70 |
| 2 | D | 17 | LYS | CG-CD-CE | 7.89 | 135.58 | 111.90 |
| 1 | C | 98 | PHE | CE1-CZ-CE2 | -7.89 | 105.80 | 120.00 |
| 2 | B | 79 | ASP | N-CA-CB | -7.88 | 96.41 | 110.60 |
| 1 | C | 114 | PRO | N-CA-C | -7.88 | 91.61 | 112.10 |
| 1 | C | 12 | ALA | CB-CA-C | -7.88 | 98.28 | 110.10 |
| 1 | A | 63 | ALA | N-CA-CB | -7.88 | 99.07 | 110.10 |
| 1 | A | 110 | ALA | C-N-CA | 7.87 | 141.36 | 121.70 |
| 1 | A | 4 | PRO | CA-CB-CG | -7.86 | 89.06 | 104.00 |
| 2 | D | 15 | TRP | NE1-CE2-CZ2 | 7.86 | 139.04 | 130.40 |
| 1 | A | 106 | LEU | O-C-N | -7.86 | 110.13 | 122.70 |
| 2 | B | 78 | LEU | CA-CB-CG | -7.85 | 97.24 | 115.30 |
| 1 | C | 14 | TRP | CE2-CD2-CG | -7.85 | 101.02 | 107.30 |
| 2 | D | 72 | SER | CA-CB-OG | -7.85 | 90.01 | 111.20 |
| 2 | B | 26 | GLU | O-C-N | 7.83 | 135.23 | 122.70 |
| 1 | C | 110 | ALA | O-C-N | -7.83 | 110.17 | 122.70 |
| 2 | B | 87 | THR | CB-CA-C | -7.83 | 90.46 | 111.60 |
| 2 | B | 57 | ASN | O-C-N | -7.82 | 106.24 | 121.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 92 | HIS | N-CA-CB | -7.82 | 96.53 | 110.60 |
| 1 | A | 117 | PHE | CB-CG-CD1 | -7.82 | 115.33 | 120.80 |
| 2 | D | 40 | ARG | CA-C-N | 7.82 | 134.39 | 117.20 |
| 1 | A | 19 | ALA | N-CA-C | -7.81 | 89.91 | 111.00 |
| 1 | A | 27 | GLU | OE1-CD-OE2 | 7.81 | 132.67 | 123.30 |
| 2 | D | 9 | SER | C-N-CA | -7.79 | 102.22 | 121.70 |
| 1 | A | 21 | ALA | N-CA-CB | 7.78 | 120.99 | 110.10 |
| 2 | B | 99 | ASP | CB-CG-OD1 | -7.78 | 111.30 | 118.30 |
| 1 | C | 43 | PHE | CG-CD1-CE1 | -7.78 | 112.24 | 120.80 |
| 1 | A | 16 | LYS | CD-CE-NZ | 7.78 | 129.59 | 111.70 |
| 2 | B | 66 | LYS | CG-CD-CE | -7.77 | 88.60 | 111.90 |
| 2 | D | 66 | LYS | CG-CD-CE | -7.76 | 88.63 | 111.90 |
| 1 | C | 115 | ALA | N-CA-CB | 7.75 | 120.95 | 110.10 |
| 2 | D | 99 | ASP | CB-CG-OD2 | -7.74 | 111.34 | 118.30 |
| 1 | A | 93 | VAL | O-C-N | -7.73 | 110.33 | 122.70 |
| 1 | A | 98 | PHE | CZ-CE2-CD2 | -7.73 | 110.82 | 120.10 |
| 2 | D | 78 | LEU | C-N-CA | -7.73 | 102.37 | 121.70 |
| 1 | A | 132 | VAL | CG1-CB-CG2 | -7.71 | 98.56 | 110.90 |
| 1 | A | 20 | HIS | CG-CD2-NE2 | -7.71 | 94.56 | 109.20 |
| 1 | A | 92 | ARG | O-C-N | -7.70 | 110.38 | 122.70 |
| 1 | C | 42 | TYR | CD1-CE1-CZ | 7.70 | 126.73 | 119.80 |
| 2 | D | 50 | THR | CA-CB-OG1 | 7.70 | 125.17 | 109.00 |
| 2 | D | 146 | HIS | CA-C-O | 7.70 | 136.26 | 120.10 |
| 1 | A | 3 | SER | O-C-N | -7.69 | 106.49 | 121.10 |
| 1 | A | 75 | ASP | CA-C-N | -7.69 | 100.29 | 117.20 |
| 2 | B | 79 | ASP | OD1-CG-OD2 | -7.69 | 108.70 | 123.30 |
| 1 | C | 17 | VAL | CB-CA-C | 7.68 | 126.00 | 111.40 |
| 1 | A | 51 | GLY | O-C-N | 7.68 | 134.98 | 122.70 |
| 1 | A | 56 | LYS | CD-CE-NZ | -7.68 | 94.05 | 111.70 |
| 2 | D | 141 | LEU | CB-CG-CD2 | -7.68 | 97.95 | 111.00 |
| 2 | D | 122 | PHE | CD1-CG-CD2 | -7.67 | 108.32 | 118.30 |
| 1 | A | 69 | ALA | N-CA-CB | -7.67 | 99.36 | 110.10 |
| 1 | C | 23 | GLU | CB-CG-CD | -7.67 | 93.49 | 114.20 |
| 1 | A | 8 | THR | CA-CB-CG2 | -7.67 | 101.67 | 112.40 |
| 2 | B | 80 | ASN | CA-C-O | -7.67 | 104.00 | 120.10 |
| 2 | B | 122 | PHE | CD1-CE1-CZ | -7.67 | 110.90 | 120.10 |
| 2 | D | 3 | LEU | CD1-CG-CD2 | -7.66 | 87.51 | 110.50 |
| 1 | A | 48 | LEU | CB-CG-CD1 | -7.64 | 98.01 | 111.00 |
| 2 | B | 45 | PHE | O-C-N | -7.63 | 110.23 | 123.20 |
| 2 | B | 55 | MET | O-C-N | 7.63 | 136.17 | 123.20 |
| 1 | A | 2 | LEU | CB-CG-CD1 | 7.63 | 123.96 | 111.00 |
| 1 | A | 108 | THR | CA-CB-CG2 | -7.62 | 101.73 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 3 | SER | CB-CA-C | 7.61 | 124.56 | 110.10 |
| 2 | B | 99 | ASP | OD1-CG-OD2 | 7.61 | 137.76 | 123.30 |
| 1 | A | 17 | VAL | C-N-CA | -7.60 | 106.33 | 122.30 |
| 1 | C | 63 | ALA | CA-C-O | 7.60 | 136.07 | 120.10 |
| 1 | A | 3 | SER | CA-C-O | 7.58 | 136.03 | 120.10 |
| 2 | B | 130 | TYR | CD1-CE1-CZ | 7.58 | 126.62 | 119.80 |
| 1 | C | 3 | SER | O-C-N | -7.58 | 106.71 | 121.10 |
| 2 | D | 89 | SER | O-C-N | -7.57 | 110.59 | 122.70 |
| 1 | A | 101 | LEU | O-C-N | -7.56 | 110.60 | 122.70 |
| 2 | D | 97 | HIS | ND1-CG-CD2 | 7.56 | 119.38 | 108.80 |
| 1 | C | 49 | SER | O-C-N | -7.55 | 110.61 | 122.70 |
| 2 | D | 131 | GLN | CG-CD-OE1 | -7.55 | 106.50 | 121.60 |
| 2 | D | 94 | ASP | N-CA-CB | -7.55 | 97.01 | 110.60 |
| 1 | C | 99 | LYS | CG-CD-CE | -7.55 | 89.25 | 111.90 |
| 2 | D | 72 | SER | CA-C-N | -7.54 | 100.60 | 117.20 |
| 1 | C | 74 | ASP | CB-CG-OD1 | 7.54 | 125.08 | 118.30 |
| 1 | C | 72 | HIS | CA-C-O | 7.53 | 135.91 | 120.10 |
| 2 | B | 13 | ALA | O-C-N | -7.53 | 110.66 | 122.70 |
| 1 | C | 106 | LEU | C-N-CA | 7.53 | 140.52 | 121.70 |
| 2 | D | 48 | LEU | CA-CB-CG | -7.52 | 98.00 | 115.30 |
| 1 | A | 7 | LYS | N-CA-CB | -7.51 | 97.08 | 110.60 |
| 1 | C | 67 | THR | CA-CB-CG2 | -7.51 | 101.88 | 112.40 |
| 1 | C | 42 | TYR | CA-CB-CG | -7.51 | 99.12 | 113.40 |
| 2 | D | 92 | HIS | CG-ND1-CE1 | -7.51 | 95.94 | 105.70 |
| 2 | D | 50 | THR | CA-CB-CG2 | -7.50 | 101.90 | 112.40 |
| 2 | D | 117 | HIS | O-C-N | -7.50 | 110.71 | 122.70 |
| 1 | C | 137 | THR | CA-CB-CG2 | -7.49 | 101.91 | 112.40 |
| 1 | A | 61 | LYS | CB-CA-C | -7.49 | 95.42 | 110.40 |
| 1 | A | 84 | SER | O-C-N | 7.48 | 134.67 | 122.70 |
| 1 | C | 17 | VAL | CA-C-N | -7.48 | 101.24 | 116.20 |
| 1 | C | 75 | ASP | CB-CG-OD1 | -7.48 | 111.57 | 118.30 |
| 1 | C | 110 | ALA | CB-CA-C | 7.48 | 121.32 | 110.10 |
| 1 | A | 85 | ASP | OD1-CG-OD2 | -7.48 | 109.09 | 123.30 |
| 2 | B | 3 | LEU | O-C-N | 7.45 | 134.62 | 122.70 |
| 2 | B | 140 | ALA | O-C-N | -7.44 | 110.79 | 122.70 |
| 1 | C | 95 | PRO | O-C-N | -7.44 | 110.80 | 122.70 |
| 1 | C | 51 | GLY | CA-C-O | 7.43 | 133.98 | 120.60 |
| 1 | C | 40 | LYS | CD-CE-NZ | -7.43 | 94.61 | 111.70 |
| 2 | D | 98 | VAL | CA-CB-CG2 | -7.43 | 99.76 | 110.90 |
| 2 | D | 17 | LYS | CB-CG-CD | -7.42 | 92.30 | 111.60 |
| 2 | D | 2 | HIS | N-CA-C | 7.41 | 131.02 | 111.00 |
| 1 | A | 77 | PRO | O-C-N | -7.41 | 110.84 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 46 | GLY | O-C-N | 7.40 | 134.55 | 122.70 |
| 2 | B | 17 | LYS | CA-C-N | 7.38 | 133.42 | 117.20 |
| 1 | C | 56 | LYS | CA-C-O | 7.37 | 135.58 | 120.10 |
| 1 | C | 107 | VAL | O-C-N | -7.37 | 110.90 | 122.70 |
| 2 | D | 47 | ASP | C-N-CA | -7.37 | 103.27 | 121.70 |
| 1 | A | 28 | ALA | CA-C-N | -7.37 | 100.99 | 117.20 |
| 2 | B | 71 | PHE | CG-CD2-CE2 | -7.37 | 112.69 | 120.80 |
| 1 | C | 141 | ARG | NH1-CZ-NH2 | 7.36 | 127.50 | 119.40 |
| 1 | A | 87 | HIS | CA-CB-CG | -7.36 | 101.09 | 113.60 |
| 1 | C | 24 | TYR | OH-CZ-CE2 | -7.36 | 100.24 | 120.10 |
| 2 | D | 110 | LEU | O-C-N | -7.35 | 110.93 | 122.70 |
| 1 | C | 99 | LYS | CA-C-N | -7.35 | 101.03 | 117.20 |
| 2 | B | 77 | HIS | ND1-CE1-NE2 | 7.35 | 126.07 | 109.90 |
| 1 | A | 105 | LEU | O-C-N | 7.34 | 134.45 | 122.70 |
| 1 | A | 61 | LYS | CD-CE-NZ | 7.33 | 128.55 | 111.70 |
| 1 | A | 65 | ALA | C-N-CA | -7.32 | 103.39 | 121.70 |
| 2 | B | 38 | THR | CA-CB-CG2 | -7.32 | 102.15 | 112.40 |
| 2 | D | 130 | TYR | CZ-CE2-CD2 | 7.32 | 126.39 | 119.80 |
| 1 | A | 127 | LYS | CG-CD-CE | -7.31 | 89.96 | 111.90 |
| 2 | D | 6 | GLU | C-N-CA | -7.31 | 103.42 | 121.70 |
| 2 | D | 131 | GLN | OE1-CD-NE2 | 7.31 | 138.72 | 121.90 |
| 1 | C | 44 | PRO | N-CD-CG | -7.31 | 92.24 | 103.20 |
| 1 | A | 89 | HIS | CG-CD2-NE2 | -7.29 | 95.36 | 109.20 |
| 2 | D | 5 | PRO | O-C-N | -7.29 | 111.04 | 122.70 |
| 1 | C | 24 | TYR | CG-CD2-CE2 | -7.28 | 115.47 | 121.30 |
| 2 | D | 57 | ASN | C-N-CD | 7.27 | 143.66 | 128.40 |
| 2 | D | 126 | VAL | O-C-N | 7.27 | 134.33 | 122.70 |
| 1 | A | 136 | LEU | CD1-CG-CD2 | 7.26 | 132.29 | 110.50 |
| 1 | C | 15 | GLY | O-C-N | -7.26 | 111.09 | 122.70 |
| 2 | D | 35 | TYR | CG-CD1-CE1 | 7.25 | 127.10 | 121.30 |
| 2 | D | 36 | PRO | N-CD-CG | 7.24 | 114.06 | 103.20 |
| 1 | A | 6 | ASP | CB-CG-OD1 | 7.24 | 124.81 | 118.30 |
| 2 | D | 65 | LYS | N-CA-CB | -7.23 | 97.58 | 110.60 |
| 2 | D | 144 | LYS | O-C-N | -7.23 | 111.13 | 122.70 |
| 2 | D | 7 | GLU | CA-C-O | -7.23 | 104.92 | 120.10 |
| 2 | B | 95 | LYS | N-CA-CB | -7.22 | 97.60 | 110.60 |
| 1 | C | 74 | ASP | CA-C-N | -7.22 | 101.31 | 117.20 |
| 2 | B | 35 | TYR | CZ-CE2-CD2 | 7.21 | 126.29 | 119.80 |
| 2 | D | 112 | CYS | CA-C-N | -7.21 | 101.34 | 117.20 |
| 2 | D | 141 | LEU | CB-CG-CD1 | -7.20 | 98.75 | 111.00 |
| 1 | A | 5 | ALA | CB-CA-C | -7.20 | 99.31 | 110.10 |
| 2 | B | 84 | THR | CA-C-O | 7.19 | 135.19 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 143 | HIS | ND1-CG-CD2 | 7.18 | 118.85 | 108.80 |
| 1 | C | 60 | LYS | CA-CB-CG | -7.17 | 97.62 | 113.40 |
| 2 | D | 38 | THR | CA-CB-CG2 | -7.17 | 102.37 | 112.40 |
| 2 | B | 20 | VAL | CA-C-N | 7.16 | 132.96 | 117.20 |
| 2 | B | 36 | PRO | CA-N-CD | -7.16 | 101.48 | 111.50 |
| 2 | B | 61 | LYS | O-C-N | -7.16 | 111.25 | 122.70 |
| 1 | C | 117 | PHE | CE1-CZ-CE2 | 7.16 | 132.88 | 120.00 |
| 1 | A | 23 | GLU | N-CA-CB | -7.16 | 97.72 | 110.60 |
| 2 | D | 43 | GLU | CB-CG-CD | -7.16 | 94.88 | 114.20 |
| 2 | D | 144 | LYS | CB-CA-C | 7.15 | 124.70 | 110.40 |
| 2 | B | 126 | VAL | O-C-N | -7.15 | 111.26 | 122.70 |
| 1 | A | 103 | HIS | CA-C-O | 7.15 | 135.11 | 120.10 |
| 2 | D | 122 | PHE | CG-CD1-CE1 | 7.14 | 128.66 | 120.80 |
| 1 | C | 37 | PRO | N-CD-CG | 7.13 | 113.90 | 103.20 |
| 2 | B | 77 | HIS | CB-CG-CD2 | -7.13 | 108.70 | 130.80 |
| 1 | A | 134 | THR | N-CA-CB | -7.13 | 96.76 | 110.30 |
| 2 | D | 45 | PHE | CG-CD1-CE1 | -7.13 | 112.96 | 120.80 |
| 1 | A | 83 | LEU | CD1-CG-CD2 | -7.13 | 89.12 | 110.50 |
| 2 | D | 93 | CYS | CA-C-N | -7.12 | 101.54 | 117.20 |
| 2 | B | 9 | SER | CA-C-N | -7.12 | 101.54 | 117.20 |
| 1 | A | 10 | VAL | O-C-N | 7.11 | 134.08 | 122.70 |
| 1 | A | 42 | TYR | CA-CB-CG | -7.11 | 99.89 | 113.40 |
| 1 | A | 17 | VAL | CA-CB-CG2 | 7.10 | 121.54 | 110.90 |
| 1 | C | 49 | SER | N-CA-C | -7.09 | 91.86 | 111.00 |
| 2 | D | 3 | LEU | CB-CG-CD1 | -7.09 | 98.95 | 111.00 |
| 2 | B | 6 | GLU | CG-CD-OE2 | 7.08 | 132.46 | 118.30 |
| 1 | A | 49 | SER | CA-C-O | 7.08 | 134.96 | 120.10 |
| 1 | C | 118 | THR | N-CA-CB | -7.07 | 96.87 | 110.30 |
| 1 | C | 94 | ASP | CB-CG-OD1 | 7.07 | 124.66 | 118.30 |
| 1 | A | 50 | HIS | O-C-N | -7.06 | 111.19 | 123.20 |
| 2 | B | 12 | THR | CA-CB-OG1 | -7.06 | 94.17 | 109.00 |
| 1 | C | 47 | ASP | N-CA-CB | -7.06 | 97.90 | 110.60 |
| 2 | B | 31 | LEU | CB-CG-CD1 | -7.05 | 99.02 | 111.00 |
| 2 | B | 130 | TYR | CB-CG-CD2 | -7.05 | 116.77 | 121.00 |
| 2 | D | 80 | ASN | CB-CA-C | -7.05 | 96.31 | 110.40 |
| 2 | D | 92 | HIS | CA-C-O | -7.05 | 105.30 | 120.10 |
| 1 | C | 17 | VAL | CA-C-O | 7.04 | 134.88 | 120.10 |
| 2 | D | 1 | VAL | CB-CA-C | -7.04 | 98.03 | 111.40 |
| 1 | C | 78 | ASN | N-CA-C | 7.03 | 129.98 | 111.00 |
| 2 | D | 13 | ALA | CA-C-O | 7.03 | 134.86 | 120.10 |
| 2 | B | 50 | THR | CA-CB-OG1 | 7.01 | 123.72 | 109.00 |
| 1 | C | 86 | LEU | CA-C-N | -7.00 | 101.81 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 137 | VAL | CB-CA-C | -7.00 | 98.10 | 111.40 |
| 1 | C | 129 | LEU | O-C-N | -7.00 | 111.51 | 122.70 |
| 1 | C | 112 | HIS | CG-CD2-NE2 | 6.99 | 122.48 | 109.20 |
| 1 | A | 58 | HIS | CA-CB-CG | -6.98 | 101.73 | 113.60 |
| 1 | C | 14 | TRP | CD2-CE3-CZ3 | 6.98 | 127.87 | 118.80 |
| 1 | C | 99 | LYS | CB-CG-CD | 6.97 | 129.72 | 111.60 |
| 1 | A | 39 | THR | O-C-N | 6.96 | 133.84 | 122.70 |
| 2 | B | 65 | LYS | CB-CG-CD | -6.96 | 93.49 | 111.60 |
| 1 | A | 17 | VAL | N-CA-CB | 6.95 | 126.78 | 111.50 |
| 1 | A | 81 | SER | CA-C-N | 6.94 | 132.47 | 117.20 |
| 2 | B | 15 | TRP | CG-CD1-NE1 | 6.94 | 117.04 | 110.10 |
| 2 | B | 28 | LEU | CA-C-O | 6.94 | 134.67 | 120.10 |
| 2 | D | 45 | PHE | C-N-CA | -6.94 | 107.73 | 122.30 |
| 2 | B | 82 | LYS | O-C-N | -6.92 | 111.43 | 123.20 |
| 2 | D | 85 | PHE | CB-CG-CD2 | 6.92 | 125.65 | 120.80 |
| 2 | D | 19 | ASN | CB-CG-ND2 | -6.91 | 100.11 | 116.70 |
| 1 | A | 61 | LYS | CA-C-N | -6.91 | 102.01 | 117.20 |
| 1 | A | 138 | SER | CB-CA-C | -6.90 | 96.98 | 110.10 |
| 2 | B | 112 | CYS | N-CA-CB | 6.90 | 123.02 | 110.60 |
| 1 | C | 99 | LYS | CA-CB-CG | 6.89 | 128.57 | 113.40 |
| 1 | C | 107 | VAL | CA-C-O | 6.89 | 134.58 | 120.10 |
| 1 | A | 60 | LYS | CA-C-N | -6.89 | 102.04 | 117.20 |
| 1 | A | 105 | LEU | N-CA-CB | -6.88 | 96.63 | 110.40 |
| 2 | D | 14 | LEU | O-C-N | 6.88 | 133.70 | 122.70 |
| 2 | D | 71 | PHE | CD1-CE1-CZ | 6.87 | 128.34 | 120.10 |
| 1 | C | 52 | SER | CA-C-N | 6.87 | 132.31 | 117.20 |
| 2 | B | 126 | VAL | CA-C-N | 6.87 | 132.31 | 117.20 |
| 2 | D | 56 | GLY | CA-C-O | 6.86 | 132.95 | 120.60 |
| 1 | C | 76 | MET | N-CA-CB | -6.86 | 98.25 | 110.60 |
| 1 | A | 43 | PHE | CG-CD1-CE1 | -6.86 | 113.25 | 120.80 |
| 2 | B | 76 | ALA | CA-C-O | 6.86 | 134.50 | 120.10 |
| 2 | B | 69 | GLY | CA-C-N | -6.86 | 102.11 | 117.20 |
| 2 | B | 77 | HIS | CB-CG-ND1 | 6.86 | 140.34 | 123.20 |
| 1 | A | 18 | GLY | CA-C-O | -6.86 | 108.26 | 120.60 |
| 2 | D | 39 | GLN | O-C-N | -6.86 | 111.73 | 122.70 |
| 2 | D | 52 | ASP | CA-CB-CG | 6.85 | 128.48 | 113.40 |
| 1 | C | 43 | PHE | CE1-CZ-CE2 | -6.85 | 107.67 | 120.00 |
| 2 | B | 15 | TRP | NE1-CE2-CD2 | -6.84 | 100.46 | 107.30 |
| 2 | B | 20 | VAL | CA-CB-CG1 | -6.84 | 100.64 | 110.90 |
| 2 | B | 84 | THR | N-CA-CB | 6.83 | 123.29 | 110.30 |
| 1 | C | 128 | PHE | O-C-N | 6.83 | 133.64 | 122.70 |
| 2 | D | 76 | ALA | N-CA-C | -6.83 | 92.55 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | C | 33 | PHE | CZ-CE2-CD2 | 6.83 | 128.29 | 120.10 |
| 1 | A | 73 | VAL | CA-CB-CG1 | 6.82 | 121.14 | 110.90 |
| 2 | B | 66 | LYS | O-C-N | 6.81 | 133.60 | 122.70 |
| 1 | A | 31 | ARG | O-C-N | 6.81 | 133.59 | 122.70 |
| 2 | B | 80 | ASN | N-CA-C | -6.80 | 92.63 | 111.00 |
| 2 | D | 4 | THR | OG1-CB-CG2 | 6.79 | 125.62 | 110.00 |
| 2 | D | 42 | PHE | C-N-CA | -6.79 | 104.73 | 121.70 |
| 2 | B | 52 | ASP | OD1-CG-OD2 | -6.79 | 110.41 | 123.30 |
| 1 | C | 141 | ARG | CG-CD-NE | -6.79 | 97.55 | 111.80 |
| 1 | A | 113 | LEU | CB-CG-CD1 | 6.78 | 122.53 | 111.00 |
| 1 | C | 131 | SER | CB-CA-C | -6.77 | 97.23 | 110.10 |
| 2 | D | 76 | ALA | CA-C-O | -6.77 | 105.88 | 120.10 |
| 1 | A | 68 | ASN | O-C-N | -6.76 | 111.88 | 122.70 |
| 1 | A | 129 | LEU | CB-CG-CD2 | -6.76 | 99.51 | 111.00 |
| 2 | B | 49 | SER | N-CA-C | -6.76 | 92.75 | 111.00 |
| 2 | B | 2 | HIS | ND1-CG-CD2 | 6.76 | 118.26 | 108.80 |
| 2 | B | 41 | PHE | CA-C-O | -6.76 | 105.91 | 120.10 |
| 2 | B | 84 | THR | O-C-N | -6.76 | 111.89 | 122.70 |
| 2 | B | 142 | ALA | CA-C-O | -6.75 | 105.93 | 120.10 |
| 2 | D | 60 | VAL | O-C-N | -6.75 | 111.90 | 122.70 |
| 2 | B | 58 | PRO | O-C-N | 6.75 | 133.50 | 122.70 |
| 2 | D | 81 | LEU | CB-CG-CD2 | 6.75 | 122.47 | 111.00 |
| 2 | B | 113 | VAL | CA-C-N | 6.75 | 132.04 | 117.20 |
| 1 | C | 45 | HIS | CB-CG-ND1 | -6.74 | 106.34 | 123.20 |
| 2 | D | 84 | THR | CA-C-N | -6.74 | 102.38 | 117.20 |
| 2 | D | 48 | LEU | C-N-CA | -6.73 | 104.88 | 121.70 |
| 2 | D | 85 | PHE | CE1-CZ-CE2 | -6.72 | 107.89 | 120.00 |
| 2 | D | 126 | VAL | CA-CB-CG1 | -6.72 | 100.81 | 110.90 |
| 1 | C | 21 | ALA | N-CA-CB | -6.72 | 100.69 | 110.10 |
| 1 | C | 55 | VAL | CA-CB-CG1 | -6.72 | 100.82 | 110.90 |
| 1 | C | 31 | ARG | NH1-CZ-NH2 | 6.72 | 126.79 | 119.40 |
| 1 | C | 58 | HIS | O-C-N | 6.71 | 134.62 | 123.20 |
| 1 | C | 29 | LEU | CA-C-O | 6.71 | 134.19 | 120.10 |
| 1 | A | 61 | LYS | C-N-CA | -6.70 | 104.94 | 121.70 |
| 1 | C | 4 | PRO | CA-C-N | -6.70 | 102.46 | 117.20 |
| 2 | D | 40 | ARG | NH1-CZ-NH2 | 6.70 | 126.77 | 119.40 |
| 2 | D | 92 | HIS | CE1-NE2-CD2 | -6.70 | 89.85 | 106.60 |
| 2 | D | 100 | PRO | O-C-N | 6.70 | 133.41 | 122.70 |
| 1 | C | 83 | LEU | N-CA-CB | -6.69 | 97.01 | 110.40 |
| 2 | D | 41 | PHE | C-N-CA | -6.69 | 104.97 | 121.70 |
| 2 | D | 26 | GLU | O-C-N | 6.69 | 133.41 | 122.70 |
| 2 | B | 139 | ASN | CA-CB-CG | -6.68 | 98.70 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 19 | ASN | CB-CA-C | 6.67 | 123.74 | 110.40 |
| 2 | D | 75 | LEU | CB-CA-C | 6.67 | 122.87 | 110.20 |
| 1 | A | 96 | VAL | CA-CB-CG1 | 6.67 | 120.90 | 110.90 |
| 2 | B | 66 | LYS | CB-CA-C | -6.67 | 97.07 | 110.40 |
| 2 | B | 90 | GLU | CG-CD-OE2 | -6.67 | 104.97 | 118.30 |
| 2 | B | 90 | GLU | CA-CB-CG | -6.65 | 98.76 | 113.40 |
| 2 | D | 80 | ASN | C-N-CA | -6.65 | 105.07 | 121.70 |
| 2 | D | 91 | LEU | CA-C-O | 6.65 | 134.06 | 120.10 |
| 1 | A | 33 | PHE | CD1-CE1-CZ | -6.64 | 112.13 | 120.10 |
| 2 | B | 44 | SER | CA-C-O | -6.64 | 106.15 | 120.10 |
| 1 | C | 7 | LYS | CA-C-N | -6.64 | 102.59 | 117.20 |
| 1 | C | 10 | VAL | CG1-CB-CG2 | -6.64 | 100.28 | 110.90 |
| 1 | C | 38 | THR | CB-CA-C | 6.63 | 129.49 | 111.60 |
| 1 | C | 130 | ALA | N-CA-CB | 6.62 | 119.37 | 110.10 |
| 2 | B | 141 | LEU | CB-CA-C | 6.62 | 122.78 | 110.20 |
| 1 | A | 24 | TYR | CA-CB-CG | -6.62 | 100.83 | 113.40 |
| 2 | B | 88 | LEU | CB-CG-CD1 | -6.62 | 99.75 | 111.00 |
| 1 | A | 78 | ASN | O-C-N | -6.59 | 112.15 | 122.70 |
| 1 | C | 64 | ASP | CA-CB-CG | 6.59 | 127.89 | 113.40 |
| 1 | C | 140 | TYR | CD1-CG-CD2 | -6.59 | 110.65 | 117.90 |
| 2 | D | 13 | ALA | CA-C-N | -6.59 | 102.71 | 117.20 |
| 2 | D | 23 | VAL | CG1-CB-CG2 | 6.58 | 121.43 | 110.90 |
| 2 | D | 1 | VAL | CG1-CB-CG2 | -6.58 | 100.37 | 110.90 |
| 1 | A | 84 | SER | CB-CA-C | -6.57 | 97.62 | 110.10 |
| 2 | D | 103 | PHE | N-CA-CB | 6.57 | 122.42 | 110.60 |
| 1 | A | 77 | PRO | N-CA-CB | 6.56 | 111.17 | 103.30 |
| 2 | B | 28 | LEU | O-C-N | -6.56 | 112.05 | 123.20 |
| 2 | D | 137 | VAL | CG1-CB-CG2 | 6.56 | 121.39 | 110.90 |
| 2 | B | 74 | GLY | N-CA-C | 6.56 | 129.49 | 113.10 |
| 1 | C | 139 | LYS | CA-CB-CG | -6.56 | 98.97 | 113.40 |
| 1 | A | 81 | SER | C-N-CA | 6.55 | 138.09 | 121.70 |
| 2 | B | 141 | LEU | O-C-N | -6.55 | 112.22 | 122.70 |
| 1 | A | 126 | ASP | CA-C-O | 6.55 | 133.86 | 120.10 |
| 1 | A | 140 | TYR | CD1-CG-CD2 | -6.55 | 110.69 | 117.90 |
| 2 | B | 101 | GLU | O-C-N | -6.55 | 112.22 | 122.70 |
| 2 | D | 8 | LYS | CA-C-O | 6.55 | 133.85 | 120.10 |
| 2 | D | 51 | PRO | CA-C-O | 6.54 | 135.90 | 120.20 |
| 1 | A | 50 | HIS | ND1-CG-CD2 | -6.54 | 96.84 | 106.00 |
| 2 | B | 101 | GLU | CG-CD-OE1 | -6.54 | 105.22 | 118.30 |
| 2 | B | 17 | LYS | C-N-CA | 6.54 | 138.04 | 121.70 |
| 2 | B | 103 | PHE | N-CA-CB | 6.54 | 122.36 | 110.60 |
| 1 | C | 140 | TYR | O-C-N | 6.53 | 133.15 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 144 | LYS | N-CA-CB | 6.53 | 122.36 | 110.60 |
| 2 | B | 95 | LYS | O-C-N | -6.53 | 112.25 | 122.70 |
| 1 | C | 6 | ASP | CB-CG-OD2 | -6.53 | 112.42 | 118.30 |
| 1 | A | 83 | LEU | CB-CA-C | -6.52 | 97.81 | 110.20 |
| 1 | A | 46 | PHE | CD1-CE1-CZ | 6.52 | 127.92 | 120.10 |
| 2 | D | 92 | HIS | CB-CG-CD2 | 6.51 | 150.99 | 130.80 |
| 1 | C | 42 | TYR | CB-CG-CD2 | 6.51 | 124.91 | 121.00 |
| 2 | D | 66 | LYS | CB-CA-C | 6.51 | 123.42 | 110.40 |
| 2 | B | 27 | ALA | N-CA-CB | -6.51 | 100.99 | 110.10 |
| 1 | A | 71 | ALA | CB-CA-C | 6.50 | 119.86 | 110.10 |
| 2 | B | 7 | GLU | N-CA-C | -6.50 | 93.45 | 111.00 |
| 2 | B | 132 | LYS | CG-CD-CE | -6.50 | 92.40 | 111.90 |
| 1 | A | 23 | GLU | CG-CD-OE2 | -6.50 | 105.30 | 118.30 |
| 2 | D | 51 | PRO | O-C-N | -6.50 | 112.30 | 122.70 |
| 1 | A | 3 | SER | N-CA-CB | -6.49 | 100.76 | 110.50 |
| 2 | B | 138 | ALA | CA-C-O | 6.49 | 133.73 | 120.10 |
| 1 | A | 84 | SER | N-CA-CB | 6.48 | 120.22 | 110.50 |
| 2 | B | 24 | GLY | CA-C-O | 6.48 | 132.26 | 120.60 |
| 1 | A | 36 | PHE | O-C-N | 6.47 | 133.40 | 121.10 |
| 1 | A | 51 | GLY | C-N-CA | -6.47 | 105.52 | 121.70 |
| 2 | B | 90 | GLU | CA-C-O | 6.47 | 133.69 | 120.10 |
| 2 | B | 91 | LEU | C-N-CA | -6.47 | 105.53 | 121.70 |
| 2 | D | 100 | PRO | CA-N-CD | -6.46 | 102.45 | 111.50 |
| 2 | D | 135 | ALA | N-CA-CB | 6.45 | 119.14 | 110.10 |
| 2 | D | 145 | TYR | CD1-CE1-CZ | -6.45 | 113.99 | 119.80 |
| 2 | B | 2 | HIS | CA-C-O | 6.45 | 133.65 | 120.10 |
| 2 | D | 49 | SER | CA-C-N | -6.45 | 103.01 | 117.20 |
| 2 | B | 99 | ASP | N-CA-C | -6.45 | 93.59 | 111.00 |
| 2 | B | 65 | LYS | CA-CB-CG | -6.45 | 99.22 | 113.40 |
| 2 | B | 3 | LEU | CB-CG-CD2 | -6.44 | 100.05 | 111.00 |
| 1 | C | 1 | VAL | CA-C-O | 6.44 | 133.62 | 120.10 |
| 1 | C | 96 | VAL | CA-CB-CG1 | -6.44 | 101.25 | 110.90 |
| 2 | D | 15 | TRP | CZ3-CH2-CZ2 | 6.44 | 129.32 | 121.60 |
| 1 | C | 36 | PHE | C-N-CD | 6.43 | 141.89 | 128.40 |
| 1 | A | 76 | MET | N-CA-CB | -6.42 | 99.03 | 110.60 |
| 2 | B | 37 | TRP | CD2-CE3-CZ3 | -6.42 | 110.45 | 118.80 |
| 2 | B | 81 | LEU | CB-CG-CD1 | 6.42 | 121.92 | 111.00 |
| 2 | D | 105 | LEU | CA-CB-CG | 6.42 | 130.07 | 115.30 |
| 2 | D | 100 | PRO | CB-CA-C | 6.42 | 128.05 | 112.00 |
| 1 | C | 61 | LYS | O-C-N | 6.42 | 132.97 | 122.70 |
| 1 | A | 72 | HIS | ND1-CE1-NE2 | -6.42 | 95.79 | 109.90 |
| 2 | B | 59 | LYS | CG-CD-CE | -6.41 | 92.66 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | C | 58 | HIS | CE1-NE2-CD2 | -6.41 | 90.57 | 106.60 |
| 1 | C | 107 | VAL | N-CA-CB | 6.41 | 125.61 | 111.50 |
| 2 | B | 118 | PHE | CZ-CE2-CD2 | 6.40 | 127.78 | 120.10 |
| 1 | C | 11 | LYS | CB-CA-C | 6.39 | 123.19 | 110.40 |
| 2 | D | 59 | LYS | CD-CE-NZ | -6.39 | 97.00 | 111.70 |
| 2 | D | 122 | PHE | N-CA-CB | -6.39 | 99.10 | 110.60 |
| 2 | D | 90 | GLU | C-N-CA | -6.39 | 105.73 | 121.70 |
| 2 | B | 142 | ALA | N-CA-CB | 6.38 | 119.04 | 110.10 |
| 1 | C | 18 | GLY | C-N-CA | -6.38 | 105.75 | 121.70 |
| 1 | A | 125 | LEU | O-C-N | -6.38 | 112.50 | 122.70 |
| 1 | C | 16 | LYS | N-CA-C | -6.38 | 93.78 | 111.00 |
| 1 | C | 112 | HIS | CA-CB-CG | -6.38 | 102.76 | 113.60 |
| 2 | D | 24 | GLY | CA-C-N | 6.37 | 128.94 | 116.20 |
| 1 | A | 86 | LEU | C-N-CA | -6.37 | 105.78 | 121.70 |
| 1 | C | 91 | LEU | N-CA-CB | -6.37 | 97.67 | 110.40 |
| 1 | C | 133 | SER | N-CA-CB | 6.37 | 120.05 | 110.50 |
| 2 | B | 80 | ASN | C-N-CA | -6.36 | 105.79 | 121.70 |
| 1 | C | 2 | LEU | CB-CG-CD2 | 6.36 | 121.81 | 111.00 |
| 1 | C | 80 | LEU | CB-CG-CD2 | -6.36 | 100.19 | 111.00 |
| 2 | D | 18 | VAL | CG1-CB-CG2 | -6.36 | 100.73 | 110.90 |
| 1 | C | 13 | ALA | CB-CA-C | 6.36 | 119.63 | 110.10 |
| 2 | B | 79 | ASP | CB-CG-OD2 | 6.35 | 124.02 | 118.30 |
| 2 | D | 60 | VAL | CA-CB-CG2 | 6.35 | 120.42 | 110.90 |
| 2 | B | 13 | ALA | N-CA-C | 6.34 | 128.12 | 111.00 |
| 1 | C | 47 | ASP | CA-CB-CG | -6.34 | 99.45 | 113.40 |
| 1 | A | 33 | PHE | CA-C-O | 6.34 | 133.41 | 120.10 |
| 2 | D | 45 | PHE | CE1-CZ-CE2 | -6.34 | 108.59 | 120.00 |
| 2 | B | 14 | LEU | CD1-CG-CD2 | 6.34 | 129.51 | 110.50 |
| 1 | A | 74 | ASP | OD1-CG-OD2 | -6.33 | 111.27 | 123.30 |
| 2 | B | 36 | PRO | N-CA-CB | 6.32 | 110.89 | 103.30 |
| 2 | B | 5 | PRO | N-CD-CG | -6.32 | 93.72 | 103.20 |
| 2 | D | 74 | GLY | CA-C-O | 6.32 | 131.97 | 120.60 |
| 2 | B | 37 | TRP | CD1-CG-CD2 | -6.31 | 101.25 | 106.30 |
| 2 | B | 103 | PHE | CG-CD2-CE2 | -6.31 | 113.86 | 120.80 |
| 2 | D | 64 | GLY | CA-C-O | 6.31 | 131.96 | 120.60 |
| 1 | C | 109 | LEU | CD1-CG-CD2 | 6.31 | 129.43 | 110.50 |
| 1 | A | 99 | LYS | CB-CG-CD | 6.31 | 128.00 | 111.60 |
| 2 | B | 66 | LYS | CA-CB-CG | 6.31 | 127.27 | 113.40 |
| 1 | A | 64 | ASP | CB-CA-C | -6.30 | 97.79 | 110.40 |
| 2 | B | 6 | GLU | CB-CA-C | -6.30 | 97.80 | 110.40 |
| 1 | C | 98 | PHE | CB-CG-CD1 | -6.30 | 116.39 | 120.80 |
| 1 | C | 103 | HIS | O-C-N | -6.30 | 112.62 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 118 | THR | O-C-N | 6.30 | 133.07 | 121.10 |
| 2 | B | 71 | PHE | CG-CD1-CE1 | 6.30 | 127.72 | 120.80 |
| 1 | A | 22 | GLY | N-CA-C | 6.29 | 128.83 | 113.10 |
| 1 | A | 30 | GLU | CG-CD-OE2 | -6.29 | 105.72 | 118.30 |
| 1 | A | 56 | LYS | CA-C-N | -6.29 | 103.63 | 116.20 |
| 1 | A | 112 | HIS | CB-CG-ND1 | -6.28 | 107.49 | 123.20 |
| 1 | C | 50 | HIS | CA-C-O | -6.28 | 106.91 | 120.10 |
| 2 | D | 139 | ASN | CA-C-O | 6.27 | 133.28 | 120.10 |
| 1 | C | 69 | ALA | CB-CA-C | 6.27 | 119.51 | 110.10 |
| 2 | B | 78 | LEU | CA-C-O | -6.27 | 106.93 | 120.10 |
| 1 | C | 65 | ALA | CB-CA-C | -6.27 | 100.69 | 110.10 |
| 1 | A | 7 | LYS | C-N-CA | -6.26 | 106.04 | 121.70 |
| 1 | C | 47 | ASP | CA-C-N | -6.25 | 103.44 | 117.20 |
| 2 | D | 4 | THR | CA-C-N | 6.25 | 134.61 | 117.10 |
| 2 | D | 96 | LEU | O-C-N | 6.25 | 132.71 | 122.70 |
| 1 | A | 86 | LEU | CD1-CG-CD2 | -6.25 | 91.75 | 110.50 |
| 1 | A | 64 | ASP | N-CA-C | 6.25 | 127.87 | 111.00 |
| 1 | A | 132 | VAL | CA-CB-CG1 | 6.24 | 120.26 | 110.90 |
| 1 | C | 58 | HIS | CG-CD2-NE2 | 6.24 | 121.05 | 109.20 |
| 1 | A | 99 | LYS | CD-CE-NZ | -6.24 | 97.36 | 111.70 |
| 2 | D | 6 | GLU | N-CA-C | -6.24 | 94.16 | 111.00 |
| 2 | B | 61 | LYS | CG-CD-CE | -6.23 | 93.21 | 111.90 |
| 2 | D | 85 | PHE | CA-CB-CG | -6.23 | 98.96 | 113.90 |
| 1 | A | 83 | LEU | O-C-N | -6.22 | 112.74 | 122.70 |
| 1 | A | 128 | PHE | CG-CD1-CE1 | -6.22 | 113.95 | 120.80 |
| 1 | A | 15 | GLY | O-C-N | -6.22 | 112.75 | 122.70 |
| 2 | D | 39 | GLN | N-CA-CB | -6.21 | 99.42 | 110.60 |
| 2 | B | 95 | LYS | N-CA-C | 6.21 | 127.77 | 111.00 |
| 1 | A | 138 | SER | O-C-N | 6.20 | 132.62 | 122.70 |
| 2 | D | 141 | LEU | CD1-CG-CD2 | -6.20 | 91.89 | 110.50 |
| 1 | C | 1 | VAL | CB-CA-C | -6.20 | 99.62 | 111.40 |
| 1 | C | 5 | ALA | CA-C-N | -6.20 | 103.56 | 117.20 |
| 2 | B | 145 | TYR | O-C-N | 6.20 | 132.62 | 122.70 |
| 2 | D | 77 | HIS | CG-ND1-CE1 | -6.20 | 97.65 | 105.70 |
| 1 | C | 54 | GLN | CA-C-N | -6.19 | 103.57 | 117.20 |
| 2 | D | 80 | ASN | CB-CG-OD1 | -6.19 | 109.21 | 121.60 |
| 1 | C | 74 | ASP | N-CA-CB | -6.19 | 99.46 | 110.60 |
| 1 | A | 75 | ASP | C-N-CA | -6.19 | 106.23 | 121.70 |
| 1 | A | 4 | PRO | O-C-N | -6.18 | 112.81 | 122.70 |
| 2 | D | 41 | PHE | CB-CG-CD1 | -6.18 | 116.47 | 120.80 |
| 2 | D | 131 | GLN | CA-C-O | 6.18 | 133.09 | 120.10 |
| 2 | B | 63 | HIS | CA-CB-CG | 6.18 | 124.11 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | A | 24 | TYR | CB-CG-CD1 | -6.18 | 117.29 | 121.00 |
| 1 | A | 117 | PHE | CZ-CE2-CD2 | -6.18 | 112.69 | 120.10 |
| 1 | A | 28 | ALA | C-N-CA | -6.18 | 106.26 | 121.70 |
| 1 | C | 50 | HIS | CA-CB-CG | -6.18 | 103.10 | 113.60 |
| 2 | B | 81 | LEU | C-N-CA | -6.17 | 106.27 | 121.70 |
| 1 | C | 141 | ARG | CB-CG-CD | -6.17 | 95.55 | 111.60 |
| 2 | D | 31 | LEU | CA-C-N | -6.17 | 103.62 | 117.20 |
| 2 | B | 21 | ASP | OD1-CG-OD2 | 6.17 | 135.02 | 123.30 |
| 2 | B | 8 | LYS | CG-CD-CE | 6.17 | 130.40 | 111.90 |
| 2 | B | 93 | CYS | O-C-N | 6.17 | 132.57 | 122.70 |
| 2 | B | 61 | LYS | CB-CA-C | -6.16 | 98.08 | 110.40 |
| 2 | D | 15 | TRP | NE1-CE2-CD2 | -6.16 | 101.14 | 107.30 |
| 2 | B | 103 | PHE | CD1-CG-CD2 | 6.16 | 126.30 | 118.30 |
| 2 | D | 7 | GLU | CB-CG-CD | -6.15 | 97.58 | 114.20 |
| 2 | B | 14 | LEU | N-CA-CB | -6.15 | 98.09 | 110.40 |
| 2 | B | 19 | ASN | CB-CG-OD1 | 6.15 | 133.91 | 121.60 |
| 2 | B | 37 | TRP | N-CA-CB | -6.15 | 99.53 | 110.60 |
| 2 | D | 24 | GLY | C-N-CA | 6.15 | 135.21 | 122.30 |
| 2 | B | 44 | SER | C-N-CA | 6.15 | 137.07 | 121.70 |
| 1 | C | 100 | LEU | CB-CA-C | 6.14 | 121.86 | 110.20 |
| 2 | D | 1 | VAL | C-N-CA | -6.14 | 106.36 | 121.70 |
| 2 | D | 19 | ASN | CA-C-O | -6.14 | 107.21 | 120.10 |
| 2 | B | 120 | LYS | CG-CD-CE | -6.13 | 93.51 | 111.90 |
| 2 | B | 120 | LYS | CB-CA-C | -6.13 | 98.14 | 110.40 |
| 2 | B | 35 | TYR | O-C-N | 6.12 | 132.74 | 121.10 |
| 1 | C | 122 | HIS | CB-CA-C | 6.12 | 122.65 | 110.40 |
| 1 | A | 79 | ALA | O-C-N | 6.11 | 132.48 | 122.70 |
| 2 | B | 76 | ALA | N-CA-C | 6.11 | 127.50 | 111.00 |
| 1 | A | 58 | HIS | CG-ND1-CE1 | -6.11 | 97.76 | 105.70 |
| 1 | A | 96 | VAL | CA-C-O | 6.11 | 132.93 | 120.10 |
| 1 | C | 38 | THR | N-CA-CB | -6.11 | 98.69 | 110.30 |
| 1 | C | 21 | ALA | CA-C-N | 6.11 | 128.42 | 116.20 |
| 1 | C | 11 | LYS | O-C-N | -6.11 | 112.93 | 122.70 |
| 2 | D | 48 | LEU | CB-CG-CD1 | -6.10 | 100.63 | 111.00 |
| 2 | D | 93 | CYS | C-N-CA | -6.10 | 106.45 | 121.70 |
| 2 | B | 90 | GLU | OE1-CD-OE2 | 6.09 | 130.61 | 123.30 |
| 2 | B | 73 | ASP | C-N-CA | 6.09 | 135.10 | 122.30 |
| 1 | C | 77 | PRO | CA-C-O | 6.09 | 134.81 | 120.20 |
| 2 | B | 41 | PHE | CG-CD1-CE1 | -6.09 | 114.10 | 120.80 |
| 1 | A | 58 | HIS | CA-C-N | -6.07 | 104.06 | 116.20 |
| 1 | C | 43 | PHE | CD1-CG-CD2 | 6.07 | 126.19 | 118.30 |
| 2 | B | 50 | THR | N-CA-C | 6.06 | 127.37 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | B | 12 | THR | CA-C-O | 6.06 | 132.82 | 120.10 |
| 2 | D | 7 | GLU | CA-CB-CG | -6.06 | 100.08 | 113.40 |
| 1 | A | 1 | VAL | CA-C-N | -6.05 | 103.88 | 117.20 |
| 1 | A | 83 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | C | 25 | GLY | C-N-CA | 6.05 | 136.83 | 121.70 |
| 1 | C | 72 | HIS | CE1-NE2-CD2 | -6.05 | 91.47 | 106.60 |
| 1 | C | 103 | HIS | ND1-CE1-NE2 | 6.05 | 123.21 | 109.90 |
| 1 | A | 89 | HIS | C-N-CA | 6.05 | 136.82 | 121.70 |
| 2 | B | 36 | PRO | O-C-N | -6.05 | 113.03 | 122.70 |
| 2 | D | 12 | THR | N-CA-CB | -6.04 | 98.82 | 110.30 |
| 2 | D | 102 | ASN | CA-C-N | 6.04 | 130.50 | 117.20 |
| 2 | B | 104 | ARG | CG-CD-NE | -6.04 | 99.11 | 111.80 |
| 1 | C | 47 | ASP | O-C-N | 6.03 | 132.35 | 122.70 |
| 1 | A | 18 | GLY | CA-C-N | -6.03 | 103.93 | 117.20 |
| 1 | C | 138 | SER | CB-CA-C | -6.03 | 98.64 | 110.10 |
| 2 | B | 97 | HIS | CG-CD2-NE2 | -6.03 | 97.75 | 109.20 |
| 1 | A | 15 | GLY | C-N-CA | 6.02 | 136.76 | 121.70 |
| 1 | A | 45 | HIS | CB-CG-ND1 | -6.02 | 108.14 | 123.20 |
| 2 | D | 92 | HIS | CA-CB-CG | -6.02 | 103.37 | 113.60 |
| 1 | A | 56 | LYS | CB-CA-C | 6.02 | 122.43 | 110.40 |
| 2 | B | 30 | ARG | CD-NE-CZ | 6.02 | 132.02 | 123.60 |
| 1 | A | 85 | ASP | CA-CB-CG | -6.01 | 100.18 | 113.40 |
| 1 | A | 109 | LEU | CD1-CG-CD2 | 6.01 | 128.53 | 110.50 |
| 1 | A | 99 | LYS | CA-CB-CG | 6.01 | 126.62 | 113.40 |
| 1 | C | 39 | THR | CA-CB-CG2 | -6.00 | 103.99 | 112.40 |
| 2 | D | 125 | PRO | CA-C-N | -6.00 | 104.01 | 117.20 |
| 1 | A | 40 | LYS | CB-CA-C | -5.99 | 98.41 | 110.40 |
| 1 | C | 75 | ASP | N-CA-CB | -5.99 | 99.81 | 110.60 |
| 2 | D | 17 | LYS | N-CA-CB | 5.99 | 121.38 | 110.60 |
| 1 | A | 26 | ALA | O-C-N | -5.98 | 113.13 | 122.70 |
| 2 | B | 108 | ASN | CB-CG-OD1 | -5.96 | 109.68 | 121.60 |
| 1 | A | 27 | GLU | N-CA-CB | -5.96 | 99.87 | 110.60 |
| 1 | A | 117 | PHE | O-C-N | 5.95 | 132.22 | 122.70 |
| 2 | B | 46 | GLY | CA-C-O | -5.95 | 109.89 | 120.60 |
| 2 | D | 103 | PHE | CG-CD2-CE2 | -5.95 | 114.25 | 120.80 |
| 1 | A | 46 | PHE | CG-CD1-CE1 | 5.95 | 127.34 | 120.80 |
| 2 | B | 140 | ALA | CA-C-N | 5.95 | 130.28 | 117.20 |
| 1 | A | 84 | SER | CA-CB-OG | -5.95 | 95.14 | 111.20 |
| 1 | A | 49 | SER | N-CA-C | -5.94 | 94.96 | 111.00 |
| 1 | C | 45 | HIS | CA-C-O | -5.94 | 107.63 | 120.10 |
| 2 | B | 91 | LEU | N-CA-CB | -5.94 | 98.53 | 110.40 |
| 1 | C | 77 | PRO | CA-CB-CG | 5.94 | 116.08 | 104.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 124 | SER | CA-C-O | -5.93 | 107.64 | 120.10 |
| 2 | D | 126 | VAL | CA-C-N | -5.93 | 104.14 | 117.20 |
| 2 | D | 78 | LEU | CA-CB-CG | 5.93 | 128.94 | 115.30 |
| 1 | A | 14 | TRP | CB-CG-CD1 | -5.93 | 119.29 | 127.00 |
| 2 | D | 21 | ASP | C-N-CA | 5.93 | 136.52 | 121.70 |
| 2 | D | 19 | ASN | O-C-N | -5.93 | 113.22 | 122.70 |
| 2 | D | 88 | LEU | CB-CG-CD1 | -5.93 | 100.93 | 111.00 |
| 1 | A | 54 | GLN | OE1-CD-NE2 | -5.92 | 108.29 | 121.90 |
| 2 | B | 28 | LEU | CB-CA-C | 5.92 | 121.44 | 110.20 |
| 1 | A | 89 | HIS | CA-C-O | 5.92 | 132.52 | 120.10 |
| 2 | B | 33 | VAL | O-C-N | 5.92 | 132.16 | 122.70 |
| 1 | A | 126 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 1 | A | 134 | THR | CA-C-N | 5.91 | 130.20 | 117.20 |
| 2 | D | 57 | ASN | CB-CG-OD1 | 5.91 | 133.42 | 121.60 |
| 1 | A | 134 | THR | CA-CB-OG1 | 5.91 | 121.40 | 109.00 |
| 2 | B | 69 | GLY | CA-C-O | 5.91 | 131.23 | 120.60 |
| 2 | D | 103 | PHE | CZ-CE2-CD2 | 5.90 | 127.18 | 120.10 |
| 1 | A | 28 | ALA | CA-C-O | 5.90 | 132.49 | 120.10 |
| 1 | A | 131 | SER | CA-C-O | -5.89 | 107.72 | 120.10 |
| 1 | C | 37 | PRO | CA-N-CD | -5.89 | 103.25 | 111.50 |
| 1 | C | 14 | TRP | CA-CB-CG | -5.89 | 102.51 | 113.70 |
| 2 | B | 24 | GLY | O-C-N | -5.89 | 113.19 | 123.20 |
| 2 | D | 91 | LEU | CB-CG-CD2 | 5.89 | 121.01 | 111.00 |
| 1 | A | 67 | THR | CA-CB-OG1 | 5.89 | 121.36 | 109.00 |
| 2 | D | 95 | LYS | CG-CD-CE | 5.89 | 129.56 | 111.90 |
| 2 | B | 50 | THR | CA-C-O | -5.89 | 107.74 | 120.10 |
| 1 | A | 135 | VAL | CA-C-N | 5.88 | 130.14 | 117.20 |
| 2 | B | 11 | VAL | O-C-N | 5.88 | 132.11 | 122.70 |
| 1 | C | 50 | HIS | CB-CG-ND1 | -5.88 | 108.51 | 123.20 |
| 1 | C | 77 | PRO | N-CA-CB | -5.87 | 96.14 | 102.60 |
| 2 | B | 123 | THR | O-C-N | 5.87 | 132.25 | 121.10 |
| 1 | C | 89 | HIS | CB-CA-C | 5.87 | 122.14 | 110.40 |
| 2 | D | 130 | TYR | CD1-CG-CD2 | -5.87 | 111.44 | 117.90 |
| 1 | A | 7 | LYS | O-C-N | 5.87 | 132.09 | 122.70 |
| 1 | A | 8 | THR | N-CA-CB | -5.86 | 99.16 | 110.30 |
| 1 | C | 92 | ARG | CG-CD-NE | -5.86 | 99.50 | 111.80 |
| 1 | C | 90 | LYS | CA-CB-CG | -5.85 | 100.53 | 113.40 |
| 1 | A | 81 | SER | CB-CA-C | -5.85 | 98.99 | 110.10 |
| 2 | D | 141 | LEU | O-C-N | -5.84 | 113.35 | 122.70 |
| 2 | B | 79 | ASP | CA-CB-CG | -5.84 | 100.55 | 113.40 |
| 1 | A | 64 | ASP | N-CA-CB | -5.84 | 100.09 | 110.60 |
| 2 | B | 132 | LYS | O-C-N | -5.83 | 113.37 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 137 | VAL | CA-CB-CG2 | -5.83 | 102.15 | 110.90 |
| 1 | A | 98 | PHE | N-CA-CB | 5.83 | 121.09 | 110.60 |
| 1 | C | 136 | LEU | CB-CG-CD1 | -5.83 | 101.10 | 111.00 |
| 1 | A | 73 | VAL | CB-CA-C | 5.82 | 122.46 | 111.40 |
| 2 | B | 17 | LYS | CA-CB-CG | -5.82 | 100.60 | 113.40 |
| 2 | D | 60 | VAL | CA-C-O | 5.81 | 132.31 | 120.10 |
| 1 | A | 44 | PRO | CA-N-CD | 5.81 | 119.83 | 111.70 |
| 1 | A | 103 | HIS | CG-ND1-CE1 | -5.81 | 98.15 | 105.70 |
| 1 | A | 11 | LYS | CD-CE-NZ | -5.80 | 98.36 | 111.70 |
| 2 | D | 53 | ALA | CA-C-N | -5.80 | 104.44 | 117.20 |
| 2 | D | 12 | THR | C-N-CA | 5.80 | 136.20 | 121.70 |
| 1 | A | 132 | VAL | CA-C-N | 5.79 | 129.95 | 117.20 |
| 1 | A | 54 | GLN | CA-C-O | -5.79 | 107.94 | 120.10 |
| 1 | C | 11 | LYS | CA-C-O | 5.79 | 132.25 | 120.10 |
| 2 | D | 97 | HIS | N-CA-CB | 5.79 | 121.01 | 110.60 |
| 1 | A | 16 | LYS | CA-C-N | -5.78 | 104.48 | 117.20 |
| 1 | A | 21 | ALA | N-CA-C | -5.78 | 95.41 | 111.00 |
| 2 | B | 37 | TRP | CE3-CZ3-CH2 | 5.78 | 127.55 | 121.20 |
| 1 | C | 46 | PHE | CA-C-O | 5.77 | 132.21 | 120.10 |
| 2 | D | 82 | LYS | CA-C-N | 5.76 | 127.72 | 116.20 |
| 1 | C | 89 | HIS | ND1-CG-CD2 | 5.76 | 116.86 | 108.80 |
| 2 | D | 68 | LEU | CB-CA-C | -5.76 | 99.26 | 110.20 |
| 1 | C | 83 | LEU | CB-CG-CD1 | -5.76 | 101.21 | 111.00 |
| 1 | C | 15 | GLY | CA-C-N | 5.75 | 129.86 | 117.20 |
| 2 | D | 22 | GLU | CB-CA-C | 5.75 | 121.91 | 110.40 |
| 1 | C | 12 | ALA | N-CA-CB | 5.75 | 118.16 | 110.10 |
| 1 | C | 118 | THR | CB-CA-C | -5.75 | 96.08 | 111.60 |
| 2 | B | 9 | SER | C-N-CA | -5.74 | 107.35 | 121.70 |
| 2 | B | 36 | PRO | CA-C-N | 5.74 | 129.83 | 117.20 |
| 2 | B | 8 | LYS | CA-C-N | 5.74 | 129.82 | 117.20 |
| 2 | B | 75 | LEU | CD1-CG-CD2 | -5.74 | 93.29 | 110.50 |
| 2 | D | 112 | CYS | CA-C-O | 5.74 | 132.15 | 120.10 |
| 1 | A | 4 | PRO | CA-C-N | -5.73 | 104.59 | 117.20 |
| 2 | B | 96 | LEU | N-CA-C | 5.73 | 126.48 | 111.00 |
| 1 | A | 103 | HIS | N-CA-CB | 5.73 | 120.92 | 110.60 |
| 1 | A | 14 | TRP | NE1-CE2-CD2 | -5.73 | 101.57 | 107.30 |
| 1 | C | 47 | ASP | CB-CA-C | -5.73 | 98.94 | 110.40 |
| 2 | D | 56 | GLY | C-N-CA | 5.72 | 136.01 | 121.70 |
| 1 | C | 78 | ASN | CB-CA-C | 5.72 | 121.85 | 110.40 |
| 2 | B | 17 | LYS | CB-CA-C | -5.72 | 98.96 | 110.40 |
| 1 | A | 32 | MET | CA-CB-CG | 5.72 | 123.02 | 113.30 |
| 2 | B | 13 | ALA | CB-CA-C | -5.71 | 101.53 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | A | 137 | THR | CA-C-N | 5.71 | 129.76 | 117.20 |
| 1 | A | 104 | CYS | CA-C-O | -5.71 | 108.12 | 120.10 |
| 1 | C | 27 | GLU | OE1-CD-OE2 | -5.71 | 116.45 | 123.30 |
| 2 | D | 108 | ASN | CB-CG-OD1 | -5.71 | 110.19 | 121.60 |
| 2 | B | 39 | GLN | OE1-CD-NE2 | 5.70 | 135.01 | 121.90 |
| 2 | B | 97 | HIS | ND1-CG-CD2 | 5.70 | 116.78 | 108.80 |
| 1 | C | 41 | THR | C-N-CA | 5.70 | 135.95 | 121.70 |
| 1 | C | 36 | PHE | CZ-CE2-CD2 | 5.70 | 126.94 | 120.10 |
| 2 | D | 28 | LEU | O-C-N | -5.70 | 113.51 | 123.20 |
| 1 | C | 116 | GLU | CA-C-O | -5.70 | 108.14 | 120.10 |
| 2 | B | 62 | ALA | C-N-CA | -5.70 | 107.46 | 121.70 |
| 2 | B | 110 | LEU | CB-CA-C | 5.69 | 121.01 | 110.20 |
| 2 | D | 13 | ALA | CB-CA-C | -5.69 | 101.57 | 110.10 |
| 2 | D | 20 | VAL | CA-C-N | -5.68 | 104.69 | 117.20 |
| 2 | D | 92 | HIS | ND1-CG-CD2 | -5.68 | 98.04 | 106.00 |
| 2 | D | 54 | VAL | CA-C-N | 5.68 | 129.69 | 117.20 |
| 2 | D | 143 | HIS | CB-CG-CD2 | -5.68 | 113.20 | 130.80 |
| 1 | A | 52 | SER | N-CA-CB | -5.67 | 102.00 | 110.50 |
| 2 | B | 50 | THR | O-C-N | 5.67 | 131.87 | 121.10 |
| 2 | D | 15 | TRP | CE3-CZ3-CH2 | -5.67 | 114.96 | 121.20 |
| 1 | A | 2 | LEU | C-N-CA | -5.67 | 107.53 | 121.70 |
| 1 | A | 88 | ALA | N-CA-CB | 5.67 | 118.03 | 110.10 |
| 2 | B | 131 | GLN | CG-CD-NE2 | 5.67 | 130.30 | 116.70 |
| 1 | A | 35 | SER | CB-CA-C | -5.67 | 99.34 | 110.10 |
| 2 | B | 91 | LEU | CB-CA-C | 5.66 | 120.96 | 110.20 |
| 1 | A | 33 | PHE | O-C-N | -5.66 | 113.64 | 122.70 |
| 2 | D | 54 | VAL | CA-CB-CG2 | 5.66 | 119.39 | 110.90 |
| 2 | B | 131 | GLN | CG-CD-OE1 | -5.66 | 110.29 | 121.60 |
| 2 | D | 121 | GLU | CA-C-N | -5.65 | 104.76 | 117.20 |
| 2 | B | 39 | GLN | CG-CD-OE1 | -5.65 | 110.30 | 121.60 |
| 1 | A | 8 | THR | O-C-N | -5.65 | 113.67 | 122.70 |
| 2 | D | 33 | VAL | CA-CB-CG1 | -5.64 | 102.44 | 110.90 |
| 1 | A | 77 | PRO | N-CA-C | 5.64 | 126.75 | 112.10 |
| 1 | C | 47 | ASP | C-N-CA | -5.63 | 107.61 | 121.70 |
| 2 | D | 143 | HIS | CA-C-O | -5.63 | 108.27 | 120.10 |
| 1 | A | 98 | PHE | CE1-CZ-CE2 | 5.63 | 130.14 | 120.00 |
| 2 | B | 11 | VAL | CB-CA-C | 5.63 | 122.10 | 111.40 |
| 1 | C | 125 | LEU | O-C-N | -5.63 | 113.69 | 122.70 |
| 2 | D | 39 | GLN | C-N-CA | 5.63 | 135.77 | 121.70 |
| 1 | C | 88 | ALA | CA-C-N | -5.63 | 104.82 | 117.20 |
| 1 | A | 55 | VAL | CA-C-O | 5.62 | 131.91 | 120.10 |
| 1 | A | 71 | ALA | CA-C-O | -5.62 | 108.29 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 83 | LEU | CA-CB-CG | -5.62 | 102.37 | 115.30 |
| 1 | A | 64 | ASP | C-N-CA | -5.62 | 107.65 | 121.70 |
| 1 | A | 13 | ALA | C-N-CA | -5.62 | 107.66 | 121.70 |
| 2 | D | 6 | GLU | CB-CG-CD | 5.62 | 129.37 | 114.20 |
| 1 | A | 13 | ALA | CA-C-N | -5.61 | 104.85 | 117.20 |
| 2 | D | 63 | HIS | CB-CG-ND1 | -5.61 | 109.17 | 123.20 |
| 2 | B | 4 | THR | O-C-N | -5.61 | 110.44 | 121.10 |
| 2 | B | 92 | HIS | CB-CA-C | -5.61 | 99.18 | 110.40 |
| 1 | C | 3 | SER | N-CA-CB | -5.61 | 102.09 | 110.50 |
| 1 | C | 69 | ALA | CA-C-O | -5.61 | 108.33 | 120.10 |
| 2 | D | 58 | PRO | CA-C-O | -5.61 | 106.75 | 120.20 |
| 1 | A | 48 | LEU | CA-C-N | -5.60 | 104.87 | 117.20 |
| 1 | A | 113 | LEU | CB-CA-C | -5.60 | 99.57 | 110.20 |
| 2 | B | 143 | HIS | CB-CG-CD2 | -5.60 | 113.45 | 130.80 |
| 1 | C | 72 | HIS | CG-CD2-NE2 | 5.59 | 119.82 | 109.20 |
| 1 | A | 8 | THR | CA-C-N | -5.59 | 104.91 | 117.20 |
| 1 | C | 131 | SER | CA-CB-OG | -5.58 | 96.12 | 111.20 |
| 2 | B | 33 | VAL | CA-CB-CG2 | -5.58 | 102.53 | 110.90 |
| 1 | C | 35 | SER | N-CA-C | 5.57 | 126.05 | 111.00 |
| 1 | C | 106 | LEU | CA-CB-CG | 5.57 | 128.12 | 115.30 |
| 2 | B | 91 | LEU | CB-CG-CD2 | 5.57 | 120.47 | 111.00 |
| 2 | B | 79 | ASP | N-CA-C | -5.57 | 95.96 | 111.00 |
| 2 | B | 124 | PRO | CA-C-N | 5.57 | 132.69 | 117.10 |
| 2 | D | 139 | ASN | O-C-N | -5.56 | 113.80 | 122.70 |
| 2 | B | 3 | LEU | CB-CA-C | -5.56 | 99.64 | 110.20 |
| 2 | B | 80 | ASN | O-C-N | 5.56 | 131.59 | 122.70 |
| 2 | B | 117 | HIS | C-N-CA | 5.56 | 135.60 | 121.70 |
| 1 | C | 44 | PRO | CA-C-O | -5.56 | 106.86 | 120.20 |
| 2 | B | 80 | ASN | CB-CA-C | 5.55 | 121.50 | 110.40 |
| 1 | A | 131 | SER | C-N-CA | -5.55 | 107.83 | 121.70 |
| 2 | B | 135 | ALA | CB-CA-C | 5.53 | 118.40 | 110.10 |
| 1 | A | 26 | ALA | CA-C-N | -5.53 | 105.04 | 117.20 |
| 2 | B | 13 | ALA | CA-C-O | 5.53 | 131.70 | 120.10 |
| 1 | A | 94 | ASP | CB-CG-OD1 | 5.52 | 123.27 | 118.30 |
| 1 | C | 98 | PHE | N-CA-CB | 5.52 | 120.53 | 110.60 |
| 2 | D | 72 | SER | O-C-N | -5.52 | 113.87 | 122.70 |
| 1 | C | 99 | LYS | CA-C-O | 5.51 | 131.66 | 120.10 |
| 2 | D | 44 | SER | CA-CB-OG | 5.50 | 126.06 | 111.20 |
| 1 | A | 116 | GLU | CB-CG-CD | -5.50 | 99.34 | 114.20 |
| 2 | D | 44 | SER | N-CA-CB | 5.50 | 118.75 | 110.50 |
| 2 | D | 45 | PHE | CD1-CG-CD2 | -5.50 | 111.15 | 118.30 |
| 2 | D | 11 | VAL | CA-CB-CG1 | -5.49 | 102.66 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 118 | PHE | CA-C-N | 5.49 | 127.18 | 116.20 |
| 1 | A | 109 | LEU | O-C-N | 5.49 | 131.48 | 122.70 |
| 2 | B | 68 | LEU | CB-CG-CD2 | 5.48 | 120.32 | 111.00 |
| 1 | C | 19 | ALA | CA-C-O | 5.48 | 131.61 | 120.10 |
| 2 | D | 62 | ALA | CA-C-N | -5.48 | 105.14 | 117.20 |
| 1 | A | 57 | GLY | CA-C-O | -5.48 | 110.74 | 120.60 |
| 2 | D | 64 | GLY | CA-C-N | -5.48 | 105.14 | 117.20 |
| 1 | C | 89 | HIS | CB-CG-CD2 | -5.47 | 113.83 | 130.80 |
| 1 | A | 16 | LYS | CB-CG-CD | -5.47 | 97.38 | 111.60 |
| 1 | C | 24 | TYR | CA-C-O | 5.47 | 131.58 | 120.10 |
| 1 | C | 29 | LEU | C-N-CA | 5.46 | 135.35 | 121.70 |
| 1 | A | 20 | HIS | ND1-CG-CD2 | -5.46 | 98.36 | 106.00 |
| 1 | C | 121 | VAL | CB-CA-C | 5.46 | 121.77 | 111.40 |
| 2 | D | 59 | LYS | C-N-CA | -5.46 | 108.05 | 121.70 |
| 1 | C | 113 | LEU | CD1-CG-CD2 | 5.45 | 126.86 | 110.50 |
| 1 | A | 139 | LYS | CA-C-N | 5.45 | 129.18 | 117.20 |
| 1 | C | 65 | ALA | O-C-N | -5.44 | 113.99 | 122.70 |
| 1 | C | 133 | SER | CA-CB-OG | -5.44 | 96.51 | 111.20 |
| 1 | C | 58 | HIS | ND1-CE1-NE2 | 5.44 | 121.87 | 109.90 |
| 2 | B | 124 | PRO | N-CD-CG | -5.43 | 95.05 | 103.20 |
| 2 | B | 143 | HIS | ND1-CE1-NE2 | 5.43 | 121.86 | 109.90 |
| 1 | C | 14 | TRP | CB-CA-C | -5.43 | 99.53 | 110.40 |
| 2 | D | 73 | ASP | CB-CA-C | -5.43 | 99.54 | 110.40 |
| 1 | A | 5 | ALA | N-CA-CB | -5.42 | 102.51 | 110.10 |
| 2 | B | 92 | HIS | CG-ND1-CE1 | -5.42 | 98.65 | 105.70 |
| 2 | B | 91 | LEU | CA-CB-CG | -5.42 | 102.83 | 115.30 |
| 1 | C | 14 | TRP | CE2-CD2-CE3 | 5.42 | 125.20 | 118.70 |
| 2 | D | 85 | PHE | CG-CD2-CE2 | -5.42 | 114.84 | 120.80 |
| 1 | A | 84 | SER | C-N-CA | -5.42 | 108.16 | 121.70 |
| 2 | D | 66 | LYS | N-CA-C | -5.41 | 96.38 | 111.00 |
| 1 | C | 53 | ALA | C-N-CA | -5.41 | 108.18 | 121.70 |
| 1 | C | 98 | PHE | CG-CD1-CE1 | 5.40 | 126.74 | 120.80 |
| 1 | A | 12 | ALA | CA-C-N | 5.40 | 129.08 | 117.20 |
| 2 | D | 3 | LEU | CB-CA-C | 5.40 | 120.46 | 110.20 |
| 1 | C | 111 | ALA | CA-C-O | -5.39 | 108.78 | 120.10 |
| 1 | A | 85 | ASP | O-C-N | -5.39 | 114.08 | 122.70 |
| 1 | C | 12 | ALA | CA-C-N | -5.38 | 105.36 | 117.20 |
| 1 | A | 4 | PRO | C-N-CA | -5.38 | 108.26 | 121.70 |
| 1 | A | 61 | LYS | CA-C-O | -5.37 | 108.81 | 120.10 |
| 2 | D | 91 | LEU | N-CA-C | 5.37 | 125.51 | 111.00 |
| 2 | D | 74 | GLY | CA-C-N | -5.37 | 105.39 | 117.20 |
| 1 | A | 112 | HIS | O-C-N | 5.36 | 131.28 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | A | 60 | LYS | N-CA-C | 5.36 | 125.48 | 111.00 |
| 2 | B | 84 | THR | CA-CB-OG1 | -5.36 | 97.74 | 109.00 |
| 1 | A | 88 | ALA | CA-C-O | -5.36 | 108.85 | 120.10 |
| 1 | C | 119 | PRO | N-CA-CB | 5.36 | 109.73 | 103.30 |
| 1 | C | 79 | ALA | O-C-N | 5.36 | 131.27 | 122.70 |
| 1 | A | 10 | VAL | CA-CB-CG2 | 5.35 | 118.92 | 110.90 |
| 1 | C | 92 | ARG | CA-C-O | 5.35 | 131.34 | 120.10 |
| 1 | A | 67 | THR | CA-CB-CG2 | -5.35 | 104.91 | 112.40 |
| 2 | D | 119 | GLY | CA-C-N | -5.35 | 105.44 | 117.20 |
| 2 | B | 41 | PHE | CD1-CE1-CZ | 5.34 | 126.51 | 120.10 |
| 2 | D | 75 | LEU | N-CA-CB | -5.34 | 99.72 | 110.40 |
| 2 | B | 77 | HIS | N-CA-C | -5.34 | 96.58 | 111.00 |
| 2 | D | 5 | PRO | CB-CG-CD | 5.34 | 127.31 | 106.50 |
| 2 | D | 68 | LEU | CA-C-O | 5.33 | 131.30 | 120.10 |
| 1 | C | 48 | LEU | N-CA-CB | -5.33 | 99.74 | 110.40 |
| 1 | C | 35 | SER | CA-C-O | 5.33 | 131.29 | 120.10 |
| 2 | B | 71 | PHE | N-CA-CB | -5.32 | 101.02 | 110.60 |
| 1 | A | 64 | ASP | CA-C-N | -5.32 | 105.50 | 117.20 |
| 2 | B | 124 | PRO | N-CA-CB | 5.32 | 109.68 | 103.30 |
| 1 | C | 78 | ASN | CA-C-N | -5.32 | 105.50 | 117.20 |
| 2 | B | 118 | PHE | CB-CA-C | 5.30 | 121.01 | 110.40 |
| 2 | D | 78 | LEU | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | A | 89 | HIS | ND1-CG-CD2 | -5.30 | 98.58 | 106.00 |
| 2 | D | 54 | VAL | N-CA-CB | -5.30 | 99.84 | 111.50 |
| 1 | C | 139 | LYS | CB-CG-CD | -5.29 | 97.84 | 111.60 |
| 1 | C | 50 | HIS | ND1-CE1-NE2 | 5.29 | 121.54 | 109.90 |
| 1 | A | 89 | HIS | N-CA-C | 5.29 | 125.28 | 111.00 |
| 2 | D | 92 | HIS | N-CA-C | -5.28 | 96.73 | 111.00 |
| 1 | A | 71 | ALA | N-CA-CB | -5.28 | 102.71 | 110.10 |
| 1 | A | 24 | TYR | CB-CA-C | -5.27 | 99.86 | 110.40 |
| 2 | D | 66 | LYS | CB-CG-CD | 5.27 | 125.30 | 111.60 |
| 2 | D | 117 | HIS | ND1-CE1-NE2 | 5.27 | 121.49 | 109.90 |
| 2 | D | 83 | GLY | CA-C-N | 5.27 | 128.79 | 117.20 |
| 2 | B | 101 | GLU | CA-C-O | 5.27 | 131.16 | 120.10 |
| 1 | C | 20 | HIS | ND1-CG-CD2 | 5.26 | 116.17 | 108.80 |
| 2 | D | 117 | HIS | CB-CG-CD2 | 5.26 | 147.11 | 130.80 |
| 2 | B | 77 | HIS | CE1-NE2-CD2 | 5.26 | 119.75 | 106.60 |
| 1 | A | 62 | VAL | CA-CB-CG2 | -5.25 | 103.02 | 110.90 |
| 1 | A | 83 | LEU | CA-C-N | 5.25 | 128.76 | 117.20 |
| 2 | B | 89 | SER | CB-CA-C | 5.25 | 120.08 | 110.10 |
| 2 | B | 122 | PHE | CZ-CE2-CD2 | -5.25 | 113.80 | 120.10 |
| 1 | C | 20 | HIS | ND1-CE1-NE2 | -5.25 | 98.36 | 109.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | D | 75 | LEU | CA-CB-CG | 5.25 | 127.36 | 115.30 |
| 2 | B | 20 | VAL | C-N-CA | 5.24 | 134.81 | 121.70 |
| 2 | D | 74 | GLY | C-N-CA | -5.24 | 108.60 | 121.70 |
| 1 | A | 140 | TYR | N-CA-CB | 5.24 | 120.03 | 110.60 |
| 1 | A | 141 | ARG | CB-CG-CD | -5.24 | 97.98 | 111.60 |
| 1 | A | 2 | LEU | CA-C-N | -5.24 | 105.68 | 117.20 |
| 1 | C | 7 | LYS | N-CA-CB | -5.24 | 101.18 | 110.60 |
| 1 | A | 95 | PRO | CA-C-N | 5.23 | 128.72 | 117.20 |
| 2 | D | 63 | HIS | C-N-CA | -5.23 | 111.32 | 122.30 |
| 1 | A | 50 | HIS | CA-CB-CG | -5.23 | 104.71 | 113.60 |
| 1 | A | 90 | LYS | CG-CD-CE | -5.23 | 96.21 | 111.90 |
| 2 | D | 139 | ASN | CB-CG-ND2 | -5.23 | 104.15 | 116.70 |
| 2 | D | 77 | HIS | CB-CG-ND1 | -5.23 | 110.13 | 123.20 |
| 2 | D | 41 | PHE | CD1-CG-CD2 | 5.22 | 125.09 | 118.30 |
| 1 | A | 71 | ALA | C-N-CA | 5.22 | 134.75 | 121.70 |
| 1 | C | 140 | TYR | CD1-CE1-CZ | 5.22 | 124.50 | 119.80 |
| 1 | A | 82 | ALA | O-C-N | -5.22 | 114.35 | 122.70 |
| 1 | C | 28 | ALA | O-C-N | 5.21 | 131.04 | 122.70 |
| 1 | A | 112 | HIS | CE1-NE2-CD2 | -5.21 | 93.57 | 106.60 |
| 2 | B | 54 | VAL | O-C-N | -5.21 | 114.37 | 122.70 |
| 2 | D | 102 | ASN | C-N-CA | 5.21 | 134.72 | 121.70 |
| 2 | D | 127 | GLN | CB-CA-C | 5.21 | 120.82 | 110.40 |
| 1 | A | 24 | TYR | CA-C-N | 5.21 | 126.61 | 116.20 |
| 1 | A | 41 | THR | CA-C-N | 5.21 | 128.65 | 117.20 |
| 1 | C | 137 | THR | O-C-N | 5.21 | 131.03 | 122.70 |
| 2 | B | 54 | VAL | CA-CB-CG1 | -5.21 | 103.09 | 110.90 |
| 1 | A | 11 | LYS | O-C-N | -5.20 | 114.38 | 122.70 |
| 1 | A | 23 | GLU | CB-CG-CD | -5.20 | 100.16 | 114.20 |
| 1 | A | 72 | HIS | CB-CA-C | -5.20 | 100.00 | 110.40 |
| 2 | B | 7 | GLU | CA-CB-CG | 5.20 | 124.83 | 113.40 |
| 2 | D | 91 | LEU | CA-C-N | -5.19 | 105.77 | 117.20 |
| 2 | B | 119 | GLY | O-C-N | -5.19 | 114.39 | 122.70 |
| 1 | A | 73 | VAL | CG1-CB-CG2 | 5.19 | 119.20 | 110.90 |
| 2 | B | 17 | LYS | N-CA-CB | 5.19 | 119.94 | 110.60 |
| 1 | C | 75 | ASP | CA-C-N | -5.19 | 105.78 | 117.20 |
| 2 | D | 100 | PRO | N-CA-CB | 5.19 | 109.53 | 103.30 |
| 1 | C | 76 | MET | CB-CG-SD | -5.18 | 96.86 | 112.40 |
| 2 | B | 85 | PHE | CB-CA-C | 5.18 | 120.76 | 110.40 |
| 2 | B | 22 | GLU | N-CA-CB | -5.17 | 101.29 | 110.60 |
| 1 | A | 139 | LYS | CD-CE-NZ | -5.17 | 99.81 | 111.70 |
| 2 | B | 15 | TRP | CZ3-CH2-CZ2 | 5.16 | 127.80 | 121.60 |
| 2 | B | 82 | LYS | CG-CD-CE | -5.16 | 96.42 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | D | 90 | GLU | N-CA-CB | -5.16 | 101.31 | 110.60 |
| 2 | D | 143 | HIS | CB-CA-C | 5.16 | 120.72 | 110.40 |
| 1 | A | 101 | LEU | CB-CG-CD1 | 5.16 | 119.77 | 111.00 |
| 2 | B | 45 | PHE | CD1-CG-CD2 | -5.16 | 111.60 | 118.30 |
| 1 | C | 75 | ASP | N-CA-C | -5.16 | 97.08 | 111.00 |
| 1 | A | 19 | ALA | CA-C-N | 5.15 | 128.53 | 117.20 |
| 2 | B | 95 | LYS | CA-C-O | 5.15 | 130.92 | 120.10 |
| 2 | B | 89 | SER | CA-CB-OG | -5.15 | 97.29 | 111.20 |
| 2 | D | 106 | LEU | CB-CG-CD2 | -5.15 | 102.25 | 111.00 |
| 1 | C | 58 | HIS | C-N-CA | -5.15 | 111.49 | 122.30 |
| 1 | C | 40 | LYS | CB-CG-CD | -5.14 | 98.23 | 111.60 |
| 2 | D | 58 | PRO | N-CA-CB | 5.14 | 109.47 | 103.30 |
| 2 | B | 75 | LEU | CB-CA-C | -5.14 | 100.44 | 110.20 |
| 1 | C | 17 | VAL | N-CA-CB | 5.14 | 122.81 | 111.50 |
| 2 | D | 44 | SER | C-N-CA | 5.14 | 134.55 | 121.70 |
| 1 | A | 74 | ASP | C-N-CA | 5.14 | 134.54 | 121.70 |
| 2 | B | 66 | LYS | C-N-CA | -5.14 | 108.86 | 121.70 |
| 1 | C | 36 | PHE | O-C-N | 5.14 | 130.86 | 121.10 |
| 1 | A | 106 | LEU | CB-CG-CD2 | 5.13 | 119.73 | 111.00 |
| 1 | A | 30 | GLU | CA-CB-CG | -5.13 | 102.11 | 113.40 |
| 1 | A | 39 | THR | C-N-CA | -5.12 | 108.89 | 121.70 |
| 1 | C | 65 | ALA | CA-C-O | 5.12 | 130.86 | 120.10 |
| 2 | B | 26 | GLU | C-N-CA | -5.12 | 108.89 | 121.70 |
| 1 | A | 14 | TRP | O-C-N | 5.12 | 131.91 | 123.20 |
| 2 | B | 55 | MET | C-N-CA | -5.12 | 111.55 | 122.30 |
| 2 | B | 145 | TYR | CB-CG-CD1 | -5.12 | 117.93 | 121.00 |
| 1 | A | 16 | LYS | CA-C-O | 5.12 | 130.85 | 120.10 |
| 2 | B | 106 | LEU | O-C-N | -5.11 | 114.51 | 123.20 |
| 2 | D | 9 | SER | CA-C-O | -5.11 | 109.37 | 120.10 |
| 2 | D | 83 | GLY | N-CA-C | -5.11 | 100.33 | 113.10 |
| 1 | C | 62 | VAL | CA-C-O | 5.11 | 130.82 | 120.10 |
| 1 | C | 3 | SER | CA-C-O | 5.10 | 130.81 | 120.10 |
| 2 | B | 62 | ALA | O-C-N | 5.09 | 130.85 | 122.70 |
| 2 | D | 132 | LYS | CG-CD-CE | -5.09 | 96.62 | 111.90 |
| 2 | B | 93 | CYS | N-CA-CB | -5.09 | 101.43 | 110.60 |
| 1 | C | 75 | ASP | CA-CB-CG | 5.09 | 124.60 | 113.40 |
| 2 | B | 145 | TYR | C-N-CA | 5.09 | 134.42 | 121.70 |
| 1 | A | 25 | GLY | CA-C-O | 5.08 | 129.75 | 120.60 |
| 1 | A | 59 | GLY | CA-C-O | 5.08 | 129.75 | 120.60 |
| 2 | B | 116 | HIS | CG-CD2-NE2 | 5.08 | 118.86 | 109.20 |
| 2 | D | 77 | HIS | O-C-N | -5.08 | 114.57 | 122.70 |
| 1 | C | 117 | PHE | CD1-CE1-CZ | -5.08 | 114.01 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | A | 44 | PRO | CB-CA-C | -5.08 | 99.31 | 112.00 |
| 2 | B | 35 | TYR | CB-CG-CD1 | 5.07 | 124.04 | 121.00 |
| 2 | B | 111 | VAL | CA-CB-CG1 | -5.07 | 103.29 | 110.90 |
| 2 | B | 145 | TYR | CA-CB-CG | 5.07 | 123.04 | 113.40 |
| 1 | A | 83 | LEU | N-CA-CB | -5.07 | 100.26 | 110.40 |
| 1 | A | 92 | ARG | C-N-CA | 5.07 | 134.38 | 121.70 |
| 1 | C | 35 | SER | O-C-N | -5.07 | 114.59 | 122.70 |
| 1 | A | 58 | HIS | CA-C-O | -5.07 | 109.46 | 120.10 |
| 1 | A | 103 | HIS | ND1-CE1-NE2 | 5.06 | 121.04 | 109.90 |
| 2 | D | 73 | ASP | N-CA-CB | 5.06 | 119.71 | 110.60 |
| 2 | B | 1 | VAL | O-C-N | 5.06 | 130.79 | 122.70 |
| 2 | B | 76 | ALA | CA-C-N | -5.06 | 106.07 | 117.20 |
| 2 | D | 9 | SER | N-CA-CB | -5.06 | 102.91 | 110.50 |
| 1 | A | 47 | ASP | CA-C-N | -5.05 | 106.08 | 117.20 |
| 1 | A | 14 | TRP | CD1-CG-CD2 | -5.05 | 102.26 | 106.30 |
| 1 | C | 36 | PHE | CA-C-N | -5.04 | 102.98 | 117.10 |
| 2 | D | 42 | PHE | CD1-CG-CD2 | 5.04 | 124.85 | 118.30 |
| 1 | A | 88 | ALA | CA-C-N | -5.04 | 106.12 | 117.20 |
| 1 | A | 119 | PRO | O-C-N | -5.04 | 114.64 | 122.70 |
| 2 | B | 103 | PHE | CG-CD1-CE1 | -5.04 | 115.26 | 120.80 |
| 2 | D | 40 | ARG | N-CA-C | -5.04 | 97.40 | 111.00 |
| 1 | A | 136 | LEU | CB-CG-CD2 | 5.04 | 119.56 | 111.00 |
| 1 | A | 82 | ALA | CA-C-O | 5.04 | 130.68 | 120.10 |
| 1 | A | 109 | LEU | C-N-CA | -5.03 | 109.11 | 121.70 |
| 2 | B | 8 | LYS | C-N-CA | 5.03 | 134.28 | 121.70 |
| 2 | B | 27 | ALA | O-C-N | -5.03 | 114.65 | 122.70 |
| 2 | B | 15 | TRP | CB-CG-CD2 | -5.03 | 120.06 | 126.60 |
| 1 | A | 90 | LYS | CB-CG-CD | 5.03 | 124.67 | 111.60 |
| 2 | B | 3 | LEU | CD1-CG-CD2 | -5.03 | 95.42 | 110.50 |
| 1 | A | 34 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 2 | D | 88 | LEU | CD1-CG-CD2 | 5.03 | 125.58 | 110.50 |
| 1 | C | 26 | ALA | O-C-N | -5.02 | 114.67 | 122.70 |
| 2 | D | 48 | LEU | CA-C-N | -5.02 | 106.16 | 117.20 |
| 1 | A | 100 | LEU | CD1-CG-CD2 | -5.01 | 95.47 | 110.50 |
| 2 | D | 137 | VAL | N-CA-C | 5.01 | 124.53 | 111.00 |
| 2 | B | 2 | HIS | CE1-NE2-CD2 | -5.01 | 94.08 | 106.60 |
| 2 | B | 37 | TRP | O-C-N | -5.00 | 114.70 | 122.70 |
| 2 | D | 12 | THR | CA-C-N | 5.00 | 128.21 | 117.20 |

All (10) chirality outliers are listed below:

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
|-----|-------|-----|------|------|

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 137 | THR | CB |
| 2 | B | 12 | THR | CB |
| 2 | B | 50 | THR | CB |
| 1 | C | 78 | ASN | CA |
| 1 | C | 118 | THR | CB |
| 2 | D | 2 | HIS | CA |
| 2 | D | 72 | SER | CA |
| 2 | D | 73 | ASP | CA |
| 2 | D | 78 | LEU | CA |
| 2 | D | 144 | LYS | CA |

All (207) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 1 | VAL | Mainchain |
| 1 | A | 101 | LEU | Mainchain |
| 1 | A | 106 | LEU | Mainchain |
| 1 | A | 11 | LYS | Mainchain |
| 1 | A | 111 | ALA | Mainchain |
| 1 | A | 114 | PRO | Mainchain |
| 1 | A | 118 | THR | Mainchain |
| 1 | A | 12 | ALA | Mainchain |
| 1 | A | 122 | HIS | Mainchain |
| 1 | A | 126 | ASP | Sidechain |
| 1 | A | 141 | ARG | Sidechain |
| 1 | A | 15 | GLY | Mainchain |
| 1 | A | 18 | GLY | Peptide |
| 1 | A | 19 | ALA | Mainchain |
| 1 | A | 20 | HIS | Sidechain |
| 1 | A | 21 | ALA | Mainchain |
| 1 | A | 22 | GLY | Mainchain |
| 1 | A | 23 | GLU | Sidechain |
| 1 | A | 24 | TYR | Sidechain |
| 1 | A | 3 | SER | Mainchain |
| 1 | A | 36 | PHE | Sidechain |
| 1 | A | 4 | PRO | Mainchain |
| 1 | A | 41 | THR | Mainchain |
| 1 | A | 45 | HIS | Sidechain |
| 1 | A | 46 | PHE | Mainchain |
| 1 | A | 48 | LEU | Mainchain |
| 1 | A | 50 | HIS | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 1 | A | 52 | SER | Mainchain |
| 1 | A | 54 | GLN | Sidechain |
| 1 | A | 56 | LYS | Mainchain |
| 1 | A | 59 | GLY | Mainchain |
| 1 | A | 61 | LYS | Mainchain |
| 1 | A | 63 | ALA | Mainchain |
| 1 | A | 64 | ASP | Sidechain |
| 1 | A | 72 | HIS | Sidechain |
| 1 | A | 74 | ASP | Mainchain |
| 1 | A | 75 | ASP | Mainchain |
| 1 | A | 76 | MET | Mainchain |
| 1 | A | 78 | ASN | Sidechain,Mainchain |
| 1 | A | 81 | SER | Mainchain |
| 1 | A | 82 | ALA | Mainchain |
| 1 | A | 83 | LEU | Mainchain |
| 1 | A | 85 | ASP | Sidechain,Mainchain |
| 1 | A | 88 | ALA | Mainchain |
| 1 | A | 9 | ASN | Mainchain |
| 1 | A | 90 | LYS | Mainchain |
| 1 | A | 92 | ARG | Sidechain |
| 1 | A | 97 | ASN | Mainchain |
| 1 | A | 99 | LYS | Mainchain |
| 2 | B | 1 | VAL | Mainchain |
| 2 | B | 100 | PRO | Mainchain |
| 2 | B | 101 | GLU | Mainchain |
| 2 | B | 104 | ARG | Sidechain |
| 2 | B | 114 | LEU | Mainchain |
| 2 | B | 117 | HIS | Sidechain |
| 2 | B | 118 | PHE | Sidechain |
| 2 | B | 121 | GLU | Sidechain |
| 2 | B | 123 | THR | Mainchain |
| 2 | B | 126 | VAL | Mainchain |
| 2 | B | 131 | GLN | Mainchain |
| 2 | B | 139 | ASN | Mainchain |
| 2 | B | 14 | LEU | Mainchain |
| 2 | B | 141 | LEU | Mainchain |
| 2 | B | 143 | HIS | Sidechain |
| 2 | B | 146 | HIS | Sidechain |
| 2 | B | 19 | ASN | Sidechain |
| 2 | B | 2 | HIS | Sidechain |
| 2 | B | 21 | ASP | Sidechain,Mainchain |
| 2 | B | 22 | GLU | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 2 | B | 26 | GLU | Sidechain |
| 2 | B | 3 | LEU | Mainchain |
| 2 | B | 38 | THR | Mainchain |
| 2 | B | 4 | THR | Mainchain |
| 2 | B | 43 | GLU | Mainchain |
| 2 | B | 44 | SER | Mainchain |
| 2 | B | 47 | ASP | Sidechain,Mainchain |
| 2 | B | 49 | SER | Mainchain,Peptide |
| 2 | B | 52 | ASP | Sidechain |
| 2 | B | 56 | GLY | Mainchain |
| 2 | B | 59 | LYS | Mainchain |
| 2 | B | 6 | GLU | Sidechain |
| 2 | B | 60 | VAL | Mainchain |
| 2 | B | 61 | LYS | Mainchain |
| 2 | B | 62 | ALA | Mainchain |
| 2 | B | 63 | HIS | Sidechain,Mainchain |
| 2 | B | 7 | GLU | Mainchain |
| 2 | B | 78 | LEU | Mainchain |
| 2 | B | 79 | ASP | Sidechain,Mainchain |
| 2 | B | 80 | ASN | Sidechain,Mainchain |
| 2 | B | 84 | THR | Mainchain |
| 2 | B | 90 | GLU | Sidechain,Mainchain |
| 1 | C | 109 | LEU | Mainchain |
| 1 | C | 110 | ALA | Mainchain |
| 1 | C | 111 | ALA | Mainchain |
| 1 | C | 112 | HIS | Mainchain |
| 1 | C | 113 | LEU | Mainchain |
| 1 | C | 114 | PRO | Mainchain |
| 1 | C | 116 | GLU | Sidechain,Mainchain |
| 1 | C | 119 | PRO | Mainchain |
| 1 | C | 125 | LEU | Mainchain |
| 1 | C | 126 | ASP | Sidechain |
| 1 | C | 135 | VAL | Mainchain |
| 1 | C | 138 | SER | Mainchain |
| 1 | C | 14 | TRP | Mainchain |
| 1 | C | 141 | ARG | Sidechain |
| 1 | C | 17 | VAL | Mainchain |
| 1 | C | 18 | GLY | Mainchain |
| 1 | C | 20 | HIS | Sidechain |
| 1 | C | 21 | ALA | Mainchain |
| 1 | C | 23 | GLU | Sidechain |
| 1 | C | 25 | GLY | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 1 | C | 3 | SER | Mainchain |
| 1 | C | 44 | PRO | Mainchain |
| 1 | C | 45 | HIS | Sidechain,Mainchain |
| 1 | C | 46 | PHE | Sidechain,Mainchain |
| 1 | C | 47 | ASP | Sidechain,Mainchain |
| 1 | C | 48 | LEU | Mainchain |
| 1 | C | 5 | ALA | Mainchain |
| 1 | C | 64 | ASP | Sidechain |
| 1 | C | 69 | ALA | Mainchain |
| 1 | C | 71 | ALA | Mainchain |
| 1 | C | 72 | HIS | Mainchain |
| 1 | C | 74 | ASP | Mainchain |
| 1 | C | 75 | ASP | Sidechain,Mainchain |
| 1 | C | 78 | ASN | Sidechain |
| 1 | C | 80 | LEU | Mainchain |
| 1 | C | 83 | LEU | Mainchain |
| 1 | C | 88 | ALA | Mainchain |
| 1 | C | 9 | ASN | Sidechain |
| 1 | C | 92 | ARG | Sidechain |
| 1 | C | 95 | PRO | Mainchain |
| 2 | D | 1 | VAL | Mainchain |
| 2 | D | 101 | GLU | Sidechain |
| 2 | D | 104 | ARG | Sidechain |
| 2 | D | 108 | ASN | Sidechain |
| 2 | D | 117 | HIS | Sidechain,Mainchain |
| 2 | D | 118 | PHE | Sidechain |
| 2 | D | 120 | LYS | Mainchain |
| 2 | D | 121 | GLU | Sidechain |
| 2 | D | 127 | GLN | Sidechain |
| 2 | D | 137 | VAL | Mainchain |
| 2 | D | 139 | ASN | Sidechain |
| 2 | D | 143 | HIS | Sidechain |
| 2 | D | 144 | LYS | Mainchain |
| 2 | D | 146 | HIS | Sidechain |
| 2 | D | 17 | LYS | Mainchain |
| 2 | D | 18 | VAL | Peptide |
| 2 | D | 19 | ASN | Sidechain |
| 2 | D | 2 | HIS | Sidechain,Mainchain |
| 2 | D | 21 | ASP | Sidechain,Mainchain |
| 2 | D | 22 | GLU | Sidechain,Mainchain |
| 2 | D | 26 | GLU | Sidechain |
| 2 | D | 3 | LEU | Mainchain,Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------------------|
| 2 | D | 33 | VAL | Mainchain |
| 2 | D | 34 | VAL | Mainchain |
| 2 | D | 40 | ARG | Sidechain |
| 2 | D | 42 | PHE | Mainchain |
| 2 | D | 43 | GLU | Sidechain |
| 2 | D | 46 | GLY | Mainchain |
| 2 | D | 48 | LEU | Mainchain,Peptide |
| 2 | D | 49 | SER | Mainchain,Peptide |
| 2 | D | 5 | PRO | Mainchain |
| 2 | D | 52 | ASP | Sidechain,Mainchain |
| 2 | D | 56 | GLY | Mainchain |
| 2 | D | 6 | GLU | Sidechain |
| 2 | D | 60 | VAL | Mainchain |
| 2 | D | 63 | HIS | Sidechain |
| 2 | D | 64 | GLY | Mainchain |
| 2 | D | 66 | LYS | Mainchain |
| 2 | D | 7 | GLU | Sidechain |
| 2 | D | 73 | ASP | Mainchain |
| 2 | D | 75 | LEU | Mainchain |
| 2 | D | 76 | ALA | Mainchain |
| 2 | D | 77 | HIS | Sidechain |
| 2 | D | 79 | ASP | Sidechain,Mainchain |
| 2 | D | 8 | LYS | Mainchain |
| 2 | D | 80 | ASN | Mainchain |
| 2 | D | 83 | GLY | Mainchain |
| 2 | D | 84 | THR | Mainchain |
| 2 | D | 90 | GLU | Sidechain |
| 2 | D | 92 | HIS | Sidechain,Mainchain |
| 2 | D | 94 | ASP | Sidechain |
| 2 | D | 96 | LEU | Mainchain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1069 | 0 | 1061 | 239 | 0 |
| 1 | C | 1069 | 0 | 1063 | 255 | 1 |
| 2 | B | 1123 | 0 | 1104 | 323 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | D | 1123 | 0 | 1108 | 419 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 43 | 0 | 30 | 6 | 0 |
| 4 | B | 43 | 0 | 30 | 10 | 0 |
| 4 | C | 43 | 0 | 30 | 14 | 0 |
| 4 | D | 43 | 0 | 30 | 11 | 0 |
| 5 | A | 56 | 0 | 0 | 1 | 0 |
| 5 | B | 57 | 0 | 0 | 1 | 2 |
| 5 | C | 59 | 0 | 0 | 0 | 1 |
| 5 | D | 49 | 0 | 0 | 1 | 0 |
| All | All | 4779 | 0 | 4456 | 1268 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 141.

All (1268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 2:B:3:LEU:CA | 2:B:3:LEU:CB | 1.77 | 1.63 |
| 2:D:77:HIS:CB | 2:D:77:HIS:CA | 1.75 | 1.62 |
| 2:B:104:ARG:CD | 2:B:104:ARG:CG | 1.76 | 1.62 |
| 1:A:5:ALA:CB | 1:A:5:ALA:CA | 1.77 | 1.62 |
| 1:C:48:LEU:CG | 1:C:48:LEU:CD2 | 1.74 | 1.62 |
| 2:B:7:GLU:CB | 2:B:7:GLU:CG | 1.77 | 1.61 |
| 1:A:40:LYS:CB | 1:A:40:LYS:CA | 1.75 | 1.60 |
| 2:D:8:LYS:CB | 2:D:8:LYS:CG | 1.79 | 1.60 |
| 2:D:18:VAL:CB | 2:D:18:VAL:CG2 | 1.80 | 1.60 |
| 1:C:113:LEU:CD1 | 1:C:113:LEU:CG | 1.75 | 1.60 |
| 2:B:8:LYS:CB | 2:B:8:LYS:CA | 1.74 | 1.60 |
| 2:D:113:VAL:CG2 | 2:D:113:VAL:CB | 1.74 | 1.59 |
| 2:D:48:LEU:CG | 2:D:48:LEU:CD1 | 1.75 | 1.59 |
| 1:C:118:THR:CB | 1:C:118:THR:CA | 1.75 | 1.59 |
| 1:A:72:HIS:CB | 1:A:72:HIS:CA | 1.78 | 1.59 |
| 2:D:123:THR:CG2 | 2:D:123:THR:CB | 1.80 | 1.59 |
| 2:D:2:HIS:CG | 2:D:2:HIS:CD2 | 1.85 | 1.59 |
| 2:D:141:LEU:CD2 | 2:D:141:LEU:CG | 1.78 | 1.59 |
| 2:D:126:VAL:CA | 2:D:126:VAL:CB | 1.81 | 1.58 |
| 1:A:84:SER:CA | 1:A:84:SER:CB | 1.82 | 1.58 |
| 2:B:50:THR:CG2 | 2:B:50:THR:CB | 1.75 | 1.58 |
| 2:B:65:LYS:CB | 2:B:65:LYS:CA | 1.80 | 1.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:141:ARG:CB | 1:A:141:ARG:CG | 1.79 | 1.57 |
| 2:D:78:LEU:CA | 2:D:78:LEU:CB | 1.79 | 1.57 |
| 2:D:4:THR:CA | 2:D:4:THR:CB | 1.82 | 1.57 |
| 2:D:121:GLU:CA | 2:D:121:GLU:CB | 1.79 | 1.57 |
| 1:A:14:TRP:CB | 1:A:14:TRP:CA | 1.83 | 1.57 |
| 2:B:77:HIS:CG | 2:B:77:HIS:CD2 | 1.84 | 1.56 |
| 1:C:99:LYS:CG | 1:C:99:LYS:CD | 1.82 | 1.56 |
| 2:D:8:LYS:CA | 2:D:8:LYS:N | 1.68 | 1.56 |
| 2:D:67:VAL:CB | 2:D:67:VAL:CA | 1.76 | 1.56 |
| 2:B:143:HIS:ND1 | 2:B:143:HIS:CG | 1.70 | 1.56 |
| 1:C:73:VAL:CA | 1:C:73:VAL:CB | 1.80 | 1.56 |
| 1:C:70:VAL:CA | 1:C:70:VAL:C | 1.74 | 1.56 |
| 2:B:47:ASP:N | 2:B:47:ASP:CA | 1.67 | 1.56 |
| 1:A:1:VAL:CA | 1:A:1:VAL:CB | 1.84 | 1.56 |
| 1:C:105:LEU:CD1 | 1:C:105:LEU:CG | 1.79 | 1.56 |
| 1:A:56:LYS:CD | 1:A:56:LYS:CE | 1.84 | 1.56 |
| 1:A:31:ARG:CD | 1:A:31:ARG:NE | 1.68 | 1.55 |
| 2:D:18:VAL:N | 2:D:18:VAL:CA | 1.70 | 1.55 |
| 1:A:29:LEU:CB | 1:A:29:LEU:CA | 1.79 | 1.55 |
| 2:D:94:ASP:N | 2:D:94:ASP:CA | 1.68 | 1.55 |
| 2:B:8:LYS:CD | 2:B:8:LYS:CG | 1.78 | 1.55 |
| 1:C:40:LYS:CE | 1:C:40:LYS:NZ | 1.69 | 1.54 |
| 1:C:84:SER:CB | 1:C:84:SER:CA | 1.79 | 1.54 |
| 2:B:9:SER:CA | 2:B:9:SER:CB | 1.79 | 1.54 |
| 1:C:61:LYS:CD | 1:C:61:LYS:CE | 1.81 | 1.54 |
| 2:B:49:SER:CA | 2:B:49:SER:N | 1.67 | 1.54 |
| 2:B:90:GLU:CB | 2:B:90:GLU:CA | 1.84 | 1.54 |
| 2:B:80:ASN:CG | 2:B:80:ASN:CB | 1.75 | 1.54 |
| 2:D:53:ALA:C | 2:D:53:ALA:CA | 1.76 | 1.54 |
| 2:B:1:VAL:CA | 2:B:1:VAL:N | 1.69 | 1.54 |
| 2:D:7:GLU:CA | 2:D:7:GLU:C | 1.75 | 1.54 |
| 1:C:16:LYS:CE | 1:C:16:LYS:NZ | 1.71 | 1.54 |
| 2:B:49:SER:CB | 2:B:49:SER:CA | 1.83 | 1.53 |
| 2:B:81:LEU:N | 2:B:81:LEU:CA | 1.68 | 1.53 |
| 4:B:148:HEM:CBD | 4:B:148:HEM:CGD | 1.85 | 1.53 |
| 1:C:38:THR:CB | 1:C:38:THR:CA | 1.81 | 1.53 |
| 1:A:62:VAL:CA | 1:A:62:VAL:C | 1.75 | 1.53 |
| 1:C:78:ASN:CB | 1:C:78:ASN:CG | 1.76 | 1.53 |
| 1:C:75:ASP:CA | 1:C:75:ASP:N | 1.71 | 1.53 |
| 2:D:12:THR:N | 2:D:12:THR:CA | 1.68 | 1.53 |
| 1:C:54:GLN:CA | 1:C:54:GLN:C | 1.75 | 1.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:58:HIS:CA | 1:A:58:HIS:C | 1.76 | 1.53 |
| 2:B:47:ASP:CA | 2:B:47:ASP:C | 1.75 | 1.52 |
| 1:A:87:HIS:CA | 1:A:87:HIS:C | 1.75 | 1.52 |
| 2:B:145:TYR:CA | 2:B:145:TYR:C | 1.75 | 1.52 |
| 1:A:90:LYS:CD | 1:A:90:LYS:CE | 1.84 | 1.52 |
| 2:B:1:VAL:CA | 2:B:1:VAL:CB | 1.86 | 1.52 |
| 2:D:22:GLU:CG | 2:D:22:GLU:CA | 1.85 | 1.52 |
| 1:C:137:THR:CA | 1:C:137:THR:C | 1.74 | 1.52 |
| 2:D:92:HIS:CA | 2:D:92:HIS:C | 1.76 | 1.52 |
| 2:B:10:ALA:C | 2:B:10:ALA:CA | 1.78 | 1.52 |
| 2:B:52:ASP:CB | 2:B:52:ASP:CG | 1.77 | 1.52 |
| 2:B:117:HIS:ND1 | 2:B:117:HIS:CE1 | 1.75 | 1.52 |
| 2:D:52:ASP:CG | 2:D:52:ASP:CB | 1.75 | 1.51 |
| 2:D:10:ALA:C | 2:D:10:ALA:CA | 1.75 | 1.51 |
| 2:B:6:GLU:C | 2:B:6:GLU:CA | 1.77 | 1.51 |
| 2:D:45:PHE:C | 2:D:46:GLY:CA | 1.78 | 1.51 |
| 2:D:131:GLN:CG | 2:D:131:GLN:CD | 1.77 | 1.51 |
| 2:D:59:LYS:C | 2:D:59:LYS:CA | 1.76 | 1.51 |
| 1:C:16:LYS:CD | 1:C:16:LYS:CG | 1.81 | 1.51 |
| 1:C:70:VAL:CA | 1:C:70:VAL:N | 1.68 | 1.50 |
| 1:C:8:THR:CB | 1:C:8:THR:CA | 1.84 | 1.50 |
| 2:D:8:LYS:CA | 2:D:8:LYS:CB | 1.85 | 1.50 |
| 2:B:61:LYS:NZ | 2:B:61:LYS:CE | 1.75 | 1.50 |
| 1:C:131:SER:C | 1:C:131:SER:CA | 1.76 | 1.50 |
| 2:D:47:ASP:CB | 2:D:47:ASP:CG | 1.76 | 1.50 |
| 1:C:61:LYS:CA | 1:C:61:LYS:C | 1.76 | 1.50 |
| 2:D:73:ASP:CA | 2:D:73:ASP:CB | 1.86 | 1.50 |
| 1:C:72:HIS:CA | 1:C:72:HIS:CB | 1.85 | 1.50 |
| 2:D:48:LEU:N | 2:D:48:LEU:CA | 1.72 | 1.50 |
| 2:D:59:LYS:CE | 2:D:59:LYS:CD | 1.88 | 1.50 |
| 1:C:56:LYS:CE | 1:C:56:LYS:NZ | 1.72 | 1.50 |
| 2:D:50:THR:CA | 2:D:50:THR:N | 1.71 | 1.49 |
| 2:B:143:HIS:CA | 2:B:143:HIS:C | 1.76 | 1.49 |
| 2:D:21:ASP:CB | 2:D:21:ASP:CG | 1.78 | 1.49 |
| 2:D:117:HIS:ND1 | 2:D:117:HIS:CG | 1.74 | 1.49 |
| 2:B:12:THR:CA | 2:B:12:THR:CG2 | 1.89 | 1.49 |
| 1:C:10:VAL:C | 1:C:10:VAL:CA | 1.81 | 1.49 |
| 2:B:124:PRO:N | 2:B:124:PRO:CD | 1.70 | 1.48 |
| 2:D:80:ASN:CA | 2:D:80:ASN:N | 1.75 | 1.48 |
| 2:B:5:PRO:C | 2:B:5:PRO:CA | 1.78 | 1.48 |
| 2:D:1:VAL:N | 2:D:1:VAL:CA | 1.77 | 1.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:7:LYS:N | 1:C:7:LYS:CA | 1.75 | 1.48 |
| 2:D:82:LYS:CD | 2:D:82:LYS:CG | 1.89 | 1.48 |
| 1:C:2:LEU:C | 1:C:2:LEU:CA | 1.79 | 1.48 |
| 2:B:80:ASN:C | 2:B:80:ASN:CA | 1.80 | 1.48 |
| 1:C:16:LYS:C | 1:C:16:LYS:CA | 1.82 | 1.48 |
| 2:D:52:ASP:CA | 2:D:52:ASP:N | 1.76 | 1.48 |
| 1:A:2:LEU:C | 1:A:2:LEU:CA | 1.77 | 1.48 |
| 1:C:87:HIS:CA | 1:C:87:HIS:C | 1.82 | 1.48 |
| 2:B:80:ASN:N | 2:B:80:ASN:CA | 1.73 | 1.47 |
| 2:D:7:GLU:CG | 2:D:7:GLU:CB | 1.88 | 1.47 |
| 2:D:108:ASN:CB | 2:D:108:ASN:CG | 1.83 | 1.47 |
| 1:C:90:LYS:CE | 1:C:90:LYS:CD | 1.91 | 1.47 |
| 1:A:61:LYS:CE | 1:A:61:LYS:NZ | 1.74 | 1.47 |
| 4:B:148:HEM:CBA | 4:B:148:HEM:CGA | 1.91 | 1.47 |
| 2:B:41:PHE:C | 2:B:41:PHE:CA | 1.77 | 1.47 |
| 2:B:82:LYS:CG | 2:B:82:LYS:CE | 1.93 | 1.47 |
| 1:A:52:SER:N | 1:A:52:SER:CA | 1.75 | 1.47 |
| 2:B:21:ASP:CB | 2:B:21:ASP:CG | 1.84 | 1.46 |
| 1:A:60:LYS:CE | 1:A:60:LYS:CD | 1.93 | 1.46 |
| 1:A:16:LYS:CE | 1:A:16:LYS:CD | 1.92 | 1.46 |
| 1:A:74:ASP:CG | 1:A:74:ASP:CB | 1.80 | 1.46 |
| 2:B:142:ALA:CA | 2:B:142:ALA:C | 1.82 | 1.46 |
| 1:A:137:THR:CA | 1:A:137:THR:CB | 1.91 | 1.46 |
| 2:D:47:ASP:CB | 2:D:47:ASP:CA | 1.94 | 1.45 |
| 1:C:90:LYS:CG | 1:C:90:LYS:CD | 1.90 | 1.45 |
| 2:D:46:GLY:CA | 2:D:46:GLY:C | 1.82 | 1.45 |
| 1:C:16:LYS:CG | 1:C:16:LYS:CB | 1.93 | 1.45 |
| 2:B:74:GLY:C | 2:B:75:LEU:N | 1.70 | 1.45 |
| 1:A:76:MET:CG | 1:A:76:MET:SD | 2.02 | 1.45 |
| 1:A:44:PRO:C | 1:A:44:PRO:CA | 1.83 | 1.45 |
| 2:D:43:GLU:CG | 2:D:43:GLU:CA | 1.95 | 1.45 |
| 2:B:22:GLU:CG | 2:B:22:GLU:CD | 1.85 | 1.45 |
| 2:B:2:HIS:CG | 2:B:2:HIS:CD2 | 2.05 | 1.44 |
| 2:B:87:THR:CB | 2:B:87:THR:CA | 1.95 | 1.44 |
| 4:C:142:HEM:CGD | 4:C:142:HEM:CBD | 1.93 | 1.44 |
| 1:C:1:VAL:CA | 1:C:1:VAL:C | 1.83 | 1.44 |
| 2:B:108:ASN:CG | 2:B:108:ASN:CB | 1.84 | 1.44 |
| 1:C:20:HIS:CE1 | 1:C:20:HIS:ND1 | 1.79 | 1.44 |
| 2:D:22:GLU:C | 2:D:22:GLU:CA | 1.83 | 1.44 |
| 2:B:61:LYS:CD | 2:B:61:LYS:CG | 1.93 | 1.44 |
| 2:B:2:HIS:C | 2:B:2:HIS:CA | 1.84 | 1.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:D:79:ASP:CA | 2:D:79:ASP:C | 1.83 | 1.44 |
| 1:A:99:LYS:CD | 1:A:99:LYS:CE | 1.95 | 1.44 |
| 2:D:12:THR:CA | 2:D:12:THR:CB | 1.93 | 1.43 |
| 1:C:76:MET:CG | 1:C:76:MET:SD | 2.05 | 1.43 |
| 2:D:49:SER:C | 2:D:49:SER:CA | 1.86 | 1.43 |
| 1:C:82:ALA:C | 1:C:83:LEU:N | 1.69 | 1.43 |
| 2:B:139:ASN:CA | 2:B:139:ASN:CG | 1.87 | 1.43 |
| 2:B:9:SER:CA | 2:B:9:SER:C | 1.87 | 1.43 |
| 1:C:7:LYS:CG | 1:C:7:LYS:CD | 1.95 | 1.43 |
| 2:D:143:HIS:CD2 | 2:D:143:HIS:CG | 1.85 | 1.42 |
| 1:A:11:LYS:CE | 1:A:11:LYS:CD | 1.96 | 1.42 |
| 2:B:65:LYS:CA | 2:B:65:LYS:CG | 1.98 | 1.42 |
| 1:A:20:HIS:CG | 1:A:20:HIS:ND1 | 1.71 | 1.42 |
| 1:A:137:THR:OG1 | 1:A:137:THR:CB | 1.66 | 1.42 |
| 2:D:19:ASN:CG | 2:D:19:ASN:ND2 | 1.71 | 1.42 |
| 1:A:18:GLY:C | 1:A:18:GLY:CA | 1.86 | 1.42 |
| 2:D:146:HIS:CG | 2:D:146:HIS:ND1 | 1.85 | 1.41 |
| 1:C:139:LYS:CD | 1:C:139:LYS:CE | 1.95 | 1.41 |
| 1:C:139:LYS:CE | 1:C:139:LYS:NZ | 1.84 | 1.41 |
| 1:C:72:HIS:CG | 1:C:72:HIS:ND1 | 1.80 | 1.41 |
| 1:A:75:ASP:CA | 1:A:75:ASP:CG | 1.88 | 1.40 |
| 1:A:75:ASP:CB | 1:A:75:ASP:CA | 1.97 | 1.40 |
| 1:A:138:SER:OG | 1:A:138:SER:CA | 1.68 | 1.40 |
| 2:D:5:PRO:N | 2:D:5:PRO:CA | 1.84 | 1.40 |
| 2:D:26:GLU:CD | 2:D:26:GLU:CG | 1.90 | 1.40 |
| 2:D:2:HIS:CE1 | 2:D:2:HIS:NE2 | 1.90 | 1.40 |
| 2:B:66:LYS:CE | 2:B:66:LYS:NZ | 1.81 | 1.40 |
| 1:A:127:LYS:CG | 1:A:127:LYS:CD | 1.97 | 1.40 |
| 2:B:2:HIS:CG | 2:B:2:HIS:ND1 | 1.89 | 1.39 |
| 2:D:77:HIS:NE2 | 2:D:77:HIS:CD2 | 1.88 | 1.39 |
| 2:D:2:HIS:CE1 | 2:D:2:HIS:ND1 | 1.90 | 1.39 |
| 1:A:16:LYS:CG | 1:A:16:LYS:CD | 2.01 | 1.39 |
| 2:D:58:PRO:CD | 2:D:58:PRO:N | 1.71 | 1.39 |
| 2:D:55:MET:CA | 2:D:55:MET:C | 1.90 | 1.39 |
| 2:B:125:PRO:N | 2:B:125:PRO:CD | 1.67 | 1.39 |
| 2:B:144:LYS:CE | 2:B:144:LYS:CD | 2.01 | 1.38 |
| 1:A:127:LYS:CG | 1:A:127:LYS:CA | 2.02 | 1.38 |
| 2:D:77:HIS:CE1 | 2:D:77:HIS:ND1 | 1.91 | 1.38 |
| 2:B:146:HIS:CG | 2:B:146:HIS:CB | 2.04 | 1.38 |
| 2:D:43:GLU:CD | 2:D:43:GLU:CG | 1.92 | 1.38 |
| 2:B:2:HIS:CA | 2:B:2:HIS:CB | 2.01 | 1.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:81:SER:CA | 1:A:81:SER:CB | 2.00 | 1.37 |
| 1:A:92:ARG:CD | 1:A:92:ARG:CZ | 2.01 | 1.37 |
| 1:C:114:PRO:C | 1:C:114:PRO:CA | 1.91 | 1.37 |
| 1:C:92:ARG:CZ | 1:C:92:ARG:NH1 | 1.87 | 1.37 |
| 1:C:138:SER:OG | 1:C:138:SER:CA | 1.72 | 1.37 |
| 2:B:87:THR:CG2 | 2:B:87:THR:CB | 2.02 | 1.37 |
| 2:B:104:ARG:NH1 | 2:B:104:ARG:CZ | 1.87 | 1.36 |
| 2:B:49:SER:CB | 2:B:49:SER:OG | 1.71 | 1.36 |
| 2:D:8:LYS:CE | 2:D:8:LYS:CD | 2.03 | 1.36 |
| 2:D:146:HIS:CD2 | 2:D:146:HIS:ND1 | 1.91 | 1.36 |
| 2:D:104:ARG:NE | 2:D:104:ARG:CD | 1.84 | 1.36 |
| 4:D:148:HEM:CBD | 4:D:148:HEM:CGD | 2.01 | 1.35 |
| 1:A:50:HIS:CA | 1:A:50:HIS:CB | 2.02 | 1.35 |
| 2:D:43:GLU:CA | 2:D:43:GLU:C | 1.94 | 1.35 |
| 2:B:1:VAL:CG1 | 2:B:1:VAL:CB | 2.03 | 1.35 |
| 2:D:80:ASN:CG | 2:D:80:ASN:OD1 | 1.66 | 1.34 |
| 1:A:17:VAL:CA | 1:A:17:VAL:C | 1.96 | 1.34 |
| 2:B:132:LYS:CE | 2:B:132:LYS:NZ | 1.88 | 1.34 |
| 1:C:30:GLU:CG | 1:C:30:GLU:CD | 1.96 | 1.34 |
| 1:A:56:LYS:CD | 1:A:56:LYS:CG | 2.06 | 1.34 |
| 1:A:16:LYS:CG | 1:A:16:LYS:CE | 2.06 | 1.34 |
| 2:D:20:VAL:CA | 2:D:20:VAL:CB | 2.05 | 1.34 |
| 2:D:90:GLU:OE1 | 2:D:90:GLU:CD | 1.64 | 1.33 |
| 2:D:6:GLU:CD | 2:D:6:GLU:CG | 1.97 | 1.33 |
| 2:B:117:HIS:ND1 | 2:B:117:HIS:CG | 1.94 | 1.33 |
| 2:D:66:LYS:CD | 2:D:66:LYS:CG | 2.06 | 1.33 |
| 1:A:64:ASP:CG | 1:A:64:ASP:CB | 1.95 | 1.33 |
| 2:B:6:GLU:CD | 2:B:6:GLU:OE1 | 1.67 | 1.33 |
| 2:B:59:LYS:NZ | 2:B:59:LYS:CE | 1.92 | 1.33 |
| 1:A:78:ASN:CB | 1:A:78:ASN:ND2 | 1.87 | 1.33 |
| 1:A:72:HIS:CG | 1:A:72:HIS:CA | 2.12 | 1.32 |
| 1:A:61:LYS:CE | 1:A:61:LYS:CG | 2.06 | 1.32 |
| 1:C:114:PRO:CA | 1:C:114:PRO:N | 1.72 | 1.31 |
| 2:D:139:ASN:OD1 | 2:D:139:ASN:CG | 1.68 | 1.31 |
| 1:C:11:LYS:CE | 1:C:11:LYS:NZ | 1.91 | 1.31 |
| 1:C:40:LYS:CG | 1:C:40:LYS:CE | 2.07 | 1.30 |
| 2:D:8:LYS:CE | 2:D:8:LYS:NZ | 1.94 | 1.30 |
| 2:D:82:LYS:CE | 2:D:82:LYS:NZ | 1.94 | 1.30 |
| 2:B:143:HIS:ND1 | 2:B:143:HIS:CE1 | 1.99 | 1.30 |
| 4:D:148:HEM:CGA | 4:D:148:HEM:O2A | 1.77 | 1.30 |
| 2:D:20:VAL:CA | 2:D:20:VAL:CG1 | 2.10 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:139:LYS:NZ | 1:A:139:LYS:CE | 1.96 | 1.29 |
| 1:A:15:GLY:O | 1:A:15:GLY:C | 1.67 | 1.29 |
| 2:B:1:VAL:C | 2:B:1:VAL:O | 1.70 | 1.29 |
| 1:C:112:HIS:CG | 1:C:112:HIS:ND1 | 1.78 | 1.29 |
| 2:D:76:ALA:N | 2:D:76:ALA:CA | 1.94 | 1.29 |
| 4:A:142:HEM:CBD | 4:A:142:HEM:CGD | 2.09 | 1.29 |
| 2:D:50:THR:CA | 2:D:50:THR:CB | 2.11 | 1.29 |
| 2:B:79:ASP:CG | 2:B:79:ASP:OD2 | 1.67 | 1.29 |
| 2:D:66:LYS:CE | 2:D:66:LYS:NZ | 1.95 | 1.29 |
| 2:D:43:GLU:HB2 | 2:D:43:GLU:C | 1.53 | 1.29 |
| 2:D:121:GLU:CD | 2:D:121:GLU:CG | 2.01 | 1.28 |
| 2:D:1:VAL:C | 2:D:1:VAL:CA | 2.02 | 1.28 |
| 2:D:26:GLU:OE2 | 2:D:26:GLU:CD | 1.71 | 1.28 |
| 1:C:40:LYS:NZ | 1:C:40:LYS:CD | 1.95 | 1.28 |
| 2:B:146:HIS:ND1 | 2:B:146:HIS:CE1 | 1.84 | 1.28 |
| 1:A:30:GLU:CG | 1:A:30:GLU:CD | 2.00 | 1.28 |
| 2:B:101:GLU:CG | 2:B:101:GLU:CD | 2.02 | 1.28 |
| 1:A:23:GLU:CD | 1:A:23:GLU:OE1 | 1.72 | 1.27 |
| 2:B:104:ARG:NH2 | 2:B:104:ARG:CZ | 1.97 | 1.27 |
| 1:C:105:LEU:CG | 1:C:105:LEU:CD2 | 2.12 | 1.27 |
| 1:C:61:LYS:CE | 1:C:61:LYS:NZ | 1.98 | 1.27 |
| 2:B:12:THR:CG2 | 2:B:12:THR:OG1 | 1.78 | 1.27 |
| 2:D:4:THR:HB | 2:D:6:GLU:OE2 | 1.30 | 1.27 |
| 1:A:138:SER:CB | 1:A:138:SER:CA | 2.12 | 1.26 |
| 1:C:138:SER:CA | 1:C:138:SER:CB | 2.14 | 1.26 |
| 1:A:1:VAL:CG2 | 1:A:1:VAL:CA | 2.13 | 1.26 |
| 2:D:95:LYS:NZ | 2:D:95:LYS:CE | 1.99 | 1.25 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:CG2 | 2.13 | 1.25 |
| 2:B:8:LYS:CA | 2:B:8:LYS:CG | 2.13 | 1.25 |
| 2:B:144:LYS:CE | 2:B:144:LYS:NZ | 1.99 | 1.25 |
| 2:D:17:LYS:CE | 2:D:17:LYS:NZ | 1.98 | 1.25 |
| 1:C:1:VAL:CG2 | 1:C:1:VAL:HG13 | 1.64 | 1.25 |
| 1:A:85:ASP:CG | 1:A:85:ASP:OD2 | 1.73 | 1.24 |
| 1:A:72:HIS:CG | 1:A:72:HIS:ND1 | 1.85 | 1.24 |
| 2:D:125:PRO:N | 2:D:125:PRO:CD | 1.67 | 1.24 |
| 2:B:90:GLU:CG | 2:B:90:GLU:CD | 2.07 | 1.24 |
| 2:D:95:LYS:CG | 2:D:95:LYS:CD | 2.17 | 1.23 |
| 2:B:6:GLU:CD | 2:B:6:GLU:CG | 2.07 | 1.23 |
| 2:B:22:GLU:CD | 2:B:22:GLU:OE1 | 1.77 | 1.23 |
| 2:D:101:GLU:CD | 2:D:101:GLU:CG | 2.06 | 1.22 |
| 2:B:5:PRO:CD | 2:B:5:PRO:N | 1.81 | 1.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:121:GLU:CD | 2:B:121:GLU:CG | 2.07 | 1.22 |
| 2:D:26:GLU:CB | 2:D:26:GLU:CG | 2.18 | 1.22 |
| 2:B:1:VAL:C | 2:B:1:VAL:CA | 2.09 | 1.21 |
| 1:A:21:ALA:CA | 1:A:21:ALA:C | 2.09 | 1.21 |
| 1:C:60:LYS:NZ | 1:C:60:LYS:CE | 2.02 | 1.21 |
| 2:D:3:LEU:O | 2:D:3:LEU:C | 1.77 | 1.21 |
| 2:B:49:SER:O | 2:B:49:SER:C | 1.79 | 1.21 |
| 2:B:2:HIS:NE2 | 2:B:2:HIS:CD2 | 2.09 | 1.20 |
| 1:A:92:ARG:NH1 | 1:A:92:ARG:CD | 2.03 | 1.20 |
| 1:A:14:TRP:CG | 1:A:14:TRP:CA | 2.22 | 1.20 |
| 1:C:99:LYS:CG | 1:C:99:LYS:CA | 2.17 | 1.20 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:CA | 2.18 | 1.20 |
| 2:B:47:ASP:OD2 | 2:B:47:ASP:CG | 1.78 | 1.19 |
| 1:A:23:GLU:CG | 1:A:23:GLU:CD | 2.10 | 1.19 |
| 1:A:78:ASN:CG | 1:A:78:ASN:CA | 2.11 | 1.19 |
| 2:D:65:LYS:CD | 2:D:65:LYS:CE | 2.20 | 1.19 |
| 2:D:2:HIS:CB | 2:D:2:HIS:CA | 2.21 | 1.19 |
| 2:D:26:GLU:OE1 | 2:D:26:GLU:CD | 1.79 | 1.19 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:CB | 2.22 | 1.18 |
| 2:D:58:PRO:CD | 2:D:58:PRO:CB | 2.20 | 1.18 |
| 2:B:58:PRO:CD | 2:B:58:PRO:N | 1.78 | 1.18 |
| 1:C:90:LYS:CE | 1:C:90:LYS:NZ | 2.06 | 1.18 |
| 1:C:16:LYS:CD | 1:C:16:LYS:CE | 2.23 | 1.17 |
| 2:D:43:GLU:CD | 2:D:43:GLU:CB | 2.13 | 1.17 |
| 1:A:75:ASP:OD1 | 1:A:75:ASP:CG | 1.82 | 1.17 |
| 1:A:127:LYS:CB | 1:A:127:LYS:CD | 2.23 | 1.17 |
| 1:A:92:ARG:HD3 | 1:A:92:ARG:NH1 | 1.60 | 1.16 |
| 1:C:92:ARG:NE | 1:C:92:ARG:HH21 | 1.42 | 1.16 |
| 2:D:73:ASP:CG | 2:D:73:ASP:CA | 2.14 | 1.16 |
| 2:B:26:GLU:OE2 | 2:B:26:GLU:HG2 | 1.45 | 1.16 |
| 1:C:113:LEU:CB | 1:C:113:LEU:CD1 | 2.22 | 1.15 |
| 2:B:104:ARG:CD | 2:B:104:ARG:CZ | 2.24 | 1.15 |
| 2:D:47:ASP:N | 2:D:47:ASP:CA | 2.09 | 1.15 |
| 1:C:23:GLU:CG | 1:C:23:GLU:CD | 2.15 | 1.15 |
| 1:A:1:VAL:CG2 | 1:A:1:VAL:N | 2.09 | 1.14 |
| 2:D:77:HIS:CG | 2:D:77:HIS:NE2 | 2.15 | 1.14 |
| 1:C:99:LYS:CD | 1:C:99:LYS:CE | 2.26 | 1.14 |
| 2:B:139:ASN:ND2 | 2:B:139:ASN:CG | 2.01 | 1.14 |
| 2:B:26:GLU:OE2 | 2:B:26:GLU:CG | 1.95 | 1.13 |
| 1:C:73:VAL:CA | 1:C:73:VAL:CG1 | 2.26 | 1.13 |
| 1:C:56:LYS:CD | 1:C:56:LYS:CG | 2.27 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:121:GLU:CD | 2:B:121:GLU:OE1 | 1.87 | 1.13 |
| 1:C:46:PHE:CE2 | 1:C:46:PHE:CG | 2.02 | 1.13 |
| 1:A:1:VAL:HG23 | 1:A:1:VAL:N | 1.61 | 1.13 |
| 2:B:108:ASN:ND2 | 2:B:108:ASN:CB | 2.10 | 1.13 |
| 2:D:49:SER:C | 2:D:50:THR:CA | 2.17 | 1.13 |
| 2:D:6:GLU:CG | 2:D:6:GLU:CA | 2.28 | 1.12 |
| 2:D:66:LYS:CE | 2:D:66:LYS:CD | 2.27 | 1.12 |
| 2:B:2:HIS:ND1 | 2:B:2:HIS:CE1 | 2.18 | 1.12 |
| 2:B:104:ARG:NE | 2:B:104:ARG:CZ | 2.13 | 1.12 |
| 2:D:65:LYS:CG | 2:D:65:LYS:CD | 2.27 | 1.12 |
| 2:D:82:LYS:NZ | 2:D:82:LYS:CD | 2.12 | 1.12 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:HG22 | 1.77 | 1.12 |
| 2:B:49:SER:CB | 2:B:49:SER:C | 2.15 | 1.12 |
| 4:C:142:HEM:O2A | 4:C:142:HEM:CGA | 0.82 | 1.11 |
| 2:D:8:LYS:CA | 2:D:8:LYS:CG | 2.29 | 1.10 |
| 2:D:46:GLY:C | 2:D:47:ASP:CA | 2.20 | 1.10 |
| 1:A:16:LYS:CG | 1:A:16:LYS:HE2 | 1.82 | 1.10 |
| 4:C:142:HEM:CBA | 4:C:142:HEM:CGA | 2.29 | 1.10 |
| 2:D:43:GLU:CD | 2:D:43:GLU:HB3 | 1.71 | 1.09 |
| 2:D:5:PRO:CB | 2:D:5:PRO:CA | 2.31 | 1.09 |
| 1:A:90:LYS:CG | 1:A:90:LYS:CE | 2.30 | 1.09 |
| 2:B:117:HIS:CD2 | 2:B:117:HIS:NE2 | 2.21 | 1.09 |
| 2:D:4:THR:CB | 2:D:6:GLU:OE2 | 2.00 | 1.08 |
| 2:D:78:LEU:CD2 | 2:D:78:LEU:CD1 | 2.30 | 1.08 |
| 4:A:142:HEM:CGA | 4:A:142:HEM:CBA | 2.32 | 1.07 |
| 2:D:144:LYS:CE | 2:D:144:LYS:NZ | 2.16 | 1.07 |
| 1:C:16:LYS:CD | 1:C:16:LYS:CB | 2.33 | 1.07 |
| 2:D:22:GLU:HG3 | 2:D:22:GLU:CA | 1.61 | 1.07 |
| 2:D:43:GLU:CB | 2:D:43:GLU:C | 2.23 | 1.07 |
| 2:D:8:LYS:CD | 2:D:8:LYS:CB | 2.33 | 1.06 |
| 2:D:78:LEU:CD2 | 2:D:78:LEU:CB | 2.33 | 1.06 |
| 2:D:10:ALA:C | 2:D:10:ALA:CB | 2.23 | 1.06 |
| 2:D:76:ALA:N | 2:D:76:ALA:CB | 2.17 | 1.06 |
| 1:A:75:ASP:OD2 | 1:A:75:ASP:CB | 2.02 | 1.06 |
| 1:A:78:ASN:HB3 | 1:A:78:ASN:CG | 1.50 | 1.06 |
| 1:C:84:SER:OG | 1:C:84:SER:CA | 2.04 | 1.05 |
| 1:A:99:LYS:NZ | 1:A:99:LYS:CE | 2.20 | 1.05 |
| 2:D:26:GLU:OE1 | 2:D:26:GLU:CG | 2.05 | 1.05 |
| 1:C:116:GLU:CB | 1:C:116:GLU:CG | 2.33 | 1.04 |
| 2:B:65:LYS:CE | 2:B:65:LYS:CD | 2.35 | 1.04 |
| 1:A:78:ASN:HB2 | 1:A:78:ASN:CG | 1.51 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:D:6:GLU:CG | 2:D:6:GLU:HB3 | 1.55 | 1.04 |
| 2:D:141:LEU:CD2 | 2:D:141:LEU:CD1 | 2.34 | 1.04 |
| 1:A:92:ARG:HH11 | 1:A:92:ARG:CD | 1.66 | 1.04 |
| 2:B:59:LYS:CD | 2:B:59:LYS:CE | 2.36 | 1.04 |
| 2:B:8:LYS:HB2 | 2:B:8:LYS:CG | 1.52 | 1.03 |
| 1:A:75:ASP:HB2 | 1:A:75:ASP:CG | 1.42 | 1.03 |
| 2:B:48:LEU:C | 2:B:49:SER:CA | 2.27 | 1.03 |
| 2:D:4:THR:C | 2:D:5:PRO:CA | 2.27 | 1.03 |
| 2:D:6:GLU:HG3 | 2:D:6:GLU:CB | 1.51 | 1.03 |
| 1:C:38:THR:HG22 | 1:C:38:THR:H | 1.22 | 1.03 |
| 1:A:16:LYS:HE2 | 1:A:16:LYS:HG3 | 1.38 | 1.03 |
| 2:D:58:PRO:CA | 2:D:58:PRO:CD | 2.37 | 1.03 |
| 2:B:66:LYS:CE | 2:B:66:LYS:CD | 2.37 | 1.02 |
| 1:C:92:ARG:CD | 1:C:92:ARG:HH21 | 1.72 | 1.02 |
| 1:C:99:LYS:CB | 1:C:99:LYS:CD | 2.36 | 1.02 |
| 1:A:75:ASP:OD2 | 1:A:75:ASP:HB3 | 1.54 | 1.02 |
| 2:D:6:GLU:CB | 2:D:6:GLU:HG2 | 1.51 | 1.02 |
| 1:C:40:LYS:HE2 | 1:C:40:LYS:CD | 1.53 | 1.02 |
| 2:B:81:LEU:CB | 2:B:81:LEU:N | 2.23 | 1.02 |
| 1:C:1:VAL:CB | 1:C:1:VAL:N | 2.22 | 1.02 |
| 1:A:75:ASP:HB3 | 1:A:75:ASP:CG | 1.42 | 1.02 |
| 1:C:40:LYS:CE | 1:C:40:LYS:HD2 | 1.50 | 1.02 |
| 2:B:139:ASN:ND2 | 2:B:139:ASN:OD1 | 1.91 | 1.02 |
| 1:C:40:LYS:HE3 | 1:C:40:LYS:CD | 1.53 | 1.01 |
| 2:D:6:GLU:CG | 2:D:6:GLU:HB2 | 1.55 | 1.01 |
| 2:D:79:ASP:OD1 | 2:D:79:ASP:CG | 1.99 | 1.01 |
| 2:D:79:ASP:CG | 2:D:79:ASP:OD2 | 1.98 | 1.01 |
| 1:C:90:LYS:CB | 1:C:90:LYS:CD | 2.39 | 1.01 |
| 2:B:1:VAL:CA | 2:B:2:HIS:N | 2.23 | 1.01 |
| 4:D:148:HEM:CGA | 4:D:148:HEM:CBA | 2.39 | 1.01 |
| 2:D:1:VAL:CA | 2:D:2:HIS:N | 2.23 | 1.01 |
| 1:C:56:LYS:CD | 1:C:56:LYS:CE | 2.39 | 1.00 |
| 1:C:40:LYS:CE | 1:C:40:LYS:HD3 | 1.50 | 1.00 |
| 2:B:46:GLY:C | 2:B:47:ASP:CA | 2.29 | 1.00 |
| 2:D:18:VAL:CG2 | 2:D:18:VAL:CG1 | 2.40 | 1.00 |
| 1:A:74:ASP:CG | 1:A:74:ASP:OD1 | 0.80 | 1.00 |
| 1:A:92:ARG:NH2 | 1:A:92:ARG:CZ | 0.85 | 1.00 |
| 1:C:30:GLU:OE2 | 1:C:30:GLU:CD | 0.80 | 1.00 |
| 2:D:77:HIS:C | 2:D:77:HIS:CB | 2.29 | 0.99 |
| 2:D:47:ASP:C | 2:D:48:LEU:CA | 2.30 | 0.99 |
| 1:A:1:VAL:H3 | 1:A:1:VAL:HG23 | 1.12 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:D:12:THR:CG2 | 2:D:12:THR:CA | 2.39 | 0.99 |
| 2:B:101:GLU:CG | 2:B:101:GLU:OE2 | 2.09 | 0.99 |
| 2:B:8:LYS:HB3 | 2:B:8:LYS:CG | 1.52 | 0.99 |
| 2:D:47:ASP:N | 2:D:47:ASP:CB | 2.25 | 0.99 |
| 1:A:92:ARG:NH1 | 1:A:92:ARG:HD2 | 1.75 | 0.99 |
| 2:D:78:LEU:HD21 | 2:D:78:LEU:CG | 1.51 | 0.99 |
| 2:D:6:GLU:CA | 2:D:6:GLU:C | 2.31 | 0.99 |
| 2:D:79:ASP:CB | 2:D:79:ASP:C | 2.31 | 0.99 |
| 2:B:132:LYS:CD | 2:B:132:LYS:NZ | 2.26 | 0.99 |
| 2:D:146:HIS:NE2 | 2:D:146:HIS:ND1 | 2.10 | 0.98 |
| 2:D:53:ALA:C | 2:D:53:ALA:CB | 2.30 | 0.98 |
| 2:D:104:ARG:HH11 | 2:D:104:ARG:CD | 1.76 | 0.98 |
| 2:D:82:LYS:CE | 2:D:82:LYS:CD | 2.42 | 0.98 |
| 2:D:43:GLU:HG3 | 2:D:43:GLU:CB | 1.47 | 0.98 |
| 1:A:78:ASN:CB | 1:A:78:ASN:CG | 0.88 | 0.98 |
| 2:B:2:HIS:CA | 2:B:3:LEU:N | 2.28 | 0.97 |
| 2:B:82:LYS:CG | 2:B:82:LYS:HE2 | 1.74 | 0.97 |
| 1:A:2:LEU:CA | 1:A:3:SER:N | 2.27 | 0.97 |
| 2:B:8:LYS:CE | 2:B:8:LYS:NZ | 2.27 | 0.97 |
| 2:D:52:ASP:CB | 2:D:52:ASP:N | 2.28 | 0.97 |
| 2:D:43:GLU:HG2 | 2:D:43:GLU:CB | 1.47 | 0.97 |
| 2:B:139:ASN:HB3 | 2:B:139:ASN:CG | 1.37 | 0.97 |
| 2:B:9:SER:CA | 2:B:9:SER:OG | 2.13 | 0.96 |
| 2:D:45:PHE:C | 2:D:46:GLY:HA3 | 1.85 | 0.96 |
| 2:B:49:SER:C | 2:B:49:SER:N | 2.18 | 0.96 |
| 2:B:90:GLU:CG | 2:B:90:GLU:CA | 2.41 | 0.96 |
| 1:C:139:LYS:CD | 1:C:139:LYS:NZ | 2.27 | 0.96 |
| 4:B:148:HEM:CGA | 4:B:148:HEM:O2A | 0.66 | 0.96 |
| 1:C:38:THR:CA | 1:C:38:THR:CG2 | 2.44 | 0.96 |
| 2:D:45:PHE:CA | 2:D:46:GLY:N | 2.27 | 0.96 |
| 2:D:78:LEU:HD22 | 2:D:78:LEU:HG | 0.96 | 0.96 |
| 1:C:61:LYS:CD | 1:C:61:LYS:NZ | 2.29 | 0.95 |
| 2:D:120:LYS:CE | 2:D:120:LYS:NZ | 2.29 | 0.95 |
| 1:A:85:ASP:CG | 1:A:85:ASP:OD1 | 0.75 | 0.95 |
| 4:C:142:HEM:CBA | 4:C:142:HEM:O2A | 2.14 | 0.95 |
| 1:A:127:LYS:CE | 1:A:127:LYS:CG | 2.44 | 0.95 |
| 2:B:8:LYS:HG3 | 2:B:8:LYS:CB | 1.44 | 0.95 |
| 2:D:121:GLU:CA | 2:D:121:GLU:CG | 2.45 | 0.95 |
| 2:B:139:ASN:HB2 | 2:B:139:ASN:CG | 1.37 | 0.94 |
| 1:A:17:VAL:O | 1:A:17:VAL:C | 0.75 | 0.94 |
| 2:B:8:LYS:HG2 | 2:B:8:LYS:CB | 1.44 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:75:ASP:OD2 | 1:A:75:ASP:CG | 2.04 | 0.94 |
| 2:D:77:HIS:CE1 | 2:D:77:HIS:CG | 2.52 | 0.94 |
| 2:D:141:LEU:CD2 | 2:D:141:LEU:CB | 2.45 | 0.94 |
| 2:D:126:VAL:CA | 2:D:126:VAL:CG2 | 2.46 | 0.94 |
| 1:C:1:VAL:HG13 | 1:C:1:VAL:HG22 | 0.95 | 0.94 |
| 2:D:79:ASP:C | 2:D:80:ASN:CA | 2.35 | 0.94 |
| 2:D:6:GLU:CG | 2:D:6:GLU:CB | 0.94 | 0.94 |
| 1:A:61:LYS:CD | 1:A:61:LYS:HE2 | 1.42 | 0.94 |
| 1:C:7:LYS:CG | 1:C:7:LYS:CE | 2.45 | 0.93 |
| 1:A:61:LYS:HD3 | 1:A:61:LYS:CE | 1.44 | 0.93 |
| 1:A:92:ARG:HD2 | 1:A:92:ARG:CZ | 1.94 | 0.93 |
| 2:D:20:VAL:CA | 2:D:20:VAL:CG2 | 2.45 | 0.93 |
| 1:A:78:ASN:CG | 1:A:78:ASN:OD1 | 2.07 | 0.93 |
| 1:C:1:VAL:HB | 1:C:1:VAL:N | 1.81 | 0.93 |
| 1:A:61:LYS:HD2 | 1:A:61:LYS:CE | 1.44 | 0.93 |
| 1:A:137:THR:OG1 | 1:A:137:THR:CG2 | 2.14 | 0.93 |
| 2:B:87:THR:CG2 | 2:B:87:THR:OG1 | 2.16 | 0.93 |
| 1:A:92:ARG:HD3 | 1:A:92:ARG:HH11 | 1.21 | 0.93 |
| 4:B:148:HEM:CBA | 4:B:148:HEM:O2A | 2.15 | 0.93 |
| 2:D:22:GLU:HB3 | 2:D:22:GLU:CG | 1.43 | 0.93 |
| 1:A:61:LYS:HE3 | 1:A:61:LYS:CD | 1.42 | 0.93 |
| 2:D:7:GLU:C | 2:D:8:LYS:CA | 2.37 | 0.92 |
| 2:B:2:HIS:CD2 | 2:B:2:HIS:CB | 2.52 | 0.92 |
| 2:D:22:GLU:HB2 | 2:D:22:GLU:CG | 1.43 | 0.92 |
| 1:A:85:ASP:CB | 1:A:85:ASP:OD1 | 2.15 | 0.92 |
| 2:D:52:ASP:OD1 | 2:D:52:ASP:CB | 2.17 | 0.92 |
| 2:B:82:LYS:CE | 2:B:82:LYS:HD3 | 1.40 | 0.92 |
| 1:A:127:LYS:HG2 | 1:A:127:LYS:CB | 1.40 | 0.92 |
| 4:D:148:HEM:CBA | 4:D:148:HEM:O1A | 2.18 | 0.92 |
| 2:D:92:HIS:CB | 2:D:92:HIS:C | 2.37 | 0.92 |
| 1:C:1:VAL:CB | 1:C:1:VAL:C | 2.38 | 0.92 |
| 1:C:46:PHE:CD2 | 1:C:46:PHE:CE2 | 0.92 | 0.92 |
| 2:D:67:VAL:CG1 | 2:D:67:VAL:CA | 2.47 | 0.92 |
| 2:D:73:ASP:C | 2:D:73:ASP:CB | 2.38 | 0.92 |
| 2:D:20:VAL:CA | 2:D:20:VAL:HG12 | 1.99 | 0.92 |
| 1:C:1:VAL:CA | 1:C:1:VAL:N | 2.33 | 0.91 |
| 1:A:90:LYS:HG3 | 1:A:90:LYS:CE | 1.98 | 0.91 |
| 2:D:79:ASP:CA | 2:D:80:ASN:N | 2.33 | 0.91 |
| 2:D:45:PHE:C | 2:D:46:GLY:N | 0.87 | 0.91 |
| 1:C:84:SER:C | 1:C:84:SER:CB | 2.39 | 0.91 |
| 2:B:82:LYS:HD2 | 2:B:82:LYS:CE | 1.40 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:82:LYS:HE3 | 2:B:82:LYS:CD | 1.39 | 0.91 |
| 2:D:20:VAL:CA | 2:D:20:VAL:HG13 | 1.99 | 0.91 |
| 2:D:65:LYS:CD | 2:D:65:LYS:CB | 2.49 | 0.91 |
| 2:D:139:ASN:CB | 2:D:139:ASN:OD1 | 2.19 | 0.91 |
| 2:B:2:HIS:C | 2:B:2:HIS:CB | 2.39 | 0.90 |
| 2:B:104:ARG:HD3 | 2:B:104:ARG:CZ | 1.98 | 0.90 |
| 2:D:108:ASN:CB | 2:D:108:ASN:ND2 | 2.33 | 0.90 |
| 2:B:8:LYS:CB | 2:B:8:LYS:CD | 2.49 | 0.90 |
| 2:D:22:GLU:CD | 2:D:22:GLU:CG | 2.39 | 0.90 |
| 2:D:126:VAL:CA | 2:D:126:VAL:CG1 | 2.48 | 0.90 |
| 2:B:65:LYS:CA | 2:B:65:LYS:HG3 | 2.01 | 0.90 |
| 1:A:56:LYS:CD | 1:A:56:LYS:CB | 2.49 | 0.90 |
| 1:C:1:VAL:CB | 1:C:1:VAL:CG2 | 2.48 | 0.90 |
| 1:A:137:THR:CG2 | 1:A:137:THR:CA | 2.45 | 0.90 |
| 2:D:3:LEU:O | 2:D:4:THR:N | 2.03 | 0.90 |
| 2:B:65:LYS:CG | 2:B:65:LYS:CD | 2.49 | 0.90 |
| 1:C:72:HIS:CG | 1:C:72:HIS:CA | 2.54 | 0.90 |
| 1:A:62:VAL:CA | 1:A:63:ALA:N | 2.33 | 0.90 |
| 2:D:22:GLU:HG2 | 2:D:22:GLU:CB | 1.39 | 0.90 |
| 1:A:61:LYS:CD | 1:A:61:LYS:NZ | 2.34 | 0.90 |
| 2:B:82:LYS:NZ | 2:B:82:LYS:CE | 2.35 | 0.90 |
| 2:B:82:LYS:HE2 | 2:B:82:LYS:CD | 1.39 | 0.90 |
| 1:C:30:GLU:OE2 | 1:C:30:GLU:CG | 2.20 | 0.90 |
| 1:A:127:LYS:HG3 | 1:A:127:LYS:CB | 1.40 | 0.89 |
| 2:D:26:GLU:OE2 | 2:D:26:GLU:CG | 2.20 | 0.89 |
| 2:D:22:GLU:HG3 | 2:D:22:GLU:CB | 1.39 | 0.89 |
| 2:D:67:VAL:N | 2:D:67:VAL:CB | 2.36 | 0.89 |
| 2:B:65:LYS:HG2 | 2:B:65:LYS:CA | 2.01 | 0.89 |
| 2:B:80:ASN:ND2 | 2:B:80:ASN:CB | 2.33 | 0.89 |
| 2:B:12:THR:HG23 | 2:B:12:THR:C | 1.93 | 0.89 |
| 2:B:80:ASN:C | 2:B:81:LEU:CA | 2.40 | 0.89 |
| 1:C:46:PHE:CE2 | 1:C:46:PHE:HD2 | 1.60 | 0.89 |
| 2:B:10:ALA:C | 2:B:10:ALA:CB | 2.41 | 0.88 |
| 1:A:127:LYS:HB2 | 1:A:127:LYS:CG | 1.37 | 0.88 |
| 2:B:47:ASP:CB | 2:B:47:ASP:C | 2.41 | 0.88 |
| 1:A:1:VAL:CG1 | 1:A:1:VAL:CA | 2.50 | 0.88 |
| 2:D:66:LYS:NZ | 4:D:148:HEM:O1A | 2.06 | 0.88 |
| 2:B:2:HIS:CG | 2:B:2:HIS:CB | 0.83 | 0.88 |
| 2:D:78:LEU:CD2 | 2:D:78:LEU:CG | 0.88 | 0.88 |
| 2:D:76:ALA:N | 2:D:76:ALA:C | 2.26 | 0.88 |
| 1:A:127:LYS:HB3 | 1:A:127:LYS:CG | 1.37 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:1:VAL:CA | 1:C:1:VAL:CG2 | 2.51 | 0.88 |
| 2:B:22:GLU:OE2 | 2:B:22:GLU:CD | 2.12 | 0.88 |
| 1:C:99:LYS:CG | 1:C:99:LYS:HB3 | 1.36 | 0.88 |
| 1:C:99:LYS:CB | 1:C:99:LYS:HG3 | 1.36 | 0.87 |
| 1:A:51:GLY:C | 1:A:52:SER:CA | 2.43 | 0.87 |
| 2:D:47:ASP:C | 2:D:47:ASP:CA | 2.43 | 0.87 |
| 2:B:117:HIS:CB | 2:B:117:HIS:ND1 | 2.37 | 0.87 |
| 2:D:90:GLU:CG | 2:D:90:GLU:CD | 2.43 | 0.87 |
| 1:C:72:HIS:C | 1:C:72:HIS:CB | 2.41 | 0.87 |
| 1:A:72:HIS:CB | 1:A:72:HIS:C | 2.42 | 0.87 |
| 2:B:43:GLU:CG | 2:B:43:GLU:CD | 2.42 | 0.87 |
| 2:B:2:HIS:CG | 2:B:2:HIS:HB2 | 1.42 | 0.87 |
| 1:C:16:LYS:CD | 1:C:16:LYS:HB3 | 2.03 | 0.87 |
| 4:C:142:HEM:O1A | 4:C:142:HEM:O2A | 1.92 | 0.87 |
| 2:D:80:ASN:N | 2:D:80:ASN:HB3 | 1.89 | 0.87 |
| 1:A:50:HIS:CB | 1:A:50:HIS:N | 2.37 | 0.87 |
| 2:B:8:LYS:HG3 | 2:B:8:LYS:CA | 2.02 | 0.87 |
| 2:B:8:LYS:CB | 2:B:8:LYS:CG | 0.87 | 0.87 |
| 1:C:38:THR:H | 1:C:38:THR:CG2 | 1.88 | 0.87 |
| 2:B:139:ASN:OD1 | 2:B:139:ASN:CB | 2.20 | 0.86 |
| 2:D:146:HIS:CE1 | 2:D:146:HIS:ND1 | 0.67 | 0.86 |
| 1:C:99:LYS:CB | 1:C:99:LYS:HG2 | 1.36 | 0.86 |
| 2:B:2:HIS:CG | 2:B:2:HIS:HB3 | 1.42 | 0.86 |
| 2:D:78:LEU:HD22 | 2:D:78:LEU:CG | 1.51 | 0.86 |
| 1:C:38:THR:N | 1:C:38:THR:HG22 | 1.91 | 0.86 |
| 1:A:127:LYS:HB2 | 1:A:127:LYS:CD | 2.06 | 0.86 |
| 2:B:47:ASP:N | 2:B:47:ASP:CB | 2.39 | 0.86 |
| 1:A:141:ARG:CA | 1:A:141:ARG:CG | 2.53 | 0.86 |
| 1:C:99:LYS:CG | 1:C:99:LYS:HB2 | 1.36 | 0.86 |
| 2:D:94:ASP:N | 2:D:94:ASP:CB | 2.38 | 0.86 |
| 2:D:104:ARG:HH11 | 2:D:104:ARG:HD2 | 1.36 | 0.86 |
| 2:D:49:SER:C | 2:D:49:SER:CB | 2.44 | 0.86 |
| 1:A:31:ARG:CZ | 1:A:31:ARG:CD | 2.54 | 0.85 |
| 2:B:108:ASN:HD22 | 2:B:108:ASN:CB | 1.88 | 0.85 |
| 1:A:58:HIS:CA | 1:A:59:GLY:N | 2.39 | 0.85 |
| 1:A:17:VAL:CA | 1:A:18:GLY:N | 2.38 | 0.85 |
| 1:C:8:THR:CG2 | 1:C:8:THR:CA | 2.55 | 0.85 |
| 1:C:40:LYS:CE | 1:C:40:LYS:CD | 0.85 | 0.85 |
| 1:A:138:SER:HG | 1:A:138:SER:CA | 1.85 | 0.85 |
| 1:C:38:THR:N | 1:C:38:THR:CG2 | 2.39 | 0.85 |
| 2:D:7:GLU:CD | 2:D:7:GLU:CB | 2.45 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:141:ARG:CB | 1:A:141:ARG:CD | 2.55 | 0.85 |
| 1:A:137:THR:OG1 | 1:A:137:THR:CA | 2.25 | 0.84 |
| 2:D:20:VAL:C | 2:D:20:VAL:CB | 2.45 | 0.84 |
| 2:D:93:CYS:C | 2:D:94:ASP:CA | 2.45 | 0.84 |
| 2:B:12:THR:CG2 | 2:B:12:THR:C | 2.45 | 0.84 |
| 2:D:146:HIS:HE1 | 2:D:146:HIS:ND1 | 1.35 | 0.84 |
| 2:B:7:GLU:CA | 2:B:7:GLU:CG | 2.47 | 0.84 |
| 2:D:77:HIS:CG | 2:D:77:HIS:CA | 2.61 | 0.84 |
| 2:B:5:PRO:C | 2:B:5:PRO:N | 2.31 | 0.84 |
| 2:B:49:SER:O | 2:B:49:SER:CA | 2.25 | 0.84 |
| 2:D:59:LYS:CA | 2:D:60:VAL:N | 2.40 | 0.84 |
| 1:C:56:LYS:CG | 1:C:56:LYS:CE | 2.55 | 0.84 |
| 1:A:75:ASP:CB | 1:A:75:ASP:C | 2.45 | 0.84 |
| 1:C:118:THR:CB | 1:C:118:THR:N | 2.40 | 0.84 |
| 1:A:44:PRO:CB | 1:A:44:PRO:C | 2.46 | 0.83 |
| 2:D:19:ASN:OD1 | 2:D:19:ASN:ND2 | 2.10 | 0.83 |
| 2:B:65:LYS:CB | 2:B:65:LYS:HG3 | 1.32 | 0.83 |
| 1:C:70:VAL:CA | 1:C:71:ALA:N | 2.36 | 0.83 |
| 1:C:105:LEU:CB | 1:C:105:LEU:CD2 | 2.56 | 0.83 |
| 2:D:78:LEU:CD2 | 2:D:78:LEU:HG | 0.56 | 0.83 |
| 2:D:77:HIS:NE2 | 2:D:77:HIS:ND1 | 2.18 | 0.83 |
| 2:B:5:PRO:CA | 2:B:6:GLU:N | 2.40 | 0.83 |
| 4:B:148:HEM:CBA | 4:B:148:HEM:O1A | 2.24 | 0.83 |
| 1:C:48:LEU:CD2 | 1:C:48:LEU:CD1 | 2.57 | 0.83 |
| 1:C:40:LYS:NZ | 1:C:40:LYS:HD3 | 1.92 | 0.83 |
| 2:B:47:ASP:CA | 2:B:48:LEU:N | 2.41 | 0.83 |
| 2:B:65:LYS:CB | 2:B:65:LYS:HG2 | 1.32 | 0.82 |
| 1:A:60:LYS:CG | 1:A:60:LYS:CE | 2.57 | 0.82 |
| 2:B:61:LYS:NZ | 2:B:61:LYS:CD | 2.42 | 0.82 |
| 1:A:99:LYS:CG | 1:A:99:LYS:CE | 2.52 | 0.82 |
| 2:B:65:LYS:CG | 2:B:65:LYS:HB2 | 1.31 | 0.82 |
| 1:C:105:LEU:CB | 1:C:105:LEU:CD1 | 2.57 | 0.82 |
| 1:C:60:LYS:NZ | 1:C:60:LYS:CD | 2.41 | 0.82 |
| 2:D:4:THR:CA | 2:D:4:THR:CG2 | 2.54 | 0.82 |
| 1:A:84:SER:CA | 1:A:84:SER:OG | 2.28 | 0.82 |
| 2:D:78:LEU:HG | 2:D:78:LEU:HD23 | 0.83 | 0.82 |
| 2:B:3:LEU:CB | 2:B:3:LEU:N | 2.42 | 0.82 |
| 2:D:113:VAL:CG1 | 2:D:113:VAL:CG2 | 2.58 | 0.82 |
| 2:D:2:HIS:CG | 2:D:2:HIS:ND1 | 2.48 | 0.81 |
| 2:D:48:LEU:CB | 2:D:48:LEU:CD1 | 2.58 | 0.81 |
| 1:A:61:LYS:CD | 1:A:61:LYS:CE | 0.81 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:5:ALA:N | 1:A:5:ALA:CB | 2.43 | 0.81 |
| 2:D:48:LEU:N | 2:D:48:LEU:CB | 2.42 | 0.81 |
| 1:C:105:LEU:CD1 | 1:C:105:LEU:CD2 | 2.58 | 0.81 |
| 2:D:80:ASN:N | 2:D:80:ASN:CB | 2.40 | 0.81 |
| 2:B:121:GLU:OE2 | 2:B:121:GLU:CG | 2.27 | 0.81 |
| 1:C:23:GLU:OE2 | 1:C:23:GLU:CB | 2.29 | 0.81 |
| 1:A:21:ALA:CA | 1:A:22:GLY:N | 2.43 | 0.81 |
| 1:C:23:GLU:CG | 1:C:23:GLU:OE2 | 2.28 | 0.81 |
| 2:B:65:LYS:CG | 2:B:65:LYS:HB3 | 1.31 | 0.81 |
| 1:C:76:MET:CB | 1:C:76:MET:SD | 2.68 | 0.81 |
| 2:D:18:VAL:CG2 | 2:D:18:VAL:CA | 2.58 | 0.81 |
| 1:A:72:HIS:N | 1:A:72:HIS:CG | 2.48 | 0.81 |
| 2:B:65:LYS:CE | 2:B:65:LYS:CG | 2.58 | 0.81 |
| 1:A:92:ARG:HH21 | 1:A:92:ARG:CZ | 1.48 | 0.81 |
| 2:B:143:HIS:ND1 | 2:B:143:HIS:CB | 2.43 | 0.81 |
| 1:A:50:HIS:CB | 1:A:50:HIS:C | 2.50 | 0.81 |
| 1:A:92:ARG:HH22 | 1:A:92:ARG:CZ | 1.48 | 0.80 |
| 2:D:49:SER:O | 2:D:50:THR:HA | 1.81 | 0.80 |
| 1:C:139:LYS:CG | 1:C:139:LYS:CE | 2.56 | 0.80 |
| 2:B:12:THR:CB | 2:B:12:THR:HG22 | 1.28 | 0.80 |
| 1:A:76:MET:CB | 1:A:76:MET:SD | 2.66 | 0.80 |
| 2:B:65:LYS:CB | 2:B:65:LYS:CD | 2.59 | 0.80 |
| 2:D:43:GLU:CG | 2:D:43:GLU:HB2 | 1.29 | 0.80 |
| 2:B:8:LYS:HG2 | 2:B:8:LYS:CA | 2.09 | 0.80 |
| 2:D:45:PHE:O | 2:D:46:GLY:N | 2.14 | 0.80 |
| 1:C:73:VAL:CA | 1:C:73:VAL:CG2 | 2.59 | 0.80 |
| 2:D:43:GLU:HB3 | 2:D:43:GLU:CG | 1.29 | 0.80 |
| 2:D:55:MET:CA | 2:D:56:GLY:N | 2.43 | 0.80 |
| 1:A:1:VAL:CA | 1:A:1:VAL:HG22 | 2.12 | 0.80 |
| 1:C:1:VAL:HA | 1:C:1:VAL:CG2 | 2.12 | 0.80 |
| 1:A:138:SER:OG | 1:A:138:SER:HA | 1.81 | 0.79 |
| 2:D:59:LYS:CE | 2:D:59:LYS:CG | 2.52 | 0.79 |
| 2:D:20:VAL:CG2 | 2:D:20:VAL:HA | 2.13 | 0.79 |
| 4:A:142:HEM:O1A | 4:A:142:HEM:CBA | 2.31 | 0.79 |
| 1:A:74:ASP:OD2 | 1:A:74:ASP:OD1 | 2.00 | 0.79 |
| 2:B:146:HIS:CD2 | 2:B:146:HIS:CB | 2.66 | 0.79 |
| 1:A:81:SER:CB | 1:A:81:SER:N | 2.45 | 0.79 |
| 2:D:49:SER:O | 2:D:50:THR:CA | 2.31 | 0.79 |
| 2:D:82:LYS:HD2 | 2:D:82:LYS:NZ | 1.98 | 0.79 |
| 2:D:17:LYS:CD | 2:D:17:LYS:NZ | 2.46 | 0.79 |
| 1:C:61:LYS:CE | 1:C:61:LYS:CG | 2.59 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:12:THR:HG23 | 2:B:12:THR:CB | 1.28 | 0.79 |
| 2:D:8:LYS:CE | 2:D:8:LYS:CG | 2.59 | 0.78 |
| 2:D:50:THR:CB | 2:D:50:THR:C | 2.50 | 0.78 |
| 1:C:69:ALA:C | 1:C:70:VAL:CA | 2.50 | 0.78 |
| 2:B:2:HIS:ND1 | 2:B:2:HIS:CB | 2.44 | 0.78 |
| 2:B:2:HIS:CG | 2:B:2:HIS:CA | 2.65 | 0.78 |
| 1:C:70:VAL:O | 1:C:70:VAL:CA | 2.32 | 0.78 |
| 1:C:74:ASP:C | 1:C:75:ASP:CA | 2.51 | 0.78 |
| 2:B:59:LYS:CG | 2:B:59:LYS:CE | 2.61 | 0.78 |
| 2:B:65:LYS:HG3 | 2:B:65:LYS:C | 2.03 | 0.78 |
| 2:B:117:HIS:NE2 | 2:B:117:HIS:CG | 2.52 | 0.78 |
| 2:D:6:GLU:OE2 | 2:D:6:GLU:OE1 | 2.02 | 0.78 |
| 1:C:46:PHE:CD2 | 1:C:46:PHE:HE2 | 1.48 | 0.78 |
| 1:A:75:ASP:CB | 1:A:75:ASP:CG | 0.68 | 0.77 |
| 2:D:7:GLU:CA | 2:D:7:GLU:CG | 2.63 | 0.77 |
| 2:D:43:GLU:CG | 2:D:43:GLU:CB | 0.78 | 0.77 |
| 1:C:118:THR:CB | 1:C:118:THR:C | 2.52 | 0.77 |
| 2:D:11:VAL:C | 2:D:12:THR:CA | 2.52 | 0.77 |
| 2:B:87:THR:CB | 2:B:87:THR:C | 2.52 | 0.77 |
| 2:B:2:HIS:CD2 | 2:B:2:HIS:CE1 | 2.72 | 0.77 |
| 2:B:82:LYS:HE2 | 2:B:82:LYS:CB | 2.14 | 0.77 |
| 1:A:133:SER:O | 1:A:137:THR:HG22 | 1.85 | 0.77 |
| 1:C:92:ARG:NE | 1:C:92:ARG:NH2 | 2.27 | 0.76 |
| 2:D:132:LYS:NZ | 2:D:132:LYS:CE | 2.49 | 0.76 |
| 1:C:90:LYS:CG | 1:C:90:LYS:CE | 2.63 | 0.76 |
| 2:B:41:PHE:CA | 2:B:42:PHE:N | 2.46 | 0.76 |
| 2:B:41:PHE:O | 2:B:41:PHE:CA | 2.31 | 0.76 |
| 1:A:18:GLY:CA | 1:A:19:ALA:N | 2.49 | 0.76 |
| 4:D:148:HEM:CBD | 4:D:148:HEM:O1D | 2.34 | 0.76 |
| 2:B:80:ASN:O | 2:B:80:ASN:CA | 2.31 | 0.76 |
| 2:B:87:THR:OG1 | 2:B:87:THR:CA | 2.32 | 0.76 |
| 1:A:40:LYS:CA | 1:A:40:LYS:CG | 2.61 | 0.76 |
| 1:C:131:SER:O | 1:C:131:SER:CA | 2.34 | 0.76 |
| 1:A:2:LEU:O | 1:A:2:LEU:CA | 2.33 | 0.76 |
| 2:B:139:ASN:ND2 | 2:B:139:ASN:CB | 2.47 | 0.76 |
| 4:A:142:HEM:O2A | 4:A:142:HEM:CBA | 2.33 | 0.76 |
| 2:D:12:THR:HG22 | 2:D:12:THR:C | 2.07 | 0.76 |
| 2:B:121:GLU:CD | 2:B:121:GLU:CB | 2.52 | 0.76 |
| 1:A:40:LYS:CB | 1:A:40:LYS:C | 2.53 | 0.76 |
| 2:D:22:GLU:CB | 2:D:22:GLU:CG | 0.76 | 0.76 |
| 2:D:46:GLY:CA | 2:D:46:GLY:O | 2.33 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:61:LYS:CE | 2:B:61:LYS:CG | 2.64 | 0.76 |
| 2:B:139:ASN:CB | 2:B:139:ASN:CG | 0.66 | 0.76 |
| 1:A:92:ARG:HD3 | 1:A:92:ARG:CZ | 1.95 | 0.75 |
| 2:D:47:ASP:OD1 | 2:D:47:ASP:CB | 2.34 | 0.75 |
| 2:D:104:ARG:CG | 2:D:104:ARG:NE | 2.49 | 0.75 |
| 4:A:142:HEM:CBD | 4:A:142:HEM:O1D | 2.35 | 0.75 |
| 2:D:101:GLU:CG | 2:D:101:GLU:OE2 | 2.33 | 0.75 |
| 1:C:70:VAL:CB | 1:C:70:VAL:N | 2.49 | 0.75 |
| 1:A:17:VAL:CA | 1:A:17:VAL:O | 2.34 | 0.75 |
| 2:B:8:LYS:CB | 2:B:8:LYS:N | 2.49 | 0.75 |
| 2:B:43:GLU:O | 2:B:44:SER:C | 2.23 | 0.75 |
| 2:D:143:HIS:CB | 2:D:143:HIS:CD2 | 2.67 | 0.75 |
| 2:D:2:HIS:CG | 2:D:2:HIS:CA | 2.70 | 0.74 |
| 1:C:7:LYS:N | 1:C:7:LYS:CB | 2.49 | 0.74 |
| 4:B:148:HEM:CBD | 4:B:148:HEM:O1D | 2.35 | 0.74 |
| 1:C:99:LYS:CG | 1:C:99:LYS:CB | 0.74 | 0.74 |
| 1:C:30:GLU:OE1 | 1:C:30:GLU:CG | 2.35 | 0.74 |
| 2:D:22:GLU:HG3 | 2:D:22:GLU:C | 2.09 | 0.73 |
| 2:D:82:LYS:HZ2 | 2:D:82:LYS:CD | 1.99 | 0.73 |
| 2:B:7:GLU:CB | 2:B:7:GLU:CD | 2.56 | 0.73 |
| 2:D:113:VAL:CG2 | 2:D:113:VAL:CA | 2.65 | 0.73 |
| 1:C:2:LEU:CA | 1:C:2:LEU:O | 2.36 | 0.73 |
| 2:B:49:SER:O | 2:B:50:THR:N | 2.19 | 0.73 |
| 1:C:54:GLN:CA | 1:C:55:VAL:N | 2.51 | 0.73 |
| 2:D:95:LYS:CD | 2:D:95:LYS:CB | 2.67 | 0.73 |
| 2:D:78:LEU:N | 2:D:78:LEU:CB | 2.49 | 0.73 |
| 1:A:11:LYS:CE | 1:A:11:LYS:CG | 2.64 | 0.73 |
| 1:A:50:HIS:CG | 1:A:50:HIS:CA | 2.68 | 0.73 |
| 2:D:7:GLU:CB | 2:D:7:GLU:C | 2.57 | 0.73 |
| 2:D:73:ASP:OD2 | 2:D:73:ASP:CG | 2.26 | 0.73 |
| 2:B:12:THR:HB | 2:B:12:THR:HG21 | 0.75 | 0.73 |
| 1:A:81:SER:CA | 1:A:81:SER:OG | 2.35 | 0.73 |
| 2:B:43:GLU:OE2 | 2:B:43:GLU:CG | 2.36 | 0.73 |
| 2:B:5:PRO:C | 2:B:5:PRO:CB | 2.54 | 0.73 |
| 1:A:74:ASP:OD1 | 1:A:74:ASP:CB | 2.37 | 0.73 |
| 2:B:61:LYS:CB | 2:B:61:LYS:CD | 2.62 | 0.73 |
| 2:D:7:GLU:CA | 2:D:7:GLU:O | 2.38 | 0.72 |
| 1:C:10:VAL:CA | 1:C:11:LYS:N | 2.52 | 0.72 |
| 1:A:56:LYS:CD | 1:A:56:LYS:NZ | 2.52 | 0.72 |
| 1:A:1:VAL:CG2 | 1:A:1:VAL:H1 | 1.99 | 0.72 |
| 2:D:47:ASP:HB3 | 2:D:47:ASP:N | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:12:THR:HG21 | 2:B:12:THR:CB | 1.28 | 0.72 |
| 2:B:6:GLU:C | 2:B:6:GLU:CB | 2.58 | 0.72 |
| 2:B:7:GLU:HA | 2:B:7:GLU:CG | 2.19 | 0.72 |
| 2:D:82:LYS:CD | 2:D:82:LYS:HZ3 | 1.99 | 0.72 |
| 1:C:75:ASP:C | 1:C:75:ASP:N | 2.43 | 0.72 |
| 1:A:84:SER:CB | 1:A:84:SER:C | 2.57 | 0.72 |
| 1:C:16:LYS:N | 1:C:16:LYS:C | 2.43 | 0.72 |
| 4:B:148:HEM:O2D | 4:B:148:HEM:CBD | 2.38 | 0.72 |
| 2:D:131:GLN:CG | 2:D:131:GLN:NE2 | 2.49 | 0.72 |
| 2:D:79:ASP:CB | 2:D:79:ASP:OD2 | 2.37 | 0.72 |
| 1:C:116:GLU:CB | 1:C:116:GLU:CD | 2.57 | 0.71 |
| 1:C:16:LYS:HB3 | 1:C:16:LYS:HD3 | 1.70 | 0.71 |
| 2:D:50:THR:CB | 2:D:50:THR:N | 2.53 | 0.71 |
| 2:D:12:THR:CG2 | 2:D:12:THR:C | 2.58 | 0.71 |
| 2:D:22:GLU:CA | 2:D:23:VAL:N | 2.53 | 0.71 |
| 2:D:104:ARG:NH1 | 2:D:104:ARG:CD | 2.52 | 0.71 |
| 2:D:132:LYS:CD | 2:D:132:LYS:NZ | 2.53 | 0.71 |
| 2:B:146:HIS:CG | 2:B:146:HIS:CA | 2.73 | 0.71 |
| 2:B:59:LYS:CD | 2:B:59:LYS:NZ | 2.53 | 0.71 |
| 2:D:7:GLU:CA | 2:D:8:LYS:N | 2.49 | 0.71 |
| 2:D:45:PHE:O | 2:D:46:GLY:HA3 | 1.90 | 0.71 |
| 2:B:145:TYR:O | 2:B:145:TYR:CA | 2.38 | 0.71 |
| 1:A:127:LYS:CB | 1:A:127:LYS:CG | 0.71 | 0.71 |
| 2:B:2:HIS:CG | 2:B:2:HIS:CE1 | 2.77 | 0.71 |
| 1:C:92:ARG:CD | 1:C:92:ARG:NH2 | 2.52 | 0.71 |
| 2:D:10:ALA:C | 2:D:10:ALA:HB3 | 2.08 | 0.71 |
| 1:C:75:ASP:CB | 1:C:75:ASP:N | 2.54 | 0.71 |
| 2:B:146:HIS:CB | 2:B:146:HIS:ND1 | 2.42 | 0.71 |
| 2:D:1:VAL:HB | 2:D:2:HIS:N | 2.06 | 0.71 |
| 2:B:49:SER:OG | 2:B:49:SER:C | 2.29 | 0.71 |
| 1:C:2:LEU:CB | 1:C:2:LEU:C | 2.57 | 0.71 |
| 2:B:74:GLY:CA | 2:B:75:LEU:N | 2.51 | 0.71 |
| 1:A:87:HIS:CB | 1:A:87:HIS:C | 2.60 | 0.70 |
| 1:A:50:HIS:CG | 1:A:50:HIS:C | 2.64 | 0.70 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:C | 2.59 | 0.70 |
| 1:A:52:SER:N | 1:A:52:SER:CB | 2.54 | 0.70 |
| 2:D:43:GLU:CA | 2:D:44:SER:N | 2.53 | 0.70 |
| 1:A:87:HIS:CA | 1:A:88:ALA:N | 2.50 | 0.70 |
| 2:D:59:LYS:CB | 2:D:59:LYS:C | 2.57 | 0.70 |
| 1:C:16:LYS:HA | 1:C:16:LYS:CG | 2.22 | 0.70 |
| 4:C:142:HEM:O1D | 4:C:142:HEM:CBD | 2.33 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:82:ALA:C | 1:C:83:LEU:CA | 2.58 | 0.70 |
| 2:B:6:GLU:C | 2:B:6:GLU:N | 2.43 | 0.70 |
| 2:B:82:LYS:CE | 2:B:82:LYS:CD | 0.70 | 0.70 |
| 2:D:49:SER:CA | 2:D:50:THR:N | 2.52 | 0.70 |
| 1:C:30:GLU:CD | 1:C:50:HIS:HD2 | 1.94 | 0.70 |
| 1:A:85:ASP:OD2 | 1:A:85:ASP:OD1 | 2.10 | 0.70 |
| 2:B:5:PRO:N | 2:B:6:GLU:N | 2.40 | 0.70 |
| 2:D:8:LYS:CB | 2:D:8:LYS:N | 2.55 | 0.70 |
| 2:D:123:THR:CG2 | 2:D:123:THR:CA | 2.70 | 0.70 |
| 2:D:17:LYS:HD3 | 2:D:17:LYS:NZ | 2.07 | 0.69 |
| 1:C:40:LYS:NZ | 1:C:40:LYS:HD2 | 2.01 | 0.69 |
| 2:D:8:LYS:HD3 | 2:D:8:LYS:CB | 2.21 | 0.69 |
| 2:D:12:THR:CA | 2:D:12:THR:OG1 | 2.40 | 0.69 |
| 2:D:73:ASP:OD2 | 5:D:174:HOH:O | 2.10 | 0.69 |
| 1:A:137:THR:HG22 | 1:A:137:THR:OG1 | 1.93 | 0.69 |
| 2:B:2:HIS:C | 2:B:2:HIS:CG | 2.66 | 0.69 |
| 2:B:8:LYS:HG2 | 2:B:8:LYS:C | 2.12 | 0.69 |
| 2:D:47:ASP:CA | 2:D:48:LEU:N | 2.55 | 0.69 |
| 2:D:141:LEU:CD2 | 2:D:141:LEU:HD13 | 2.20 | 0.69 |
| 2:B:90:GLU:CG | 2:B:90:GLU:OE1 | 2.38 | 0.69 |
| 2:B:145:TYR:CB | 2:B:145:TYR:C | 2.55 | 0.69 |
| 1:C:56:LYS:CD | 1:C:56:LYS:NZ | 2.56 | 0.69 |
| 1:A:92:ARG:NH2 | 1:A:92:ARG:CD | 2.56 | 0.69 |
| 2:D:139:ASN:HB3 | 2:D:139:ASN:OD1 | 1.91 | 0.69 |
| 2:D:4:THR:O | 2:D:5:PRO:CA | 2.40 | 0.69 |
| 1:A:127:LYS:HA | 1:A:127:LYS:CG | 2.15 | 0.69 |
| 1:C:1:VAL:CA | 1:C:2:LEU:N | 2.55 | 0.68 |
| 1:C:56:LYS:CD | 1:C:56:LYS:CB | 2.70 | 0.68 |
| 2:D:121:GLU:OE2 | 2:D:121:GLU:CG | 2.42 | 0.68 |
| 1:A:29:LEU:CA | 1:A:29:LEU:CG | 2.70 | 0.68 |
| 1:C:1:VAL:HG12 | 1:C:1:VAL:C | 2.12 | 0.68 |
| 1:A:11:LYS:NZ | 1:A:11:LYS:CD | 2.56 | 0.68 |
| 2:D:78:LEU:C | 2:D:78:LEU:CB | 2.58 | 0.68 |
| 2:B:52:ASP:OD2 | 2:B:52:ASP:CB | 2.41 | 0.68 |
| 1:A:78:ASN:ND2 | 1:A:78:ASN:OD1 | 2.27 | 0.68 |
| 2:B:143:HIS:C | 2:B:143:HIS:CB | 2.60 | 0.68 |
| 2:B:117:HIS:CE1 | 2:B:117:HIS:CG | 2.82 | 0.68 |
| 1:A:74:ASP:CG | 1:A:74:ASP:CA | 2.60 | 0.68 |
| 2:B:3:LEU:CB | 2:B:3:LEU:C | 2.61 | 0.68 |
| 2:B:65:LYS:CG | 2:B:65:LYS:C | 2.60 | 0.68 |
| 2:B:49:SER:CB | 2:B:49:SER:N | 2.57 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:16:LYS:CB | 1:C:16:LYS:HD3 | 2.23 | 0.68 |
| 1:C:138:SER:CA | 1:C:138:SER:HG | 2.05 | 0.68 |
| 1:C:131:SER:CB | 1:C:131:SER:C | 2.61 | 0.68 |
| 1:A:5:ALA:CB | 1:A:5:ALA:C | 2.62 | 0.67 |
| 1:C:118:THR:HB | 1:C:118:THR:CA | 2.16 | 0.67 |
| 2:B:1:VAL:CA | 2:B:1:VAL:CG2 | 2.64 | 0.67 |
| 1:A:139:LYS:CD | 1:A:139:LYS:NZ | 2.57 | 0.67 |
| 2:D:24:GLY:CA | 2:D:68:LEU:HD22 | 2.24 | 0.67 |
| 4:C:142:HEM:CBD | 4:C:142:HEM:O2D | 2.35 | 0.67 |
| 2:B:9:SER:CA | 2:B:10:ALA:N | 2.56 | 0.67 |
| 2:B:74:GLY:O | 2:B:75:LEU:N | 2.28 | 0.67 |
| 2:D:1:VAL:CB | 2:D:2:HIS:N | 2.58 | 0.67 |
| 1:C:113:LEU:CD1 | 1:C:113:LEU:HB3 | 2.21 | 0.67 |
| 1:C:48:LEU:CD2 | 1:C:48:LEU:CB | 2.66 | 0.67 |
| 2:B:65:LYS:CE | 2:B:65:LYS:HG3 | 2.24 | 0.67 |
| 1:C:38:THR:OG1 | 1:C:38:THR:CA | 2.42 | 0.67 |
| 2:D:104:ARG:CZ | 2:D:104:ARG:NE | 2.58 | 0.67 |
| 2:D:20:VAL:HG12 | 2:D:20:VAL:HA | 1.73 | 0.67 |
| 2:D:123:THR:OG1 | 2:D:123:THR:CG2 | 2.42 | 0.67 |
| 1:C:113:LEU:HD22 | 1:C:116:GLU:HG3 | 1.77 | 0.66 |
| 1:C:61:LYS:CB | 1:C:61:LYS:C | 2.60 | 0.66 |
| 2:D:82:LYS:CE | 2:D:82:LYS:CG | 2.73 | 0.66 |
| 2:D:82:LYS:CB | 2:D:82:LYS:CD | 2.68 | 0.66 |
| 2:D:24:GLY:HA2 | 2:D:68:LEU:HD22 | 1.76 | 0.66 |
| 2:D:65:LYS:NZ | 2:D:65:LYS:CD | 2.59 | 0.66 |
| 1:A:127:LYS:HG3 | 1:A:127:LYS:HA | 1.77 | 0.66 |
| 2:D:101:GLU:CG | 2:D:101:GLU:OE1 | 2.43 | 0.66 |
| 1:C:54:GLN:CB | 1:C:54:GLN:C | 2.59 | 0.66 |
| 2:D:79:ASP:N | 2:D:80:ASN:N | 2.43 | 0.66 |
| 2:D:43:GLU:HG3 | 2:D:43:GLU:HB2 | 1.34 | 0.66 |
| 2:D:55:MET:CA | 2:D:55:MET:O | 2.42 | 0.66 |
| 2:B:6:GLU:CA | 2:B:7:GLU:N | 2.54 | 0.66 |
| 2:D:43:GLU:HB3 | 2:D:43:GLU:OE1 | 1.95 | 0.66 |
| 2:B:50:THR:CG2 | 2:B:50:THR:OG1 | 2.43 | 0.66 |
| 2:B:65:LYS:CE | 2:B:65:LYS:NZ | 2.59 | 0.66 |
| 1:C:10:VAL:C | 1:C:10:VAL:CB | 2.65 | 0.66 |
| 1:C:135:VAL:O | 1:C:138:SER:HB2 | 1.95 | 0.66 |
| 2:D:92:HIS:CA | 2:D:92:HIS:O | 2.40 | 0.66 |
| 1:C:6:ASP:C | 1:C:7:LYS:CA | 2.62 | 0.66 |
| 2:D:26:GLU:OE2 | 2:D:26:GLU:CB | 2.43 | 0.66 |
| 2:B:12:THR:CA | 2:B:12:THR:HG23 | 1.88 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:44:PRO:CA | 1:A:45:HIS:N | 2.55 | 0.66 |
| 1:A:75:ASP:CB | 1:A:75:ASP:OD1 | 2.44 | 0.66 |
| 1:A:92:ARG:NE | 1:A:92:ARG:CZ | 2.57 | 0.66 |
| 1:A:30:GLU:CD | 1:A:30:GLU:CB | 2.63 | 0.65 |
| 2:D:92:HIS:C | 2:D:92:HIS:N | 2.49 | 0.65 |
| 2:D:8:LYS:CB | 2:D:8:LYS:C | 2.61 | 0.65 |
| 2:D:48:LEU:CD2 | 2:D:48:LEU:CD1 | 2.72 | 0.65 |
| 1:C:38:THR:N | 1:C:38:THR:CB | 2.56 | 0.65 |
| 2:D:1:VAL:CA | 2:D:2:HIS:H | 2.07 | 0.65 |
| 1:A:15:GLY:O | 1:A:16:LYS:N | 2.19 | 0.65 |
| 1:A:62:VAL:CB | 1:A:62:VAL:C | 2.63 | 0.65 |
| 4:C:142:HEM:HBB2 | 4:C:142:HEM:CMB | 2.25 | 0.65 |
| 2:D:78:LEU:CG | 2:D:78:LEU:HD23 | 1.51 | 0.65 |
| 1:C:23:GLU:OE2 | 1:C:23:GLU:HB2 | 1.96 | 0.65 |
| 2:B:82:LYS:NZ | 2:B:82:LYS:CD | 2.59 | 0.65 |
| 2:B:108:ASN:CA | 2:B:108:ASN:CG | 2.64 | 0.65 |
| 2:B:21:ASP:CB | 2:B:21:ASP:OD1 | 2.42 | 0.64 |
| 2:D:8:LYS:C | 2:D:8:LYS:CG | 2.65 | 0.64 |
| 1:C:92:ARG:HD2 | 1:C:92:ARG:NH1 | 2.12 | 0.64 |
| 1:C:27:GLU:OE2 | 1:C:112:HIS:HE1 | 1.80 | 0.64 |
| 2:B:104:ARG:NE | 2:B:104:ARG:CG | 2.60 | 0.64 |
| 2:D:131:GLN:CG | 2:D:131:GLN:OE1 | 2.39 | 0.64 |
| 1:A:137:THR:CB | 1:A:137:THR:C | 2.64 | 0.64 |
| 1:A:21:ALA:O | 1:A:21:ALA:CA | 2.44 | 0.64 |
| 2:B:57:ASN:C | 2:B:58:PRO:CD | 2.64 | 0.64 |
| 2:D:80:ASN:CB | 2:D:80:ASN:OD1 | 2.39 | 0.64 |
| 1:A:127:LYS:HE2 | 1:A:127:LYS:CG | 2.27 | 0.64 |
| 1:C:7:LYS:HE3 | 1:C:7:LYS:CG | 2.27 | 0.64 |
| 1:A:1:VAL:CG2 | 1:A:1:VAL:H3 | 1.89 | 0.64 |
| 1:C:1:VAL:H1 | 1:C:1:VAL:HB | 1.63 | 0.64 |
| 1:C:105:LEU:HD13 | 1:C:105:LEU:CD2 | 2.28 | 0.63 |
| 2:D:65:LYS:CG | 2:D:65:LYS:CE | 2.77 | 0.63 |
| 4:C:142:HEM:HBB2 | 4:C:142:HEM:HMB1 | 1.80 | 0.63 |
| 1:C:1:VAL:CG1 | 1:C:1:VAL:HA | 2.23 | 0.63 |
| 2:D:46:GLY:CA | 2:D:47:ASP:N | 2.60 | 0.63 |
| 1:C:60:LYS:NZ | 1:C:60:LYS:HD3 | 2.13 | 0.63 |
| 2:D:67:VAL:C | 2:D:67:VAL:CG1 | 2.66 | 0.63 |
| 2:B:80:ASN:N | 2:B:80:ASN:CB | 2.57 | 0.63 |
| 1:A:90:LYS:NZ | 1:A:90:LYS:CD | 2.62 | 0.63 |
| 2:B:48:LEU:O | 2:B:49:SER:CA | 2.47 | 0.63 |
| 2:B:52:ASP:CA | 2:B:52:ASP:CG | 2.64 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:52:ASP:HB2 | 2:D:52:ASP:N | 2.12 | 0.63 |
| 1:C:87:HIS:CB | 1:C:87:HIS:C | 2.66 | 0.63 |
| 2:B:82:LYS:CE | 2:B:82:LYS:HG2 | 2.20 | 0.63 |
| 2:D:2:HIS:CG | 2:D:2:HIS:NE2 | 2.67 | 0.63 |
| 2:B:90:GLU:C | 2:B:90:GLU:CB | 2.67 | 0.62 |
| 2:B:142:ALA:CA | 2:B:143:HIS:N | 2.54 | 0.62 |
| 1:C:87:HIS:CA | 1:C:88:ALA:N | 2.61 | 0.62 |
| 2:D:58:PRO:CG | 2:D:58:PRO:HD3 | 1.11 | 0.62 |
| 2:D:104:ARG:HD2 | 2:D:104:ARG:NH1 | 2.10 | 0.62 |
| 2:D:5:PRO:C | 2:D:5:PRO:CB | 2.68 | 0.62 |
| 2:D:12:THR:N | 2:D:12:THR:C | 2.49 | 0.62 |
| 1:C:73:VAL:HG12 | 1:C:73:VAL:H | 1.64 | 0.62 |
| 2:B:80:ASN:CG | 2:B:80:ASN:CA | 2.62 | 0.62 |
| 1:C:61:LYS:CA | 1:C:62:VAL:N | 2.62 | 0.62 |
| 2:D:4:THR:CA | 2:D:4:THR:OG1 | 2.46 | 0.62 |
| 2:D:76:ALA:N | 2:D:76:ALA:HB2 | 2.13 | 0.62 |
| 1:A:40:LYS:CB | 1:A:40:LYS:N | 2.59 | 0.62 |
| 2:B:65:LYS:HE2 | 2:B:65:LYS:HG3 | 1.82 | 0.62 |
| 2:D:58:PRO:HD2 | 2:D:58:PRO:CG | 1.11 | 0.62 |
| 2:D:6:GLU:CD | 2:D:6:GLU:CB | 2.67 | 0.62 |
| 2:D:53:ALA:CA | 2:D:54:VAL:N | 2.63 | 0.62 |
| 1:A:81:SER:CB | 1:A:81:SER:C | 2.66 | 0.61 |
| 1:C:137:THR:O | 1:C:137:THR:CA | 2.42 | 0.61 |
| 1:C:23:GLU:CD | 1:C:23:GLU:OE1 | 2.37 | 0.61 |
| 1:C:113:LEU:CD1 | 1:C:113:LEU:HB2 | 2.28 | 0.61 |
| 1:A:58:HIS:O | 1:A:58:HIS:CA | 2.45 | 0.61 |
| 2:B:12:THR:CA | 2:B:12:THR:HG22 | 1.88 | 0.61 |
| 2:B:80:ASN:HA | 2:B:80:ASN:OD1 | 2.00 | 0.61 |
| 2:D:76:ALA:N | 2:D:76:ALA:HB3 | 2.13 | 0.61 |
| 2:D:141:LEU:HD22 | 2:D:141:LEU:HD13 | 1.82 | 0.61 |
| 2:D:94:ASP:C | 2:D:94:ASP:N | 2.50 | 0.61 |
| 2:D:59:LYS:CD | 2:D:59:LYS:NZ | 2.63 | 0.61 |
| 4:C:142:HEM:O1A | 4:C:142:HEM:CBA | 2.48 | 0.61 |
| 2:D:19:ASN:ND2 | 2:D:19:ASN:CB | 2.63 | 0.61 |
| 1:A:99:LYS:HG3 | 1:A:99:LYS:CE | 2.29 | 0.61 |
| 2:D:121:GLU:CB | 2:D:121:GLU:C | 2.68 | 0.61 |
| 1:C:105:LEU:HB2 | 1:C:105:LEU:CD2 | 2.29 | 0.61 |
| 2:B:41:PHE:C | 2:B:41:PHE:CB | 2.67 | 0.61 |
| 1:A:16:LYS:CB | 1:A:16:LYS:CD | 2.78 | 0.61 |
| 2:D:21:ASP:OD2 | 2:D:21:ASP:CB | 2.42 | 0.60 |
| 2:B:82:LYS:HB3 | 2:B:82:LYS:HE2 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:D:8:LYS:CA | 2:D:8:LYS:HG3 | 2.26 | 0.60 |
| 1:A:17:VAL:N | 1:A:18:GLY:N | 2.48 | 0.60 |
| 2:B:80:ASN:C | 2:B:80:ASN:N | 2.55 | 0.60 |
| 2:D:12:THR:C | 2:D:12:THR:CB | 2.66 | 0.60 |
| 4:C:142:HEM:CGD | 4:C:142:HEM:CAD | 2.73 | 0.60 |
| 2:B:66:LYS:CE | 2:B:66:LYS:HG3 | 2.31 | 0.60 |
| 2:B:6:GLU:OE1 | 2:B:6:GLU:OE2 | 2.09 | 0.60 |
| 2:D:77:HIS:CE1 | 2:D:77:HIS:CD2 | 2.70 | 0.60 |
| 1:C:82:ALA:CA | 1:C:83:LEU:N | 2.58 | 0.60 |
| 1:C:73:VAL:HG12 | 1:C:73:VAL:CA | 2.30 | 0.60 |
| 1:A:75:ASP:CB | 1:A:75:ASP:N | 2.64 | 0.60 |
| 1:C:92:ARG:HH11 | 1:C:92:ARG:HD2 | 1.65 | 0.60 |
| 1:C:56:LYS:CD | 1:C:56:LYS:HB3 | 2.32 | 0.59 |
| 2:B:63:HIS:HE1 | 4:B:148:HEM:C4D | 2.20 | 0.59 |
| 2:B:65:LYS:CB | 2:B:65:LYS:C | 2.66 | 0.59 |
| 2:B:66:LYS:CE | 2:B:66:LYS:CG | 2.80 | 0.59 |
| 2:D:4:THR:OG1 | 2:D:6:GLU:OE2 | 2.19 | 0.59 |
| 2:B:80:ASN:CB | 2:B:80:ASN:OD1 | 2.50 | 0.59 |
| 1:A:127:LYS:HB3 | 1:A:127:LYS:CD | 2.28 | 0.59 |
| 2:D:20:VAL:HA | 2:D:20:VAL:HG22 | 1.84 | 0.59 |
| 1:C:8:THR:OG1 | 1:C:8:THR:CA | 2.46 | 0.59 |
| 1:A:137:THR:HG1 | 1:A:137:THR:CB | 2.10 | 0.58 |
| 1:A:16:LYS:CE | 1:A:16:LYS:HG2 | 2.22 | 0.58 |
| 2:D:132:LYS:NZ | 2:D:132:LYS:HD3 | 2.18 | 0.58 |
| 2:D:1:VAL:HB | 2:D:2:HIS:H | 1.67 | 0.58 |
| 1:A:52:SER:N | 1:A:52:SER:C | 2.46 | 0.58 |
| 1:C:138:SER:OG | 1:C:138:SER:HA | 1.96 | 0.58 |
| 2:D:7:GLU:N | 2:D:7:GLU:C | 2.55 | 0.58 |
| 1:A:90:LYS:NZ | 1:A:90:LYS:CE | 2.67 | 0.58 |
| 2:D:76:ALA:CB | 2:D:76:ALA:H | 2.12 | 0.58 |
| 2:B:65:LYS:CB | 2:B:65:LYS:CG | 0.58 | 0.58 |
| 2:B:12:THR:CG2 | 2:B:12:THR:CB | 0.58 | 0.58 |
| 1:A:62:VAL:CA | 1:A:62:VAL:O | 2.44 | 0.58 |
| 2:B:26:GLU:OE2 | 2:B:26:GLU:CB | 2.52 | 0.58 |
| 2:D:10:ALA:C | 2:D:10:ALA:N | 2.57 | 0.57 |
| 1:C:137:THR:CA | 1:C:138:SER:N | 2.58 | 0.57 |
| 2:D:52:ASP:C | 2:D:52:ASP:N | 2.56 | 0.57 |
| 1:C:73:VAL:HG12 | 1:C:73:VAL:N | 2.19 | 0.57 |
| 2:B:9:SER:C | 2:B:9:SER:OG | 2.43 | 0.57 |
| 2:D:79:ASP:O | 2:D:80:ASN:CA | 2.51 | 0.57 |
| 1:A:75:ASP:CB | 1:A:75:ASP:O | 2.53 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:73:VAL:HG13 | 1:C:73:VAL:CA | 2.30 | 0.57 |
| 2:D:79:ASP:C | 2:D:79:ASP:HB2 | 2.25 | 0.57 |
| 2:B:77:HIS:CB | 2:B:77:HIS:CD2 | 2.84 | 0.57 |
| 2:B:142:ALA:N | 2:B:142:ALA:C | 2.54 | 0.57 |
| 2:B:90:GLU:CB | 2:B:90:GLU:CD | 2.69 | 0.57 |
| 2:B:2:HIS:N | 2:B:2:HIS:CB | 2.66 | 0.57 |
| 2:D:78:LEU:HD21 | 2:D:78:LEU:CD1 | 2.19 | 0.56 |
| 1:C:16:LYS:CD | 1:C:16:LYS:NZ | 2.68 | 0.56 |
| 2:B:146:HIS:CG | 2:B:146:HIS:C | 2.79 | 0.56 |
| 1:C:2:LEU:N | 1:C:2:LEU:C | 2.54 | 0.56 |
| 2:D:90:GLU:CG | 2:D:90:GLU:OE1 | 2.53 | 0.56 |
| 2:B:143:HIS:CA | 2:B:144:LYS:N | 2.62 | 0.56 |
| 2:D:21:ASP:OD1 | 2:D:65:LYS:HG3 | 2.06 | 0.56 |
| 2:B:90:GLU:N | 2:B:90:GLU:CG | 2.68 | 0.56 |
| 1:A:87:HIS:CA | 1:A:87:HIS:O | 2.44 | 0.56 |
| 1:A:60:LYS:NZ | 1:A:60:LYS:CE | 2.68 | 0.56 |
| 1:C:92:ARG:HD2 | 1:C:92:ARG:HH21 | 1.68 | 0.56 |
| 2:D:51:PRO:C | 2:D:52:ASP:CA | 2.71 | 0.56 |
| 2:D:52:ASP:OD2 | 2:D:52:ASP:CG | 2.44 | 0.56 |
| 1:A:14:TRP:CB | 1:A:14:TRP:N | 2.63 | 0.56 |
| 2:D:22:GLU:N | 2:D:22:GLU:C | 2.53 | 0.55 |
| 2:D:82:LYS:HZ2 | 2:D:82:LYS:HD2 | 1.62 | 0.55 |
| 1:A:75:ASP:C | 1:A:75:ASP:CG | 2.65 | 0.55 |
| 1:C:47:ASP:OD1 | 1:C:47:ASP:C | 2.44 | 0.55 |
| 2:D:50:THR:CG2 | 2:D:50:THR:CA | 2.81 | 0.55 |
| 1:C:118:THR:HG23 | 1:C:121:VAL:H | 1.71 | 0.55 |
| 1:C:78:ASN:CB | 1:C:78:ASN:OD1 | 2.48 | 0.55 |
| 1:C:7:LYS:HE2 | 1:C:7:LYS:CG | 2.34 | 0.55 |
| 2:D:47:ASP:CG | 2:D:47:ASP:CA | 2.74 | 0.55 |
| 1:C:118:THR:CA | 1:C:118:THR:CG2 | 2.59 | 0.55 |
| 2:D:43:GLU:HB2 | 2:D:44:SER:N | 2.16 | 0.55 |
| 1:C:114:PRO:C | 1:C:114:PRO:N | 2.60 | 0.55 |
| 2:B:4:THR:C | 2:B:5:PRO:CD | 2.73 | 0.55 |
| 2:B:143:HIS:HB3 | 2:B:143:HIS:ND1 | 2.21 | 0.55 |
| 2:B:12:THR:CG2 | 2:B:12:THR:HB | 1.04 | 0.55 |
| 2:D:47:ASP:N | 2:D:47:ASP:C | 2.60 | 0.54 |
| 1:C:131:SER:CA | 1:C:132:VAL:N | 2.60 | 0.54 |
| 2:D:79:ASP:N | 2:D:80:ASN:H | 2.04 | 0.54 |
| 2:B:26:GLU:OE2 | 2:B:26:GLU:CD | 2.43 | 0.54 |
| 1:A:15:GLY:CA | 1:A:15:GLY:O | 2.56 | 0.54 |
| 1:C:84:SER:HB2 | 1:C:139:LYS:HD2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:75:ASP:O | 1:A:75:ASP:HB3 | 2.07 | 0.54 |
| 2:D:58:PRO:HG2 | 2:D:58:PRO:CD | 1.03 | 0.54 |
| 2:B:81:LEU:N | 2:B:81:LEU:HB2 | 2.18 | 0.54 |
| 2:B:21:ASP:CB | 2:B:21:ASP:OD2 | 2.56 | 0.54 |
| 2:D:104:ARG:HH21 | 2:D:104:ARG:NE | 2.06 | 0.54 |
| 1:C:40:LYS:HZ3 | 1:C:40:LYS:HD3 | 1.72 | 0.54 |
| 2:D:121:GLU:N | 2:D:121:GLU:CB | 2.60 | 0.54 |
| 2:D:18:VAL:N | 2:D:18:VAL:CB | 2.54 | 0.54 |
| 4:A:142:HEM:CGA | 4:A:142:HEM:CAA | 2.82 | 0.54 |
| 2:B:2:HIS:ND1 | 2:B:2:HIS:HB3 | 2.20 | 0.54 |
| 1:A:64:ASP:CB | 1:A:64:ASP:OD2 | 2.51 | 0.54 |
| 2:D:18:VAL:HG11 | 2:D:18:VAL:CG2 | 2.37 | 0.54 |
| 2:B:41:PHE:C | 2:B:41:PHE:N | 2.57 | 0.54 |
| 2:B:108:ASN:HB2 | 2:B:108:ASN:HD22 | 1.70 | 0.54 |
| 1:A:20:HIS:O | 1:A:21:ALA:C | 2.46 | 0.54 |
| 1:C:61:LYS:HD2 | 1:C:61:LYS:NZ | 2.19 | 0.53 |
| 1:C:8:THR:CB | 1:C:8:THR:C | 2.67 | 0.53 |
| 2:D:3:LEU:O | 2:D:4:THR:CA | 2.55 | 0.53 |
| 1:C:8:THR:CB | 1:C:8:THR:N | 2.67 | 0.53 |
| 1:C:90:LYS:CD | 1:C:90:LYS:NZ | 2.71 | 0.53 |
| 1:A:1:VAL:HG22 | 1:A:1:VAL:H1 | 1.70 | 0.53 |
| 2:D:59:LYS:CE | 2:D:59:LYS:HG2 | 2.38 | 0.53 |
| 1:C:76:MET:CG | 1:C:76:MET:CE | 2.81 | 0.53 |
| 2:B:3:LEU:CG | 2:B:3:LEU:CA | 2.81 | 0.53 |
| 2:D:126:VAL:N | 2:D:126:VAL:CB | 2.65 | 0.53 |
| 2:B:124:PRO:C | 2:B:125:PRO:CD | 2.60 | 0.53 |
| 2:B:142:ALA:CA | 2:B:142:ALA:O | 2.55 | 0.53 |
| 1:C:73:VAL:CG1 | 1:C:73:VAL:N | 2.68 | 0.53 |
| 2:B:90:GLU:HG3 | 2:B:90:GLU:H | 1.72 | 0.53 |
| 2:D:73:ASP:O | 2:D:76:ALA:HB3 | 2.08 | 0.53 |
| 2:B:101:GLU:CD | 2:B:101:GLU:CB | 2.75 | 0.53 |
| 2:D:121:GLU:CA | 2:D:121:GLU:HG3 | 2.37 | 0.53 |
| 2:B:47:ASP:HB3 | 2:B:47:ASP:C | 2.29 | 0.53 |
| 2:D:2:HIS:ND1 | 2:D:2:HIS:NE2 | 2.57 | 0.53 |
| 1:C:139:LYS:CD | 1:C:139:LYS:HZ3 | 2.15 | 0.53 |
| 2:D:102:ASN:HB3 | 4:D:148:HEM:HMC1 | 1.90 | 0.53 |
| 2:B:79:ASP:CA | 2:B:79:ASP:OD2 | 2.56 | 0.52 |
| 1:A:23:GLU:CG | 1:A:23:GLU:OE1 | 2.57 | 0.52 |
| 2:D:92:HIS:HB3 | 2:D:92:HIS:C | 2.29 | 0.52 |
| 2:D:79:ASP:O | 2:D:80:ASN:HA | 2.10 | 0.52 |
| 2:B:41:PHE:N | 2:B:42:PHE:N | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:81:SER:H | 1:A:81:SER:CB | 2.22 | 0.52 |
| 1:A:14:TRP:HA | 1:A:14:TRP:CG | 2.34 | 0.52 |
| 2:D:67:VAL:C | 2:D:67:VAL:HG12 | 2.29 | 0.52 |
| 2:D:58:PRO:CD | 2:D:58:PRO:HG3 | 1.03 | 0.52 |
| 2:B:8:LYS:C | 2:B:8:LYS:CG | 2.70 | 0.52 |
| 1:C:92:ARG:HD2 | 1:C:92:ARG:CZ | 2.40 | 0.52 |
| 2:D:90:GLU:CB | 2:D:90:GLU:OE2 | 2.58 | 0.52 |
| 2:D:95:LYS:HA | 2:D:95:LYS:HD3 | 1.91 | 0.52 |
| 1:A:61:LYS:HE2 | 1:A:61:LYS:CG | 2.11 | 0.52 |
| 4:D:148:HEM:CAA | 4:D:148:HEM:O1A | 2.56 | 0.52 |
| 2:B:1:VAL:CA | 2:B:1:VAL:CG1 | 2.88 | 0.52 |
| 2:D:65:LYS:HB3 | 2:D:65:LYS:CD | 2.36 | 0.52 |
| 2:B:22:GLU:OE2 | 2:B:22:GLU:OE1 | 2.28 | 0.52 |
| 2:B:80:ASN:CA | 2:B:80:ASN:OD1 | 2.57 | 0.52 |
| 2:D:10:ALA:HB3 | 2:D:11:VAL:N | 2.24 | 0.51 |
| 2:D:3:LEU:CA | 2:D:3:LEU:O | 2.58 | 0.51 |
| 1:C:138:SER:CB | 1:C:138:SER:N | 2.72 | 0.51 |
| 1:A:133:SER:O | 1:A:137:THR:CG2 | 2.57 | 0.51 |
| 2:D:58:PRO:HG2 | 2:D:58:PRO:HD3 | 1.04 | 0.51 |
| 2:B:22:GLU:CG | 2:B:22:GLU:OE1 | 2.59 | 0.51 |
| 2:D:5:PRO:CG | 2:D:5:PRO:CA | 2.81 | 0.51 |
| 1:C:99:LYS:CG | 1:C:99:LYS:CE | 2.88 | 0.51 |
| 1:C:139:LYS:HD2 | 1:C:139:LYS:NZ | 2.20 | 0.51 |
| 2:D:73:ASP:OD2 | 2:D:73:ASP:CB | 2.59 | 0.50 |
| 1:A:50:HIS:CB | 1:A:50:HIS:H | 2.23 | 0.50 |
| 1:C:72:HIS:N | 1:C:72:HIS:CB | 2.63 | 0.50 |
| 1:C:82:ALA:O | 1:C:83:LEU:CA | 2.59 | 0.50 |
| 2:D:26:GLU:OE1 | 2:D:26:GLU:OE2 | 2.30 | 0.50 |
| 2:D:104:ARG:NH2 | 2:D:104:ARG:NE | 2.59 | 0.50 |
| 1:C:78:ASN:CB | 1:C:78:ASN:ND2 | 2.66 | 0.50 |
| 1:C:137:THR:C | 1:C:137:THR:N | 2.59 | 0.50 |
| 1:A:2:LEU:HA | 1:A:3:SER:N | 2.21 | 0.50 |
| 1:C:40:LYS:HG2 | 1:C:48:LEU:HD13 | 1.94 | 0.50 |
| 2:D:67:VAL:C | 2:D:67:VAL:CB | 2.64 | 0.50 |
| 2:B:142:ALA:CB | 2:B:142:ALA:C | 2.72 | 0.50 |
| 2:D:82:LYS:HG3 | 2:D:82:LYS:CE | 2.41 | 0.50 |
| 1:C:92:ARG:CD | 1:C:92:ARG:CZ | 2.89 | 0.50 |
| 2:B:10:ALA:CA | 2:B:11:VAL:N | 2.66 | 0.50 |
| 2:D:67:VAL:CG2 | 2:D:67:VAL:CA | 2.77 | 0.50 |
| 2:B:143:HIS:C | 2:B:143:HIS:N | 2.60 | 0.50 |
| 1:C:103:HIS:HE1 | 2:D:131:GLN:OE1 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:LYS:HB3 | 1:C:90:LYS:CD | 2.38 | 0.50 |
| 1:A:78:ASN:CG | 1:A:78:ASN:HA | 2.20 | 0.50 |
| 2:B:1:VAL:O | 2:B:2:HIS:HA | 2.11 | 0.50 |
| 2:D:8:LYS:HA | 2:D:8:LYS:CG | 2.38 | 0.50 |
| 2:D:1:VAL:CB | 2:D:2:HIS:H | 2.23 | 0.50 |
| 2:B:50:THR:O | 2:B:54:VAL:HG23 | 2.11 | 0.50 |
| 2:D:12:THR:N | 2:D:12:THR:CB | 2.75 | 0.50 |
| 2:B:8:LYS:CB | 2:B:8:LYS:C | 2.69 | 0.49 |
| 2:D:73:ASP:OD2 | 2:D:73:ASP:OD1 | 2.30 | 0.49 |
| 2:D:10:ALA:O | 2:D:10:ALA:CA | 2.52 | 0.49 |
| 1:C:7:LYS:CD | 1:C:7:LYS:CB | 2.80 | 0.49 |
| 1:C:105:LEU:HD13 | 1:C:105:LEU:HD22 | 1.92 | 0.49 |
| 2:B:145:TYR:CA | 2:B:146:HIS:N | 2.46 | 0.49 |
| 2:D:22:GLU:C | 2:D:22:GLU:CG | 2.80 | 0.49 |
| 2:D:55:MET:N | 2:D:56:GLY:N | 2.59 | 0.49 |
| 2:B:8:LYS:HG2 | 2:B:8:LYS:CD | 2.21 | 0.49 |
| 1:C:82:ALA:O | 1:C:83:LEU:N | 2.36 | 0.49 |
| 2:B:80:ASN:ND2 | 2:B:80:ASN:HB3 | 2.27 | 0.49 |
| 1:C:7:LYS:CG | 1:C:7:LYS:N | 2.76 | 0.49 |
| 2:D:108:ASN:CA | 2:D:108:ASN:CG | 2.73 | 0.49 |
| 1:A:2:LEU:CB | 1:A:2:LEU:C | 2.75 | 0.49 |
| 1:A:51:GLY:C | 1:A:52:SER:C | 2.71 | 0.49 |
| 2:B:5:PRO:N | 2:B:6:GLU:H | 2.10 | 0.49 |
| 2:D:18:VAL:N | 2:D:18:VAL:C | 2.63 | 0.49 |
| 1:C:16:LYS:N | 1:C:17:VAL:N | 2.61 | 0.49 |
| 2:D:73:ASP:CG | 2:D:73:ASP:N | 2.65 | 0.49 |
| 1:A:44:PRO:C | 1:A:44:PRO:HB2 | 2.33 | 0.49 |
| 2:D:123:THR:HB | 2:D:124:PRO:CD | 2.43 | 0.48 |
| 2:B:65:LYS:CE | 2:B:65:LYS:CB | 2.91 | 0.48 |
| 1:A:50:HIS:HA | 5:A:173:HOH:O | 2.13 | 0.48 |
| 1:C:10:VAL:O | 1:C:10:VAL:CA | 2.47 | 0.48 |
| 2:B:22:GLU:OE2 | 2:B:22:GLU:CG | 2.61 | 0.48 |
| 2:D:121:GLU:CG | 2:D:121:GLU:OE1 | 2.60 | 0.48 |
| 2:B:96:LEU:HD13 | 4:B:148:HEM:C3D | 2.48 | 0.48 |
| 1:C:60:LYS:HD3 | 1:C:60:LYS:HZ2 | 1.79 | 0.48 |
| 2:D:8:LYS:HA | 2:D:8:LYS:HG3 | 1.95 | 0.48 |
| 2:D:47:ASP:CA | 2:D:47:ASP:OD2 | 2.62 | 0.48 |
| 2:D:67:VAL:CB | 2:D:67:VAL:H | 2.24 | 0.48 |
| 1:A:16:LYS:CG | 1:A:16:LYS:NZ | 2.71 | 0.48 |
| 2:B:87:THR:CG2 | 2:B:87:THR:CA | 2.92 | 0.48 |
| 1:A:17:VAL:CG1 | 1:A:17:VAL:C | 2.81 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:6:GLU:CB | 2:D:6:GLU:C | 2.81 | 0.48 |
| 1:A:72:HIS:CB | 1:A:72:HIS:O | 2.62 | 0.48 |
| 1:A:92:ARG:HH11 | 1:A:92:ARG:HD2 | 1.47 | 0.48 |
| 2:D:1:VAL:O | 2:D:1:VAL:CA | 2.61 | 0.48 |
| 2:D:4:THR:CB | 2:D:4:THR:C | 2.76 | 0.47 |
| 4:C:142:HEM:CBB | 4:C:142:HEM:HMB1 | 2.44 | 0.47 |
| 2:D:8:LYS:HG2 | 2:D:8:LYS:C | 2.33 | 0.47 |
| 1:C:118:THR:CA | 1:C:118:THR:OG1 | 2.54 | 0.47 |
| 1:A:137:THR:CG2 | 1:A:137:THR:N | 2.78 | 0.47 |
| 1:A:75:ASP:OD2 | 1:A:75:ASP:OD1 | 2.33 | 0.47 |
| 2:B:90:GLU:CB | 2:B:90:GLU:OE1 | 2.63 | 0.47 |
| 2:B:4:THR:HA | 2:B:5:PRO:CD | 2.44 | 0.47 |
| 1:C:16:LYS:C | 1:C:16:LYS:CB | 2.71 | 0.47 |
| 1:A:84:SER:HB2 | 1:A:139:LYS:HD2 | 1.97 | 0.47 |
| 2:B:49:SER:CB | 2:B:49:SER:HG | 2.14 | 0.47 |
| 2:D:49:SER:N | 2:D:50:THR:N | 2.63 | 0.47 |
| 1:A:138:SER:CB | 1:A:138:SER:C | 2.81 | 0.47 |
| 1:C:113:LEU:HD13 | 1:C:113:LEU:HB3 | 1.96 | 0.47 |
| 1:C:61:LYS:CD | 1:C:61:LYS:HZ3 | 2.25 | 0.47 |
| 1:C:56:LYS:CG | 1:C:56:LYS:HE3 | 2.42 | 0.47 |
| 2:D:45:PHE:O | 2:D:46:GLY:CA | 2.44 | 0.46 |
| 2:D:47:ASP:C | 2:D:47:ASP:CB | 2.84 | 0.46 |
| 1:C:56:LYS:HE3 | 1:C:56:LYS:HG3 | 1.98 | 0.46 |
| 1:A:76:MET:O | 1:A:77:PRO:C | 2.49 | 0.46 |
| 2:D:5:PRO:HA | 2:D:8:LYS:HB3 | 1.96 | 0.46 |
| 2:B:12:THR:HG1 | 2:B:12:THR:CG2 | 2.16 | 0.46 |
| 2:D:15:TRP:HE1 | 2:D:72:SER:HB3 | 1.80 | 0.46 |
| 1:C:70:VAL:CB | 1:C:70:VAL:C | 2.70 | 0.46 |
| 1:A:23:GLU:CB | 1:A:23:GLU:CD | 2.80 | 0.46 |
| 1:C:116:GLU:CB | 1:C:116:GLU:OE1 | 2.63 | 0.46 |
| 2:B:2:HIS:O | 2:B:2:HIS:ND1 | 2.48 | 0.46 |
| 2:B:2:HIS:CG | 2:B:2:HIS:O | 2.69 | 0.46 |
| 2:B:6:GLU:C | 2:B:6:GLU:HB2 | 2.36 | 0.46 |
| 2:D:82:LYS:HD3 | 2:D:143:HIS:NE2 | 2.31 | 0.46 |
| 1:A:87:HIS:N | 1:A:87:HIS:C | 2.62 | 0.46 |
| 2:B:74:GLY:C | 2:B:75:LEU:CA | 2.73 | 0.46 |
| 1:A:64:ASP:OD1 | 1:A:64:ASP:CB | 2.62 | 0.46 |
| 1:C:3:SER:O | 1:C:7:LYS:HG3 | 2.16 | 0.45 |
| 2:B:1:VAL:O | 2:B:2:HIS:CA | 2.63 | 0.45 |
| 2:D:48:LEU:N | 2:D:49:SER:N | 2.63 | 0.45 |
| 1:A:1:VAL:HG23 | 1:A:1:VAL:H1 | 1.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:76:MET:SD | 1:C:76:MET:HB3 | 2.55 | 0.45 |
| 4:D:148:HEM:CGD | 4:D:148:HEM:CAD | 2.85 | 0.45 |
| 1:A:85:ASP:CB | 1:A:85:ASP:OD2 | 2.62 | 0.45 |
| 1:C:92:ARG:NH2 | 1:C:92:ARG:HD2 | 2.28 | 0.45 |
| 2:B:6:GLU:CD | 2:B:6:GLU:CB | 2.69 | 0.45 |
| 2:D:2:HIS:CB | 2:D:2:HIS:ND1 | 2.77 | 0.45 |
| 2:B:52:ASP:OD1 | 2:B:52:ASP:CB | 2.44 | 0.45 |
| 1:A:16:LYS:HG2 | 1:A:16:LYS:NZ | 2.31 | 0.45 |
| 2:D:90:GLU:CB | 2:D:90:GLU:CD | 2.85 | 0.45 |
| 2:B:57:ASN:CA | 2:B:58:PRO:CD | 2.95 | 0.45 |
| 2:B:1:VAL:N | 5:B:197:HOH:O | 2.50 | 0.45 |
| 2:D:121:GLU:OE2 | 2:D:121:GLU:CB | 2.65 | 0.45 |
| 2:D:1:VAL:C | 2:D:1:VAL:CB | 2.81 | 0.45 |
| 1:C:137:THR:CB | 1:C:137:THR:C | 2.76 | 0.45 |
| 2:B:139:ASN:OD1 | 2:B:139:ASN:CA | 2.61 | 0.45 |
| 1:A:103:HIS:HE1 | 2:B:131:GLN:OE1 | 2.00 | 0.45 |
| 1:A:29:LEU:C | 1:A:29:LEU:CB | 2.74 | 0.45 |
| 2:B:89:SER:OG | 2:B:144:LYS:HB2 | 2.17 | 0.45 |
| 1:A:55:VAL:O | 1:A:56:LYS:C | 2.53 | 0.44 |
| 2:D:10:ALA:CA | 2:D:11:VAL:N | 2.65 | 0.44 |
| 1:A:17:VAL:C | 1:A:18:GLY:C | 2.74 | 0.44 |
| 2:B:82:LYS:CE | 2:B:82:LYS:CB | 2.78 | 0.44 |
| 1:A:18:GLY:C | 1:A:18:GLY:N | 2.61 | 0.44 |
| 2:D:124:PRO:C | 2:D:125:PRO:CD | 2.67 | 0.44 |
| 2:D:12:THR:HG23 | 2:D:12:THR:CA | 2.41 | 0.44 |
| 1:C:30:GLU:OE2 | 1:C:50:HIS:HD2 | 1.99 | 0.44 |
| 2:B:79:ASP:HA | 2:B:79:ASP:OD2 | 2.16 | 0.44 |
| 2:B:80:ASN:O | 2:B:81:LEU:CA | 2.63 | 0.44 |
| 1:A:28:ALA:CB | 1:A:105:LEU:HD23 | 2.48 | 0.44 |
| 1:C:105:LEU:HD23 | 1:C:129:LEU:HD22 | 2.00 | 0.44 |
| 2:D:94:ASP:N | 2:D:94:ASP:HB2 | 2.29 | 0.44 |
| 1:A:29:LEU:CB | 1:A:29:LEU:N | 2.74 | 0.44 |
| 2:D:43:GLU:CG | 2:D:43:GLU:N | 2.78 | 0.44 |
| 2:D:6:GLU:HB2 | 2:D:6:GLU:C | 2.38 | 0.43 |
| 2:B:65:LYS:HE2 | 2:B:65:LYS:CG | 2.39 | 0.43 |
| 1:A:43:PHE:N | 1:A:44:PRO:CD | 2.80 | 0.43 |
| 2:B:6:GLU:N | 2:B:7:GLU:N | 2.65 | 0.43 |
| 2:D:47:ASP:CA | 2:D:48:LEU:H | 2.29 | 0.43 |
| 2:B:90:GLU:N | 2:B:90:GLU:CB | 2.64 | 0.43 |
| 2:D:20:VAL:HG23 | 2:D:20:VAL:N | 2.33 | 0.43 |
| 2:D:17:LYS:HE3 | 2:D:121:GLU:OE1 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:144:LYS:HD3 | 2:B:144:LYS:CE | 2.29 | 0.43 |
| 2:B:2:HIS:O | 2:B:2:HIS:CB | 2.66 | 0.43 |
| 2:B:79:ASP:O | 2:B:80:ASN:CA | 2.65 | 0.43 |
| 2:D:63:HIS:CE1 | 4:D:148:HEM:C4D | 3.06 | 0.43 |
| 1:C:113:LEU:HD13 | 1:C:116:GLU:HB2 | 1.99 | 0.43 |
| 2:D:47:ASP:HB3 | 2:D:47:ASP:O | 2.19 | 0.43 |
| 2:B:41:PHE:N | 2:B:42:PHE:H | 2.16 | 0.43 |
| 4:C:142:HEM:CAA | 4:C:142:HEM:CGA | 2.95 | 0.43 |
| 2:B:63:HIS:CE1 | 4:B:148:HEM:C4D | 3.05 | 0.43 |
| 1:C:86:LEU:CD2 | 4:C:142:HEM:HBA2 | 2.49 | 0.43 |
| 2:D:17:LYS:HD3 | 2:D:17:LYS:HZ2 | 1.81 | 0.42 |
| 2:B:74:GLY:O | 2:B:75:LEU:CA | 2.67 | 0.42 |
| 1:C:94:ASP:OD2 | 1:C:96:VAL:HG13 | 2.18 | 0.42 |
| 2:D:53:ALA:HB1 | 2:D:53:ALA:C | 2.33 | 0.42 |
| 2:B:123:THR:CA | 2:B:124:PRO:CD | 2.97 | 0.42 |
| 2:D:80:ASN:HB2 | 2:D:80:ASN:OD1 | 2.18 | 0.42 |
| 1:A:78:ASN:ND2 | 1:A:78:ASN:HA | 2.30 | 0.42 |
| 2:D:6:GLU:N | 2:D:7:GLU:N | 2.67 | 0.42 |
| 2:D:79:ASP:C | 2:D:80:ASN:HB3 | 2.39 | 0.42 |
| 1:C:30:GLU:OE1 | 1:C:30:GLU:CB | 2.66 | 0.42 |
| 1:A:56:LYS:CD | 1:A:56:LYS:HB3 | 2.44 | 0.42 |
| 2:D:59:LYS:N | 2:D:60:VAL:N | 2.67 | 0.42 |
| 2:D:6:GLU:CA | 2:D:7:GLU:N | 2.77 | 0.42 |
| 2:D:47:ASP:H | 2:D:47:ASP:HB3 | 1.80 | 0.42 |
| 2:B:10:ALA:C | 2:B:10:ALA:N | 2.54 | 0.42 |
| 1:A:7:LYS:O | 1:A:11:LYS:HG3 | 2.19 | 0.42 |
| 1:A:87:HIS:N | 1:A:88:ALA:N | 2.67 | 0.42 |
| 1:C:56:LYS:CE | 1:C:56:LYS:HG3 | 2.46 | 0.42 |
| 1:A:16:LYS:O | 1:A:16:LYS:HG3 | 2.20 | 0.42 |
| 2:D:123:THR:HB | 2:D:124:PRO:HD2 | 2.02 | 0.42 |
| 1:A:56:LYS:CG | 1:A:56:LYS:CE | 2.98 | 0.42 |
| 2:B:101:GLU:CG | 2:B:101:GLU:OE1 | 2.59 | 0.42 |
| 2:B:65:LYS:CD | 2:B:65:LYS:HB2 | 2.46 | 0.41 |
| 2:D:52:ASP:HB2 | 2:D:52:ASP:H | 1.84 | 0.41 |
| 2:D:121:GLU:CD | 2:D:121:GLU:CB | 2.68 | 0.41 |
| 2:D:141:LEU:HA | 2:D:141:LEU:HD23 | 2.03 | 0.41 |
| 1:C:43:PHE:N | 1:C:44:PRO:CD | 2.84 | 0.41 |
| 2:D:22:GLU:CD | 2:D:22:GLU:CB | 2.87 | 0.41 |
| 1:C:2:LEU:CB | 1:C:2:LEU:O | 2.69 | 0.41 |
| 2:B:65:LYS:CB | 2:B:65:LYS:N | 2.65 | 0.41 |
| 1:C:138:SER:CB | 1:C:138:SER:C | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:117:HIS:ND1 | 2:B:117:HIS:NE2 | 2.57 | 0.41 |
| 1:A:60:LYS:NZ | 1:A:60:LYS:CD | 2.84 | 0.41 |
| 2:D:88:LEU:HA | 2:D:88:LEU:HD23 | 1.92 | 0.41 |
| 2:D:92:HIS:HA | 2:D:96:LEU:HB2 | 2.02 | 0.41 |
| 2:D:79:ASP:CA | 2:D:79:ASP:OD2 | 2.69 | 0.41 |
| 1:C:105:LEU:HB2 | 1:C:105:LEU:CD1 | 2.49 | 0.40 |
| 2:D:52:ASP:H | 2:D:52:ASP:CB | 2.28 | 0.40 |
| 1:A:85:ASP:CA | 1:A:85:ASP:OD1 | 2.67 | 0.40 |
| 2:D:17:LYS:O | 2:D:18:VAL:CA | 2.68 | 0.40 |
| 2:B:142:ALA:N | 2:B:143:HIS:N | 2.69 | 0.40 |
| 2:B:145:TYR:N | 2:B:145:TYR:C | 2.61 | 0.40 |
| 2:B:101:GLU:CB | 2:B:101:GLU:OE1 | 2.70 | 0.40 |
| 2:B:77:HIS:HA | 2:B:77:HIS:CD2 | 2.56 | 0.40 |
| 1:C:2:LEU:HD23 | 1:C:2:LEU:HA | 1.95 | 0.40 |
| 1:A:21:ALA:N | 1:A:21:ALA:C | 2.72 | 0.40 |
| 4:D:148:HEM:HBD1 | 4:D:148:HEM:O1D | 2.17 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------------|--------------------------|-------------------|
| 1:C:85:ASP:OD2 | 5:B:204:HOH:O[2_657] | 1.41 | 0.79 |
| 5:B:204:HOH:O | 5:C:161:HOH:O[2_647] | 2.02 | 0.18 |

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 | 139/141 (99%) | 122 (88%) | 14 (10%) | 3 (2%) | 8 | 1 |
| 1 | C | 139/141 (99%) | 126 (91%) | 13 (9%) | 0 | 100 | 100 |
| 2 | B | 144/146 (99%) | 129 (90%) | 14 (10%) | 1 (1%) | 26 | 9 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2 | D | 144/146 (99%) | 128 (89%) | 13 (9%) | 3 (2%) | 9 | 1 |
| All | All | 566/574 (99%) | 505 (89%) | 54 (10%) | 7 (1%) | 16 | 3 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | LYS |
| 2 | D | 73 | ASP |
| 1 | A | 21 | ALA |
| 2 | D | 77 | HIS |
| 2 | B | 4 | THR |
| 2 | D | 78 | LEU |
| 1 | A | 3 | SER |

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 | 113/113 (100%) | 105 (93%) | 8 (7%) | 18 | 3 |
| 1 | C | 113/113 (100%) | 110 (97%) | 3 (3%) | 52 | 26 |
| 2 | B | 118/118 (100%) | 106 (90%) | 12 (10%) | 9 | 1 |
| 2 | D | 118/118 (100%) | 101 (86%) | 17 (14%) | 4 | 0 |
| All | All | 462/462 (100%) | 422 (91%) | 40 (9%) | 13 | 2 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | LEU |
| 1 | A | 4 | PRO |
| 1 | A | 45 | HIS |
| 1 | A | 52 | SER |
| 1 | A | 75 | ASP |
| 1 | A | 84 | SER |
| 1 | A | 95 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 138 | SER |
| 2 | B | 1 | VAL |
| 2 | B | 6 | GLU |
| 2 | B | 9 | SER |
| 2 | B | 26 | GLU |
| 2 | B | 32 | LEU |
| 2 | B | 36 | PRO |
| 2 | B | 50 | THR |
| 2 | B | 51 | PRO |
| 2 | B | 65 | LYS |
| 2 | B | 68 | LEU |
| 2 | B | 117 | HIS |
| 2 | B | 146 | HIS |
| 1 | C | 16 | LYS |
| 1 | C | 114 | PRO |
| 1 | C | 138 | SER |
| 2 | D | 1 | VAL |
| 2 | D | 6 | GLU |
| 2 | D | 9 | SER |
| 2 | D | 21 | ASP |
| 2 | D | 22 | GLU |
| 2 | D | 26 | GLU |
| 2 | D | 43 | GLU |
| 2 | D | 47 | ASP |
| 2 | D | 66 | LYS |
| 2 | D | 68 | LEU |
| 2 | D | 72 | SER |
| 2 | D | 75 | LEU |
| 2 | D | 79 | ASP |
| 2 | D | 80 | ASN |
| 2 | D | 92 | HIS |
| 2 | D | 139 | ASN |
| 2 | D | 144 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 72 | HIS |
| 1 | A | 103 | HIS |
| 2 | B | 63 | HIS |
| 1 | C | 50 | HIS |
| 1 | C | 68 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 72 | HIS |
| 1 | C | 103 | HIS |
| 1 | C | 112 | HIS |
| 2 | D | 63 | HIS |
| 2 | D | 80 | ASN |
| 2 | D | 139 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

Of 6 ligands modelled in this entry, 2 are modelled with single atom - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | HEM | A | 142 | 1 | 30,50,50 | 5.27 | 20 (66%) | 24,82,82 | 3.57 | 14 (58%) |
| 4 | HEM | B | 148 | 2 | 30,50,50 | 3.56 | 14 (46%) | 24,82,82 | 4.75 | 18 (75%) |
| 4 | HEM | C | 142 | 1 | 30,50,50 | 3.80 | 20 (66%) | 24,82,82 | 4.70 | 18 (75%) |
| 4 | HEM | D | 148 | 2 | 30,50,50 | 4.80 | 21 (70%) | 24,82,82 | 3.71 | 14 (58%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | HEM | A | 142 | 1 | - | 0/10/54/54 | 0/0/8/8 |
| 4 | HEM | B | 148 | 2 | - | 0/10/54/54 | 0/0/8/8 |
| 4 | HEM | C | 142 | 1 | - | 0/10/54/54 | 0/0/8/8 |
| 4 | HEM | D | 148 | 2 | - | 0/10/54/54 | 0/0/8/8 |

All (75) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4 | A | 142 | HEM | C3D-C4D | -16.80 | 1.30 | 1.51 |
| 4 | C | 142 | HEM | C3D-C4D | -10.99 | 1.37 | 1.51 |
| 4 | A | 142 | HEM | C3B-C4B | -10.58 | 1.42 | 1.51 |
| 4 | D | 148 | HEM | C3D-C4D | -10.21 | 1.38 | 1.51 |
| 4 | D | 148 | HEM | C3C-CAC | -8.10 | 1.36 | 1.51 |
| 4 | A | 142 | HEM | C2D-C3D | -7.49 | 1.32 | 1.54 |
| 4 | B | 148 | HEM | CMB-C2B | -7.23 | 1.36 | 1.53 |
| 4 | D | 148 | HEM | C3B-C4B | -6.81 | 1.45 | 1.51 |
| 4 | C | 142 | HEM | C3C-CAC | -6.75 | 1.38 | 1.51 |
| 4 | C | 142 | HEM | C2D-C3D | -6.34 | 1.35 | 1.54 |
| 4 | C | 142 | HEM | CMB-C2B | -6.28 | 1.38 | 1.53 |
| 4 | A | 142 | HEM | C2C-C1C | -6.26 | 1.40 | 1.52 |
| 4 | D | 148 | HEM | C2B-C1B | -5.57 | 1.33 | 1.51 |
| 4 | A | 142 | HEM | CAD-CBD | -5.45 | 1.26 | 1.52 |
| 4 | D | 148 | HEM | CBB-CAB | -5.38 | 0.98 | 1.29 |
| 4 | A | 142 | HEM | C4C-NC | -5.26 | 1.29 | 1.36 |
| 4 | D | 148 | HEM | CMB-C2B | -5.19 | 1.41 | 1.53 |
| 4 | B | 148 | HEM | C3C-CAC | -5.06 | 1.41 | 1.51 |
| 4 | B | 148 | HEM | C2D-C3D | -4.92 | 1.39 | 1.54 |
| 4 | A | 142 | HEM | C1A-CHA | -4.80 | 1.26 | 1.39 |
| 4 | A | 142 | HEM | C3B-CAB | -4.67 | 1.42 | 1.51 |
| 4 | B | 148 | HEM | CMA-C3A | -4.58 | 1.42 | 1.51 |
| 4 | A | 142 | HEM | C2B-C1B | -4.53 | 1.37 | 1.51 |
| 4 | A | 142 | HEM | C3C-CAC | -4.48 | 1.42 | 1.51 |
| 4 | D | 148 | HEM | CBA-CAA | -4.31 | 1.23 | 1.53 |
| 4 | D | 148 | HEM | CMA-C3A | -4.18 | 1.43 | 1.51 |
| 4 | D | 148 | HEM | C2D-C1D | -4.16 | 1.38 | 1.51 |
| 4 | D | 148 | HEM | CHC-C1C | -3.94 | 1.27 | 1.36 |
| 4 | C | 142 | HEM | CHC-C1C | -3.85 | 1.27 | 1.36 |
| 4 | B | 148 | HEM | C2C-C1C | -3.79 | 1.45 | 1.52 |
| 4 | A | 142 | HEM | CBA-CAA | -3.51 | 1.29 | 1.53 |
| 4 | C | 142 | HEM | CHD-C4C | -3.50 | 1.28 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | D | 148 | HEM | C2A-C3A | -3.13 | 1.28 | 1.37 |
| 4 | A | 142 | HEM | CMC-C2C | -3.03 | 1.46 | 1.53 |
| 4 | B | 148 | HEM | C3D-C4D | -2.88 | 1.47 | 1.51 |
| 4 | A | 142 | HEM | CHD-C4C | -2.77 | 1.30 | 1.36 |
| 4 | C | 142 | HEM | CMA-C3A | -2.76 | 1.46 | 1.51 |
| 4 | C | 142 | HEM | CMD-C2D | -2.70 | 1.46 | 1.53 |
| 4 | D | 148 | HEM | CAD-CBD | -2.55 | 1.40 | 1.52 |
| 4 | C | 142 | HEM | CAD-CBD | -2.50 | 1.40 | 1.52 |
| 4 | B | 148 | HEM | CMC-C2C | -2.46 | 1.47 | 1.53 |
| 4 | A | 142 | HEM | CMA-C3A | -2.27 | 1.47 | 1.51 |
| 4 | C | 142 | HEM | C2A-C3A | -2.03 | 1.31 | 1.37 |
| 4 | D | 148 | HEM | FE-ND | 2.02 | 2.08 | 1.97 |
| 4 | C | 142 | HEM | C2D-C1D | 2.11 | 1.58 | 1.51 |
| 4 | C | 142 | HEM | C4C-NC | 2.14 | 1.38 | 1.36 |
| 4 | A | 142 | HEM | CHC-C1C | 2.52 | 1.42 | 1.36 |
| 4 | C | 142 | HEM | FE-ND | 2.63 | 2.11 | 1.97 |
| 4 | D | 148 | HEM | C4C-NC | 2.70 | 1.39 | 1.36 |
| 4 | B | 148 | HEM | CAA-C2A | 2.80 | 1.56 | 1.52 |
| 4 | A | 142 | HEM | CMD-C2D | 2.84 | 1.59 | 1.53 |
| 4 | C | 142 | HEM | FE-NB | 2.87 | 2.12 | 1.97 |
| 4 | C | 142 | HEM | CAD-C3D | 3.11 | 1.60 | 1.54 |
| 4 | C | 142 | HEM | CHD-C1D | 3.12 | 1.47 | 1.38 |
| 4 | C | 142 | HEM | CBC-CAC | 3.16 | 1.47 | 1.29 |
| 4 | D | 148 | HEM | CMC-C2C | 3.35 | 1.60 | 1.53 |
| 4 | C | 142 | HEM | FE-NC | 3.41 | 2.09 | 1.95 |
| 4 | A | 142 | HEM | FE-ND | 3.48 | 2.15 | 1.97 |
| 4 | B | 148 | HEM | C1C-NC | 3.92 | 1.40 | 1.36 |
| 4 | B | 148 | HEM | CAD-C3D | 4.20 | 1.62 | 1.54 |
| 4 | D | 148 | HEM | FE-NC | 4.61 | 2.13 | 1.95 |
| 4 | C | 142 | HEM | C1C-NC | 4.67 | 1.41 | 1.36 |
| 4 | A | 142 | HEM | FE-NB | 4.72 | 2.22 | 1.97 |
| 4 | D | 148 | HEM | C3B-CAB | 5.01 | 1.60 | 1.51 |
| 4 | D | 148 | HEM | CHD-C4C | 5.27 | 1.48 | 1.36 |
| 4 | B | 148 | HEM | C3B-CAB | 5.35 | 1.61 | 1.51 |
| 4 | B | 148 | HEM | CHC-C1C | 5.86 | 1.50 | 1.36 |
| 4 | C | 142 | HEM | C3B-CAB | 6.19 | 1.62 | 1.51 |
| 4 | D | 148 | HEM | C2C-C1C | 6.29 | 1.64 | 1.52 |
| 4 | B | 148 | HEM | C3B-C4B | 6.88 | 1.58 | 1.51 |
| 4 | A | 142 | HEM | FE-NC | 6.96 | 2.23 | 1.95 |
| 4 | A | 142 | HEM | C1C-NC | 7.81 | 1.45 | 1.36 |
| 4 | D | 148 | HEM | CHD-C1D | 7.86 | 1.60 | 1.38 |
| 4 | B | 148 | HEM | CHD-C4C | 7.94 | 1.54 | 1.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | D | 148 | HEM | CAA-C2A | 9.67 | 1.68 | 1.52 |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | C | 142 | HEM | C3B-CAB-CBB | -8.50 | 111.42 | 124.46 |
| 4 | A | 142 | HEM | CAA-CBA-CGA | -7.75 | 98.55 | 112.75 |
| 4 | B | 148 | HEM | C2C-C1C-CHC | -7.65 | 112.04 | 123.68 |
| 4 | C | 142 | HEM | CAA-CBA-CGA | -7.50 | 98.99 | 112.75 |
| 4 | D | 148 | HEM | C2C-C1C-NC | -6.59 | 99.10 | 110.21 |
| 4 | D | 148 | HEM | C3B-CAB-CBB | -5.96 | 115.31 | 124.46 |
| 4 | C | 142 | HEM | CMA-C3A-C4A | -5.95 | 118.52 | 128.36 |
| 4 | B | 148 | HEM | C4B-CHC-C1C | -5.77 | 116.17 | 125.82 |
| 4 | D | 148 | HEM | C1D-CHD-C4C | -5.33 | 116.92 | 125.82 |
| 4 | C | 142 | HEM | CAA-C2A-C3A | -5.15 | 114.29 | 129.00 |
| 4 | C | 142 | HEM | C1D-CHD-C4C | -5.02 | 117.43 | 125.82 |
| 4 | A | 142 | HEM | C1D-CHD-C4C | -4.97 | 117.51 | 125.82 |
| 4 | D | 148 | HEM | CAA-C2A-C1A | -4.73 | 121.87 | 127.01 |
| 4 | D | 148 | HEM | CBA-CAA-C2A | -4.44 | 104.57 | 112.53 |
| 4 | A | 142 | HEM | C3C-CAC-CBC | -4.33 | 117.81 | 124.46 |
| 4 | B | 148 | HEM | C3B-CAB-CBB | -3.91 | 118.46 | 124.46 |
| 4 | B | 148 | HEM | CAA-C2A-C1A | -3.77 | 122.91 | 127.01 |
| 4 | A | 142 | HEM | C2C-C1C-NC | -3.70 | 103.96 | 110.21 |
| 4 | B | 148 | HEM | CAA-C2A-C3A | -3.63 | 118.65 | 129.00 |
| 4 | A | 142 | HEM | C3B-C4B-NB | -3.36 | 105.21 | 111.63 |
| 4 | C | 142 | HEM | C2C-C1C-NC | -3.33 | 104.59 | 110.21 |
| 4 | A | 142 | HEM | CAA-C2A-C1A | -3.06 | 123.69 | 127.01 |
| 4 | A | 142 | HEM | CBA-CAA-C2A | -2.42 | 108.20 | 112.53 |
| 4 | C | 142 | HEM | C3B-C4B-NB | -2.36 | 107.12 | 111.63 |
| 4 | D | 148 | HEM | CMA-C3A-C4A | -2.35 | 124.47 | 128.36 |
| 4 | B | 148 | HEM | C3B-C4B-CHC | -2.23 | 120.03 | 123.16 |
| 4 | B | 148 | HEM | CHD-C1D-ND | -2.16 | 119.31 | 124.52 |
| 4 | B | 148 | HEM | C3B-C4B-NB | -2.11 | 107.59 | 111.63 |
| 4 | C | 142 | HEM | CAD-C3D-C2D | 2.05 | 119.10 | 113.22 |
| 4 | C | 142 | HEM | CHC-C4B-NB | 2.18 | 129.76 | 124.52 |
| 4 | B | 148 | HEM | CBD-CAD-C3D | 2.19 | 119.92 | 113.55 |
| 4 | B | 148 | HEM | CMC-C2C-C3C | 2.32 | 122.32 | 116.53 |
| 4 | A | 142 | HEM | CAD-C3D-C4D | 2.64 | 121.77 | 112.47 |
| 4 | C | 142 | HEM | C3C-CAC-CBC | 2.64 | 128.51 | 124.46 |
| 4 | A | 142 | HEM | CAD-C3D-C2D | 2.80 | 121.26 | 113.22 |
| 4 | A | 142 | HEM | CHC-C4B-NB | 3.09 | 131.96 | 124.52 |
| 4 | D | 148 | HEM | CMA-C3A-C2A | 3.09 | 131.70 | 125.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | A | 142 | HEM | CMD-C2D-C3D | 3.11 | 128.09 | 114.35 |
| 4 | D | 148 | HEM | CMD-C2D-C3D | 3.13 | 128.21 | 114.35 |
| 4 | B | 148 | HEM | CHC-C4B-NB | 3.23 | 132.30 | 124.52 |
| 4 | B | 148 | HEM | CAD-C3D-C4D | 3.66 | 125.39 | 112.47 |
| 4 | D | 148 | HEM | CAD-C3D-C4D | 4.01 | 126.60 | 112.47 |
| 4 | C | 142 | HEM | CAD-C3D-C4D | 4.20 | 127.30 | 112.47 |
| 4 | C | 142 | HEM | CMC-C2C-C3C | 4.33 | 127.35 | 116.53 |
| 4 | D | 148 | HEM | CMC-C2C-C3C | 4.54 | 127.86 | 116.53 |
| 4 | D | 148 | HEM | CAA-CBA-CGA | 4.57 | 121.12 | 112.75 |
| 4 | C | 142 | HEM | CMD-C2D-C3D | 4.69 | 135.11 | 114.35 |
| 4 | C | 142 | HEM | CHD-C1D-ND | 4.70 | 135.83 | 124.52 |
| 4 | B | 148 | HEM | CMA-C3A-C2A | 4.71 | 135.08 | 125.24 |
| 4 | A | 142 | HEM | CHD-C1D-ND | 4.94 | 136.43 | 124.52 |
| 4 | D | 148 | HEM | CMB-C2B-C3B | 5.27 | 129.68 | 116.53 |
| 4 | D | 148 | HEM | C2C-C1C-CHC | 5.46 | 131.98 | 123.68 |
| 4 | A | 142 | HEM | CMB-C2B-C3B | 5.47 | 130.18 | 116.53 |
| 4 | B | 148 | HEM | CMD-C2D-C3D | 5.48 | 138.58 | 114.35 |
| 4 | C | 142 | HEM | CAA-C2A-C1A | 5.60 | 133.09 | 127.01 |
| 4 | D | 148 | HEM | C2D-C3D-C4D | 6.02 | 111.71 | 101.50 |
| 4 | C | 142 | HEM | CMA-C3A-C2A | 6.62 | 139.07 | 125.24 |
| 4 | C | 142 | HEM | C2D-C3D-C4D | 7.11 | 113.55 | 101.50 |
| 4 | A | 142 | HEM | C2D-C3D-C4D | 7.71 | 114.56 | 101.50 |
| 4 | B | 148 | HEM | CAA-CBA-CGA | 7.75 | 126.96 | 112.75 |
| 4 | B | 148 | HEM | C2C-C1C-NC | 7.81 | 123.37 | 110.21 |
| 4 | B | 148 | HEM | C2D-C3D-C4D | 7.85 | 114.81 | 101.50 |
| 4 | C | 142 | HEM | CMB-C2B-C3B | 8.15 | 136.86 | 116.53 |
| 4 | B | 148 | HEM | CMB-C2B-C3B | 10.99 | 143.95 | 116.53 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 41 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | A | 142 | HEM | 6 | 0 |
| 4 | B | 148 | HEM | 10 | 0 |
| 4 | C | 142 | HEM | 14 | 0 |
| 4 | D | 148 | HEM | 11 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.