



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:12 PM BST

PDB ID : 3J1E
EMDB ID: : EMD-5395
Title : Cryo-EM structure of 9-fold symmetric rATcpn-beta in apo state
Authors : Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on : 2012-02-06
Resolution : 8.30 Å(reported)
Based on PDB ID : 3KO1

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
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) : trunk27241

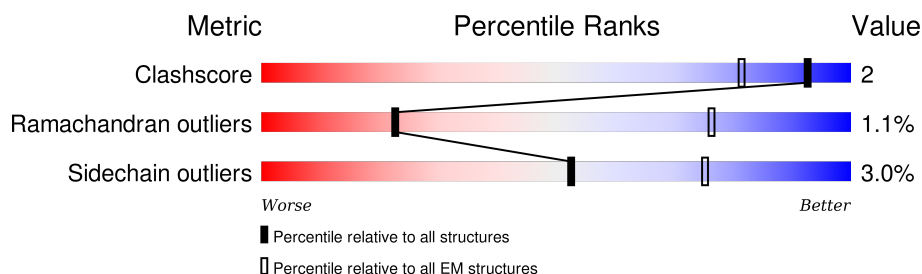
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.30 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 553 | 70% 18% • 9% |
| 1 | B | 553 | 69% 19% • 9% |
| 1 | C | 553 | 70% 20% • 9% |
| 1 | D | 553 | 69% 19% • 9% |
| 1 | E | 553 | 73% 16% • 9% |
| 1 | F | 553 | 71% 18% • 9% |
| 1 | G | 553 | 71% 17% • 9% |
| 1 | H | 553 | 69% 20% • 9% |
| 1 | I | 553 | 74% 15% • 9% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------------------------------------------------------------------|
| 1 | K | 553 | <div><div></div><div>73%</div><div>15%</div><div>•</div><div>9%</div></div> |
| 1 | L | 553 | <div><div></div><div>71%</div><div>17%</div><div>••</div><div>9%</div></div> |
| 1 | M | 553 | <div><div></div><div>72%</div><div>18%</div><div>•</div><div>9%</div></div> |
| 1 | N | 553 | <div><div></div><div>71%</div><div>18%</div><div>•</div><div>9%</div></div> |
| 1 | O | 553 | <div><div></div><div>72%</div><div>17%</div><div>•</div><div>9%</div></div> |
| 1 | P | 553 | <div><div></div><div>69%</div><div>19%</div><div>•</div><div>9%</div></div> |
| 1 | Q | 553 | <div><div></div><div>72%</div><div>17%</div><div>•</div><div>9%</div></div> |
| 1 | R | 553 | <div><div></div><div>73%</div><div>17%</div><div>•</div><div>9%</div></div> |
| 1 | S | 553 | <div><div></div><div>68%</div><div>20%</div><div>•</div><div>9%</div></div> |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 69282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chaperonin beta subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | B | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | C | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | D | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | E | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | F | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | G | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | H | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | I | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | K | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | L | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | M | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | N | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | O | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | P | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | Q | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |
| 1 | R | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |

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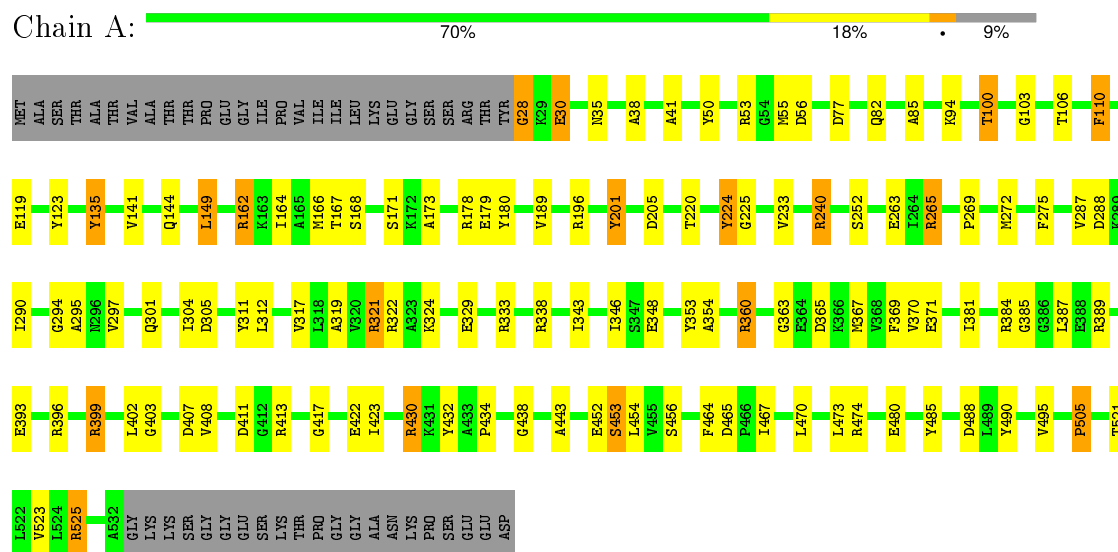
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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | S | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2423 | 658 | 757 | 11 | | |

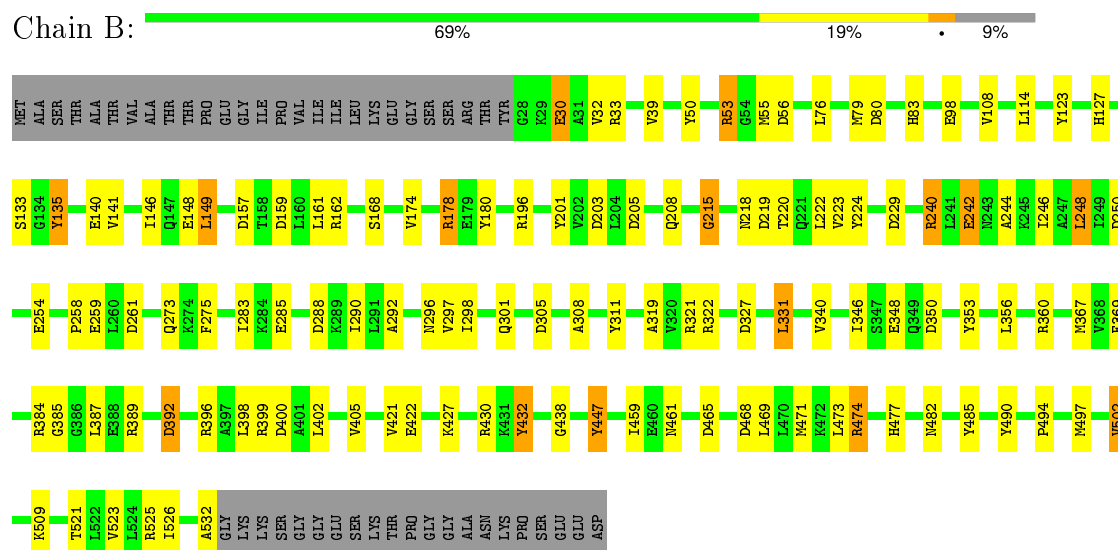
3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chaperonin beta subunit



- Molecule 1: Chaperonin beta subunit



- Molecule 1: Chaperonin beta subunit



[illegible]

Chain G:

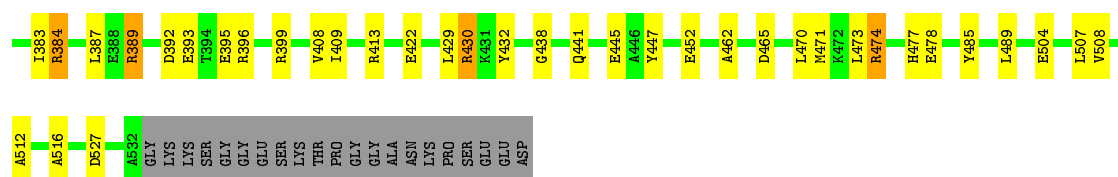
71% 17% 9%

| Amino Acid | Category | Percentage |
|------------|----------|------------|
| GLU | Green | 71% |
| SER | Green | 71% |
| LYS | Green | 71% |
| THR | Green | 71% |
| PRO | Green | 71% |
| GLY | Green | 71% |
| GLY | Green | 71% |
| ALA | Green | 71% |
| ASN | Green | 71% |
| LYS | Green | 71% |
| PRO | Green | 71% |
| SER | Green | 71% |
| GLU | Green | 71% |
| ASP | Green | 71% |
| GLU | Yellow | 17% |
| SER | Yellow | 17% |
| LYS | Yellow | 17% |
| THR | Yellow | 17% |
| PRO | Yellow | 17% |
| GLY | Yellow | 17% |
| GLU | Yellow | 17% |
| ALA | Yellow | 17% |
| ASN | Yellow | 17% |
| LYS | Yellow | 17% |
| PRO | Yellow | 17% |
| SER | Yellow | 17% |
| GLU | Yellow | 17% |
| ASP | Yellow | 17% |
| GLU | Grey | 9% |
| SER | Grey | 9% |
| LYS | Grey | 9% |
| THR | Grey | 9% |
| PRO | Grey | 9% |
| GLY | Grey | 9% |
| GLU | Grey | 9% |
| ALA | Grey | 9% |
| ASN | Grey | 9% |
| LYS | Grey | 9% |
| PRO | Grey | 9% |
| SER | Grey | 9% |
| GLU | Grey | 9% |
| ASP | Grey | 9% |

Chain H:

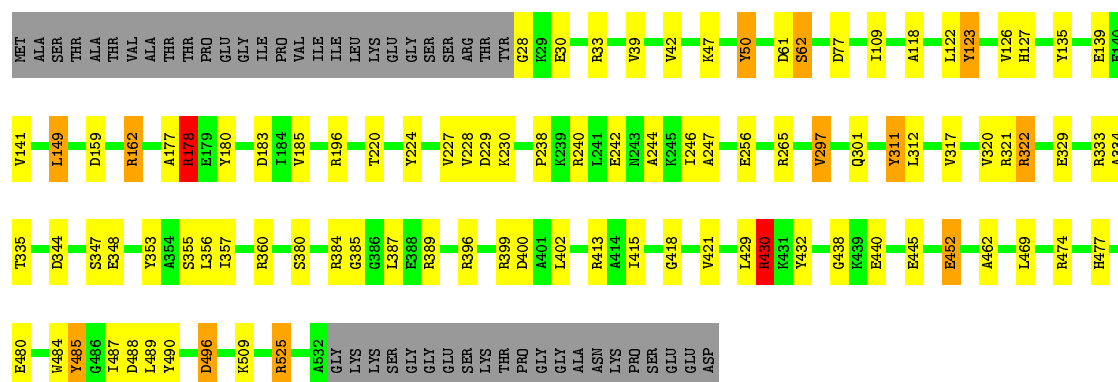
69% 20% 9%

| Position | Amino Acid | Frequency (%) |
|----------|------------|---------------|
| 1 | Met | 69% |
| 2 | Ala | 69% |
| 3 | Ser | 69% |
| 4 | Thr | 69% |
| 5 | Ala | 69% |
| 6 | Thr | 69% |
| 7 | Val | 69% |
| 8 | Thr | 69% |
| 9 | Pro | 69% |
| 10 | Glu | 69% |
| 11 | Gly | 69% |
| 12 | Ile | 69% |
| 13 | Pro | 69% |
| 14 | Val | 69% |
| 15 | Ile | 69% |
| 16 | Leu | 69% |
| 17 | Lys | 69% |
| 18 | Gly | 69% |
| 19 | Ser | 69% |
| 20 | Ser | 69% |
| 21 | Arg | 69% |
| 22 | Thr | 69% |
| 23 | Thr | 69% |
| 24 | Gln | 69% |
| 25 | Gln | 69% |
| 26 | Asp | 69% |
| 27 | Asp | 69% |
| 28 | Asp | 69% |
| 29 | Asp | 69% |
| 30 | Asp | 69% |
| 31 | Asp | 69% |
| 32 | Asp | 69% |
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| 37 | Asp | 69% |
| 38 | Asp | 69% |
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| 151 | Asp | 69% |
| 152 | Asp | 69% |
| 153 | Asp | 69% |
| 154 | Asp | 69% |
| 155 | Asp | 69% |
| 156 | Asp | 69% |
| 157 | Asp | 69% |
| 158 | Asp | |



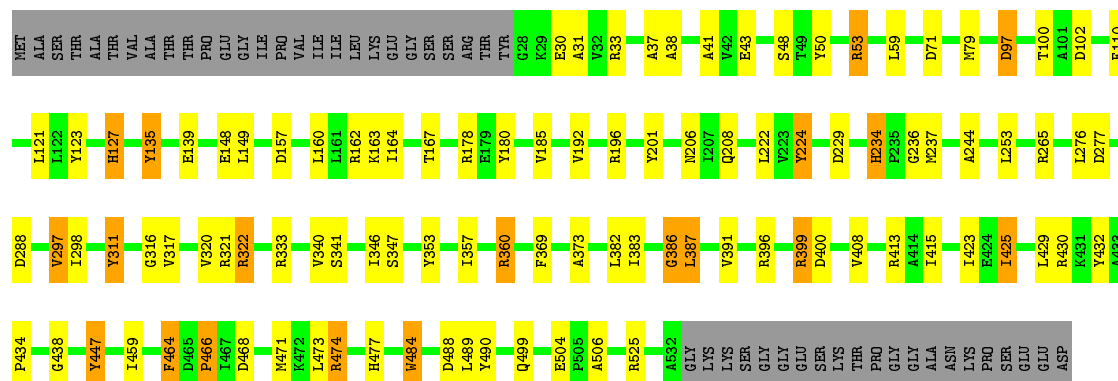
• Molecule 1: Chaperonin beta subunit

Chain I: 74% 15% 9%



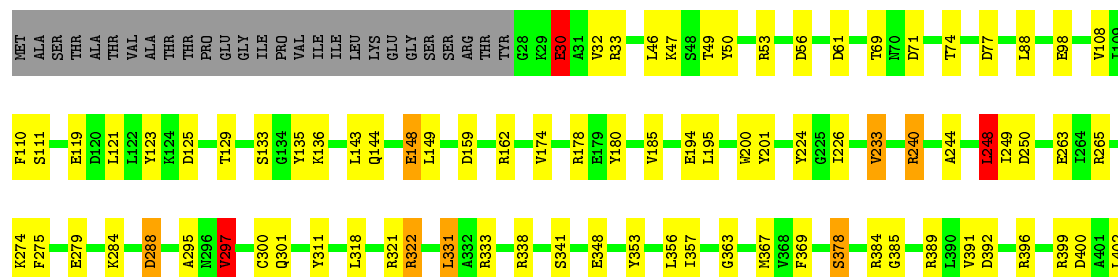
• Molecule 1: Chaperonin beta subunit

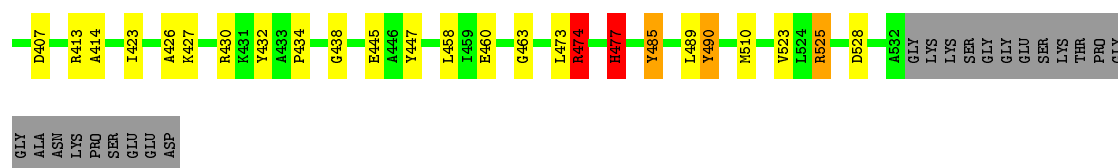
Chain K: 73% 15% 9%



• Molecule 1: Chaperonin beta subunit

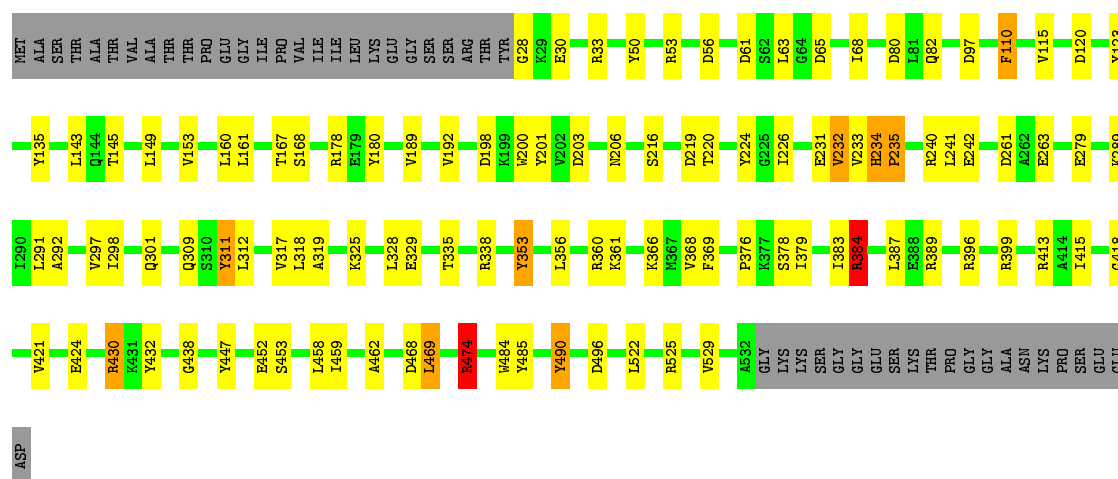
Chain L: 71% 17% 9%





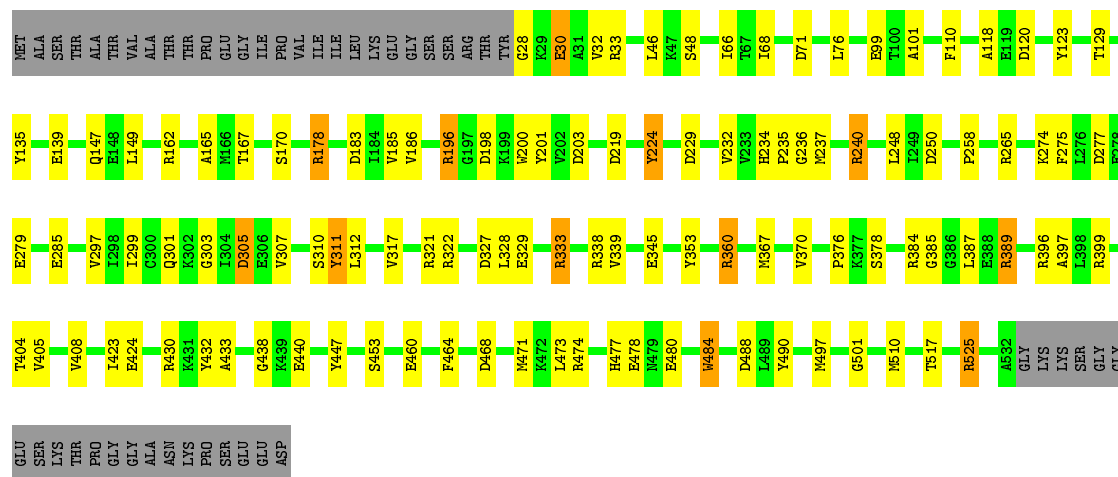
• Molecule 1: Chaperonin beta subunit

Chain M: 72% 18% 9%



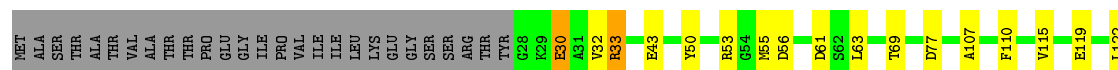
• Molecule 1: Chaperonin beta subunit

Chain N: 71% 18% 9%

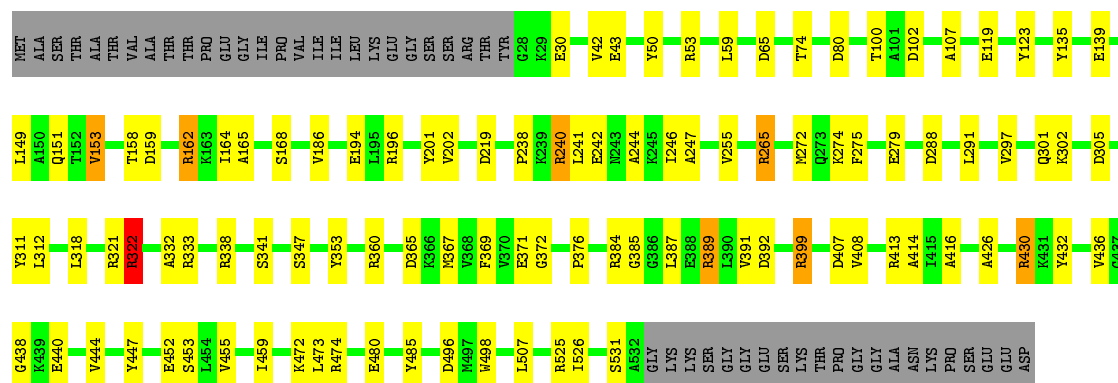


• Molecule 1: Chaperonin beta subunit

Chain O: 72% 17% 9%

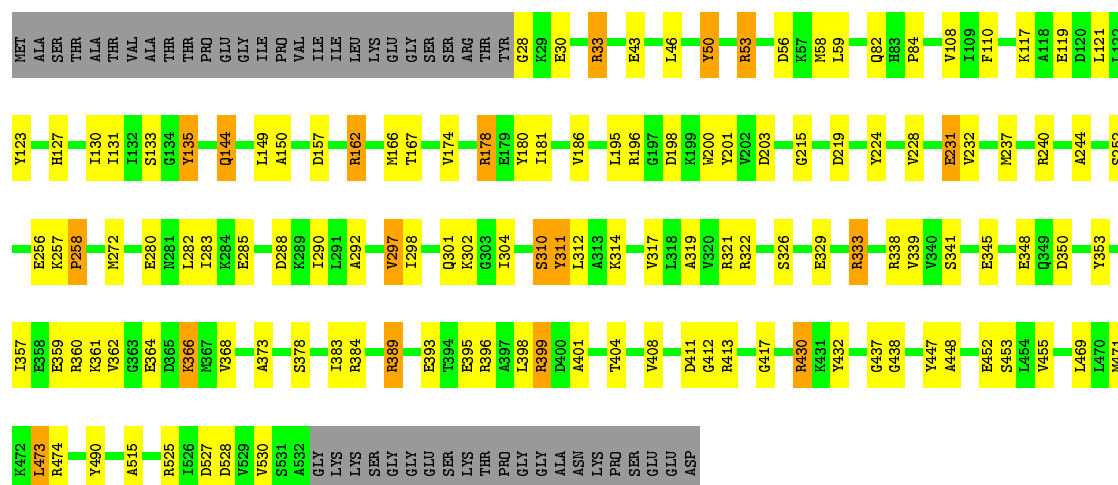


Chain R:  73% 17% 9%



• Molecule 1: Chaperonin beta subunit

Chain S:  68% 20% 9%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | The whole micrograph | Depositor |
| Microscope | FEI Titan Krios | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3500 | Depositor |
| Magnification | 96000 | Depositor |
| Image detector | Gatan Ultrascan 4000 Model 895 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 1 | A | 1.57 | 17/3886 (0.4%) | 1.94 | 86/5245 (1.6%) |
| 1 | B | 1.58 | 20/3886 (0.5%) | 1.92 | 79/5245 (1.5%) |
| 1 | C | 1.59 | 21/3886 (0.5%) | 1.95 | 95/5245 (1.8%) |
| 1 | D | 1.61 | 22/3886 (0.6%) | 1.97 | 93/5245 (1.8%) |
| 1 | E | 1.59 | 22/3886 (0.6%) | 1.94 | 94/5245 (1.8%) |
| 1 | F | 1.58 | 20/3886 (0.5%) | 1.92 | 80/5245 (1.5%) |
| 1 | G | 1.57 | 19/3886 (0.5%) | 1.90 | 80/5245 (1.5%) |
| 1 | H | 1.57 | 21/3886 (0.5%) | 1.93 | 90/5245 (1.7%) |
| 1 | I | 1.57 | 20/3886 (0.5%) | 1.95 | 82/5245 (1.6%) |
| 1 | K | 1.59 | 21/3886 (0.5%) | 1.93 | 82/5245 (1.6%) |
| 1 | L | 1.58 | 20/3886 (0.5%) | 1.93 | 84/5245 (1.6%) |
| 1 | M | 1.58 | 15/3886 (0.4%) | 1.90 | 73/5245 (1.4%) |
| 1 | N | 1.59 | 17/3886 (0.4%) | 1.99 | 85/5245 (1.6%) |
| 1 | O | 1.60 | 17/3886 (0.4%) | 1.93 | 72/5245 (1.4%) |
| 1 | P | 1.60 | 21/3886 (0.5%) | 1.91 | 74/5245 (1.4%) |
| 1 | Q | 1.60 | 21/3886 (0.5%) | 1.97 | 71/5245 (1.4%) |
| 1 | R | 1.57 | 15/3886 (0.4%) | 1.86 | 76/5245 (1.4%) |
| 1 | S | 1.59 | 18/3886 (0.5%) | 1.90 | 88/5245 (1.7%) |
| All | All | 1.58 | 347/69948 (0.5%) | 1.93 | 1484/94410 (1.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 11 |
| 1 | B | 0 | 15 |
| 1 | C | 0 | 5 |
| 1 | D | 0 | 11 |
| 1 | E | 0 | 10 |
| 1 | F | 0 | 10 |
| 1 | G | 0 | 11 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | H | 0 | 8 |
| 1 | I | 0 | 8 |
| 1 | K | 0 | 12 |
| 1 | L | 0 | 8 |
| 1 | M | 0 | 10 |
| 1 | N | 0 | 15 |
| 1 | O | 0 | 7 |
| 1 | P | 0 | 9 |
| 1 | Q | 0 | 14 |
| 1 | R | 0 | 10 |
| 1 | S | 0 | 11 |
| All | All | 0 | 185 |

All (347) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | S | 28 | GLY | N-CA | 8.99 | 1.59 | 1.46 |
| 1 | O | 347 | SER | CA-CB | 8.74 | 1.66 | 1.52 |
| 1 | B | 133 | SER | CA-CB | 8.45 | 1.65 | 1.52 |
| 1 | R | 279 | GLU | CD-OE2 | 8.16 | 1.34 | 1.25 |
| 1 | C | 28 | GLY | N-CA | 8.16 | 1.58 | 1.46 |
| 1 | G | 413 | ARG | CD-NE | 8.07 | 1.60 | 1.46 |
| 1 | F | 490 | TYR | CG-CD2 | 8.05 | 1.49 | 1.39 |
| 1 | F | 168 | SER | CA-CB | 8.01 | 1.65 | 1.52 |
| 1 | K | 48 | SER | CA-CB | 8.00 | 1.65 | 1.52 |
| 1 | R | 372 | GLY | CA-C | -7.94 | 1.39 | 1.51 |
| 1 | P | 432 | TYR | CZ-OH | 7.84 | 1.51 | 1.37 |
| 1 | N | 353 | TYR | CE1-CZ | 7.84 | 1.48 | 1.38 |
| 1 | D | 28 | GLY | N-CA | 7.78 | 1.57 | 1.46 |
| 1 | M | 28 | GLY | N-CA | 7.73 | 1.57 | 1.46 |
| 1 | D | 154 | SER | CA-CB | 7.23 | 1.63 | 1.52 |
| 1 | G | 133 | SER | CA-CB | 7.16 | 1.63 | 1.52 |
| 1 | R | 447 | TYR | CE2-CZ | 7.10 | 1.47 | 1.38 |
| 1 | N | 311 | TYR | CE2-CZ | 7.09 | 1.47 | 1.38 |
| 1 | D | 453 | SER | CA-CB | 7.04 | 1.63 | 1.52 |
| 1 | N | 170 | SER | CA-CB | 7.03 | 1.63 | 1.52 |
| 1 | E | 338 | ARG | CD-NE | 6.97 | 1.58 | 1.46 |
| 1 | P | 353 | TYR | CB-CG | -6.97 | 1.41 | 1.51 |
| 1 | C | 490 | TYR | CZ-OH | 6.87 | 1.49 | 1.37 |
| 1 | C | 180 | TYR | CE2-CZ | 6.80 | 1.47 | 1.38 |
| 1 | R | 440 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | R | 474 | ARG | CD-NE | 6.73 | 1.57 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 498 | TRP | CE3-CZ3 | 6.72 | 1.49 | 1.38 |
| 1 | S | 310 | SER | CB-OG | -6.71 | 1.33 | 1.42 |
| 1 | G | 240 | ARG | CD-NE | 6.69 | 1.57 | 1.46 |
| 1 | A | 240 | ARG | CD-NE | 6.67 | 1.57 | 1.46 |
| 1 | P | 53 | ARG | CD-NE | 6.64 | 1.57 | 1.46 |
| 1 | C | 196 | ARG | CD-NE | 6.60 | 1.57 | 1.46 |
| 1 | C | 168 | SER | CA-CB | 6.57 | 1.62 | 1.52 |
| 1 | F | 445 | GLU | CB-CG | 6.57 | 1.64 | 1.52 |
| 1 | R | 341 | SER | CA-CB | 6.56 | 1.62 | 1.52 |
| 1 | O | 119 | GLU | CB-CG | 6.55 | 1.64 | 1.52 |
| 1 | H | 285 | GLU | CD-OE1 | 6.55 | 1.32 | 1.25 |
| 1 | Q | 389 | ARG | CD-NE | 6.54 | 1.57 | 1.46 |
| 1 | P | 133 | SER | CA-CB | 6.54 | 1.62 | 1.52 |
| 1 | D | 48 | SER | CA-CB | 6.51 | 1.62 | 1.52 |
| 1 | O | 176 | GLY | CA-C | -6.51 | 1.41 | 1.51 |
| 1 | R | 369 | PHE | CG-CD1 | 6.50 | 1.48 | 1.38 |
| 1 | H | 364 | GLU | CB-CG | 6.49 | 1.64 | 1.52 |
| 1 | H | 200 | TRP | CZ2-CH2 | 6.47 | 1.49 | 1.37 |
| 1 | K | 386 | GLY | CA-C | -6.47 | 1.41 | 1.51 |
| 1 | A | 453 | SER | CB-OG | 6.46 | 1.50 | 1.42 |
| 1 | H | 311 | TYR | CE2-CZ | 6.39 | 1.46 | 1.38 |
| 1 | Q | 33 | ARG | CD-NE | 6.38 | 1.57 | 1.46 |
| 1 | S | 329 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | E | 490 | TYR | CE1-CZ | 6.37 | 1.46 | 1.38 |
| 1 | D | 275 | PHE | CE2-CZ | 6.35 | 1.49 | 1.37 |
| 1 | K | 353 | TYR | CE1-CZ | 6.33 | 1.46 | 1.38 |
| 1 | F | 287 | VAL | CB-CG1 | 6.32 | 1.66 | 1.52 |
| 1 | D | 485 | TYR | CB-CG | -6.32 | 1.42 | 1.51 |
| 1 | C | 180 | TYR | CB-CG | -6.30 | 1.42 | 1.51 |
| 1 | M | 353 | TYR | CE1-CZ | 6.30 | 1.46 | 1.38 |
| 1 | E | 83 | HIS | CB-CG | 6.29 | 1.61 | 1.50 |
| 1 | N | 345 | GLU | CA-CB | 6.28 | 1.67 | 1.53 |
| 1 | L | 333 | ARG | CD-NE | 6.25 | 1.57 | 1.46 |
| 1 | K | 447 | TYR | CZ-OH | 6.23 | 1.48 | 1.37 |
| 1 | G | 180 | TYR | CG-CD2 | 6.23 | 1.47 | 1.39 |
| 1 | K | 148 | GLU | CD-OE2 | 6.23 | 1.32 | 1.25 |
| 1 | B | 348 | GLU | CD-OE1 | 6.22 | 1.32 | 1.25 |
| 1 | N | 285 | GLU | CG-CD | 6.20 | 1.61 | 1.51 |
| 1 | A | 252 | SER | CA-CB | 6.20 | 1.62 | 1.52 |
| 1 | E | 360 | ARG | CD-NE | 6.18 | 1.56 | 1.46 |
| 1 | Q | 445 | GLU | CD-OE2 | 6.18 | 1.32 | 1.25 |
| 1 | C | 486 | GLY | CA-C | -6.17 | 1.42 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | S | 401 | ALA | CA-CB | 6.14 | 1.65 | 1.52 |
| 1 | H | 200 | TRP | CB-CG | 6.14 | 1.61 | 1.50 |
| 1 | N | 303 | GLY | CA-C | -6.13 | 1.42 | 1.51 |
| 1 | A | 403 | GLY | CA-C | -6.10 | 1.42 | 1.51 |
| 1 | D | 419 | GLY | CA-C | 6.08 | 1.61 | 1.51 |
| 1 | B | 218 | ASN | CB-CG | 6.07 | 1.65 | 1.51 |
| 1 | F | 432 | TYR | CE2-CZ | 6.06 | 1.46 | 1.38 |
| 1 | N | 432 | TYR | CG-CD2 | 6.06 | 1.47 | 1.39 |
| 1 | O | 252 | SER | CB-OG | 6.06 | 1.50 | 1.42 |
| 1 | I | 329 | GLU | CD-OE1 | 6.06 | 1.32 | 1.25 |
| 1 | S | 133 | SER | CA-CB | 6.06 | 1.62 | 1.52 |
| 1 | F | 475 | SER | CB-OG | 6.05 | 1.50 | 1.42 |
| 1 | E | 531 | SER | CB-OG | 6.04 | 1.50 | 1.42 |
| 1 | E | 254 | GLU | CD-OE1 | 6.04 | 1.32 | 1.25 |
| 1 | O | 178 | ARG | CD-NE | 6.04 | 1.56 | 1.46 |
| 1 | N | 135 | TYR | CZ-OH | 6.04 | 1.48 | 1.37 |
| 1 | R | 384 | ARG | CD-NE | 6.04 | 1.56 | 1.46 |
| 1 | B | 369 | PHE | CG-CD2 | 6.03 | 1.47 | 1.38 |
| 1 | A | 28 | GLY | N-CA | 6.03 | 1.55 | 1.46 |
| 1 | S | 258 | PRO | N-CA | -6.03 | 1.37 | 1.47 |
| 1 | A | 168 | SER | CA-CB | 6.02 | 1.61 | 1.52 |
| 1 | F | 28 | GLY | N-CA | 6.02 | 1.55 | 1.46 |
| 1 | P | 388 | GLU | CB-CG | 6.01 | 1.63 | 1.52 |
| 1 | Q | 433 | ALA | C-N | -6.01 | 1.22 | 1.34 |
| 1 | L | 430 | ARG | CD-NE | 6.01 | 1.56 | 1.46 |
| 1 | G | 353 | TYR | CG-CD2 | 6.01 | 1.47 | 1.39 |
| 1 | C | 187 | LYS | CA-CB | 6.00 | 1.67 | 1.53 |
| 1 | G | 216 | SER | CB-OG | 6.00 | 1.50 | 1.42 |
| 1 | F | 201 | TYR | CG-CD2 | 5.99 | 1.47 | 1.39 |
| 1 | I | 242 | GLU | CG-CD | 5.99 | 1.60 | 1.51 |
| 1 | F | 224 | TYR | CD2-CE2 | 5.98 | 1.48 | 1.39 |
| 1 | G | 119 | GLU | CB-CG | 5.95 | 1.63 | 1.52 |
| 1 | D | 200 | TRP | CE3-CZ3 | 5.93 | 1.48 | 1.38 |
| 1 | H | 176 | GLY | N-CA | -5.92 | 1.37 | 1.46 |
| 1 | M | 279 | GLU | CG-CD | 5.92 | 1.60 | 1.51 |
| 1 | H | 119 | GLU | CG-CD | 5.92 | 1.60 | 1.51 |
| 1 | Q | 363 | GLY | N-CA | -5.92 | 1.37 | 1.46 |
| 1 | C | 200 | TRP | CE3-CZ3 | 5.92 | 1.48 | 1.38 |
| 1 | N | 378 | SER | CB-OG | 5.91 | 1.50 | 1.42 |
| 1 | B | 322 | ARG | CD-NE | 5.91 | 1.56 | 1.46 |
| 1 | C | 243 | ASN | CA-CB | 5.91 | 1.68 | 1.53 |
| 1 | H | 447 | TYR | CD1-CE1 | 5.91 | 1.48 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | L | 224 | TYR | CG-CD2 | 5.89 | 1.46 | 1.39 |
| 1 | C | 466 | PRO | N-CD | -5.89 | 1.39 | 1.47 |
| 1 | I | 256 | GLU | CD-OE1 | 5.87 | 1.32 | 1.25 |
| 1 | D | 474 | ARG | CZ-NH1 | 5.86 | 1.40 | 1.33 |
| 1 | P | 265 | ARG | CD-NE | 5.85 | 1.56 | 1.46 |
| 1 | H | 445 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 1 | G | 253 | LEU | N-CA | -5.84 | 1.34 | 1.46 |
| 1 | O | 402 | LEU | CA-C | -5.84 | 1.37 | 1.52 |
| 1 | I | 311 | TYR | CG-CD2 | 5.84 | 1.46 | 1.39 |
| 1 | I | 347 | SER | CA-CB | 5.82 | 1.61 | 1.52 |
| 1 | K | 33 | ARG | NE-CZ | 5.82 | 1.40 | 1.33 |
| 1 | B | 174 | VAL | CB-CG2 | 5.81 | 1.65 | 1.52 |
| 1 | L | 427 | LYS | CA-CB | 5.81 | 1.66 | 1.53 |
| 1 | L | 148 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | N | 501 | GLY | CA-C | -5.80 | 1.42 | 1.51 |
| 1 | P | 119 | GLU | CG-CD | 5.80 | 1.60 | 1.51 |
| 1 | F | 140 | GLU | CB-CG | 5.78 | 1.63 | 1.52 |
| 1 | A | 399 | ARG | CD-NE | 5.78 | 1.56 | 1.46 |
| 1 | F | 259 | GLU | CG-CD | 5.77 | 1.60 | 1.51 |
| 1 | M | 338 | ARG | CD-NE | 5.76 | 1.56 | 1.46 |
| 1 | B | 180 | TYR | CE1-CZ | 5.76 | 1.46 | 1.38 |
| 1 | I | 348 | GLU | CD-OE1 | 5.74 | 1.31 | 1.25 |
| 1 | M | 168 | SER | CA-CB | 5.74 | 1.61 | 1.52 |
| 1 | I | 452 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |
| 1 | B | 254 | GLU | CB-CG | 5.72 | 1.63 | 1.52 |
| 1 | E | 140 | GLU | CB-CG | 5.72 | 1.63 | 1.52 |
| 1 | L | 119 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |
| 1 | E | 460 | GLU | CD-OE1 | 5.71 | 1.31 | 1.25 |
| 1 | A | 311 | TYR | CE1-CZ | 5.71 | 1.46 | 1.38 |
| 1 | R | 194 | GLU | CD-OE1 | 5.71 | 1.31 | 1.25 |
| 1 | K | 432 | TYR | CB-CG | -5.71 | 1.43 | 1.51 |
| 1 | I | 445 | GLU | CG-CD | 5.71 | 1.60 | 1.51 |
| 1 | C | 316 | GLY | CA-C | 5.70 | 1.60 | 1.51 |
| 1 | P | 316 | GLY | CA-C | -5.70 | 1.42 | 1.51 |
| 1 | M | 123 | TYR | CE1-CZ | 5.70 | 1.46 | 1.38 |
| 1 | M | 453 | SER | N-CA | 5.70 | 1.57 | 1.46 |
| 1 | I | 28 | GLY | N-CA | 5.69 | 1.54 | 1.46 |
| 1 | M | 216 | SER | CB-OG | 5.69 | 1.49 | 1.42 |
| 1 | P | 460 | GLU | CG-CD | 5.69 | 1.60 | 1.51 |
| 1 | N | 235 | PRO | N-CA | -5.68 | 1.37 | 1.47 |
| 1 | B | 485 | TYR | CB-CG | -5.68 | 1.43 | 1.51 |
| 1 | Q | 103 | GLY | N-CA | 5.67 | 1.54 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | Q | 280 | GLU | CD-OE2 | 5.67 | 1.31 | 1.25 |
| 1 | H | 285 | GLU | CG-CD | -5.66 | 1.43 | 1.51 |
| 1 | H | 371 | GLU | CB-CG | 5.66 | 1.62 | 1.52 |
| 1 | K | 347 | SER | CB-OG | -5.65 | 1.34 | 1.42 |
| 1 | L | 240 | ARG | CA-CB | 5.63 | 1.66 | 1.53 |
| 1 | G | 50 | TYR | CE1-CZ | 5.63 | 1.45 | 1.38 |
| 1 | C | 322 | ARG | CD-NE | 5.63 | 1.56 | 1.46 |
| 1 | I | 440 | GLU | CD-OE2 | 5.63 | 1.31 | 1.25 |
| 1 | P | 464 | PHE | CG-CD2 | 5.62 | 1.47 | 1.38 |
| 1 | L | 445 | GLU | CD-OE1 | 5.61 | 1.31 | 1.25 |
| 1 | K | 447 | TYR | CE2-CZ | 5.61 | 1.45 | 1.38 |
| 1 | Q | 279 | GLU | CG-CD | 5.61 | 1.60 | 1.51 |
| 1 | D | 321 | ARG | CD-NE | 5.59 | 1.55 | 1.46 |
| 1 | Q | 413 | ARG | CD-NE | 5.59 | 1.55 | 1.46 |
| 1 | O | 531 | SER | CA-CB | 5.59 | 1.61 | 1.52 |
| 1 | M | 180 | TYR | CB-CG | 5.59 | 1.60 | 1.51 |
| 1 | R | 371 | GLU | CD-OE1 | -5.59 | 1.19 | 1.25 |
| 1 | C | 353 | TYR | CE1-CZ | -5.58 | 1.31 | 1.38 |
| 1 | C | 53 | ARG | CD-NE | 5.57 | 1.55 | 1.46 |
| 1 | H | 201 | TYR | CZ-OH | 5.57 | 1.47 | 1.37 |
| 1 | E | 436 | VAL | CA-CB | -5.56 | 1.43 | 1.54 |
| 1 | O | 201 | TYR | CG-CD2 | 5.54 | 1.46 | 1.39 |
| 1 | D | 318 | LEU | CA-CB | 5.54 | 1.66 | 1.53 |
| 1 | P | 371 | GLU | CD-OE1 | 5.53 | 1.31 | 1.25 |
| 1 | E | 490 | TYR | CE2-CZ | 5.52 | 1.45 | 1.38 |
| 1 | G | 326 | SER | CA-CB | 5.52 | 1.61 | 1.52 |
| 1 | S | 417 | GLY | N-CA | 5.52 | 1.54 | 1.46 |
| 1 | L | 378 | SER | CA-CB | 5.52 | 1.61 | 1.52 |
| 1 | G | 51 | GLY | CA-C | -5.51 | 1.43 | 1.51 |
| 1 | A | 50 | TYR | CA-CB | 5.50 | 1.66 | 1.53 |
| 1 | I | 353 | TYR | CE2-CZ | 5.50 | 1.45 | 1.38 |
| 1 | K | 178 | ARG | CD-NE | 5.50 | 1.55 | 1.46 |
| 1 | Q | 385 | GLY | C-N | 5.49 | 1.43 | 1.33 |
| 1 | A | 396 | ARG | CD-NE | 5.49 | 1.55 | 1.46 |
| 1 | A | 294 | GLY | CA-C | -5.49 | 1.43 | 1.51 |
| 1 | B | 389 | ARG | NE-CZ | 5.49 | 1.40 | 1.33 |
| 1 | E | 345 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 1 | D | 224 | TYR | CD2-CE2 | 5.47 | 1.47 | 1.39 |
| 1 | M | 242 | GLU | CD-OE2 | 5.47 | 1.31 | 1.25 |
| 1 | F | 200 | TRP | NE1-CE2 | -5.47 | 1.30 | 1.37 |
| 1 | F | 263 | GLU | CD-OE2 | -5.47 | 1.19 | 1.25 |
| 1 | H | 201 | TYR | CD1-CE1 | 5.46 | 1.47 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | K | 148 | GLU | CB-CG | 5.45 | 1.62 | 1.52 |
| 1 | M | 418 | GLY | CA-C | 5.45 | 1.60 | 1.51 |
| 1 | H | 235 | PRO | N-CD | 5.44 | 1.55 | 1.47 |
| 1 | E | 384 | ARG | CD-NE | 5.44 | 1.55 | 1.46 |
| 1 | Q | 402 | LEU | CA-CB | 5.44 | 1.66 | 1.53 |
| 1 | C | 128 | PRO | CA-CB | -5.44 | 1.42 | 1.53 |
| 1 | K | 316 | GLY | N-CA | -5.44 | 1.37 | 1.46 |
| 1 | C | 529 | VAL | CB-CG1 | 5.43 | 1.64 | 1.52 |
| 1 | I | 360 | ARG | CD-NE | 5.43 | 1.55 | 1.46 |
| 1 | E | 376 | PRO | CA-C | -5.43 | 1.42 | 1.52 |
| 1 | B | 494 | PRO | N-CD | -5.42 | 1.40 | 1.47 |
| 1 | H | 110 | PHE | CE1-CZ | 5.42 | 1.47 | 1.37 |
| 1 | I | 380 | SER | CA-CB | 5.42 | 1.61 | 1.52 |
| 1 | B | 461 | ASN | CB-CG | 5.42 | 1.63 | 1.51 |
| 1 | P | 208 | GLN | CA-CB | 5.42 | 1.65 | 1.53 |
| 1 | Q | 380 | SER | CB-OG | -5.42 | 1.35 | 1.42 |
| 1 | H | 178 | ARG | N-CA | -5.41 | 1.35 | 1.46 |
| 1 | I | 62 | SER | CA-CB | 5.41 | 1.61 | 1.52 |
| 1 | O | 127 | HIS | CB-CG | 5.41 | 1.59 | 1.50 |
| 1 | I | 353 | TYR | CE1-CZ | 5.41 | 1.45 | 1.38 |
| 1 | Q | 133 | SER | CA-CB | 5.40 | 1.61 | 1.52 |
| 1 | B | 30 | GLU | CG-CD | 5.40 | 1.60 | 1.51 |
| 1 | R | 347 | SER | CB-OG | 5.39 | 1.49 | 1.42 |
| 1 | S | 280 | GLU | C-N | 5.38 | 1.46 | 1.34 |
| 1 | P | 33 | ARG | CG-CD | 5.38 | 1.65 | 1.51 |
| 1 | F | 192 | VAL | CB-CG1 | 5.38 | 1.64 | 1.52 |
| 1 | C | 488 | ASP | CA-CB | 5.37 | 1.65 | 1.53 |
| 1 | Q | 475 | SER | CB-OG | 5.37 | 1.49 | 1.42 |
| 1 | A | 464 | PHE | CB-CG | -5.37 | 1.42 | 1.51 |
| 1 | I | 135 | TYR | CA-CB | 5.36 | 1.65 | 1.53 |
| 1 | P | 353 | TYR | CZ-OH | 5.35 | 1.47 | 1.37 |
| 1 | E | 292 | ALA | CA-CB | 5.35 | 1.63 | 1.52 |
| 1 | P | 135 | TYR | CG-CD2 | 5.34 | 1.46 | 1.39 |
| 1 | S | 412 | GLY | CA-C | -5.33 | 1.43 | 1.51 |
| 1 | D | 490 | TYR | CD2-CE2 | 5.33 | 1.47 | 1.39 |
| 1 | E | 452 | GLU | CB-CG | 5.33 | 1.62 | 1.52 |
| 1 | A | 179 | GLU | CG-CD | 5.32 | 1.59 | 1.51 |
| 1 | G | 263 | GLU | CD-OE2 | 5.31 | 1.31 | 1.25 |
| 1 | F | 52 | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 1 | E | 349 | GLN | CG-CD | 5.31 | 1.63 | 1.51 |
| 1 | K | 396 | ARG | CD-NE | 5.30 | 1.55 | 1.46 |
| 1 | H | 504 | GLU | CD-OE1 | 5.30 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | N | 480 | GLU | CB-CG | 5.30 | 1.62 | 1.52 |
| 1 | D | 98 | GLU | CG-CD | 5.30 | 1.59 | 1.51 |
| 1 | E | 359 | GLU | CD-OE1 | 5.30 | 1.31 | 1.25 |
| 1 | L | 353 | TYR | CZ-OH | 5.29 | 1.46 | 1.37 |
| 1 | F | 471 | MET | CA-CB | 5.28 | 1.65 | 1.53 |
| 1 | D | 440 | GLU | CB-CG | 5.27 | 1.62 | 1.52 |
| 1 | Q | 461 | ASN | CA-CB | 5.27 | 1.66 | 1.53 |
| 1 | A | 467 | ILE | CA-CB | -5.27 | 1.42 | 1.54 |
| 1 | H | 447 | TYR | CZ-OH | 5.27 | 1.46 | 1.37 |
| 1 | G | 441 | GLN | CG-CD | 5.26 | 1.63 | 1.51 |
| 1 | S | 341 | SER | CA-CB | 5.26 | 1.60 | 1.52 |
| 1 | O | 171 | SER | CA-CB | 5.25 | 1.60 | 1.52 |
| 1 | Q | 453 | SER | CA-CB | 5.25 | 1.60 | 1.52 |
| 1 | I | 430 | ARG | CD-NE | 5.25 | 1.55 | 1.46 |
| 1 | Q | 492 | GLY | N-CA | 5.25 | 1.53 | 1.46 |
| 1 | A | 432 | TYR | CG-CD2 | 5.25 | 1.46 | 1.39 |
| 1 | R | 123 | TYR | CE1-CZ | 5.25 | 1.45 | 1.38 |
| 1 | L | 284 | LYS | C-N | 5.25 | 1.46 | 1.34 |
| 1 | M | 235 | PRO | N-CD | -5.24 | 1.40 | 1.47 |
| 1 | L | 348 | GLU | CB-CG | 5.24 | 1.62 | 1.52 |
| 1 | B | 180 | TYR | CZ-OH | 5.24 | 1.46 | 1.37 |
| 1 | S | 326 | SER | CA-CB | 5.23 | 1.60 | 1.52 |
| 1 | D | 168 | SER | CA-CB | -5.23 | 1.45 | 1.52 |
| 1 | D | 527 | ASP | CB-CG | -5.23 | 1.40 | 1.51 |
| 1 | G | 258 | PRO | N-CD | -5.23 | 1.40 | 1.47 |
| 1 | S | 437 | GLY | C-N | 5.23 | 1.42 | 1.33 |
| 1 | S | 364 | GLU | CG-CD | 5.23 | 1.59 | 1.51 |
| 1 | S | 119 | GLU | CB-CG | 5.23 | 1.62 | 1.52 |
| 1 | D | 194 | GLU | CD-OE1 | 5.22 | 1.31 | 1.25 |
| 1 | M | 53 | ARG | CD-NE | 5.22 | 1.55 | 1.46 |
| 1 | P | 179 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | O | 388 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | G | 525 | ARG | CZ-NH1 | -5.21 | 1.26 | 1.33 |
| 1 | S | 144 | GLN | CA-CB | 5.21 | 1.65 | 1.53 |
| 1 | P | 135 | TYR | CE1-CZ | 5.21 | 1.45 | 1.38 |
| 1 | K | 396 | ARG | CZ-NH1 | 5.20 | 1.39 | 1.33 |
| 1 | M | 200 | TRP | NE1-CE2 | 5.20 | 1.44 | 1.37 |
| 1 | A | 201 | TYR | CE1-CZ | 5.20 | 1.45 | 1.38 |
| 1 | B | 208 | GLN | N-CA | -5.20 | 1.35 | 1.46 |
| 1 | K | 50 | TYR | CB-CG | -5.20 | 1.43 | 1.51 |
| 1 | K | 504 | GLU | CB-CG | 5.20 | 1.62 | 1.52 |
| 1 | S | 180 | TYR | CE2-CZ | 5.19 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | B | 292 | ALA | CA-CB | 5.19 | 1.63 | 1.52 |
| 1 | O | 278 | GLU | CD-OE1 | 5.18 | 1.31 | 1.25 |
| 1 | F | 30 | GLU | CB-CG | 5.16 | 1.61 | 1.52 |
| 1 | B | 201 | TYR | CB-CG | 5.16 | 1.59 | 1.51 |
| 1 | I | 311 | TYR | CZ-OH | 5.16 | 1.46 | 1.37 |
| 1 | Q | 105 | LYS | CA-CB | 5.16 | 1.65 | 1.53 |
| 1 | E | 112 | GLY | CA-C | 5.16 | 1.60 | 1.51 |
| 1 | F | 278 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | M | 413 | ARG | CZ-NH1 | 5.16 | 1.39 | 1.33 |
| 1 | C | 311 | TYR | CG-CD2 | 5.15 | 1.45 | 1.39 |
| 1 | S | 348 | GLU | C-N | 5.15 | 1.45 | 1.34 |
| 1 | L | 460 | GLU | CG-CD | -5.14 | 1.44 | 1.51 |
| 1 | H | 316 | GLY | N-CA | -5.14 | 1.38 | 1.46 |
| 1 | O | 115 | VAL | CB-CG2 | 5.14 | 1.63 | 1.52 |
| 1 | B | 140 | GLU | CD-OE1 | 5.13 | 1.31 | 1.25 |
| 1 | N | 433 | ALA | C-N | 5.13 | 1.44 | 1.34 |
| 1 | C | 180 | TYR | CZ-OH | 5.13 | 1.46 | 1.37 |
| 1 | H | 393 | GLU | CB-CG | 5.13 | 1.61 | 1.52 |
| 1 | D | 224 | TYR | CB-CG | -5.12 | 1.44 | 1.51 |
| 1 | E | 303 | GLY | CA-C | -5.12 | 1.43 | 1.51 |
| 1 | R | 447 | TYR | CG-CD1 | 5.12 | 1.45 | 1.39 |
| 1 | K | 466 | PRO | N-CD | 5.12 | 1.55 | 1.47 |
| 1 | P | 518 | GLU | CD-OE2 | -5.12 | 1.20 | 1.25 |
| 1 | L | 363 | GLY | CA-C | -5.12 | 1.43 | 1.51 |
| 1 | I | 418 | GLY | CA-C | -5.11 | 1.43 | 1.51 |
| 1 | B | 168 | SER | CA-CB | 5.11 | 1.60 | 1.52 |
| 1 | G | 204 | LEU | N-CA | -5.11 | 1.36 | 1.46 |
| 1 | N | 432 | TYR | CE2-CZ | 5.11 | 1.45 | 1.38 |
| 1 | O | 197 | GLY | CA-C | 5.09 | 1.59 | 1.51 |
| 1 | I | 50 | TYR | CD2-CE2 | 5.09 | 1.47 | 1.39 |
| 1 | S | 231 | GLU | CB-CG | 5.09 | 1.61 | 1.52 |
| 1 | N | 198 | ASP | CB-CG | -5.08 | 1.41 | 1.51 |
| 1 | Q | 62 | SER | CA-CB | 5.08 | 1.60 | 1.52 |
| 1 | L | 200 | TRP | CZ2-CH2 | 5.08 | 1.47 | 1.37 |
| 1 | L | 279 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | D | 201 | TYR | CG-CD2 | 5.08 | 1.45 | 1.39 |
| 1 | B | 98 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | F | 485 | TYR | CE2-CZ | 5.07 | 1.45 | 1.38 |
| 1 | L | 434 | PRO | CA-C | -5.07 | 1.42 | 1.52 |
| 1 | L | 32 | VAL | CA-CB | -5.07 | 1.44 | 1.54 |
| 1 | Q | 464 | PHE | CG-CD1 | 5.07 | 1.46 | 1.38 |
| 1 | K | 37 | ALA | CA-CB | 5.07 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | E | 50 | TYR | CG-CD2 | 5.07 | 1.45 | 1.39 |
| 1 | E | 330 | LYS | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | H | 452 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | F | 498 | TRP | CG-CD2 | 5.07 | 1.52 | 1.43 |
| 1 | G | 110 | PHE | CA-CB | 5.07 | 1.65 | 1.53 |
| 1 | Q | 490 | TYR | CZ-OH | 5.06 | 1.46 | 1.37 |
| 1 | R | 302 | LYS | C-N | 5.06 | 1.42 | 1.33 |
| 1 | C | 123 | TYR | CB-CG | -5.06 | 1.44 | 1.51 |
| 1 | K | 163 | LYS | CA-CB | 5.06 | 1.65 | 1.53 |
| 1 | L | 338 | ARG | CA-CB | 5.06 | 1.65 | 1.53 |
| 1 | N | 484 | TRP | NE1-CE2 | 5.05 | 1.44 | 1.37 |
| 1 | K | 333 | ARG | CD-NE | 5.05 | 1.55 | 1.46 |
| 1 | P | 424 | GLU | CB-CG | 5.05 | 1.61 | 1.52 |
| 1 | D | 123 | TYR | CB-CG | -5.04 | 1.44 | 1.51 |
| 1 | O | 215 | GLY | CA-C | -5.04 | 1.43 | 1.51 |
| 1 | R | 531 | SER | CB-OG | 5.04 | 1.48 | 1.42 |
| 1 | O | 333 | ARG | CD-NE | 5.04 | 1.55 | 1.46 |
| 1 | D | 353 | TYR | CZ-OH | 5.03 | 1.46 | 1.37 |
| 1 | G | 321 | ARG | CD-NE | 5.03 | 1.54 | 1.46 |
| 1 | G | 224 | TYR | CB-CG | -5.02 | 1.44 | 1.51 |
| 1 | L | 194 | GLU | CB-CG | 5.01 | 1.61 | 1.52 |
| 1 | N | 28 | GLY | N-CA | 5.01 | 1.53 | 1.46 |
| 1 | P | 224 | TYR | CB-CG | -5.01 | 1.44 | 1.51 |
| 1 | P | 280 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |
| 1 | A | 263 | GLU | CB-CG | 5.00 | 1.61 | 1.52 |
| 1 | K | 297 | VAL | CB-CG1 | 5.00 | 1.63 | 1.52 |
| 1 | O | 123 | TYR | CE1-CZ | 5.00 | 1.45 | 1.38 |

All (1484) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | N | 265 | ARG | NE-CZ-NH2 | 21.33 | 130.97 | 120.30 |
| 1 | E | 474 | ARG | NE-CZ-NH2 | 18.96 | 129.78 | 120.30 |
| 1 | Q | 413 | ARG | NE-CZ-NH1 | -18.84 | 110.88 | 120.30 |
| 1 | C | 413 | ARG | NE-CZ-NH1 | -18.20 | 111.20 | 120.30 |
| 1 | D | 53 | ARG | NE-CZ-NH1 | 17.94 | 129.27 | 120.30 |
| 1 | M | 201 | TYR | CB-CG-CD1 | -17.71 | 110.38 | 121.00 |
| 1 | I | 178 | ARG | NE-CZ-NH2 | 17.67 | 129.13 | 120.30 |
| 1 | C | 413 | ARG | NE-CZ-NH2 | 17.06 | 128.83 | 120.30 |
| 1 | E | 384 | ARG | NE-CZ-NH1 | 16.98 | 128.79 | 120.30 |
| 1 | O | 162 | ARG | NE-CZ-NH2 | -16.42 | 112.09 | 120.30 |
| 1 | Q | 240 | ARG | NE-CZ-NH2 | -16.00 | 112.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | P | 178 | ARG | NE-CZ-NH2 | 15.77 | 128.18 | 120.30 |
| 1 | D | 525 | ARG | NE-CZ-NH1 | 15.65 | 128.13 | 120.30 |
| 1 | L | 135 | TYR | CB-CG-CD1 | -15.27 | 111.84 | 121.00 |
| 1 | I | 240 | ARG | NE-CZ-NH1 | 15.17 | 127.89 | 120.30 |
| 1 | I | 399 | ARG | NE-CZ-NH2 | 15.16 | 127.88 | 120.30 |
| 1 | P | 338 | ARG | NE-CZ-NH2 | -14.94 | 112.83 | 120.30 |
| 1 | B | 33 | ARG | NE-CZ-NH1 | 14.70 | 127.65 | 120.30 |
| 1 | P | 240 | ARG | NE-CZ-NH1 | 14.55 | 127.58 | 120.30 |
| 1 | O | 53 | ARG | NE-CZ-NH1 | 14.42 | 127.51 | 120.30 |
| 1 | N | 432 | TYR | CB-CG-CD2 | -14.41 | 112.36 | 121.00 |
| 1 | L | 338 | ARG | NE-CZ-NH2 | -14.39 | 113.10 | 120.30 |
| 1 | N | 178 | ARG | NE-CZ-NH2 | 14.38 | 127.49 | 120.30 |
| 1 | D | 196 | ARG | NE-CZ-NH1 | -14.38 | 113.11 | 120.30 |
| 1 | P | 384 | ARG | NE-CZ-NH2 | -14.36 | 113.12 | 120.30 |
| 1 | F | 389 | ARG | NE-CZ-NH1 | 14.32 | 127.46 | 120.30 |
| 1 | B | 430 | ARG | NE-CZ-NH1 | 14.28 | 127.44 | 120.30 |
| 1 | O | 360 | ARG | NE-CZ-NH1 | -14.28 | 113.16 | 120.30 |
| 1 | C | 33 | ARG | NE-CZ-NH2 | -14.21 | 113.19 | 120.30 |
| 1 | A | 338 | ARG | NE-CZ-NH2 | -14.18 | 113.21 | 120.30 |
| 1 | A | 135 | TYR | CB-CG-CD2 | 14.14 | 129.48 | 121.00 |
| 1 | N | 265 | ARG | NE-CZ-NH1 | -14.12 | 113.24 | 120.30 |
| 1 | G | 135 | TYR | CB-CG-CD2 | 14.03 | 129.42 | 121.00 |
| 1 | I | 430 | ARG | NE-CZ-NH1 | 14.01 | 127.30 | 120.30 |
| 1 | R | 413 | ARG | NE-CZ-NH2 | 14.00 | 127.30 | 120.30 |
| 1 | Q | 110 | PHE | CB-CG-CD2 | 13.89 | 130.53 | 120.80 |
| 1 | L | 240 | ARG | NE-CZ-NH2 | -13.85 | 113.37 | 120.30 |
| 1 | B | 180 | TYR | CB-CG-CD1 | -13.71 | 112.77 | 121.00 |
| 1 | P | 321 | ARG | NE-CZ-NH1 | 13.56 | 127.08 | 120.30 |
| 1 | E | 196 | ARG | NE-CZ-NH2 | 13.55 | 127.08 | 120.30 |
| 1 | G | 180 | TYR | CB-CG-CD2 | -13.56 | 112.87 | 121.00 |
| 1 | K | 399 | ARG | NE-CZ-NH2 | 13.55 | 127.08 | 120.30 |
| 1 | C | 135 | TYR | CB-CG-CD1 | -13.43 | 112.94 | 121.00 |
| 1 | I | 474 | ARG | NE-CZ-NH2 | 13.34 | 126.97 | 120.30 |
| 1 | B | 384 | ARG | NE-CZ-NH1 | 13.27 | 126.93 | 120.30 |
| 1 | N | 311 | TYR | CB-CG-CD1 | 13.26 | 128.96 | 121.00 |
| 1 | S | 360 | ARG | NE-CZ-NH2 | 13.19 | 126.90 | 120.30 |
| 1 | G | 178 | ARG | NE-CZ-NH2 | 13.19 | 126.89 | 120.30 |
| 1 | N | 389 | ARG | NE-CZ-NH1 | 13.11 | 126.85 | 120.30 |
| 1 | B | 322 | ARG | NE-CZ-NH2 | -13.07 | 113.76 | 120.30 |
| 1 | M | 178 | ARG | NE-CZ-NH2 | 13.07 | 126.84 | 120.30 |
| 1 | S | 240 | ARG | NE-CZ-NH1 | 13.02 | 126.81 | 120.30 |
| 1 | N | 311 | TYR | CB-CG-CD2 | -13.01 | 113.19 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | K | 360 | ARG | NE-CZ-NH1 | -13.01 | 113.80 | 120.30 |
| 1 | P | 333 | ARG | NE-CZ-NH1 | 13.00 | 126.80 | 120.30 |
| 1 | G | 265 | ARG | NE-CZ-NH1 | -12.96 | 113.82 | 120.30 |
| 1 | D | 196 | ARG | NE-CZ-NH2 | 12.88 | 126.74 | 120.30 |
| 1 | Q | 240 | ARG | NE-CZ-NH1 | 12.85 | 126.73 | 120.30 |
| 1 | G | 275 | PHE | CB-CG-CD2 | 12.77 | 129.74 | 120.80 |
| 1 | B | 33 | ARG | NE-CZ-NH2 | -12.77 | 113.92 | 120.30 |
| 1 | F | 474 | ARG | NE-CZ-NH1 | -12.76 | 113.92 | 120.30 |
| 1 | G | 432 | TYR | CB-CG-CD1 | 12.71 | 128.62 | 121.00 |
| 1 | A | 135 | TYR | CB-CG-CD1 | -12.68 | 113.39 | 121.00 |
| 1 | K | 322 | ARG | NE-CZ-NH1 | 12.67 | 126.64 | 120.30 |
| 1 | R | 321 | ARG | NE-CZ-NH2 | -12.63 | 113.98 | 120.30 |
| 1 | D | 321 | ARG | NE-CZ-NH1 | 12.59 | 126.59 | 120.30 |
| 1 | H | 53 | ARG | NE-CZ-NH2 | -12.56 | 114.02 | 120.30 |
| 1 | D | 396 | ARG | NE-CZ-NH2 | -12.53 | 114.03 | 120.30 |
| 1 | B | 396 | ARG | NE-CZ-NH1 | 12.52 | 126.56 | 120.30 |
| 1 | K | 413 | ARG | NE-CZ-NH2 | 12.48 | 126.54 | 120.30 |
| 1 | R | 399 | ARG | NE-CZ-NH2 | 12.48 | 126.54 | 120.30 |
| 1 | R | 162 | ARG | NE-CZ-NH2 | -12.47 | 114.06 | 120.30 |
| 1 | H | 53 | ARG | NE-CZ-NH1 | 12.46 | 126.53 | 120.30 |
| 1 | I | 384 | ARG | NE-CZ-NH1 | 12.40 | 126.50 | 120.30 |
| 1 | M | 360 | ARG | NE-CZ-NH1 | -12.37 | 114.11 | 120.30 |
| 1 | P | 338 | ARG | NE-CZ-NH1 | 12.36 | 126.48 | 120.30 |
| 1 | Q | 360 | ARG | NE-CZ-NH1 | -12.30 | 114.15 | 120.30 |
| 1 | P | 384 | ARG | NE-CZ-NH1 | 12.28 | 126.44 | 120.30 |
| 1 | L | 135 | TYR | CB-CG-CD2 | 12.25 | 128.35 | 121.00 |
| 1 | R | 321 | ARG | NE-CZ-NH1 | 12.21 | 126.41 | 120.30 |
| 1 | K | 162 | ARG | NE-CZ-NH1 | 12.16 | 126.38 | 120.30 |
| 1 | L | 338 | ARG | NE-CZ-NH1 | 12.15 | 126.38 | 120.30 |
| 1 | K | 360 | ARG | NE-CZ-NH2 | 12.14 | 126.37 | 120.30 |
| 1 | B | 135 | TYR | CB-CG-CD1 | -12.13 | 113.72 | 121.00 |
| 1 | S | 338 | ARG | NE-CZ-NH1 | 12.07 | 126.33 | 120.30 |
| 1 | M | 490 | TYR | CB-CG-CD2 | -12.06 | 113.77 | 121.00 |
| 1 | I | 396 | ARG | NE-CZ-NH1 | 12.02 | 126.31 | 120.30 |
| 1 | O | 399 | ARG | NE-CZ-NH2 | 12.02 | 126.31 | 120.30 |
| 1 | M | 525 | ARG | NE-CZ-NH1 | -11.96 | 114.32 | 120.30 |
| 1 | K | 265 | ARG | NE-CZ-NH2 | 11.93 | 126.26 | 120.30 |
| 1 | F | 196 | ARG | NE-CZ-NH2 | 11.89 | 126.25 | 120.30 |
| 1 | Q | 201 | TYR | CB-CG-CD2 | -11.86 | 113.89 | 121.00 |
| 1 | B | 240 | ARG | NE-CZ-NH2 | -11.85 | 114.37 | 120.30 |
| 1 | C | 50 | TYR | CB-CG-CD2 | -11.85 | 113.89 | 121.00 |
| 1 | I | 224 | TYR | CB-CG-CD1 | -11.84 | 113.90 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | H | 350 | ASP | CB-CG-OD2 | 11.82 | 128.94 | 118.30 |
| 1 | L | 162 | ARG | NE-CZ-NH1 | 11.82 | 126.21 | 120.30 |
| 1 | K | 396 | ARG | NE-CZ-NH1 | 11.75 | 126.18 | 120.30 |
| 1 | N | 360 | ARG | NE-CZ-NH2 | 11.75 | 126.17 | 120.30 |
| 1 | M | 50 | TYR | CB-CG-CD2 | -11.68 | 113.99 | 121.00 |
| 1 | O | 525 | ARG | NE-CZ-NH1 | 11.66 | 126.13 | 120.30 |
| 1 | O | 180 | TYR | CB-CG-CD2 | -11.63 | 114.02 | 121.00 |
| 1 | B | 396 | ARG | NE-CZ-NH2 | -11.61 | 114.50 | 120.30 |
| 1 | B | 240 | ARG | NE-CZ-NH1 | 11.55 | 126.07 | 120.30 |
| 1 | F | 474 | ARG | NE-CZ-NH2 | 11.53 | 126.06 | 120.30 |
| 1 | H | 120 | ASP | CB-CG-OD2 | -11.49 | 107.96 | 118.30 |
| 1 | L | 33 | ARG | NE-CZ-NH2 | -11.49 | 114.56 | 120.30 |
| 1 | A | 474 | ARG | NE-CZ-NH1 | -11.46 | 114.57 | 120.30 |
| 1 | F | 333 | ARG | NE-CZ-NH1 | 11.44 | 126.02 | 120.30 |
| 1 | H | 322 | ARG | NE-CZ-NH1 | 11.44 | 126.02 | 120.30 |
| 1 | K | 399 | ARG | NE-CZ-NH1 | -11.43 | 114.59 | 120.30 |
| 1 | Q | 33 | ARG | NE-CZ-NH2 | -11.28 | 114.66 | 120.30 |
| 1 | D | 275 | PHE | CB-CG-CD1 | 11.24 | 128.67 | 120.80 |
| 1 | E | 322 | ARG | NE-CZ-NH1 | 11.20 | 125.90 | 120.30 |
| 1 | H | 311 | TYR | CB-CG-CD2 | -11.15 | 114.31 | 121.00 |
| 1 | O | 53 | ARG | NE-CZ-NH2 | -11.14 | 114.73 | 120.30 |
| 1 | Q | 110 | PHE | CB-CG-CD1 | -11.14 | 113.00 | 120.80 |
| 1 | O | 196 | ARG | NE-CZ-NH2 | 11.13 | 125.87 | 120.30 |
| 1 | M | 396 | ARG | NE-CZ-NH2 | -11.12 | 114.74 | 120.30 |
| 1 | I | 360 | ARG | NE-CZ-NH1 | -11.02 | 114.79 | 120.30 |
| 1 | D | 275 | PHE | CB-CG-CD2 | -10.94 | 113.14 | 120.80 |
| 1 | I | 311 | TYR | CB-CG-CD2 | -10.91 | 114.45 | 121.00 |
| 1 | R | 240 | ARG | NE-CZ-NH1 | 10.90 | 125.75 | 120.30 |
| 1 | D | 205 | ASP | CB-CG-OD2 | 10.90 | 128.11 | 118.30 |
| 1 | E | 321 | ARG | NE-CZ-NH2 | 10.90 | 125.75 | 120.30 |
| 1 | K | 400 | ASP | CB-CG-OD1 | -10.86 | 108.52 | 118.30 |
| 1 | E | 384 | ARG | NE-CZ-NH2 | -10.84 | 114.88 | 120.30 |
| 1 | A | 162 | ARG | NE-CZ-NH2 | 10.75 | 125.67 | 120.30 |
| 1 | P | 333 | ARG | NE-CZ-NH2 | -10.71 | 114.94 | 120.30 |
| 1 | N | 432 | TYR | CB-CG-CD1 | 10.70 | 127.42 | 121.00 |
| 1 | O | 178 | ARG | NE-CZ-NH2 | 10.68 | 125.64 | 120.30 |
| 1 | S | 178 | ARG | NE-CZ-NH2 | 10.64 | 125.62 | 120.30 |
| 1 | A | 360 | ARG | NE-CZ-NH1 | -10.63 | 114.98 | 120.30 |
| 1 | B | 305 | ASP | CB-CG-OD1 | 10.63 | 127.86 | 118.30 |
| 1 | D | 201 | TYR | CB-CG-CD2 | 10.62 | 127.37 | 121.00 |
| 1 | A | 413 | ARG | NE-CZ-NH2 | 10.62 | 125.61 | 120.30 |
| 1 | A | 322 | ARG | NE-CZ-NH2 | -10.57 | 115.02 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | F | 396 | ARG | NE-CZ-NH1 | 10.55 | 125.58 | 120.30 |
| 1 | G | 224 | TYR | CB-CG-CD1 | -10.51 | 114.70 | 121.00 |
| 1 | O | 353 | TYR | CB-CG-CD2 | 10.50 | 127.30 | 121.00 |
| 1 | Q | 344 | ASP | CB-CG-OD1 | 10.50 | 127.75 | 118.30 |
| 1 | M | 413 | ARG | NE-CZ-NH2 | 10.48 | 125.54 | 120.30 |
| 1 | Q | 196 | ARG | NE-CZ-NH2 | 10.47 | 125.53 | 120.30 |
| 1 | N | 135 | TYR | CB-CG-CD2 | 10.45 | 127.27 | 121.00 |
| 1 | N | 196 | ARG | NE-CZ-NH1 | -10.41 | 115.09 | 120.30 |
| 1 | O | 196 | ARG | NE-CZ-NH1 | -10.41 | 115.09 | 120.30 |
| 1 | H | 396 | ARG | NE-CZ-NH1 | 10.34 | 125.47 | 120.30 |
| 1 | L | 399 | ARG | NE-CZ-NH1 | -10.33 | 115.14 | 120.30 |
| 1 | B | 201 | TYR | CB-CG-CD2 | -10.32 | 114.81 | 121.00 |
| 1 | G | 275 | PHE | CB-CG-CD1 | -10.32 | 113.58 | 120.80 |
| 1 | R | 275 | PHE | CB-CG-CD2 | -10.31 | 113.58 | 120.80 |
| 1 | E | 219 | ASP | CB-CG-OD2 | 10.29 | 127.56 | 118.30 |
| 1 | O | 125 | ASP | CB-CG-OD2 | 10.28 | 127.55 | 118.30 |
| 1 | C | 135 | TYR | CB-CG-CD2 | 10.27 | 127.16 | 121.00 |
| 1 | E | 360 | ARG | NE-CZ-NH1 | -10.23 | 115.19 | 120.30 |
| 1 | F | 178 | ARG | NE-CZ-NH2 | 10.22 | 125.41 | 120.30 |
| 1 | Q | 344 | ASP | CB-CG-OD2 | -10.19 | 109.13 | 118.30 |
| 1 | K | 311 | TYR | CB-CG-CD2 | 10.18 | 127.11 | 121.00 |
| 1 | D | 178 | ARG | NE-CZ-NH2 | 10.13 | 125.37 | 120.30 |
| 1 | N | 162 | ARG | NE-CZ-NH2 | -10.13 | 115.24 | 120.30 |
| 1 | A | 413 | ARG | NE-CZ-NH1 | -10.10 | 115.25 | 120.30 |
| 1 | A | 338 | ARG | NE-CZ-NH1 | 10.09 | 125.34 | 120.30 |
| 1 | F | 53 | ARG | NE-CZ-NH1 | 10.09 | 125.34 | 120.30 |
| 1 | D | 353 | TYR | CB-CG-CD1 | -10.06 | 114.96 | 121.00 |
| 1 | F | 447 | TYR | CB-CG-CD2 | -10.06 | 114.96 | 121.00 |
| 1 | K | 474 | ARG | NE-CZ-NH1 | -10.04 | 115.28 | 120.30 |
| 1 | M | 65 | ASP | CB-CG-OD1 | 10.02 | 127.32 | 118.30 |
| 1 | P | 430 | ARG | NE-CZ-NH1 | 9.96 | 125.28 | 120.30 |
| 1 | S | 123 | TYR | CB-CG-CD1 | -9.95 | 115.03 | 121.00 |
| 1 | L | 224 | TYR | CB-CG-CD2 | -9.86 | 115.09 | 121.00 |
| 1 | O | 413 | ARG | NE-CZ-NH1 | -9.85 | 115.37 | 120.30 |
| 1 | C | 224 | TYR | CB-CG-CD1 | -9.85 | 115.09 | 121.00 |
| 1 | K | 178 | ARG | NE-CZ-NH1 | 9.85 | 125.22 | 120.30 |
| 1 | S | 178 | ARG | NE-CZ-NH1 | -9.81 | 115.40 | 120.30 |
| 1 | G | 162 | ARG | NE-CZ-NH1 | 9.80 | 125.20 | 120.30 |
| 1 | C | 384 | ARG | NE-CZ-NH1 | 9.79 | 125.19 | 120.30 |
| 1 | N | 322 | ARG | NE-CZ-NH1 | 9.77 | 125.19 | 120.30 |
| 1 | R | 196 | ARG | NE-CZ-NH2 | 9.76 | 125.18 | 120.30 |
| 1 | B | 322 | ARG | NE-CZ-NH1 | 9.76 | 125.18 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | F | 430 | ARG | NE-CZ-NH1 | 9.76 | 125.18 | 120.30 |
| 1 | L | 384 | ARG | NE-CZ-NH1 | 9.73 | 125.17 | 120.30 |
| 1 | H | 183 | ASP | CB-CG-OD2 | -9.71 | 109.56 | 118.30 |
| 1 | C | 53 | ARG | NE-CZ-NH2 | -9.71 | 115.44 | 120.30 |
| 1 | N | 353 | TYR | CB-CG-CD2 | -9.68 | 115.19 | 121.00 |
| 1 | A | 322 | ARG | NE-CZ-NH1 | 9.65 | 125.12 | 120.30 |
| 1 | S | 353 | TYR | CB-CG-CD2 | -9.64 | 115.22 | 121.00 |
| 1 | A | 474 | ARG | NE-CZ-NH2 | 9.64 | 125.12 | 120.30 |
| 1 | D | 201 | TYR | CB-CG-CD1 | -9.62 | 115.23 | 121.00 |
| 1 | I | 178 | ARG | NE-CZ-NH1 | -9.62 | 115.49 | 120.30 |
| 1 | L | 162 | ARG | NE-CZ-NH2 | -9.61 | 115.50 | 120.30 |
| 1 | F | 396 | ARG | NE-CZ-NH2 | -9.56 | 115.52 | 120.30 |
| 1 | D | 53 | ARG | NE-CZ-NH2 | -9.54 | 115.53 | 120.30 |
| 1 | P | 389 | ARG | NE-CZ-NH1 | 9.54 | 125.07 | 120.30 |
| 1 | G | 447 | TYR | CB-CG-CD2 | -9.49 | 115.31 | 121.00 |
| 1 | F | 240 | ARG | NE-CZ-NH1 | 9.48 | 125.04 | 120.30 |
| 1 | C | 490 | TYR | CB-CG-CD2 | -9.45 | 115.33 | 121.00 |
| 1 | M | 432 | TYR | CG-CD2-CE2 | -9.44 | 113.75 | 121.30 |
| 1 | A | 240 | ARG | NE-CZ-NH2 | 9.41 | 125.00 | 120.30 |
| 1 | H | 485 | TYR | CB-CG-CD1 | 9.39 | 126.64 | 121.00 |
| 1 | G | 360 | ARG | NE-CZ-NH1 | -9.32 | 115.64 | 120.30 |
| 1 | R | 53 | ARG | NE-CZ-NH2 | -9.32 | 115.64 | 120.30 |
| 1 | F | 201 | TYR | CB-CG-CD2 | 9.32 | 126.59 | 121.00 |
| 1 | I | 474 | ARG | NE-CZ-NH1 | -9.32 | 115.64 | 120.30 |
| 1 | Q | 338 | ARG | NE-CZ-NH2 | -9.30 | 115.65 | 120.30 |
| 1 | A | 201 | TYR | CG-CD1-CE1 | -9.29 | 113.86 | 121.30 |
| 1 | H | 71 | ASP | CB-CG-OD2 | -9.28 | 109.95 | 118.30 |
| 1 | S | 399 | ARG | NE-CZ-NH1 | -9.26 | 115.67 | 120.30 |
| 1 | L | 224 | TYR | CG-CD2-CE2 | -9.26 | 113.89 | 121.30 |
| 1 | C | 196 | ARG | NE-CZ-NH2 | 9.25 | 124.92 | 120.30 |
| 1 | D | 447 | TYR | CB-CG-CD1 | 9.25 | 126.55 | 121.00 |
| 1 | I | 196 | ARG | NE-CZ-NH1 | -9.22 | 115.69 | 120.30 |
| 1 | S | 490 | TYR | CB-CG-CD2 | -9.22 | 115.47 | 121.00 |
| 1 | K | 321 | ARG | NE-CZ-NH2 | 9.21 | 124.91 | 120.30 |
| 1 | D | 178 | ARG | NE-CZ-NH1 | -9.20 | 115.70 | 120.30 |
| 1 | L | 240 | ARG | NE-CZ-NH1 | 9.19 | 124.90 | 120.30 |
| 1 | N | 430 | ARG | NE-CZ-NH2 | -9.18 | 115.71 | 120.30 |
| 1 | F | 360 | ARG | NE-CZ-NH1 | -9.14 | 115.73 | 120.30 |
| 1 | M | 240 | ARG | NE-CZ-NH1 | 9.13 | 124.86 | 120.30 |
| 1 | F | 360 | ARG | NE-CZ-NH2 | 9.11 | 124.85 | 120.30 |
| 1 | Q | 224 | TYR | CB-CG-CD2 | 9.09 | 126.46 | 121.00 |
| 1 | P | 288 | ASP | CB-CG-OD1 | 9.08 | 126.47 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | H | 373 | ALA | N-CA-CB | -9.08 | 97.39 | 110.10 |
| 1 | Q | 79 | MET | CG-SD-CE | -9.07 | 85.69 | 100.20 |
| 1 | F | 203 | ASP | CB-CG-OD2 | 9.05 | 126.45 | 118.30 |
| 1 | C | 369 | PHE | CB-CG-CD2 | 9.00 | 127.10 | 120.80 |
| 1 | H | 432 | TYR | CB-CG-CD1 | -9.00 | 115.60 | 121.00 |
| 1 | I | 123 | TYR | CB-CG-CD2 | -8.96 | 115.62 | 121.00 |
| 1 | R | 196 | ARG | NE-CZ-NH1 | -8.96 | 115.82 | 120.30 |
| 1 | I | 50 | TYR | CB-CG-CD1 | -8.95 | 115.63 | 121.00 |
| 1 | D | 305 | ASP | CB-CG-OD2 | -8.94 | 110.25 | 118.30 |
| 1 | M | 110 | PHE | CB-CG-CD1 | -8.93 | 114.55 | 120.80 |
| 1 | S | 360 | ARG | NE-CZ-NH1 | -8.93 | 115.83 | 120.30 |
| 1 | D | 33 | ARG | NE-CZ-NH2 | -8.92 | 115.84 | 120.30 |
| 1 | L | 430 | ARG | NE-CZ-NH1 | 8.92 | 124.76 | 120.30 |
| 1 | B | 180 | TYR | CB-CG-CD2 | 8.91 | 126.35 | 121.00 |
| 1 | N | 497 | MET | CG-SD-CE | -8.89 | 85.97 | 100.20 |
| 1 | N | 488 | ASP | CB-CG-OD2 | 8.87 | 126.29 | 118.30 |
| 1 | Q | 490 | TYR | CB-CG-CD1 | -8.87 | 115.68 | 121.00 |
| 1 | N | 277 | ASP | CB-CG-OD1 | 8.86 | 126.27 | 118.30 |
| 1 | F | 525 | ARG | NE-CZ-NH1 | 8.85 | 124.72 | 120.30 |
| 1 | A | 201 | TYR | CB-CG-CD1 | -8.81 | 115.71 | 121.00 |
| 1 | K | 102 | ASP | CB-CG-OD2 | -8.79 | 110.39 | 118.30 |
| 1 | Q | 322 | ARG | NE-CZ-NH1 | 8.77 | 124.69 | 120.30 |
| 1 | C | 321 | ARG | NE-CZ-NH1 | 8.75 | 124.67 | 120.30 |
| 1 | H | 183 | ASP | CB-CG-OD1 | 8.74 | 126.16 | 118.30 |
| 1 | R | 219 | ASP | CB-CG-OD2 | -8.72 | 110.45 | 118.30 |
| 1 | L | 311 | TYR | CG-CD2-CE2 | -8.71 | 114.33 | 121.30 |
| 1 | E | 447 | TYR | CB-CG-CD2 | -8.70 | 115.78 | 121.00 |
| 1 | L | 485 | TYR | CB-CG-CD2 | -8.70 | 115.78 | 121.00 |
| 1 | D | 447 | TYR | CB-CG-CD2 | -8.64 | 115.82 | 121.00 |
| 1 | I | 396 | ARG | NE-CZ-NH2 | -8.64 | 115.98 | 120.30 |
| 1 | P | 430 | ARG | NE-CZ-NH2 | -8.63 | 115.99 | 120.30 |
| 1 | F | 180 | TYR | CB-CG-CD2 | -8.62 | 115.83 | 121.00 |
| 1 | G | 399 | ARG | NE-CZ-NH1 | -8.62 | 115.99 | 120.30 |
| 1 | A | 178 | ARG | NE-CZ-NH1 | -8.60 | 116.00 | 120.30 |
| 1 | H | 430 | ARG | NE-CZ-NH2 | -8.60 | 116.00 | 120.30 |
| 1 | E | 353 | TYR | CB-CG-CD1 | 8.59 | 126.15 | 121.00 |
| 1 | I | 265 | ARG | NE-CZ-NH1 | -8.58 | 116.01 | 120.30 |
| 1 | M | 384 | ARG | NE-CZ-NH1 | 8.57 | 124.59 | 120.30 |
| 1 | E | 338 | ARG | NE-CZ-NH2 | -8.56 | 116.02 | 120.30 |
| 1 | C | 396 | ARG | NE-CZ-NH1 | 8.56 | 124.58 | 120.30 |
| 1 | I | 496 | ASP | CB-CG-OD2 | 8.56 | 126.00 | 118.30 |
| 1 | M | 201 | TYR | CB-CG-CD2 | 8.55 | 126.13 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | Q | 474 | ARG | NE-CZ-NH2 | 8.52 | 124.56 | 120.30 |
| 1 | O | 180 | TYR | CG-CD1-CE1 | -8.51 | 114.50 | 121.30 |
| 1 | F | 485 | TYR | CG-CD2-CE2 | 8.50 | 128.10 | 121.30 |
| 1 | D | 333 | ARG | NE-CZ-NH1 | 8.49 | 124.55 | 120.30 |
| 1 | K | 135 | TYR | CB-CG-CD1 | -8.48 | 115.91 | 121.00 |
| 1 | E | 178 | ARG | NE-CZ-NH2 | 8.47 | 124.54 | 120.30 |
| 1 | O | 465 | ASP | CB-CG-OD1 | 8.47 | 125.92 | 118.30 |
| 1 | L | 178 | ARG | NE-CZ-NH1 | -8.47 | 116.07 | 120.30 |
| 1 | G | 327 | ASP | CB-CG-OD1 | 8.45 | 125.90 | 118.30 |
| 1 | R | 219 | ASP | CB-CG-OD1 | 8.45 | 125.90 | 118.30 |
| 1 | E | 413 | ARG | NE-CZ-NH2 | 8.44 | 124.52 | 120.30 |
| 1 | I | 50 | TYR | CG-CD2-CE2 | -8.44 | 114.55 | 121.30 |
| 1 | K | 400 | ASP | CB-CG-OD2 | 8.43 | 125.89 | 118.30 |
| 1 | K | 320 | VAL | CA-CB-CG1 | 8.42 | 123.53 | 110.90 |
| 1 | L | 413 | ARG | NE-CZ-NH1 | -8.41 | 116.09 | 120.30 |
| 1 | K | 180 | TYR | CB-CG-CD2 | 8.41 | 126.04 | 121.00 |
| 1 | L | 430 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 1 | O | 389 | ARG | NE-CZ-NH1 | 8.38 | 124.49 | 120.30 |
| 1 | I | 322 | ARG | NE-CZ-NH1 | 8.37 | 124.48 | 120.30 |
| 1 | F | 490 | TYR | CB-CG-CD2 | -8.36 | 115.99 | 121.00 |
| 1 | H | 485 | TYR | CB-CG-CD2 | -8.33 | 116.00 | 121.00 |
| 1 | C | 474 | ARG | NE-CZ-NH1 | -8.32 | 116.14 | 120.30 |
| 1 | I | 228 | VAL | CA-CB-CG2 | -8.32 | 98.42 | 110.90 |
| 1 | O | 288 | ASP | CB-CG-OD2 | 8.32 | 125.79 | 118.30 |
| 1 | K | 53 | ARG | NE-CZ-NH2 | -8.31 | 116.14 | 120.30 |
| 1 | I | 488 | ASP | CB-CG-OD2 | -8.29 | 110.83 | 118.30 |
| 1 | E | 277 | ASP | CB-CG-OD2 | 8.29 | 125.76 | 118.30 |
| 1 | P | 322 | ARG | NE-CZ-NH1 | 8.28 | 124.44 | 120.30 |
| 1 | B | 275 | PHE | CB-CG-CD1 | -8.28 | 115.01 | 120.80 |
| 1 | D | 360 | ARG | NE-CZ-NH1 | -8.25 | 116.17 | 120.30 |
| 1 | A | 525 | ARG | NE-CZ-NH1 | 8.24 | 124.42 | 120.30 |
| 1 | H | 353 | TYR | CB-CG-CD2 | -8.24 | 116.05 | 121.00 |
| 1 | K | 464 | PHE | CB-CG-CD2 | -8.24 | 115.03 | 120.80 |
| 1 | B | 201 | TYR | CD1-CE1-CZ | -8.24 | 112.39 | 119.80 |
| 1 | F | 178 | ARG | NE-CZ-NH1 | -8.23 | 116.18 | 120.30 |
| 1 | R | 407 | ASP | CB-CG-OD1 | 8.23 | 125.70 | 118.30 |
| 1 | Q | 353 | TYR | CB-CG-CD1 | -8.22 | 116.07 | 121.00 |
| 1 | A | 490 | TYR | CB-CG-CD1 | -8.21 | 116.07 | 121.00 |
| 1 | E | 61 | ASP | CB-CG-OD1 | 8.21 | 125.69 | 118.30 |
| 1 | P | 490 | TYR | CB-CG-CD2 | 8.21 | 125.92 | 121.00 |
| 1 | A | 224 | TYR | CB-CG-CD2 | -8.20 | 116.08 | 121.00 |
| 1 | C | 201 | TYR | CB-CG-CD1 | 8.19 | 125.91 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | P | 237 | MET | CG-SD-CE | -8.18 | 87.11 | 100.20 |
| 1 | P | 490 | TYR | CB-CG-CD1 | -8.18 | 116.09 | 121.00 |
| 1 | S | 53 | ARG | NE-CZ-NH1 | 8.18 | 124.39 | 120.30 |
| 1 | Q | 365 | ASP | CB-CG-OD2 | -8.16 | 110.96 | 118.30 |
| 1 | G | 413 | ARG | NE-CZ-NH1 | -8.16 | 116.22 | 120.30 |
| 1 | S | 50 | TYR | CG-CD1-CE1 | -8.15 | 114.78 | 121.30 |
| 1 | N | 360 | ARG | NE-CZ-NH1 | -8.15 | 116.22 | 120.30 |
| 1 | A | 110 | PHE | CB-CG-CD2 | 8.13 | 126.49 | 120.80 |
| 1 | O | 33 | ARG | NE-CZ-NH2 | -8.13 | 116.23 | 120.30 |
| 1 | D | 220 | THR | CA-CB-CG2 | -8.13 | 101.02 | 112.40 |
| 1 | O | 311 | TYR | CB-CG-CD2 | -8.13 | 116.12 | 121.00 |
| 1 | I | 162 | ARG | NE-CZ-NH2 | 8.12 | 124.36 | 120.30 |
| 1 | P | 307 | VAL | CG1-CB-CG2 | -8.11 | 97.92 | 110.90 |
| 1 | A | 205 | ASP | CB-CG-OD2 | 8.11 | 125.60 | 118.30 |
| 1 | D | 338 | ARG | NE-CZ-NH1 | 8.10 | 124.35 | 120.30 |
| 1 | M | 219 | ASP | CB-CG-OD1 | -8.10 | 111.01 | 118.30 |
| 1 | S | 162 | ARG | NE-CZ-NH1 | 8.10 | 124.35 | 120.30 |
| 1 | E | 485 | TYR | CB-CG-CD2 | -8.09 | 116.14 | 121.00 |
| 1 | B | 311 | TYR | CB-CG-CD1 | 8.09 | 125.85 | 121.00 |
| 1 | L | 400 | ASP | CB-CG-OD2 | 8.08 | 125.57 | 118.30 |
| 1 | K | 237 | MET | CG-SD-CE | -8.08 | 87.27 | 100.20 |
| 1 | S | 201 | TYR | CB-CG-CD2 | -8.07 | 116.16 | 121.00 |
| 1 | C | 224 | TYR | CB-CG-CD2 | 8.07 | 125.84 | 121.00 |
| 1 | F | 50 | TYR | CB-CG-CD1 | -8.06 | 116.16 | 121.00 |
| 1 | K | 157 | ASP | CB-CG-OD2 | 8.05 | 125.55 | 118.30 |
| 1 | C | 157 | ASP | CB-CG-OD2 | 8.04 | 125.53 | 118.30 |
| 1 | H | 327 | ASP | CB-CG-OD2 | -8.04 | 111.07 | 118.30 |
| 1 | B | 135 | TYR | CG-CD2-CE2 | -8.03 | 114.88 | 121.30 |
| 1 | G | 413 | ARG | NE-CZ-NH2 | 8.03 | 124.31 | 120.30 |
| 1 | F | 50 | TYR | CG-CD2-CE2 | -8.01 | 114.89 | 121.30 |
| 1 | C | 157 | ASP | CB-CG-OD1 | -8.01 | 111.09 | 118.30 |
| 1 | A | 384 | ARG | NE-CZ-NH1 | 8.01 | 124.30 | 120.30 |
| 1 | F | 407 | ASP | CB-CG-OD2 | 7.99 | 125.49 | 118.30 |
| 1 | O | 353 | TYR | CB-CG-CD1 | -7.98 | 116.21 | 121.00 |
| 1 | H | 97 | ASP | CB-CG-OD1 | 7.98 | 125.48 | 118.30 |
| 1 | O | 110 | PHE | CB-CG-CD2 | 7.98 | 126.39 | 120.80 |
| 1 | G | 229 | ASP | CB-CG-OD1 | 7.98 | 125.48 | 118.30 |
| 1 | S | 162 | ARG | NE-CZ-NH2 | -7.97 | 116.31 | 120.30 |
| 1 | Q | 338 | ARG | NE-CZ-NH1 | 7.96 | 124.28 | 120.30 |
| 1 | L | 396 | ARG | NE-CZ-NH1 | 7.95 | 124.28 | 120.30 |
| 1 | H | 201 | TYR | CB-CG-CD2 | -7.94 | 116.24 | 121.00 |
| 1 | H | 275 | PHE | CB-CG-CD1 | 7.94 | 126.36 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | M | 224 | TYR | CB-CG-CD1 | -7.91 | 116.25 | 121.00 |
| 1 | A | 123 | TYR | CG-CD2-CE2 | -7.90 | 114.98 | 121.30 |
| 1 | Q | 322 | ARG | NE-CZ-NH2 | -7.86 | 116.37 | 120.30 |
| 1 | O | 43 | GLU | OE1-CD-OE2 | -7.85 | 113.88 | 123.30 |
| 1 | A | 196 | ARG | NE-CZ-NH1 | -7.85 | 116.37 | 120.30 |
| 1 | F | 525 | ARG | NE-CZ-NH2 | -7.85 | 116.38 | 120.30 |
| 1 | F | 353 | TYR | CB-CG-CD2 | 7.84 | 125.70 | 121.00 |
| 1 | K | 229 | ASP | CB-CG-OD2 | 7.84 | 125.36 | 118.30 |
| 1 | K | 201 | TYR | CB-CG-CD1 | -7.83 | 116.30 | 121.00 |
| 1 | A | 321 | ARG | NE-CZ-NH1 | 7.83 | 124.22 | 120.30 |
| 1 | S | 135 | TYR | CB-CG-CD2 | 7.82 | 125.69 | 121.00 |
| 1 | F | 490 | TYR | CB-CG-CD1 | 7.81 | 125.69 | 121.00 |
| 1 | G | 123 | TYR | CB-CG-CD1 | -7.81 | 116.31 | 121.00 |
| 1 | P | 413 | ARG | NE-CZ-NH2 | 7.81 | 124.20 | 120.30 |
| 1 | A | 189 | VAL | CG1-CB-CG2 | -7.78 | 98.45 | 110.90 |
| 1 | E | 135 | TYR | CB-CG-CD1 | -7.78 | 116.33 | 121.00 |
| 1 | Q | 58 | MET | CG-SD-CE | -7.78 | 87.75 | 100.20 |
| 1 | Q | 360 | ARG | NE-CZ-NH2 | 7.78 | 124.19 | 120.30 |
| 1 | I | 196 | ARG | NE-CZ-NH2 | 7.76 | 124.18 | 120.30 |
| 1 | L | 396 | ARG | NE-CZ-NH2 | -7.76 | 116.42 | 120.30 |
| 1 | C | 240 | ARG | NE-CZ-NH2 | 7.73 | 124.16 | 120.30 |
| 1 | L | 432 | TYR | CB-CG-CD1 | 7.72 | 125.64 | 121.00 |
| 1 | O | 432 | TYR | CB-CG-CD2 | -7.72 | 116.37 | 121.00 |
| 1 | O | 360 | ARG | NE-CZ-NH2 | 7.72 | 124.16 | 120.30 |
| 1 | M | 328 | LEU | CB-CG-CD2 | 7.71 | 124.10 | 111.00 |
| 1 | E | 490 | TYR | CB-CG-CD2 | -7.69 | 116.39 | 121.00 |
| 1 | R | 413 | ARG | NE-CZ-NH1 | -7.68 | 116.46 | 120.30 |
| 1 | R | 525 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 1 | O | 50 | TYR | CD1-CE1-CZ | -7.68 | 112.89 | 119.80 |
| 1 | C | 322 | ARG | NE-CZ-NH1 | 7.65 | 124.13 | 120.30 |
| 1 | N | 229 | ASP | CB-CG-OD1 | 7.65 | 125.18 | 118.30 |
| 1 | G | 407 | ASP | CB-CG-OD1 | 7.63 | 125.17 | 118.30 |
| 1 | E | 344 | ASP | CB-CG-OD1 | -7.63 | 111.44 | 118.30 |
| 1 | K | 525 | ARG | NE-CZ-NH1 | 7.62 | 124.11 | 120.30 |
| 1 | K | 373 | ALA | N-CA-CB | 7.62 | 120.76 | 110.10 |
| 1 | D | 80 | ASP | CB-CG-OD2 | 7.61 | 125.15 | 118.30 |
| 1 | K | 31 | ALA | N-CA-CB | -7.60 | 99.45 | 110.10 |
| 1 | D | 77 | ASP | CB-CG-OD2 | 7.60 | 125.14 | 118.30 |
| 1 | Q | 201 | TYR | CG-CD2-CE2 | -7.59 | 115.23 | 121.30 |
| 1 | G | 485 | TYR | CB-CG-CD1 | 7.58 | 125.55 | 121.00 |
| 1 | O | 55 | MET | CG-SD-CE | -7.58 | 88.07 | 100.20 |
| 1 | G | 265 | ARG | NE-CZ-NH2 | 7.58 | 124.09 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | E | 178 | ARG | NE-CZ-NH1 | -7.57 | 116.52 | 120.30 |
| 1 | N | 322 | ARG | NE-CZ-NH2 | -7.57 | 116.52 | 120.30 |
| 1 | I | 224 | TYR | CB-CG-CD2 | 7.54 | 125.53 | 121.00 |
| 1 | N | 203 | ASP | CB-CG-OD1 | 7.54 | 125.09 | 118.30 |
| 1 | F | 389 | ARG | NE-CZ-NH2 | -7.53 | 116.54 | 120.30 |
| 1 | Q | 424 | GLU | OE1-CD-OE2 | -7.53 | 114.27 | 123.30 |
| 1 | P | 525 | ARG | NE-CZ-NH2 | -7.52 | 116.54 | 120.30 |
| 1 | B | 162 | ARG | O-C-N | -7.52 | 110.67 | 122.70 |
| 1 | S | 123 | TYR | CB-CG-CD2 | 7.52 | 125.51 | 121.00 |
| 1 | C | 525 | ARG | NE-CZ-NH1 | 7.51 | 124.06 | 120.30 |
| 1 | Q | 384 | ARG | NE-CZ-NH2 | -7.51 | 116.55 | 120.30 |
| 1 | B | 465 | ASP | CB-CG-OD1 | 7.50 | 125.05 | 118.30 |
| 1 | H | 196 | ARG | NE-CZ-NH2 | 7.49 | 124.04 | 120.30 |
| 1 | R | 311 | TYR | CB-CG-CD1 | -7.48 | 116.51 | 121.00 |
| 1 | M | 120 | ASP | CB-CG-OD2 | 7.48 | 125.03 | 118.30 |
| 1 | M | 485 | TYR | CB-CG-CD2 | -7.47 | 116.52 | 121.00 |
| 1 | N | 333 | ARG | NE-CZ-NH2 | -7.47 | 116.56 | 120.30 |
| 1 | M | 161 | LEU | CB-CG-CD2 | 7.47 | 123.69 | 111.00 |
| 1 | E | 490 | TYR | CB-CG-CD1 | 7.44 | 125.47 | 121.00 |
| 1 | N | 183 | ASP | CB-CG-OD1 | 7.42 | 124.98 | 118.30 |
| 1 | B | 275 | PHE | CB-CG-CD2 | 7.42 | 126.00 | 120.80 |
| 1 | D | 39 | VAL | CA-CB-CG1 | 7.41 | 122.01 | 110.90 |
| 1 | R | 274 | LYS | O-C-N | -7.40 | 110.85 | 122.70 |
| 1 | M | 110 | PHE | CB-CG-CD2 | 7.38 | 125.97 | 120.80 |
| 1 | Q | 219 | ASP | CB-CG-OD1 | 7.38 | 124.94 | 118.30 |
| 1 | Q | 224 | TYR | CB-CG-CD1 | -7.37 | 116.58 | 121.00 |
| 1 | N | 478 | GLU | OE1-CD-OE2 | -7.36 | 114.47 | 123.30 |
| 1 | A | 224 | TYR | CB-CG-CD1 | 7.35 | 125.41 | 121.00 |
| 1 | N | 399 | ARG | NE-CZ-NH1 | -7.35 | 116.63 | 120.30 |
| 1 | G | 180 | TYR | CG-CD1-CE1 | -7.34 | 115.42 | 121.30 |
| 1 | I | 126 | VAL | CG1-CB-CG2 | -7.34 | 99.15 | 110.90 |
| 1 | N | 464 | PHE | CB-CG-CD2 | -7.33 | 115.67 | 120.80 |
| 1 | S | 321 | ARG | NE-CZ-NH2 | 7.33 | 123.96 | 120.30 |
| 1 | O | 135 | TYR | CB-CG-CD1 | -7.32 | 116.61 | 121.00 |
| 1 | K | 369 | PHE | CB-CG-CD1 | 7.31 | 125.92 | 120.80 |
| 1 | I | 265 | ARG | NE-CZ-NH2 | 7.30 | 123.95 | 120.30 |
| 1 | S | 240 | ARG | CD-NE-CZ | 7.29 | 133.81 | 123.60 |
| 1 | M | 198 | ASP | CB-CG-OD1 | 7.29 | 124.86 | 118.30 |
| 1 | N | 275 | PHE | CB-CG-CD2 | 7.29 | 125.90 | 120.80 |
| 1 | L | 311 | TYR | CB-CG-CD2 | -7.26 | 116.64 | 121.00 |
| 1 | A | 287 | VAL | CA-CB-CG2 | 7.25 | 121.78 | 110.90 |
| 1 | D | 474 | ARG | NE-CZ-NH2 | 7.24 | 123.92 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 178 | ARG | NE-CZ-NH2 | 7.23 | 123.92 | 120.30 |
| 1 | D | 169 | LEU | O-C-N | -7.23 | 111.13 | 122.70 |
| 1 | D | 380 | SER | N-CA-CB | 7.23 | 121.35 | 110.50 |
| 1 | A | 333 | ARG | NE-CZ-NH1 | 7.23 | 123.92 | 120.30 |
| 1 | L | 288 | ASP | CB-CG-OD2 | -7.22 | 111.80 | 118.30 |
| 1 | I | 322 | ARG | NH1-CZ-NH2 | -7.22 | 111.46 | 119.40 |
| 1 | H | 110 | PHE | CB-CG-CD1 | -7.20 | 115.76 | 120.80 |
| 1 | A | 288 | ASP | CB-CG-OD2 | 7.20 | 124.78 | 118.30 |
| 1 | D | 240 | ARG | NE-CZ-NH2 | 7.20 | 123.90 | 120.30 |
| 1 | F | 53 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 1 | B | 53 | ARG | NE-CZ-NH2 | -7.17 | 116.72 | 120.30 |
| 1 | A | 85 | ALA | N-CA-CB | 7.16 | 120.13 | 110.10 |
| 1 | D | 525 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 1 | Q | 120 | ASP | CB-CG-OD2 | 7.15 | 124.74 | 118.30 |
| 1 | S | 348 | GLU | OE1-CD-OE2 | -7.15 | 114.72 | 123.30 |
| 1 | C | 430 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | A | 333 | ARG | NE-CZ-NH2 | -7.13 | 116.73 | 120.30 |
| 1 | M | 369 | PHE | CB-CG-CD1 | -7.13 | 115.81 | 120.80 |
| 1 | E | 196 | ARG | NE-CZ-NH1 | -7.12 | 116.74 | 120.30 |
| 1 | A | 53 | ARG | NE-CZ-NH2 | 7.11 | 123.86 | 120.30 |
| 1 | O | 56 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 1 | M | 432 | TYR | CZ-CE2-CD2 | 7.11 | 126.20 | 119.80 |
| 1 | C | 53 | ARG | NE-CZ-NH1 | 7.11 | 123.85 | 120.30 |
| 1 | C | 430 | ARG | NE-CZ-NH2 | 7.11 | 123.85 | 120.30 |
| 1 | S | 166 | MET | CG-SD-CE | -7.11 | 88.83 | 100.20 |
| 1 | N | 471 | MET | CG-SD-CE | -7.10 | 88.83 | 100.20 |
| 1 | N | 237 | MET | CG-SD-CE | -7.10 | 88.84 | 100.20 |
| 1 | P | 277 | ASP | O-C-N | -7.10 | 111.34 | 122.70 |
| 1 | C | 432 | TYR | CB-CG-CD1 | -7.10 | 116.74 | 121.00 |
| 1 | F | 141 | VAL | CA-CB-CG2 | -7.09 | 100.26 | 110.90 |
| 1 | R | 240 | ARG | NE-CZ-NH2 | -7.09 | 116.75 | 120.30 |
| 1 | Q | 389 | ARG | NE-CZ-NH2 | 7.09 | 123.84 | 120.30 |
| 1 | D | 510 | MET | CA-CB-CG | 7.09 | 125.35 | 113.30 |
| 1 | Q | 430 | ARG | NE-CZ-NH1 | 7.09 | 123.84 | 120.30 |
| 1 | R | 53 | ARG | NE-CZ-NH1 | 7.08 | 123.84 | 120.30 |
| 1 | C | 432 | TYR | CG-CD1-CE1 | -7.07 | 115.64 | 121.30 |
| 1 | Q | 452 | GLU | OE1-CD-OE2 | -7.07 | 114.81 | 123.30 |
| 1 | N | 339 | VAL | CA-CB-CG2 | 7.06 | 121.49 | 110.90 |
| 1 | I | 509 | LYS | O-C-N | -7.06 | 111.41 | 122.70 |
| 1 | E | 399 | ARG | NE-CZ-NH2 | 7.05 | 123.83 | 120.30 |
| 1 | B | 244 | ALA | N-CA-CB | -7.03 | 100.26 | 110.10 |
| 1 | S | 186 | VAL | CA-CB-CG2 | -7.03 | 100.36 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 399 | ARG | NE-CZ-NH2 | 7.03 | 123.81 | 120.30 |
| 1 | L | 447 | TYR | CZ-CE2-CD2 | -7.02 | 113.48 | 119.80 |
| 1 | A | 240 | ARG | NH1-CZ-NH2 | -7.02 | 111.68 | 119.40 |
| 1 | H | 196 | ARG | NE-CZ-NH1 | -7.01 | 116.80 | 120.30 |
| 1 | K | 123 | TYR | CG-CD2-CE2 | -7.01 | 115.69 | 121.30 |
| 1 | C | 485 | TYR | CB-CG-CD2 | -7.00 | 116.80 | 121.00 |
| 1 | B | 384 | ARG | NE-CZ-NH2 | -7.00 | 116.80 | 120.30 |
| 1 | S | 157 | ASP | CB-CG-OD2 | 7.00 | 124.60 | 118.30 |
| 1 | G | 219 | ASP | CB-CG-OD1 | -7.00 | 112.00 | 118.30 |
| 1 | I | 183 | ASP | CB-CG-OD1 | 7.00 | 124.60 | 118.30 |
| 1 | Q | 532 | ALA | CB-CA-C | -7.00 | 99.60 | 110.10 |
| 1 | D | 153 | VAL | CA-CB-CG2 | -6.98 | 100.42 | 110.90 |
| 1 | A | 265 | ARG | NE-CZ-NH2 | 6.98 | 123.79 | 120.30 |
| 1 | H | 465 | ASP | CB-CG-OD1 | 6.98 | 124.58 | 118.30 |
| 1 | O | 391 | VAL | CG1-CB-CG2 | -6.98 | 99.74 | 110.90 |
| 1 | F | 329 | GLU | OE1-CD-OE2 | -6.97 | 114.93 | 123.30 |
| 1 | L | 490 | TYR | CB-CG-CD1 | 6.97 | 125.19 | 121.00 |
| 1 | C | 396 | ARG | NE-CZ-NH2 | -6.97 | 116.82 | 120.30 |
| 1 | I | 490 | TYR | CG-CD2-CE2 | -6.97 | 115.73 | 121.30 |
| 1 | Q | 123 | TYR | CB-CG-CD1 | 6.96 | 125.18 | 121.00 |
| 1 | L | 275 | PHE | CB-CG-CD2 | 6.96 | 125.67 | 120.80 |
| 1 | D | 50 | TYR | CB-CG-CD1 | -6.96 | 116.83 | 121.00 |
| 1 | P | 396 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 1 | H | 203 | ASP | CB-CG-OD1 | 6.94 | 124.55 | 118.30 |
| 1 | N | 178 | ARG | NE-CZ-NH1 | -6.94 | 116.83 | 120.30 |
| 1 | P | 360 | ARG | CD-NE-CZ | 6.94 | 133.32 | 123.60 |
| 1 | S | 196 | ARG | NE-CZ-NH1 | -6.94 | 116.83 | 120.30 |
| 1 | K | 277 | ASP | CB-CG-OD2 | 6.94 | 124.55 | 118.30 |
| 1 | H | 80 | ASP | CB-CG-OD1 | -6.94 | 112.06 | 118.30 |
| 1 | L | 318 | LEU | CB-CG-CD2 | 6.93 | 122.79 | 111.00 |
| 1 | R | 272 | MET | CG-SD-CE | -6.93 | 89.11 | 100.20 |
| 1 | C | 159 | ASP | CB-CG-OD1 | 6.93 | 124.53 | 118.30 |
| 1 | H | 373 | ALA | CB-CA-C | 6.92 | 120.49 | 110.10 |
| 1 | K | 490 | TYR | CB-CG-CD2 | -6.92 | 116.85 | 121.00 |
| 1 | L | 201 | TYR | CB-CG-CD1 | -6.91 | 116.85 | 121.00 |
| 1 | L | 53 | ARG | NE-CZ-NH2 | -6.91 | 116.85 | 120.30 |
| 1 | K | 484 | TRP | CB-CG-CD2 | 6.90 | 135.57 | 126.60 |
| 1 | H | 399 | ARG | NE-CZ-NH1 | -6.89 | 116.86 | 120.30 |
| 1 | S | 430 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | B | 288 | ASP | CB-CG-OD2 | -6.89 | 112.10 | 118.30 |
| 1 | L | 233 | VAL | CA-CB-CG1 | 6.88 | 121.22 | 110.90 |
| 1 | Q | 399 | ARG | CD-NE-CZ | 6.88 | 133.23 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | F | 31 | ALA | CB-CA-C | -6.88 | 99.79 | 110.10 |
| 1 | D | 485 | TYR | CB-CG-CD2 | -6.88 | 116.88 | 121.00 |
| 1 | G | 135 | TYR | CB-CG-CD1 | -6.87 | 116.88 | 121.00 |
| 1 | K | 387 | LEU | CB-CG-CD1 | -6.87 | 99.32 | 111.00 |
| 1 | L | 111 | SER | N-CA-CB | 6.86 | 120.80 | 110.50 |
| 1 | L | 50 | TYR | CG-CD2-CE2 | -6.86 | 115.81 | 121.30 |
| 1 | B | 421 | VAL | CA-CB-CG2 | -6.85 | 100.62 | 110.90 |
| 1 | G | 392 | ASP | CB-CG-OD2 | 6.85 | 124.47 | 118.30 |
| 1 | N | 405 | VAL | CA-CB-CG1 | 6.85 | 121.17 | 110.90 |
| 1 | E | 33 | ARG | NE-CZ-NH2 | -6.85 | 116.88 | 120.30 |
| 1 | F | 34 | ALA | N-CA-CB | -6.84 | 100.53 | 110.10 |
| 1 | K | 490 | TYR | CB-CG-CD1 | 6.83 | 125.10 | 121.00 |
| 1 | Q | 365 | ASP | CB-CG-OD1 | 6.83 | 124.44 | 118.30 |
| 1 | B | 327 | ASP | CB-CG-OD2 | 6.82 | 124.44 | 118.30 |
| 1 | O | 123 | TYR | CB-CG-CD2 | -6.82 | 116.91 | 121.00 |
| 1 | P | 380 | SER | N-CA-CB | 6.82 | 120.72 | 110.50 |
| 1 | S | 196 | ARG | NE-CZ-NH2 | 6.80 | 123.70 | 120.30 |
| 1 | L | 133 | SER | N-CA-CB | -6.79 | 100.31 | 110.50 |
| 1 | S | 525 | ARG | NE-CZ-NH2 | -6.79 | 116.91 | 120.30 |
| 1 | C | 265 | ARG | NE-CZ-NH2 | 6.76 | 123.68 | 120.30 |
| 1 | I | 335 | THR | CA-CB-CG2 | -6.76 | 102.94 | 112.40 |
| 1 | Q | 97 | ASP | CB-CG-OD1 | 6.76 | 124.38 | 118.30 |
| 1 | E | 485 | TYR | CB-CG-CD1 | 6.75 | 125.05 | 121.00 |
| 1 | O | 123 | TYR | CZ-CE2-CD2 | -6.75 | 113.73 | 119.80 |
| 1 | S | 333 | ARG | NE-CZ-NH2 | -6.75 | 116.93 | 120.30 |
| 1 | I | 301 | GLN | C-N-CA | 6.75 | 138.57 | 121.70 |
| 1 | K | 311 | TYR | CB-CG-CD1 | -6.75 | 116.95 | 121.00 |
| 1 | P | 71 | ASP | CB-CG-OD1 | -6.72 | 112.25 | 118.30 |
| 1 | I | 220 | THR | CA-CB-CG2 | -6.70 | 103.02 | 112.40 |
| 1 | C | 344 | ASP | CB-CG-OD2 | 6.70 | 124.33 | 118.30 |
| 1 | G | 261 | ASP | CB-CG-OD1 | -6.69 | 112.28 | 118.30 |
| 1 | B | 525 | ARG | O-C-N | -6.67 | 112.02 | 122.70 |
| 1 | K | 110 | PHE | CB-CG-CD1 | -6.67 | 116.13 | 120.80 |
| 1 | R | 444 | VAL | CG1-CB-CG2 | -6.66 | 100.24 | 110.90 |
| 1 | K | 43 | GLU | OE1-CD-OE2 | -6.65 | 115.31 | 123.30 |
| 1 | D | 384 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | C | 430 | ARG | NH1-CZ-NH2 | -6.64 | 112.09 | 119.40 |
| 1 | E | 527 | ASP | CB-CG-OD1 | 6.64 | 124.27 | 118.30 |
| 1 | G | 380 | SER | CB-CA-C | -6.63 | 97.50 | 110.10 |
| 1 | K | 391 | VAL | CA-CB-CG1 | 6.62 | 120.82 | 110.90 |
| 1 | Q | 499 | GLN | CG-CD-OE1 | 6.61 | 134.82 | 121.60 |
| 1 | O | 311 | TYR | CB-CG-CD1 | 6.61 | 124.97 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | O | 69 | THR | O-C-N | -6.60 | 112.14 | 122.70 |
| 1 | G | 123 | TYR | CB-CG-CD2 | 6.60 | 124.96 | 121.00 |
| 1 | P | 432 | TYR | CG-CD2-CE2 | -6.60 | 116.02 | 121.30 |
| 1 | E | 484 | TRP | CB-CG-CD2 | 6.60 | 135.18 | 126.60 |
| 1 | I | 320 | VAL | CA-CB-CG1 | 6.60 | 120.80 | 110.90 |
| 1 | S | 515 | ALA | N-CA-CB | -6.59 | 100.87 | 110.10 |
| 1 | N | 353 | TYR | CG-CD2-CE2 | -6.58 | 116.03 | 121.30 |
| 1 | A | 123 | TYR | CZ-CE2-CD2 | 6.58 | 125.72 | 119.80 |
| 1 | H | 322 | ARG | NH1-CZ-NH2 | -6.58 | 112.17 | 119.40 |
| 1 | N | 183 | ASP | CB-CG-OD2 | -6.56 | 112.39 | 118.30 |
| 1 | E | 474 | ARG | NH1-CZ-NH2 | -6.56 | 112.19 | 119.40 |
| 1 | R | 474 | ARG | NE-CZ-NH2 | 6.55 | 123.58 | 120.30 |
| 1 | B | 350 | ASP | CB-CG-OD2 | 6.55 | 124.19 | 118.30 |
| 1 | H | 224 | TYR | CG-CD1-CE1 | -6.55 | 116.06 | 121.30 |
| 1 | P | 180 | TYR | CG-CD2-CE2 | -6.55 | 116.06 | 121.30 |
| 1 | S | 198 | ASP | CB-CG-OD2 | 6.55 | 124.19 | 118.30 |
| 1 | C | 485 | TYR | CB-CG-CD1 | 6.55 | 124.93 | 121.00 |
| 1 | I | 229 | ASP | CB-CG-OD1 | 6.54 | 124.19 | 118.30 |
| 1 | S | 322 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | Q | 288 | ASP | CB-CG-OD2 | 6.54 | 124.19 | 118.30 |
| 1 | S | 322 | ARG | NE-CZ-NH2 | -6.53 | 117.03 | 120.30 |
| 1 | N | 339 | VAL | CG1-CB-CG2 | -6.53 | 100.45 | 110.90 |
| 1 | E | 229 | ASP | N-CA-CB | -6.53 | 98.85 | 110.60 |
| 1 | H | 166 | MET | CG-SD-CE | -6.53 | 89.76 | 100.20 |
| 1 | I | 380 | SER | O-C-N | -6.53 | 112.26 | 122.70 |
| 1 | D | 50 | TYR | CB-CG-CD2 | 6.52 | 124.91 | 121.00 |
| 1 | I | 61 | ASP | CB-CG-OD2 | 6.51 | 124.16 | 118.30 |
| 1 | M | 474 | ARG | NE-CZ-NH1 | -6.51 | 117.05 | 120.30 |
| 1 | P | 183 | ASP | CB-CG-OD1 | 6.50 | 124.15 | 118.30 |
| 1 | G | 360 | ARG | N-CA-CB | 6.50 | 122.29 | 110.60 |
| 1 | F | 203 | ASP | CB-CG-OD1 | -6.50 | 112.45 | 118.30 |
| 1 | D | 369 | PHE | CB-CG-CD2 | -6.49 | 116.25 | 120.80 |
| 1 | H | 275 | PHE | CG-CD2-CE2 | 6.49 | 127.94 | 120.80 |
| 1 | A | 180 | TYR | CG-CD1-CE1 | -6.49 | 116.11 | 121.30 |
| 1 | K | 160 | LEU | CB-CG-CD1 | 6.49 | 122.03 | 111.00 |
| 1 | D | 367 | MET | CG-SD-CE | -6.48 | 89.83 | 100.20 |
| 1 | A | 490 | TYR | CD1-CG-CD2 | 6.48 | 125.03 | 117.90 |
| 1 | R | 123 | TYR | CD1-CE1-CZ | -6.48 | 113.97 | 119.80 |
| 1 | P | 434 | PRO | N-CD-CG | 6.47 | 112.91 | 103.20 |
| 1 | N | 200 | TRP | CA-CB-CG | 6.47 | 125.99 | 113.70 |
| 1 | O | 61 | ASP | CB-CG-OD1 | 6.47 | 124.12 | 118.30 |
| 1 | F | 161 | LEU | CB-CG-CD2 | 6.47 | 122.00 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | E | 321 | ARG | NE-CZ-NH1 | -6.47 | 117.07 | 120.30 |
| 1 | E | 198 | ASP | CB-CG-OD2 | 6.46 | 124.12 | 118.30 |
| 1 | S | 180 | TYR | CB-CG-CD2 | 6.46 | 124.88 | 121.00 |
| 1 | P | 96 | GLN | O-C-N | -6.46 | 112.36 | 122.70 |
| 1 | D | 209 | ILE | O-C-N | -6.45 | 112.38 | 122.70 |
| 1 | P | 344 | ASP | O-C-N | -6.44 | 112.40 | 122.70 |
| 1 | M | 203 | ASP | CB-CG-OD2 | -6.44 | 112.51 | 118.30 |
| 1 | B | 141 | VAL | CG1-CB-CG2 | -6.43 | 100.60 | 110.90 |
| 1 | A | 360 | ARG | NE-CZ-NH2 | 6.43 | 123.52 | 120.30 |
| 1 | L | 61 | ASP | CB-CG-OD2 | -6.43 | 112.51 | 118.30 |
| 1 | M | 458 | LEU | CB-CG-CD1 | 6.43 | 121.93 | 111.00 |
| 1 | N | 468 | ASP | CB-CG-OD1 | 6.43 | 124.09 | 118.30 |
| 1 | K | 162 | ARG | NE-CZ-NH2 | -6.43 | 117.09 | 120.30 |
| 1 | L | 69 | THR | CA-CB-OG1 | 6.42 | 122.48 | 109.00 |
| 1 | N | 484 | TRP | CA-CB-CG | 6.42 | 125.90 | 113.70 |
| 1 | M | 468 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 1 | O | 454 | LEU | CB-CG-CD2 | -6.41 | 100.10 | 111.00 |
| 1 | L | 474 | ARG | NE-CZ-NH1 | -6.41 | 117.10 | 120.30 |
| 1 | L | 77 | ASP | CB-CG-OD2 | -6.41 | 112.53 | 118.30 |
| 1 | L | 288 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 1 | B | 159 | ASP | CB-CG-OD1 | 6.39 | 124.06 | 118.30 |
| 1 | F | 58 | MET | CG-SD-CE | 6.39 | 110.43 | 100.20 |
| 1 | N | 279 | GLU | O-C-N | -6.39 | 112.47 | 122.70 |
| 1 | C | 532 | ALA | N-CA-CB | -6.39 | 101.16 | 110.10 |
| 1 | S | 240 | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 1 | H | 389 | ARG | NE-CZ-NH2 | -6.39 | 117.11 | 120.30 |
| 1 | F | 50 | TYR | CB-CG-CD2 | 6.38 | 124.83 | 121.00 |
| 1 | B | 229 | ASP | CB-CG-OD2 | 6.38 | 124.04 | 118.30 |
| 1 | R | 322 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | S | 33 | ARG | NE-CZ-NH2 | 6.37 | 123.49 | 120.30 |
| 1 | C | 411 | ASP | CB-CG-OD2 | 6.37 | 124.03 | 118.30 |
| 1 | D | 283 | ILE | CA-CB-CG1 | 6.37 | 123.10 | 111.00 |
| 1 | G | 484 | TRP | CB-CG-CD1 | -6.37 | 118.72 | 127.00 |
| 1 | C | 233 | VAL | CA-CB-CG1 | 6.36 | 120.44 | 110.90 |
| 1 | O | 334 | ALA | N-CA-CB | 6.36 | 119.01 | 110.10 |
| 1 | F | 391 | VAL | CA-CB-CG1 | 6.36 | 120.44 | 110.90 |
| 1 | P | 203 | ASP | CB-CG-OD1 | 6.34 | 124.01 | 118.30 |
| 1 | D | 338 | ARG | NH1-CZ-NH2 | -6.34 | 112.43 | 119.40 |
| 1 | B | 400 | ASP | CB-CG-OD2 | -6.34 | 112.60 | 118.30 |
| 1 | H | 474 | ARG | NE-CZ-NH1 | 6.33 | 123.47 | 120.30 |
| 1 | F | 392 | ASP | CB-CG-OD1 | 6.33 | 124.00 | 118.30 |
| 1 | N | 250 | ASP | CB-CG-OD2 | -6.33 | 112.60 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | O | 485 | TYR | CB-CG-CD1 | -6.33 | 117.20 | 121.00 |
| 1 | A | 407 | ASP | CB-CG-OD2 | 6.32 | 123.99 | 118.30 |
| 1 | K | 396 | ARG | NH1-CZ-NH2 | -6.32 | 112.45 | 119.40 |
| 1 | C | 71 | ASP | C-N-CA | 6.31 | 135.54 | 122.30 |
| 1 | N | 510 | MET | CA-CB-CG | -6.31 | 102.58 | 113.30 |
| 1 | E | 348 | GLU | OE1-CD-OE2 | -6.31 | 115.73 | 123.30 |
| 1 | A | 480 | GLU | OE1-CD-OE2 | -6.30 | 115.74 | 123.30 |
| 1 | G | 288 | ASP | CB-CG-OD2 | 6.30 | 123.97 | 118.30 |
| 1 | B | 261 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | F | 421 | VAL | CG1-CB-CG2 | -6.30 | 100.83 | 110.90 |
| 1 | S | 447 | TYR | CZ-CE2-CD2 | -6.30 | 114.13 | 119.80 |
| 1 | K | 157 | ASP | CB-CG-OD1 | -6.29 | 112.63 | 118.30 |
| 1 | C | 180 | TYR | CZ-CE2-CD2 | -6.29 | 114.14 | 119.80 |
| 1 | S | 333 | ARG | NE-CZ-NH1 | 6.29 | 123.45 | 120.30 |
| 1 | G | 333 | ARG | NE-CZ-NH2 | -6.29 | 117.16 | 120.30 |
| 1 | H | 270 | THR | O-C-N | -6.29 | 112.64 | 122.70 |
| 1 | S | 393 | GLU | OE1-CD-OE2 | -6.29 | 115.76 | 123.30 |
| 1 | B | 402 | LEU | N-CA-CB | 6.28 | 122.96 | 110.40 |
| 1 | G | 219 | ASP | CB-CG-OD2 | 6.28 | 123.95 | 118.30 |
| 1 | R | 123 | TYR | CG-CD2-CE2 | -6.28 | 116.28 | 121.30 |
| 1 | E | 350 | ASP | CB-CG-OD2 | 6.27 | 123.94 | 118.30 |
| 1 | A | 417 | GLY | O-C-N | -6.27 | 112.54 | 123.20 |
| 1 | C | 33 | ARG | NE-CZ-NH1 | 6.27 | 123.43 | 120.30 |
| 1 | N | 384 | ARG | NE-CZ-NH2 | -6.27 | 117.17 | 120.30 |
| 1 | D | 523 | VAL | CA-CB-CG2 | -6.27 | 101.50 | 110.90 |
| 1 | G | 402 | LEU | CB-CG-CD2 | 6.26 | 121.65 | 111.00 |
| 1 | G | 508 | VAL | CA-CB-CG2 | -6.26 | 101.52 | 110.90 |
| 1 | K | 382 | LEU | CB-CG-CD2 | -6.25 | 100.37 | 111.00 |
| 1 | N | 307 | VAL | CG1-CB-CG2 | -6.25 | 100.89 | 110.90 |
| 1 | C | 237 | MET | CG-SD-CE | -6.25 | 90.20 | 100.20 |
| 1 | L | 528 | ASP | CB-CG-OD1 | 6.24 | 123.92 | 118.30 |
| 1 | R | 265 | ARG | NE-CZ-NH1 | -6.24 | 117.18 | 120.30 |
| 1 | D | 268 | ASP | CB-CG-OD1 | 6.24 | 123.91 | 118.30 |
| 1 | K | 489 | LEU | CB-CG-CD1 | -6.23 | 100.41 | 111.00 |
| 1 | R | 159 | ASP | CB-CG-OD2 | 6.23 | 123.90 | 118.30 |
| 1 | R | 360 | ARG | NE-CZ-NH1 | 6.23 | 123.41 | 120.30 |
| 1 | D | 125 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | A | 348 | GLU | OE1-CD-OE2 | -6.22 | 115.84 | 123.30 |
| 1 | K | 288 | ASP | CB-CG-OD2 | -6.21 | 112.71 | 118.30 |
| 1 | N | 118 | ALA | CB-CA-C | -6.21 | 100.78 | 110.10 |
| 1 | C | 180 | TYR | CB-CG-CD2 | -6.21 | 117.27 | 121.00 |
| 1 | F | 208 | GLN | CA-CB-CG | 6.21 | 127.06 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | E | 152 | THR | N-CA-CB | 6.21 | 122.09 | 110.30 |
| 1 | H | 180 | TYR | CB-CG-CD2 | 6.19 | 124.72 | 121.00 |
| 1 | D | 264 | ILE | CA-CB-CG1 | 6.19 | 122.76 | 111.00 |
| 1 | Q | 104 | THR | CA-CB-CG2 | -6.19 | 103.73 | 112.40 |
| 1 | Q | 352 | GLY | CA-C-O | 6.19 | 131.74 | 120.60 |
| 1 | F | 61 | ASP | CB-CG-OD1 | 6.19 | 123.87 | 118.30 |
| 1 | L | 407 | ASP | CB-CG-OD2 | 6.18 | 123.86 | 118.30 |
| 1 | D | 400 | ASP | CB-CG-OD1 | -6.18 | 112.74 | 118.30 |
| 1 | I | 139 | GLU | OE1-CD-OE2 | -6.18 | 115.89 | 123.30 |
| 1 | L | 477 | HIS | CA-CB-CG | 6.18 | 124.10 | 113.60 |
| 1 | I | 353 | TYR | CB-CG-CD2 | -6.17 | 117.30 | 121.00 |
| 1 | I | 141 | VAL | CG1-CB-CG2 | -6.17 | 101.03 | 110.90 |
| 1 | R | 389 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 1 | L | 33 | ARG | NE-CZ-NH1 | 6.17 | 123.38 | 120.30 |
| 1 | E | 399 | ARG | NE-CZ-NH1 | -6.17 | 117.22 | 120.30 |
| 1 | B | 178 | ARG | NE-CZ-NH1 | -6.16 | 117.22 | 120.30 |
| 1 | D | 224 | TYR | CG-CD2-CE2 | -6.16 | 116.37 | 121.30 |
| 1 | G | 266 | ILE | CG1-CB-CG2 | -6.16 | 97.86 | 111.40 |
| 1 | I | 334 | ALA | O-C-N | -6.15 | 112.86 | 122.70 |
| 1 | K | 276 | LEU | CB-CG-CD2 | 6.15 | 121.45 | 111.00 |
| 1 | M | 61 | ASP | CB-CG-OD1 | 6.15 | 123.83 | 118.30 |
| 1 | R | 50 | TYR | CG-CD2-CE2 | -6.15 | 116.38 | 121.30 |
| 1 | B | 384 | ARG | N-CA-C | -6.15 | 94.41 | 111.00 |
| 1 | M | 413 | ARG | NH1-CZ-NH2 | -6.14 | 112.64 | 119.40 |
| 1 | Q | 413 | ARG | NH1-CZ-NH2 | 6.14 | 126.16 | 119.40 |
| 1 | Q | 389 | ARG | NH1-CZ-NH2 | -6.14 | 112.64 | 119.40 |
| 1 | P | 491 | ALA | N-CA-CB | -6.14 | 101.51 | 110.10 |
| 1 | I | 149 | LEU | CB-CG-CD2 | -6.13 | 100.58 | 111.00 |
| 1 | O | 135 | TYR | CG-CD1-CE1 | -6.12 | 116.40 | 121.30 |
| 1 | M | 80 | ASP | CB-CG-OD1 | -6.12 | 112.79 | 118.30 |
| 1 | P | 210 | VAL | CG1-CB-CG2 | -6.12 | 101.10 | 110.90 |
| 1 | K | 178 | ARG | NH1-CZ-NH2 | -6.12 | 112.67 | 119.40 |
| 1 | C | 77 | ASP | CB-CG-OD1 | 6.12 | 123.80 | 118.30 |
| 1 | S | 56 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | H | 185 | VAL | CA-CB-CG2 | -6.11 | 101.73 | 110.90 |
| 1 | I | 118 | ALA | CB-CA-C | -6.11 | 100.94 | 110.10 |
| 1 | K | 471 | MET | CG-SD-CE | -6.11 | 90.43 | 100.20 |
| 1 | C | 110 | PHE | CB-CG-CD1 | -6.11 | 116.53 | 120.80 |
| 1 | A | 171 | SER | O-C-N | -6.10 | 112.94 | 122.70 |
| 1 | D | 123 | TYR | CB-CG-CD2 | -6.10 | 117.34 | 121.00 |
| 1 | N | 460 | GLU | OE1-CD-OE2 | -6.09 | 115.99 | 123.30 |
| 1 | A | 324 | LYS | O-C-N | -6.09 | 112.95 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | H | 178 | ARG | CG-CD-NE | -6.09 | 99.01 | 111.80 |
| 1 | F | 490 | TYR | CG-CD2-CE2 | -6.09 | 116.43 | 121.30 |
| 1 | A | 56 | ASP | CB-CG-OD2 | -6.08 | 112.83 | 118.30 |
| 1 | M | 33 | ARG | NE-CZ-NH2 | -6.08 | 117.26 | 120.30 |
| 1 | P | 155 | ILE | O-C-N | -6.08 | 112.98 | 122.70 |
| 1 | K | 415 | ILE | O-C-N | -6.07 | 112.98 | 122.70 |
| 1 | N | 424 | GLU | O-C-N | -6.07 | 112.98 | 122.70 |
| 1 | C | 65 | ASP | CB-CG-OD1 | -6.07 | 112.83 | 118.30 |
| 1 | R | 165 | ALA | N-CA-CB | 6.07 | 118.60 | 110.10 |
| 1 | M | 201 | TYR | CG-CD1-CE1 | -6.07 | 116.45 | 121.30 |
| 1 | F | 485 | TYR | CB-CG-CD1 | 6.06 | 124.64 | 121.00 |
| 1 | Q | 93 | ALA | N-CA-CB | -6.05 | 101.63 | 110.10 |
| 1 | B | 162 | ARG | CD-NE-CZ | 6.05 | 132.07 | 123.60 |
| 1 | S | 384 | ARG | NH1-CZ-NH2 | -6.05 | 112.75 | 119.40 |
| 1 | O | 262 | ALA | N-CA-CB | 6.05 | 118.56 | 110.10 |
| 1 | A | 55 | MET | CG-SD-CE | -6.04 | 90.53 | 100.20 |
| 1 | A | 485 | TYR | CB-CG-CD2 | 6.04 | 124.62 | 121.00 |
| 1 | A | 488 | ASP | CB-CG-OD1 | -6.04 | 112.86 | 118.30 |
| 1 | B | 482 | ASN | N-CA-CB | 6.04 | 121.47 | 110.60 |
| 1 | G | 311 | TYR | CB-CG-CD1 | -6.04 | 117.38 | 121.00 |
| 1 | S | 473 | LEU | CB-CG-CD2 | 6.04 | 121.27 | 111.00 |
| 1 | M | 424 | GLU | O-C-N | -6.04 | 113.04 | 122.70 |
| 1 | H | 353 | TYR | CG-CD1-CE1 | -6.03 | 116.48 | 121.30 |
| 1 | E | 126 | VAL | CG1-CB-CG2 | -6.03 | 101.25 | 110.90 |
| 1 | I | 413 | ARG | NE-CZ-NH2 | 6.02 | 123.31 | 120.30 |
| 1 | P | 32 | VAL | CG1-CB-CG2 | -6.02 | 101.26 | 110.90 |
| 1 | N | 423 | ILE | O-C-N | -6.02 | 113.07 | 122.70 |
| 1 | S | 368 | VAL | CG1-CB-CG2 | -6.01 | 101.28 | 110.90 |
| 1 | M | 120 | ASP | CB-CG-OD1 | -6.01 | 112.89 | 118.30 |
| 1 | M | 232 | VAL | CA-CB-CG2 | 6.01 | 119.92 | 110.90 |
| 1 | O | 110 | PHE | CB-CG-CD1 | -6.01 | 116.59 | 120.80 |
| 1 | O | 516 | ALA | N-CA-CB | -6.01 | 101.69 | 110.10 |
| 1 | G | 440 | GLU | OE1-CD-OE2 | -6.01 | 116.09 | 123.30 |
| 1 | N | 129 | THR | CA-CB-CG2 | -6.01 | 103.99 | 112.40 |
| 1 | Q | 183 | ASP | CB-CG-OD2 | 6.01 | 123.70 | 118.30 |
| 1 | Q | 490 | TYR | CA-CB-CG | -6.00 | 102.00 | 113.40 |
| 1 | I | 399 | ARG | NE-CZ-NH1 | -6.00 | 117.30 | 120.30 |
| 1 | E | 261 | ASP | CB-CG-OD1 | -6.00 | 112.90 | 118.30 |
| 1 | E | 510 | MET | CG-SD-CE | -5.99 | 90.62 | 100.20 |
| 1 | M | 311 | TYR | CG-CD1-CE1 | -5.99 | 116.51 | 121.30 |
| 1 | R | 59 | LEU | O-C-N | 5.99 | 132.28 | 122.70 |
| 1 | H | 263 | GLU | O-C-N | -5.98 | 113.13 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | E | 462 | ALA | N-CA-CB | 5.98 | 118.48 | 110.10 |
| 1 | G | 232 | VAL | CA-CB-CG2 | 5.98 | 119.88 | 110.90 |
| 1 | G | 321 | ARG | CD-NE-CZ | 5.98 | 131.98 | 123.60 |
| 1 | I | 177 | ALA | N-CA-CB | -5.98 | 101.72 | 110.10 |
| 1 | L | 485 | TYR | CB-CG-CD1 | 5.98 | 124.59 | 121.00 |
| 1 | S | 384 | ARG | NE-CZ-NH2 | 5.98 | 123.29 | 120.30 |
| 1 | E | 229 | ASP | O-C-N | -5.97 | 113.15 | 122.70 |
| 1 | P | 320 | VAL | CG1-CB-CG2 | -5.97 | 101.35 | 110.90 |
| 1 | G | 433 | ALA | CA-C-N | 5.97 | 133.81 | 117.10 |
| 1 | P | 135 | TYR | CB-CG-CD2 | 5.97 | 124.58 | 121.00 |
| 1 | S | 150 | ALA | N-CA-CB | 5.97 | 118.46 | 110.10 |
| 1 | C | 275 | PHE | CB-CG-CD2 | -5.97 | 116.62 | 120.80 |
| 1 | F | 265 | ARG | NE-CZ-NH1 | -5.97 | 117.32 | 120.30 |
| 1 | G | 338 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | I | 488 | ASP | CB-CG-OD1 | 5.96 | 123.67 | 118.30 |
| 1 | L | 525 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | K | 425 | ILE | O-C-N | -5.96 | 113.17 | 122.70 |
| 1 | H | 90 | VAL | CG1-CB-CG2 | 5.95 | 120.42 | 110.90 |
| 1 | I | 421 | VAL | CA-CB-CG2 | -5.95 | 101.98 | 110.90 |
| 1 | N | 46 | LEU | CB-CG-CD2 | 5.95 | 121.11 | 111.00 |
| 1 | S | 237 | MET | CG-SD-CE | -5.95 | 90.69 | 100.20 |
| 1 | E | 322 | ARG | NE-CZ-NH2 | -5.95 | 117.33 | 120.30 |
| 1 | H | 305 | ASP | CB-CG-OD1 | 5.95 | 123.65 | 118.30 |
| 1 | L | 274 | LYS | CA-C-O | 5.94 | 132.57 | 120.10 |
| 1 | P | 480 | GLU | CG-CD-OE2 | -5.94 | 106.42 | 118.30 |
| 1 | G | 224 | TYR | CB-CG-CD2 | 5.94 | 124.56 | 121.00 |
| 1 | E | 462 | ALA | CB-CA-C | -5.93 | 101.20 | 110.10 |
| 1 | I | 432 | TYR | CB-CG-CD1 | -5.93 | 117.44 | 121.00 |
| 1 | L | 121 | LEU | CB-CG-CD1 | -5.93 | 100.92 | 111.00 |
| 1 | Q | 265 | ARG | NE-CZ-NH2 | 5.93 | 123.26 | 120.30 |
| 1 | R | 391 | VAL | CA-CB-CG2 | -5.93 | 102.01 | 110.90 |
| 1 | E | 157 | ASP | CB-CG-OD1 | -5.92 | 112.97 | 118.30 |
| 1 | E | 373 | ALA | CB-CA-C | 5.92 | 118.98 | 110.10 |
| 1 | G | 310 | SER | N-CA-CB | 5.92 | 119.38 | 110.50 |
| 1 | I | 240 | ARG | NE-CZ-NH2 | -5.92 | 117.34 | 120.30 |
| 1 | G | 194 | GLU | OE1-CD-OE2 | -5.92 | 116.20 | 123.30 |
| 1 | H | 360 | ARG | NE-CZ-NH2 | 5.92 | 123.26 | 120.30 |
| 1 | K | 33 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | Q | 198 | ASP | CB-CG-OD1 | 5.92 | 123.63 | 118.30 |
| 1 | H | 265 | ARG | NH1-CZ-NH2 | -5.91 | 112.90 | 119.40 |
| 1 | O | 485 | TYR | CB-CG-CD2 | 5.91 | 124.55 | 121.00 |
| 1 | A | 295 | ALA | N-CA-CB | -5.91 | 101.83 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 384 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | Q | 512 | ALA | CB-CA-C | 5.90 | 118.95 | 110.10 |
| 1 | O | 265 | ARG | CD-NE-CZ | 5.90 | 131.86 | 123.60 |
| 1 | E | 33 | ARG | CG-CD-NE | -5.89 | 99.42 | 111.80 |
| 1 | H | 478 | GLU | OE1-CD-OE2 | -5.89 | 116.23 | 123.30 |
| 1 | O | 175 | ALA | CA-C-N | 5.89 | 127.99 | 116.20 |
| 1 | N | 48 | SER | O-C-N | -5.89 | 113.27 | 122.70 |
| 1 | F | 123 | TYR | CB-CG-CD2 | -5.89 | 117.47 | 121.00 |
| 1 | D | 77 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 1 | F | 293 | THR | CA-CB-OG1 | 5.89 | 121.36 | 109.00 |
| 1 | D | 414 | ALA | O-C-N | -5.88 | 113.29 | 122.70 |
| 1 | G | 432 | TYR | CB-CG-CD2 | -5.88 | 117.47 | 121.00 |
| 1 | S | 56 | ASP | CB-CG-OD2 | -5.88 | 113.00 | 118.30 |
| 1 | Q | 53 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | R | 255 | VAL | CG1-CB-CG2 | -5.88 | 101.49 | 110.90 |
| 1 | L | 322 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | N | 219 | ASP | CA-CB-CG | -5.88 | 100.47 | 113.40 |
| 1 | N | 120 | ASP | O-C-N | -5.88 | 113.30 | 122.70 |
| 1 | I | 311 | TYR | CB-CG-CD1 | 5.88 | 124.53 | 121.00 |
| 1 | K | 102 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | S | 471 | MET | CG-SD-CE | -5.88 | 90.80 | 100.20 |
| 1 | M | 317 | VAL | CA-CB-CG2 | -5.87 | 102.09 | 110.90 |
| 1 | O | 367 | MET | CG-SD-CE | -5.87 | 90.80 | 100.20 |
| 1 | G | 272 | MET | CG-SD-CE | -5.87 | 90.81 | 100.20 |
| 1 | I | 247 | ALA | C-N-CA | 5.87 | 136.38 | 121.70 |
| 1 | O | 204 | LEU | O-C-N | -5.87 | 113.31 | 122.70 |
| 1 | Q | 389 | ARG | NE-CZ-NH1 | 5.87 | 123.23 | 120.30 |
| 1 | E | 396 | ARG | NE-CZ-NH1 | 5.87 | 123.23 | 120.30 |
| 1 | F | 157 | ASP | CB-CG-OD1 | 5.86 | 123.57 | 118.30 |
| 1 | S | 396 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | S | 453 | SER | N-CA-CB | -5.85 | 101.72 | 110.50 |
| 1 | R | 247 | ALA | CB-CA-C | -5.85 | 101.32 | 110.10 |
| 1 | E | 436 | VAL | CA-CB-CG2 | 5.85 | 119.67 | 110.90 |
| 1 | K | 265 | ARG | NE-CZ-NH1 | -5.85 | 117.38 | 120.30 |
| 1 | L | 341 | SER | N-CA-CB | 5.85 | 119.27 | 110.50 |
| 1 | O | 473 | LEU | CA-CB-CG | 5.85 | 128.75 | 115.30 |
| 1 | S | 455 | VAL | CA-CB-CG1 | -5.85 | 102.13 | 110.90 |
| 1 | B | 474 | ARG | NE-CZ-NH2 | 5.84 | 123.22 | 120.30 |
| 1 | H | 527 | ASP | CB-CG-OD2 | 5.84 | 123.56 | 118.30 |
| 1 | S | 272 | MET | CG-SD-CE | -5.84 | 90.85 | 100.20 |
| 1 | S | 228 | VAL | CA-CB-CG1 | -5.84 | 102.14 | 110.90 |
| 1 | R | 50 | TYR | CZ-CE2-CD2 | 5.84 | 125.06 | 119.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 123 | TYR | CB-CG-CD1 | -5.84 | 117.50 | 121.00 |
| 1 | K | 180 | TYR | CB-CG-CD1 | -5.84 | 117.50 | 121.00 |
| 1 | S | 117 | LYS | O-C-N | -5.84 | 113.36 | 122.70 |
| 1 | M | 231 | GLU | N-CA-CB | -5.83 | 100.10 | 110.60 |
| 1 | A | 180 | TYR | CB-CG-CD2 | -5.83 | 117.50 | 121.00 |
| 1 | S | 322 | ARG | CD-NE-CZ | 5.83 | 131.76 | 123.60 |
| 1 | H | 512 | ALA | C-N-CA | 5.83 | 136.27 | 121.70 |
| 1 | P | 141 | VAL | CA-CB-CG2 | -5.83 | 102.16 | 110.90 |
| 1 | B | 319 | ALA | CB-CA-C | -5.83 | 101.36 | 110.10 |
| 1 | D | 429 | LEU | CB-CG-CD1 | 5.83 | 120.91 | 111.00 |
| 1 | H | 470 | LEU | CB-CG-CD2 | -5.82 | 101.10 | 111.00 |
| 1 | E | 331 | LEU | O-C-N | -5.82 | 113.39 | 122.70 |
| 1 | L | 110 | PHE | CB-CG-CD1 | -5.82 | 116.73 | 120.80 |
| 1 | P | 192 | VAL | CA-CB-CG2 | -5.82 | 102.18 | 110.90 |
| 1 | D | 474 | ARG | NH1-CZ-NH2 | -5.81 | 113.01 | 119.40 |
| 1 | E | 285 | GLU | OE1-CD-OE2 | -5.81 | 116.33 | 123.30 |
| 1 | A | 119 | GLU | OE1-CD-OE2 | -5.81 | 116.33 | 123.30 |
| 1 | A | 329 | GLU | O-C-N | -5.81 | 113.41 | 122.70 |
| 1 | I | 149 | LEU | O-C-N | -5.81 | 113.40 | 122.70 |
| 1 | K | 320 | VAL | CG1-CB-CG2 | -5.81 | 101.61 | 110.90 |
| 1 | O | 525 | ARG | NE-CZ-NH2 | -5.81 | 117.39 | 120.30 |
| 1 | Q | 475 | SER | N-CA-CB | 5.81 | 119.21 | 110.50 |
| 1 | C | 220 | THR | O-C-N | -5.81 | 113.41 | 122.70 |
| 1 | F | 33 | ARG | CG-CD-NE | -5.81 | 99.60 | 111.80 |
| 1 | G | 484 | TRP | CB-CG-CD2 | 5.81 | 134.15 | 126.60 |
| 1 | C | 222 | LEU | CB-CG-CD2 | 5.81 | 120.87 | 111.00 |
| 1 | D | 338 | ARG | NE-CZ-NH2 | 5.81 | 123.20 | 120.30 |
| 1 | B | 392 | ASP | CB-CG-OD2 | 5.80 | 123.52 | 118.30 |
| 1 | C | 270 | THR | O-C-N | -5.79 | 113.43 | 122.70 |
| 1 | E | 45 | ALA | N-CA-CB | -5.79 | 101.99 | 110.10 |
| 1 | H | 123 | TYR | CZ-CE2-CD2 | 5.79 | 125.01 | 119.80 |
| 1 | L | 447 | TYR | CG-CD1-CE1 | -5.79 | 116.67 | 121.30 |
| 1 | L | 195 | LEU | O-C-N | -5.79 | 113.44 | 122.70 |
| 1 | A | 505 | PRO | N-CA-CB | 5.79 | 110.24 | 103.30 |
| 1 | H | 338 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | S | 378 | SER | CB-CA-C | -5.78 | 99.12 | 110.10 |
| 1 | L | 174 | VAL | CG1-CB-CG2 | -5.78 | 101.66 | 110.90 |
| 1 | B | 430 | ARG | NE-CZ-NH2 | -5.77 | 117.41 | 120.30 |
| 1 | R | 107 | ALA | CB-CA-C | 5.77 | 118.76 | 110.10 |
| 1 | R | 43 | GLU | OE1-CD-OE2 | -5.77 | 116.38 | 123.30 |
| 1 | C | 39 | VAL | CA-CB-CG2 | -5.77 | 102.25 | 110.90 |
| 1 | K | 525 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | Q | 237 | MET | CG-SD-CE | -5.76 | 90.98 | 100.20 |
| 1 | O | 480 | GLU | O-C-N | -5.76 | 113.48 | 122.70 |
| 1 | R | 413 | ARG | CG-CD-NE | -5.76 | 99.71 | 111.80 |
| 1 | Q | 530 | VAL | O-C-N | -5.75 | 113.50 | 122.70 |
| 1 | N | 389 | ARG | CG-CD-NE | -5.75 | 99.73 | 111.80 |
| 1 | S | 59 | LEU | CB-CG-CD2 | 5.75 | 120.77 | 111.00 |
| 1 | D | 123 | TYR | CG-CD2-CE2 | -5.75 | 116.70 | 121.30 |
| 1 | H | 80 | ASP | N-CA-CB | -5.74 | 100.26 | 110.60 |
| 1 | O | 123 | TYR | CG-CD1-CE1 | -5.74 | 116.71 | 121.30 |
| 1 | D | 370 | VAL | CA-CB-CG2 | -5.74 | 102.30 | 110.90 |
| 1 | P | 369 | PHE | CB-CG-CD1 | -5.74 | 116.78 | 120.80 |
| 1 | R | 151 | GLN | CG-CD-OE1 | 5.73 | 133.06 | 121.60 |
| 1 | C | 501 | GLY | O-C-N | -5.73 | 113.53 | 122.70 |
| 1 | M | 496 | ASP | CB-CG-OD2 | 5.73 | 123.45 | 118.30 |
| 1 | Q | 470 | LEU | CB-CG-CD2 | 5.73 | 120.73 | 111.00 |
| 1 | R | 318 | LEU | CB-CG-CD2 | 5.73 | 120.73 | 111.00 |
| 1 | P | 265 | ARG | CG-CD-NE | -5.72 | 99.78 | 111.80 |
| 1 | E | 450 | ALA | CB-CA-C | 5.72 | 118.68 | 110.10 |
| 1 | B | 369 | PHE | CB-CG-CD1 | 5.72 | 124.81 | 120.80 |
| 1 | C | 407 | ASP | CB-CG-OD2 | 5.72 | 123.45 | 118.30 |
| 1 | F | 510 | MET | CG-SD-CE | -5.72 | 91.05 | 100.20 |
| 1 | L | 384 | ARG | NH1-CZ-NH2 | -5.72 | 113.11 | 119.40 |
| 1 | H | 229 | ASP | CB-CG-OD2 | 5.71 | 123.44 | 118.30 |
| 1 | H | 162 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 1 | Q | 104 | THR | N-CA-CB | 5.71 | 121.15 | 110.30 |
| 1 | Q | 185 | VAL | CA-CB-CG2 | -5.71 | 102.33 | 110.90 |
| 1 | L | 125 | ASP | CB-CG-OD1 | -5.71 | 113.16 | 118.30 |
| 1 | D | 382 | LEU | CB-CG-CD1 | 5.71 | 120.70 | 111.00 |
| 1 | G | 265 | ARG | CG-CD-NE | -5.71 | 99.81 | 111.80 |
| 1 | I | 227 | VAL | CG1-CB-CG2 | -5.70 | 101.78 | 110.90 |
| 1 | G | 311 | TYR | CB-CG-CD2 | 5.70 | 124.42 | 121.00 |
| 1 | R | 305 | ASP | CB-CG-OD1 | -5.70 | 113.17 | 118.30 |
| 1 | O | 334 | ALA | CB-CA-C | -5.70 | 101.55 | 110.10 |
| 1 | G | 180 | TYR | CG-CD2-CE2 | -5.70 | 116.74 | 121.30 |
| 1 | S | 469 | LEU | CB-CG-CD2 | 5.70 | 120.68 | 111.00 |
| 1 | B | 79 | MET | CA-CB-CG | 5.69 | 122.98 | 113.30 |
| 1 | B | 259 | GLU | O-C-N | -5.69 | 113.59 | 122.70 |
| 1 | H | 178 | ARG | NE-CZ-NH1 | -5.69 | 117.45 | 120.30 |
| 1 | E | 297 | VAL | CB-CA-C | 5.69 | 122.20 | 111.40 |
| 1 | P | 178 | ARG | NH1-CZ-NH2 | -5.69 | 113.15 | 119.40 |
| 1 | E | 333 | ARG | CD-NE-CZ | 5.68 | 131.56 | 123.60 |
| 1 | F | 76 | LEU | N-CA-CB | -5.68 | 99.03 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | F | 198 | ASP | CB-CA-C | 5.68 | 121.77 | 110.40 |
| 1 | E | 365 | ASP | CB-CG-OD1 | -5.68 | 113.19 | 118.30 |
| 1 | D | 351 | LEU | CB-CG-CD2 | -5.67 | 101.36 | 111.00 |
| 1 | G | 334 | ALA | CB-CA-C | -5.67 | 101.59 | 110.10 |
| 1 | N | 33 | ARG | NE-CZ-NH2 | 5.67 | 123.14 | 120.30 |
| 1 | C | 30 | GLU | N-CA-C | 5.67 | 126.30 | 111.00 |
| 1 | D | 365 | ASP | CB-CG-OD1 | 5.67 | 123.40 | 118.30 |
| 1 | E | 205 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 1 | H | 432 | TYR | CB-CG-CD2 | 5.66 | 124.40 | 121.00 |
| 1 | K | 224 | TYR | CA-CB-CG | -5.66 | 102.66 | 113.40 |
| 1 | R | 496 | ASP | CB-CG-OD1 | 5.65 | 123.39 | 118.30 |
| 1 | D | 422 | GLU | OE1-CD-OE2 | -5.65 | 116.52 | 123.30 |
| 1 | G | 338 | ARG | CA-CB-CG | 5.65 | 125.82 | 113.40 |
| 1 | H | 102 | ASP | CB-CG-OD2 | 5.65 | 123.38 | 118.30 |
| 1 | I | 445 | GLU | O-C-N | -5.65 | 113.66 | 122.70 |
| 1 | P | 259 | GLU | OE1-CD-OE2 | -5.65 | 116.52 | 123.30 |
| 1 | R | 426 | ALA | O-C-N | -5.65 | 113.67 | 122.70 |
| 1 | E | 70 | ASN | O-C-N | -5.64 | 113.67 | 122.70 |
| 1 | G | 432 | TYR | CG-CD2-CE2 | 5.64 | 125.81 | 121.30 |
| 1 | A | 220 | THR | CA-CB-CG2 | -5.64 | 104.51 | 112.40 |
| 1 | E | 360 | ARG | NE-CZ-NH2 | 5.64 | 123.12 | 120.30 |
| 1 | S | 311 | TYR | CG-CD2-CE2 | -5.64 | 116.79 | 121.30 |
| 1 | C | 350 | ASP | CB-CG-OD2 | 5.63 | 123.37 | 118.30 |
| 1 | L | 248 | LEU | CB-CG-CD2 | 5.63 | 120.58 | 111.00 |
| 1 | E | 358 | GLU | OE1-CD-OE2 | -5.63 | 116.54 | 123.30 |
| 1 | O | 304 | ILE | O-C-N | -5.63 | 113.70 | 122.70 |
| 1 | H | 327 | ASP | CB-CG-OD1 | 5.62 | 123.36 | 118.30 |
| 1 | G | 407 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | F | 201 | TYR | CD1-CE1-CZ | 5.62 | 124.85 | 119.80 |
| 1 | S | 345 | GLU | O-C-N | -5.61 | 113.72 | 122.70 |
| 1 | M | 180 | TYR | CB-CG-CD1 | -5.61 | 117.63 | 121.00 |
| 1 | B | 327 | ASP | CB-CG-OD1 | -5.61 | 113.25 | 118.30 |
| 1 | B | 432 | TYR | CB-CG-CD1 | -5.61 | 117.63 | 121.00 |
| 1 | N | 370 | VAL | O-C-N | -5.61 | 113.73 | 122.70 |
| 1 | S | 389 | ARG | CG-CD-NE | -5.61 | 100.03 | 111.80 |
| 1 | I | 525 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |
| 1 | F | 318 | LEU | CB-CG-CD2 | 5.60 | 120.52 | 111.00 |
| 1 | K | 413 | ARG | NE-CZ-NH1 | -5.60 | 117.50 | 120.30 |
| 1 | S | 362 | VAL | CG1-CB-CG2 | -5.59 | 101.95 | 110.90 |
| 1 | F | 427 | LYS | N-CA-CB | -5.59 | 100.54 | 110.60 |
| 1 | R | 416 | ALA | N-CA-CB | 5.59 | 117.92 | 110.10 |
| 1 | D | 353 | TYR | CG-CD2-CE2 | -5.59 | 116.83 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | P | 391 | VAL | CA-CB-CG1 | 5.58 | 119.28 | 110.90 |
| 1 | D | 528 | ASP | CB-CG-OD1 | 5.58 | 123.33 | 118.30 |
| 1 | L | 123 | TYR | CB-CG-CD2 | 5.58 | 124.35 | 121.00 |
| 1 | B | 350 | ASP | CB-CG-OD1 | -5.58 | 113.28 | 118.30 |
| 1 | C | 242 | GLU | OE1-CD-OE2 | -5.58 | 116.60 | 123.30 |
| 1 | S | 527 | ASP | N-CA-CB | -5.58 | 100.56 | 110.60 |
| 1 | R | 430 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | R | 194 | GLU | OE1-CD-OE2 | -5.58 | 116.61 | 123.30 |
| 1 | R | 498 | TRP | CB-CG-CD1 | 5.58 | 134.25 | 127.00 |
| 1 | M | 430 | ARG | NE-CZ-NH2 | -5.57 | 117.52 | 120.30 |
| 1 | A | 365 | ASP | CB-CG-OD1 | -5.57 | 113.29 | 118.30 |
| 1 | F | 250 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 1 | N | 440 | GLU | O-C-N | -5.57 | 113.80 | 122.70 |
| 1 | I | 384 | ARG | N-CA-C | -5.56 | 95.98 | 111.00 |
| 1 | I | 333 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |
| 1 | M | 65 | ASP | CB-CG-OD2 | -5.56 | 113.30 | 118.30 |
| 1 | F | 490 | TYR | CA-CB-CG | -5.55 | 102.85 | 113.40 |
| 1 | N | 185 | VAL | CA-CB-CG1 | 5.55 | 119.23 | 110.90 |
| 1 | N | 327 | ASP | CB-CG-OD2 | 5.55 | 123.30 | 118.30 |
| 1 | A | 287 | VAL | CG1-CB-CG2 | -5.55 | 102.02 | 110.90 |
| 1 | C | 175 | ALA | O-C-N | -5.55 | 113.76 | 123.20 |
| 1 | N | 328 | LEU | CB-CG-CD2 | 5.55 | 120.43 | 111.00 |
| 1 | R | 74 | THR | O-C-N | -5.55 | 113.82 | 122.70 |
| 1 | F | 44 | GLU | O-C-N | -5.55 | 113.83 | 122.70 |
| 1 | I | 50 | TYR | CD1-CG-CD2 | 5.55 | 124.00 | 117.90 |
| 1 | K | 79 | MET | CG-SD-CE | -5.54 | 91.33 | 100.20 |
| 1 | A | 353 | TYR | CG-CD1-CE1 | 5.54 | 125.73 | 121.30 |
| 1 | A | 523 | VAL | CA-CB-CG2 | -5.54 | 102.58 | 110.90 |
| 1 | C | 80 | ASP | CB-CG-OD2 | 5.54 | 123.29 | 118.30 |
| 1 | C | 148 | GLU | CA-C-O | 5.54 | 131.74 | 120.10 |
| 1 | D | 391 | VAL | C-N-CA | 5.54 | 135.56 | 121.70 |
| 1 | P | 115 | VAL | CG1-CB-CG2 | -5.54 | 102.03 | 110.90 |
| 1 | Q | 320 | VAL | CG1-CB-CG2 | -5.54 | 102.03 | 110.90 |
| 1 | K | 139 | GLU | CB-CA-C | 5.54 | 121.48 | 110.40 |
| 1 | E | 360 | ARG | O-C-N | -5.54 | 113.84 | 122.70 |
| 1 | L | 49 | THR | CA-CB-OG1 | 5.54 | 120.63 | 109.00 |
| 1 | H | 272 | MET | CG-SD-CE | -5.54 | 91.34 | 100.20 |
| 1 | R | 526 | ILE | O-C-N | -5.54 | 113.84 | 122.70 |
| 1 | H | 277 | ASP | CB-CG-OD2 | 5.53 | 123.28 | 118.30 |
| 1 | M | 484 | TRP | CH2-CZ2-CE2 | 5.53 | 122.93 | 117.40 |
| 1 | A | 465 | ASP | CB-CG-OD1 | -5.53 | 113.33 | 118.30 |
| 1 | K | 322 | ARG | NE-CZ-NH2 | -5.53 | 117.54 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | L | 426 | ALA | CB-CA-C | 5.53 | 118.39 | 110.10 |
| 1 | S | 350 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | E | 208 | GLN | O-C-N | -5.53 | 113.86 | 122.70 |
| 1 | E | 433 | ALA | CA-C-O | -5.53 | 108.50 | 120.10 |
| 1 | A | 275 | PHE | CB-CG-CD1 | -5.52 | 116.93 | 120.80 |
| 1 | N | 305 | ASP | CB-CG-OD1 | -5.52 | 113.33 | 118.30 |
| 1 | R | 119 | GLU | OE1-CD-OE2 | -5.52 | 116.67 | 123.30 |
| 1 | D | 78 | LYS | O-C-N | -5.52 | 113.86 | 122.70 |
| 1 | M | 529 | VAL | CA-CB-CG1 | -5.52 | 102.62 | 110.90 |
| 1 | P | 49 | THR | CA-CB-CG2 | -5.52 | 104.67 | 112.40 |
| 1 | C | 451 | LEU | CB-CA-C | -5.51 | 99.72 | 110.20 |
| 1 | R | 153 | VAL | CA-CB-CG2 | -5.51 | 102.63 | 110.90 |
| 1 | Q | 382 | LEU | CB-CG-CD1 | 5.51 | 120.37 | 111.00 |
| 1 | P | 425 | ILE | CA-CB-CG1 | 5.51 | 121.47 | 111.00 |
| 1 | P | 474 | ARG | NE-CZ-NH1 | -5.51 | 117.54 | 120.30 |
| 1 | R | 275 | PHE | CB-CG-CD1 | 5.51 | 124.66 | 120.80 |
| 1 | N | 101 | ALA | O-C-N | -5.51 | 113.89 | 122.70 |
| 1 | A | 180 | TYR | CD1-CE1-CZ | 5.51 | 124.76 | 119.80 |
| 1 | Q | 333 | ARG | NE-CZ-NH1 | 5.51 | 123.05 | 120.30 |
| 1 | L | 389 | ARG | CG-CD-NE | -5.50 | 100.24 | 111.80 |
| 1 | B | 219 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | G | 474 | ARG | NE-CZ-NH2 | 5.50 | 123.05 | 120.30 |
| 1 | S | 411 | ASP | CB-CA-C | 5.50 | 121.41 | 110.40 |
| 1 | P | 413 | ARG | NH1-CZ-NH2 | -5.50 | 113.35 | 119.40 |
| 1 | C | 490 | TYR | CG-CD2-CE2 | -5.50 | 116.90 | 121.30 |
| 1 | B | 502 | VAL | CA-CB-CG2 | -5.50 | 102.65 | 110.90 |
| 1 | E | 341 | SER | N-CA-CB | 5.50 | 118.75 | 110.50 |
| 1 | B | 360 | ARG | NE-CZ-NH2 | 5.50 | 123.05 | 120.30 |
| 1 | H | 57 | LYS | N-CA-CB | 5.50 | 120.50 | 110.60 |
| 1 | S | 174 | VAL | O-C-N | -5.50 | 113.91 | 122.70 |
| 1 | B | 205 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 1 | R | 244 | ALA | N-CA-CB | -5.49 | 102.41 | 110.10 |
| 1 | A | 317 | VAL | O-C-N | -5.49 | 113.92 | 122.70 |
| 1 | H | 429 | LEU | CB-CG-CD1 | 5.49 | 120.33 | 111.00 |
| 1 | Q | 50 | TYR | CG-CD2-CE2 | -5.49 | 116.91 | 121.30 |
| 1 | K | 484 | TRP | CB-CG-CD1 | -5.49 | 119.87 | 127.00 |
| 1 | P | 240 | ARG | NH1-CZ-NH2 | -5.49 | 113.37 | 119.40 |
| 1 | D | 456 | SER | N-CA-CB | 5.48 | 118.72 | 110.50 |
| 1 | R | 242 | GLU | OE1-CD-OE2 | -5.48 | 116.72 | 123.30 |
| 1 | A | 389 | ARG | NE-CZ-NH1 | -5.48 | 117.56 | 120.30 |
| 1 | F | 434 | PRO | N-CA-CB | 5.48 | 109.88 | 103.30 |
| 1 | G | 101 | ALA | CB-CA-C | 5.48 | 118.32 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | Q | 153 | VAL | CG1-CB-CG2 | -5.48 | 102.14 | 110.90 |
| 1 | C | 250 | ASP | CB-CG-OD2 | 5.47 | 123.23 | 118.30 |
| 1 | A | 495 | VAL | CA-CB-CG1 | -5.47 | 102.69 | 110.90 |
| 1 | C | 460 | GLU | OE1-CD-OE2 | 5.47 | 129.87 | 123.30 |
| 1 | H | 180 | TYR | CB-CG-CD1 | -5.47 | 117.72 | 121.00 |
| 1 | K | 222 | LEU | CB-CG-CD2 | -5.47 | 101.70 | 111.00 |
| 1 | O | 432 | TYR | CG-CD1-CE1 | -5.47 | 116.92 | 121.30 |
| 1 | B | 468 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 1 | R | 288 | ASP | O-C-N | -5.47 | 113.95 | 122.70 |
| 1 | G | 351 | LEU | O-C-N | -5.47 | 113.91 | 123.20 |
| 1 | G | 389 | ARG | NE-CZ-NH2 | 5.47 | 123.03 | 120.30 |
| 1 | A | 411 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | H | 167 | THR | O-C-N | -5.46 | 113.96 | 122.70 |
| 1 | H | 392 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 1 | K | 121 | LEU | O-C-N | -5.46 | 113.96 | 122.70 |
| 1 | N | 525 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | O | 411 | ASP | CB-CG-OD2 | 5.46 | 123.22 | 118.30 |
| 1 | D | 79 | MET | CG-SD-CE | -5.46 | 91.47 | 100.20 |
| 1 | G | 487 | ILE | CA-CB-CG1 | 5.46 | 121.37 | 111.00 |
| 1 | R | 50 | TYR | CB-CG-CD1 | -5.46 | 117.73 | 121.00 |
| 1 | A | 82 | GLN | O-C-N | -5.46 | 113.97 | 122.70 |
| 1 | N | 338 | ARG | CD-NE-CZ | 5.45 | 131.23 | 123.60 |
| 1 | L | 389 | ARG | CB-CG-CD | 5.45 | 125.77 | 111.60 |
| 1 | I | 413 | ARG | NE-CZ-NH1 | -5.45 | 117.58 | 120.30 |
| 1 | G | 211 | LYS | CA-CB-CG | 5.45 | 125.38 | 113.40 |
| 1 | P | 504 | GLU | OE1-CD-OE2 | -5.45 | 116.76 | 123.30 |
| 1 | H | 178 | ARG | CD-NE-CZ | 5.45 | 131.22 | 123.60 |
| 1 | L | 98 | GLU | O-C-N | -5.45 | 113.99 | 122.70 |
| 1 | B | 220 | THR | CA-CB-CG2 | -5.44 | 104.78 | 112.40 |
| 1 | I | 311 | TYR | CG-CD2-CE2 | -5.44 | 116.94 | 121.30 |
| 1 | Q | 512 | ALA | N-CA-CB | -5.44 | 102.48 | 110.10 |
| 1 | D | 494 | PRO | N-CA-CB | 5.44 | 109.83 | 103.30 |
| 1 | E | 447 | TYR | CB-CG-CD1 | 5.44 | 124.27 | 121.00 |
| 1 | P | 157 | ASP | CB-CG-OD1 | 5.44 | 123.20 | 118.30 |
| 1 | D | 305 | ASP | CB-CG-OD1 | 5.44 | 123.19 | 118.30 |
| 1 | L | 125 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 1 | P | 392 | ASP | CB-CG-OD1 | 5.44 | 123.19 | 118.30 |
| 1 | E | 484 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 1 | A | 470 | LEU | CB-CG-CD1 | 5.43 | 120.24 | 111.00 |
| 1 | C | 90 | VAL | CA-CB-CG1 | -5.43 | 102.75 | 110.90 |
| 1 | C | 522 | LEU | CB-CG-CD1 | 5.43 | 120.24 | 111.00 |
| 1 | D | 349 | GLN | CG-CD-OE1 | -5.43 | 110.73 | 121.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | B | 250 | ASP | CB-CA-C | 5.43 | 121.27 | 110.40 |
| 1 | B | 331 | LEU | N-CA-CB | -5.43 | 99.53 | 110.40 |
| 1 | H | 255 | VAL | CG1-CB-CG2 | -5.43 | 102.21 | 110.90 |
| 1 | P | 304 | ILE | CA-CB-CG2 | -5.43 | 100.03 | 110.90 |
| 1 | E | 481 | ASN | CA-CB-CG | -5.43 | 101.45 | 113.40 |
| 1 | I | 415 | ILE | O-C-N | -5.43 | 114.01 | 122.70 |
| 1 | D | 160 | LEU | CB-CG-CD2 | -5.43 | 101.77 | 111.00 |
| 1 | B | 55 | MET | CG-SD-CE | -5.42 | 91.52 | 100.20 |
| 1 | I | 39 | VAL | CA-CB-CG2 | -5.41 | 102.78 | 110.90 |
| 1 | K | 317 | VAL | CA-CB-CG1 | -5.41 | 102.78 | 110.90 |
| 1 | L | 333 | ARG | NE-CZ-NH2 | 5.41 | 123.01 | 120.30 |
| 1 | M | 261 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | M | 291 | LEU | C-N-CA | 5.41 | 135.22 | 121.70 |
| 1 | P | 516 | ALA | N-CA-C | 5.41 | 125.61 | 111.00 |
| 1 | H | 129 | THR | CA-CB-CG2 | -5.41 | 104.83 | 112.40 |
| 1 | N | 186 | VAL | CB-CA-C | -5.41 | 101.13 | 111.40 |
| 1 | C | 229 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 1 | C | 528 | ASP | CA-C-N | -5.40 | 105.31 | 117.20 |
| 1 | D | 406 | ALA | N-CA-CB | -5.40 | 102.53 | 110.10 |
| 1 | R | 485 | TYR | CB-CG-CD1 | -5.40 | 117.76 | 121.00 |
| 1 | N | 71 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 1 | P | 514 | LYS | N-CA-CB | 5.40 | 120.32 | 110.60 |
| 1 | H | 354 | ALA | N-CA-CB | 5.40 | 117.66 | 110.10 |
| 1 | I | 322 | ARG | NE-CZ-NH2 | 5.40 | 123.00 | 120.30 |
| 1 | S | 215 | GLY | O-C-N | -5.40 | 114.06 | 122.70 |
| 1 | B | 108 | VAL | CA-CB-CG1 | 5.40 | 119.00 | 110.90 |
| 1 | F | 384 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | L | 525 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | R | 279 | GLU | OE1-CD-OE2 | -5.39 | 116.83 | 123.30 |
| 1 | S | 292 | ALA | N-CA-CB | 5.39 | 117.65 | 110.10 |
| 1 | D | 484 | TRP | CH2-CZ2-CE2 | 5.39 | 122.79 | 117.40 |
| 1 | L | 384 | ARG | CD-NE-CZ | 5.39 | 131.15 | 123.60 |
| 1 | I | 400 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |
| 1 | I | 432 | TYR | CB-CG-CD2 | 5.39 | 124.23 | 121.00 |
| 1 | M | 369 | PHE | CB-CG-CD2 | 5.39 | 124.57 | 120.80 |
| 1 | N | 432 | TYR | CG-CD2-CE2 | -5.39 | 116.99 | 121.30 |
| 1 | R | 305 | ASP | O-C-N | -5.39 | 114.08 | 122.70 |
| 1 | F | 475 | SER | C-N-CA | 5.38 | 135.16 | 121.70 |
| 1 | C | 389 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | G | 279 | GLU | OE1-CD-OE2 | -5.38 | 116.84 | 123.30 |
| 1 | B | 296 | ASN | O-C-N | -5.38 | 114.09 | 122.70 |
| 1 | G | 401 | ALA | CB-CA-C | 5.38 | 118.17 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 100 | THR | CA-CB-CG2 | -5.38 | 104.87 | 112.40 |
| 1 | R | 353 | TYR | CB-CG-CD1 | -5.38 | 117.77 | 121.00 |
| 1 | N | 162 | ARG | CD-NE-CZ | 5.38 | 131.13 | 123.60 |
| 1 | G | 201 | TYR | CZ-CE2-CD2 | 5.37 | 124.64 | 119.80 |
| 1 | O | 224 | TYR | CB-CG-CD2 | -5.37 | 117.78 | 121.00 |
| 1 | P | 203 | ASP | CA-CB-CG | 5.37 | 125.21 | 113.40 |
| 1 | K | 506 | ALA | CB-CA-C | 5.36 | 118.14 | 110.10 |
| 1 | F | 506 | ALA | O-C-N | -5.36 | 114.12 | 122.70 |
| 1 | G | 327 | ASP | CB-CG-OD2 | -5.36 | 113.47 | 118.30 |
| 1 | S | 46 | LEU | CB-CG-CD1 | -5.36 | 101.88 | 111.00 |
| 1 | C | 256 | GLU | OE1-CD-OE2 | -5.36 | 116.87 | 123.30 |
| 1 | D | 301 | GLN | O-C-N | -5.36 | 114.13 | 122.70 |
| 1 | E | 430 | ARG | CD-NE-CZ | -5.36 | 116.10 | 123.60 |
| 1 | K | 489 | LEU | CB-CG-CD2 | 5.36 | 120.10 | 111.00 |
| 1 | G | 236 | GLY | O-C-N | -5.35 | 114.14 | 122.70 |
| 1 | M | 135 | TYR | CD1-CE1-CZ | -5.35 | 114.98 | 119.80 |
| 1 | A | 272 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | M | 224 | TYR | CD1-CE1-CZ | -5.35 | 114.98 | 119.80 |
| 1 | H | 50 | TYR | CB-CG-CD2 | -5.35 | 117.79 | 121.00 |
| 1 | C | 424 | GLU | O-C-N | -5.34 | 114.15 | 122.70 |
| 1 | O | 280 | GLU | OE1-CD-OE2 | -5.34 | 116.89 | 123.30 |
| 1 | F | 287 | VAL | CA-CB-CG2 | 5.34 | 118.91 | 110.90 |
| 1 | L | 399 | ARG | CG-CD-NE | -5.34 | 100.58 | 111.80 |
| 1 | C | 277 | ASP | CB-CG-OD1 | -5.34 | 113.50 | 118.30 |
| 1 | F | 247 | ALA | C-N-CA | 5.34 | 135.05 | 121.70 |
| 1 | C | 510 | MET | CG-SD-CE | -5.34 | 91.66 | 100.20 |
| 1 | D | 466 | PRO | N-CA-C | 5.33 | 125.97 | 112.10 |
| 1 | I | 42 | VAL | CA-CB-CG2 | -5.33 | 102.90 | 110.90 |
| 1 | S | 219 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | E | 279 | GLU | CA-CB-CG | 5.33 | 125.13 | 113.40 |
| 1 | D | 222 | LEU | CB-CA-C | 5.33 | 120.32 | 110.20 |
| 1 | E | 344 | ASP | CB-CG-OD2 | 5.33 | 123.09 | 118.30 |
| 1 | O | 122 | LEU | O-C-N | -5.33 | 114.18 | 122.70 |
| 1 | S | 244 | ALA | N-CA-CB | -5.33 | 102.64 | 110.10 |
| 1 | E | 505 | PRO | N-CD-CG | 5.33 | 111.19 | 103.20 |
| 1 | K | 208 | GLN | CA-CB-CG | 5.33 | 125.12 | 113.40 |
| 1 | E | 219 | ASP | OD1-CG-OD2 | -5.33 | 113.18 | 123.30 |
| 1 | E | 527 | ASP | CB-CG-OD2 | -5.33 | 113.51 | 118.30 |
| 1 | F | 120 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | F | 298 | ILE | O-C-N | -5.33 | 114.18 | 122.70 |
| 1 | O | 275 | PHE | CG-CD2-CE2 | -5.33 | 114.94 | 120.80 |
| 1 | D | 485 | TYR | CB-CG-CD1 | 5.32 | 124.19 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 147 | GLN | O-C-N | -5.32 | 114.19 | 122.70 |
| 1 | P | 219 | ASP | CB-CG-OD2 | -5.32 | 113.51 | 118.30 |
| 1 | N | 353 | TYR | CD1-CG-CD2 | 5.32 | 123.75 | 117.90 |
| 1 | D | 396 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 1 | Q | 277 | ASP | CB-CG-OD2 | 5.32 | 123.08 | 118.30 |
| 1 | P | 55 | MET | CA-CB-CG | 5.32 | 122.34 | 113.30 |
| 1 | C | 476 | THR | C-N-CA | 5.31 | 134.98 | 121.70 |
| 1 | D | 241 | LEU | CB-CG-CD1 | 5.31 | 120.03 | 111.00 |
| 1 | F | 65 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | G | 190 | THR | O-C-N | -5.31 | 114.20 | 122.70 |
| 1 | L | 136 | LYS | O-C-N | -5.31 | 114.20 | 122.70 |
| 1 | A | 233 | VAL | O-C-N | -5.31 | 114.21 | 122.70 |
| 1 | C | 340 | VAL | CA-CB-CG2 | -5.31 | 102.94 | 110.90 |
| 1 | S | 448 | ALA | O-C-N | -5.31 | 114.21 | 122.70 |
| 1 | D | 224 | TYR | CB-CG-CD1 | -5.30 | 117.82 | 121.00 |
| 1 | H | 384 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | C | 265 | ARG | NH1-CZ-NH2 | -5.30 | 113.57 | 119.40 |
| 1 | P | 438 | GLY | CA-C-O | 5.30 | 130.15 | 120.60 |
| 1 | D | 31 | ALA | CB-CA-C | 5.30 | 118.05 | 110.10 |
| 1 | N | 310 | SER | O-C-N | -5.30 | 114.22 | 122.70 |
| 1 | Q | 50 | TYR | CB-CG-CD1 | 5.30 | 124.18 | 121.00 |
| 1 | R | 100 | THR | O-C-N | -5.29 | 114.23 | 122.70 |
| 1 | G | 473 | LEU | CB-CG-CD2 | 5.29 | 119.99 | 111.00 |
| 1 | K | 430 | ARG | NE-CZ-NH1 | 5.29 | 122.94 | 120.30 |
| 1 | L | 74 | THR | O-C-N | -5.29 | 114.24 | 122.70 |
| 1 | L | 263 | GLU | OE1-CD-OE2 | -5.29 | 116.95 | 123.30 |
| 1 | D | 108 | VAL | CG1-CB-CG2 | -5.29 | 102.44 | 110.90 |
| 1 | R | 332 | ALA | CB-CA-C | 5.29 | 118.03 | 110.10 |
| 1 | H | 223 | VAL | O-C-N | -5.29 | 114.24 | 122.70 |
| 1 | E | 278 | GLU | N-CA-CB | -5.28 | 101.09 | 110.60 |
| 1 | M | 368 | VAL | CA-CB-CG2 | -5.28 | 102.97 | 110.90 |
| 1 | D | 150 | ALA | O-C-N | -5.28 | 114.25 | 122.70 |
| 1 | C | 528 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | I | 122 | LEU | CB-CG-CD2 | 5.28 | 119.97 | 111.00 |
| 1 | S | 232 | VAL | CA-CB-CG1 | 5.28 | 118.81 | 110.90 |
| 1 | B | 301 | GLN | N-CA-CB | -5.27 | 101.11 | 110.60 |
| 1 | Q | 262 | ALA | N-CA-CB | 5.27 | 117.48 | 110.10 |
| 1 | B | 305 | ASP | OD1-CG-OD2 | -5.27 | 113.29 | 123.30 |
| 1 | C | 305 | ASP | O-C-N | -5.27 | 114.27 | 122.70 |
| 1 | M | 189 | VAL | CG1-CB-CG2 | -5.27 | 102.47 | 110.90 |
| 1 | P | 265 | ARG | NE-CZ-NH2 | 5.27 | 122.93 | 120.30 |
| 1 | S | 359 | GLU | OE1-CD-OE2 | -5.27 | 116.98 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 443 | ALA | N-CA-CB | 5.26 | 117.47 | 110.10 |
| 1 | C | 125 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 1 | O | 232 | VAL | O-C-N | -5.26 | 114.28 | 122.70 |
| 1 | B | 215 | GLY | O-C-N | -5.26 | 114.28 | 122.70 |
| 1 | B | 485 | TYR | CB-CG-CD1 | -5.26 | 117.84 | 121.00 |
| 1 | D | 523 | VAL | O-C-N | -5.26 | 114.28 | 122.70 |
| 1 | I | 344 | ASP | CB-CA-C | -5.26 | 99.88 | 110.40 |
| 1 | I | 355 | SER | CB-CA-C | -5.26 | 100.11 | 110.10 |
| 1 | M | 224 | TYR | CG-CD2-CE2 | -5.26 | 117.09 | 121.30 |
| 1 | A | 354 | ALA | O-C-N | -5.26 | 114.29 | 122.70 |
| 1 | O | 32 | VAL | CA-CB-CG2 | -5.26 | 103.01 | 110.90 |
| 1 | H | 344 | ASP | CB-CG-OD2 | 5.26 | 123.03 | 118.30 |
| 1 | N | 32 | VAL | CA-CB-CG2 | -5.25 | 103.02 | 110.90 |
| 1 | S | 411 | ASP | CB-CG-OD1 | -5.25 | 113.57 | 118.30 |
| 1 | B | 203 | ASP | CB-CG-OD1 | -5.25 | 113.57 | 118.30 |
| 1 | B | 384 | ARG | O-C-N | -5.25 | 114.27 | 123.20 |
| 1 | E | 392 | ASP | CB-CG-OD2 | 5.25 | 123.03 | 118.30 |
| 1 | E | 305 | ASP | CB-CA-C | -5.25 | 99.90 | 110.40 |
| 1 | F | 421 | VAL | C-N-CA | 5.25 | 134.83 | 121.70 |
| 1 | G | 423 | ILE | O-C-N | -5.25 | 114.30 | 122.70 |
| 1 | O | 220 | THR | CA-CB-OG1 | 5.25 | 120.03 | 109.00 |
| 1 | S | 203 | ASP | CB-CG-OD1 | -5.25 | 113.58 | 118.30 |
| 1 | D | 477 | HIS | CA-CB-CG | 5.25 | 122.52 | 113.60 |
| 1 | E | 224 | TYR | O-C-N | -5.25 | 114.28 | 123.20 |
| 1 | N | 165 | ALA | O-C-N | -5.25 | 114.30 | 122.70 |
| 1 | E | 83 | HIS | CA-CB-CG | 5.25 | 122.52 | 113.60 |
| 1 | H | 185 | VAL | O-C-N | -5.25 | 114.31 | 122.70 |
| 1 | I | 77 | ASP | CB-CG-OD2 | -5.25 | 113.58 | 118.30 |
| 1 | O | 413 | ARG | NE-CZ-NH2 | 5.25 | 122.92 | 120.30 |
| 1 | E | 389 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | N | 224 | TYR | CB-CG-CD2 | -5.24 | 117.85 | 121.00 |
| 1 | R | 391 | VAL | CA-CB-CG1 | 5.24 | 118.77 | 110.90 |
| 1 | S | 384 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | E | 392 | ASP | CB-CG-OD1 | -5.24 | 113.58 | 118.30 |
| 1 | S | 339 | VAL | CB-CA-C | -5.24 | 101.45 | 111.40 |
| 1 | O | 416 | ALA | CA-C-N | 5.24 | 126.67 | 116.20 |
| 1 | E | 408 | VAL | CA-CB-CG2 | -5.23 | 103.05 | 110.90 |
| 1 | N | 135 | TYR | CB-CG-CD1 | -5.23 | 117.86 | 121.00 |
| 1 | R | 80 | ASP | CB-CG-OD2 | -5.23 | 113.59 | 118.30 |
| 1 | S | 359 | GLU | O-C-N | -5.23 | 114.33 | 122.70 |
| 1 | I | 347 | SER | N-CA-CB | 5.23 | 118.34 | 110.50 |
| 1 | K | 71 | ASP | CB-CG-OD2 | 5.23 | 123.00 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | S | 257 | LYS | CB-CA-C | -5.23 | 99.94 | 110.40 |
| 1 | N | 232 | VAL | CA-CB-CG2 | 5.22 | 118.74 | 110.90 |
| 1 | R | 407 | ASP | OD1-CG-OD2 | -5.22 | 113.37 | 123.30 |
| 1 | C | 296 | ASN | CB-CG-OD1 | 5.22 | 132.05 | 121.60 |
| 1 | D | 465 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | F | 443 | ALA | N-CA-CB | 5.22 | 117.41 | 110.10 |
| 1 | G | 370 | VAL | CG1-CB-CG2 | -5.22 | 102.55 | 110.90 |
| 1 | P | 55 | MET | CG-SD-CE | -5.22 | 91.85 | 100.20 |
| 1 | P | 484 | TRP | CA-CB-CG | 5.22 | 123.61 | 113.70 |
| 1 | B | 422 | GLU | OE1-CD-OE2 | -5.21 | 117.04 | 123.30 |
| 1 | K | 196 | ARG | CD-NE-CZ | 5.21 | 130.90 | 123.60 |
| 1 | P | 399 | ARG | NE-CZ-NH2 | 5.21 | 122.91 | 120.30 |
| 1 | E | 403 | GLY | O-C-N | -5.21 | 114.36 | 122.70 |
| 1 | L | 369 | PHE | CB-CG-CD1 | -5.21 | 117.15 | 120.80 |
| 1 | O | 317 | VAL | CG1-CB-CG2 | -5.21 | 102.56 | 110.90 |
| 1 | A | 141 | VAL | CA-CB-CG2 | -5.21 | 103.09 | 110.90 |
| 1 | B | 250 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | M | 63 | LEU | CB-CG-CD2 | 5.20 | 119.85 | 111.00 |
| 1 | N | 474 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | P | 53 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | M | 178 | ARG | NE-CZ-NH1 | -5.20 | 117.70 | 120.30 |
| 1 | A | 166 | MET | CA-CB-CG | 5.20 | 122.14 | 113.30 |
| 1 | B | 285 | GLU | N-CA-CB | 5.20 | 119.96 | 110.60 |
| 1 | D | 503 | ILE | CA-CB-CG1 | 5.20 | 120.88 | 111.00 |
| 1 | K | 474 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | C | 432 | TYR | CD1-CG-CD2 | 5.20 | 123.62 | 117.90 |
| 1 | L | 295 | ALA | O-C-N | -5.20 | 114.39 | 122.70 |
| 1 | I | 389 | ARG | NE-CZ-NH2 | 5.19 | 122.90 | 120.30 |
| 1 | R | 507 | LEU | CB-CG-CD2 | -5.19 | 102.17 | 111.00 |
| 1 | K | 347 | SER | N-CA-CB | 5.19 | 118.29 | 110.50 |
| 1 | N | 397 | ALA | N-CA-CB | -5.19 | 102.83 | 110.10 |
| 1 | P | 53 | ARG | NH1-CZ-NH2 | -5.19 | 113.69 | 119.40 |
| 1 | B | 219 | ASP | O-C-N | -5.19 | 114.40 | 122.70 |
| 1 | D | 524 | LEU | CB-CG-CD2 | -5.19 | 102.18 | 111.00 |
| 1 | O | 107 | ALA | O-C-N | -5.19 | 114.40 | 122.70 |
| 1 | C | 55 | MET | N-CA-CB | -5.19 | 101.26 | 110.60 |
| 1 | H | 49 | THR | CA-CB-OG1 | 5.18 | 119.88 | 109.00 |
| 1 | S | 108 | VAL | CG1-CB-CG2 | -5.18 | 102.61 | 110.90 |
| 1 | B | 157 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | A | 196 | ARG | NE-CZ-NH2 | 5.18 | 122.89 | 120.30 |
| 1 | H | 50 | TYR | C-N-CA | 5.18 | 133.17 | 122.30 |
| 1 | H | 339 | VAL | CB-CA-C | -5.17 | 101.57 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 192 | VAL | CA-CB-CG1 | 5.17 | 118.66 | 110.90 |
| 1 | N | 322 | ARG | O-C-N | -5.17 | 114.43 | 122.70 |
| 1 | L | 159 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 1 | E | 447 | TYR | CA-C-O | 5.17 | 130.96 | 120.10 |
| 1 | H | 348 | GLU | CA-CB-CG | 5.17 | 124.77 | 113.40 |
| 1 | M | 292 | ALA | CB-CA-C | -5.17 | 102.35 | 110.10 |
| 1 | N | 240 | ARG | CG-CD-NE | -5.17 | 100.94 | 111.80 |
| 1 | O | 389 | ARG | NH1-CZ-NH2 | -5.17 | 113.72 | 119.40 |
| 1 | D | 258 | PRO | N-CA-C | 5.17 | 125.53 | 112.10 |
| 1 | E | 321 | ARG | CG-CD-NE | -5.17 | 100.95 | 111.80 |
| 1 | I | 356 | LEU | O-C-N | -5.17 | 114.44 | 122.70 |
| 1 | C | 77 | ASP | CB-CG-OD2 | -5.16 | 113.65 | 118.30 |
| 1 | Q | 471 | MET | CG-SD-CE | -5.16 | 91.94 | 100.20 |
| 1 | H | 152 | THR | CA-CB-CG2 | -5.16 | 105.17 | 112.40 |
| 1 | M | 458 | LEU | CB-CG-CD2 | -5.16 | 102.23 | 111.00 |
| 1 | E | 237 | MET | CG-SD-CE | -5.16 | 91.95 | 100.20 |
| 1 | E | 498 | TRP | CB-CG-CD1 | 5.16 | 133.71 | 127.00 |
| 1 | H | 201 | TYR | CZ-CE2-CD2 | -5.16 | 115.16 | 119.80 |
| 1 | L | 250 | ASP | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | M | 50 | TYR | CB-CG-CD1 | 5.16 | 124.09 | 121.00 |
| 1 | M | 469 | LEU | CB-CG-CD1 | 5.16 | 119.77 | 111.00 |
| 1 | E | 277 | ASP | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 1 | C | 196 | ARG | CA-C-N | 5.15 | 126.51 | 116.20 |
| 1 | S | 256 | GLU | N-CA-CB | -5.15 | 101.32 | 110.60 |
| 1 | F | 125 | ASP | CB-CG-OD1 | -5.15 | 113.66 | 118.30 |
| 1 | L | 71 | ASP | CB-CG-OD1 | -5.15 | 113.66 | 118.30 |
| 1 | L | 523 | VAL | CG1-CB-CG2 | -5.15 | 102.66 | 110.90 |
| 1 | S | 447 | TYR | CG-CD1-CE1 | -5.15 | 117.18 | 121.30 |
| 1 | E | 379 | ILE | CA-CB-CG1 | 5.15 | 120.78 | 111.00 |
| 1 | S | 413 | ARG | NE-CZ-NH1 | -5.15 | 117.72 | 120.30 |
| 1 | E | 128 | PRO | CA-N-CD | 5.15 | 118.91 | 111.70 |
| 1 | H | 101 | ALA | N-CA-CB | -5.15 | 102.89 | 110.10 |
| 1 | K | 468 | ASP | O-C-N | -5.15 | 114.46 | 122.70 |
| 1 | K | 185 | VAL | CA-CB-CG1 | 5.15 | 118.62 | 110.90 |
| 1 | C | 162 | ARG | CG-CD-NE | -5.14 | 101.00 | 111.80 |
| 1 | M | 178 | ARG | NH1-CZ-NH2 | -5.14 | 113.74 | 119.40 |
| 1 | O | 162 | ARG | NH1-CZ-NH2 | 5.14 | 125.06 | 119.40 |
| 1 | Q | 484 | TRP | CB-CG-CD1 | -5.14 | 120.31 | 127.00 |
| 1 | C | 428 | LYS | CA-CB-CG | 5.14 | 124.71 | 113.40 |
| 1 | B | 521 | THR | CA-CB-CG2 | -5.14 | 105.20 | 112.40 |
| 1 | A | 149 | LEU | CB-CG-CD2 | -5.14 | 102.27 | 111.00 |
| 1 | S | 329 | GLU | OE1-CD-OE2 | -5.14 | 117.14 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 227 | VAL | CA-CB-CG2 | -5.13 | 103.20 | 110.90 |
| 1 | H | 220 | THR | CA-CB-CG2 | -5.13 | 105.21 | 112.40 |
| 1 | H | 321 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 1 | P | 203 | ASP | CB-CG-OD2 | -5.13 | 113.68 | 118.30 |
| 1 | O | 474 | ARG | NE-CZ-NH1 | -5.13 | 117.73 | 120.30 |
| 1 | S | 58 | MET | CG-SD-CE | -5.13 | 91.99 | 100.20 |
| 1 | K | 322 | ARG | CD-NE-CZ | 5.13 | 130.78 | 123.60 |
| 1 | P | 233 | VAL | O-C-N | -5.13 | 114.49 | 122.70 |
| 1 | I | 230 | LYS | CA-C-O | 5.13 | 130.87 | 120.10 |
| 1 | L | 135 | TYR | CG-CD2-CE2 | -5.13 | 117.20 | 121.30 |
| 1 | L | 224 | TYR | CZ-CE2-CD2 | 5.13 | 124.42 | 119.80 |
| 1 | M | 97 | ASP | CB-CG-OD1 | -5.13 | 113.69 | 118.30 |
| 1 | L | 399 | ARG | NH1-CZ-NH2 | 5.12 | 125.04 | 119.40 |
| 1 | C | 431 | LYS | N-CA-CB | -5.12 | 101.38 | 110.60 |
| 1 | C | 512 | ALA | CB-CA-C | -5.12 | 102.42 | 110.10 |
| 1 | A | 35 | ASN | CB-CG-OD1 | 5.12 | 131.84 | 121.60 |
| 1 | A | 490 | TYR | CG-CD2-CE2 | -5.12 | 117.21 | 121.30 |
| 1 | E | 220 | THR | CA-CB-CG2 | -5.12 | 105.23 | 112.40 |
| 1 | F | 317 | VAL | CA-CB-CG1 | 5.12 | 118.58 | 110.90 |
| 1 | G | 248 | LEU | CB-CG-CD1 | 5.12 | 119.70 | 111.00 |
| 1 | G | 288 | ASP | CB-CG-OD1 | -5.12 | 113.70 | 118.30 |
| 1 | M | 224 | TYR | CB-CG-CD2 | 5.12 | 124.07 | 121.00 |
| 1 | S | 338 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | F | 340 | VAL | CA-CB-CG2 | -5.11 | 103.23 | 110.90 |
| 1 | D | 420 | ALA | N-CA-CB | -5.11 | 102.95 | 110.10 |
| 1 | F | 102 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | M | 143 | LEU | O-C-N | -5.11 | 114.53 | 122.70 |
| 1 | Q | 126 | VAL | CA-CB-CG1 | -5.11 | 103.23 | 110.90 |
| 1 | A | 384 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | R | 202 | VAL | O-C-N | -5.11 | 114.53 | 122.70 |
| 1 | C | 288 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 1 | E | 319 | ALA | N-CA-CB | -5.11 | 102.95 | 110.10 |
| 1 | B | 174 | VAL | CA-CB-CG1 | -5.10 | 103.25 | 110.90 |
| 1 | F | 353 | TYR | CG-CD2-CE2 | 5.10 | 125.38 | 121.30 |
| 1 | P | 198 | ASP | O-C-N | -5.10 | 114.53 | 122.70 |
| 1 | R | 474 | ARG | NH1-CZ-NH2 | -5.10 | 113.79 | 119.40 |
| 1 | G | 220 | THR | CA-CB-CG2 | -5.10 | 105.26 | 112.40 |
| 1 | M | 469 | LEU | O-C-N | -5.10 | 114.54 | 122.70 |
| 1 | M | 525 | ARG | NE-CZ-NH2 | 5.10 | 122.85 | 120.30 |
| 1 | E | 141 | VAL | CA-CB-CG1 | 5.09 | 118.54 | 110.90 |
| 1 | G | 317 | VAL | CA-CB-CG2 | -5.09 | 103.26 | 110.90 |
| 1 | H | 396 | ARG | NH1-CZ-NH2 | -5.09 | 113.80 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | H | 508 | VAL | CG1-CB-CG2 | 5.09 | 119.05 | 110.90 |
| 1 | I | 109 | ILE | CB-CA-C | -5.09 | 101.41 | 111.60 |
| 1 | K | 341 | SER | CB-CA-C | -5.09 | 100.42 | 110.10 |
| 1 | P | 399 | ARG | NE-CZ-NH1 | -5.09 | 117.75 | 120.30 |
| 1 | F | 436 | VAL | CA-CB-CG1 | 5.09 | 118.53 | 110.90 |
| 1 | G | 433 | ALA | CA-C-O | -5.09 | 109.41 | 120.10 |
| 1 | M | 462 | ALA | C-N-CA | 5.09 | 132.99 | 122.30 |
| 1 | O | 461 | ASN | CA-CB-CG | -5.09 | 102.20 | 113.40 |
| 1 | A | 162 | ARG | NH1-CZ-NH2 | -5.09 | 113.80 | 119.40 |
| 1 | R | 139 | GLU | C-N-CA | 5.09 | 134.42 | 121.70 |
| 1 | C | 384 | ARG | NE-CZ-NH2 | -5.09 | 117.76 | 120.30 |
| 1 | E | 447 | TYR | O-C-N | -5.08 | 114.56 | 122.70 |
| 1 | H | 413 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |
| 1 | D | 462 | ALA | N-CA-CB | 5.08 | 117.22 | 110.10 |
| 1 | F | 427 | LYS | CB-CA-C | 5.08 | 120.57 | 110.40 |
| 1 | G | 414 | ALA | CB-CA-C | -5.08 | 102.47 | 110.10 |
| 1 | K | 488 | ASP | O-C-N | -5.08 | 114.56 | 122.70 |
| 1 | L | 50 | TYR | CZ-CE2-CD2 | 5.08 | 124.38 | 119.80 |
| 1 | O | 207 | ILE | N-CA-C | -5.08 | 97.27 | 111.00 |
| 1 | Q | 490 | TYR | CB-CG-CD2 | 5.08 | 124.05 | 121.00 |
| 1 | H | 471 | MET | CG-SD-CE | 5.08 | 108.33 | 100.20 |
| 1 | K | 229 | ASP | CB-CG-OD1 | -5.08 | 113.73 | 118.30 |
| 1 | A | 77 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | G | 528 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | C | 33 | ARG | CD-NE-CZ | 5.07 | 130.70 | 123.60 |
| 1 | B | 471 | MET | CG-SD-CE | -5.07 | 92.09 | 100.20 |
| 1 | I | 485 | TYR | CB-CG-CD2 | 5.07 | 124.04 | 121.00 |
| 1 | L | 297 | VAL | CA-CB-CG2 | 5.07 | 118.50 | 110.90 |
| 1 | Q | 430 | ARG | NH1-CZ-NH2 | -5.07 | 113.82 | 119.40 |
| 1 | R | 392 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | D | 333 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 1 | E | 403 | GLY | C-N-CA | 5.07 | 134.37 | 121.70 |
| 1 | A | 317 | VAL | C-N-CA | 5.07 | 134.37 | 121.70 |
| 1 | F | 116 | LYS | CA-CB-CG | 5.07 | 124.54 | 113.40 |
| 1 | M | 234 | HIS | CA-CB-CG | 5.07 | 122.21 | 113.60 |
| 1 | S | 110 | PHE | CB-CA-C | 5.07 | 120.53 | 110.40 |
| 1 | C | 228 | VAL | CG1-CB-CG2 | -5.06 | 102.81 | 110.90 |
| 1 | L | 414 | ALA | O-C-N | -5.06 | 114.60 | 122.70 |
| 1 | B | 427 | LYS | CA-CB-CG | 5.05 | 124.52 | 113.40 |
| 1 | C | 392 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 1 | E | 325 | LYS | C-N-CA | 5.05 | 134.32 | 121.70 |
| 1 | M | 325 | LYS | C-N-CA | 5.05 | 134.32 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | C | 464 | PHE | CZ-CE2-CD2 | 5.05 | 126.16 | 120.10 |
| 1 | E | 398 | LEU | CB-CG-CD2 | 5.05 | 119.58 | 111.00 |
| 1 | H | 114 | LEU | CB-CG-CD2 | 5.05 | 119.58 | 111.00 |
| 1 | R | 436 | VAL | CG1-CB-CG2 | -5.04 | 102.83 | 110.90 |
| 1 | B | 146 | ILE | CA-CB-CG1 | -5.04 | 101.42 | 111.00 |
| 1 | B | 288 | ASP | CB-CA-C | 5.04 | 120.49 | 110.40 |
| 1 | D | 261 | ASP | CB-CG-OD1 | 5.04 | 122.84 | 118.30 |
| 1 | C | 393 | GLU | CG-CD-OE2 | 5.04 | 128.38 | 118.30 |
| 1 | M | 289 | LYS | N-CA-CB | -5.04 | 101.52 | 110.60 |
| 1 | O | 360 | ARG | N-CA-CB | 5.04 | 119.67 | 110.60 |
| 1 | I | 525 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | B | 32 | VAL | CG1-CB-CG2 | -5.04 | 102.84 | 110.90 |
| 1 | M | 201 | TYR | CD1-CG-CD2 | 5.04 | 123.44 | 117.90 |
| 1 | H | 372 | GLY | O-C-N | -5.04 | 114.64 | 122.70 |
| 1 | M | 383 | ILE | CG1-CB-CG2 | -5.04 | 100.32 | 111.40 |
| 1 | R | 102 | ASP | CB-CG-OD1 | -5.04 | 113.77 | 118.30 |
| 1 | P | 277 | ASP | CA-C-O | 5.03 | 130.67 | 120.10 |
| 1 | O | 340 | VAL | CA-CB-CG2 | -5.03 | 103.35 | 110.90 |
| 1 | R | 65 | ASP | O-C-N | -5.03 | 114.65 | 122.70 |
| 1 | I | 159 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | L | 426 | ALA | CA-C-N | 5.03 | 128.26 | 117.20 |
| 1 | S | 290 | ILE | O-C-N | -5.03 | 114.66 | 122.70 |
| 1 | F | 389 | ARG | CB-CA-C | -5.02 | 100.36 | 110.40 |
| 1 | G | 396 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 1 | K | 400 | ASP | N-CA-CB | -5.02 | 101.56 | 110.60 |
| 1 | C | 135 | TYR | CG-CD1-CE1 | -5.02 | 117.28 | 121.30 |
| 1 | D | 360 | ARG | NH1-CZ-NH2 | 5.02 | 124.92 | 119.40 |
| 1 | M | 115 | VAL | CA-CB-CG2 | -5.02 | 103.37 | 110.90 |
| 1 | P | 340 | VAL | O-C-N | -5.02 | 114.67 | 122.70 |
| 1 | F | 240 | ARG | NH1-CZ-NH2 | -5.02 | 113.88 | 119.40 |
| 1 | N | 274 | LYS | O-C-N | -5.02 | 114.67 | 122.70 |
| 1 | G | 303 | GLY | O-C-N | 5.01 | 130.72 | 122.70 |
| 1 | I | 159 | ASP | CB-CG-OD2 | -5.01 | 113.79 | 118.30 |
| 1 | N | 265 | ARG | NH1-CZ-NH2 | -5.01 | 113.89 | 119.40 |
| 1 | H | 245 | LYS | O-C-N | -5.01 | 114.68 | 122.70 |
| 1 | R | 472 | LYS | CD-CE-NZ | -5.01 | 100.17 | 111.70 |
| 1 | A | 353 | TYR | CD1-CE1-CZ | -5.01 | 115.29 | 119.80 |
| 1 | R | 365 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 1 | F | 180 | TYR | CB-CG-CD1 | 5.01 | 124.00 | 121.00 |
| 1 | M | 311 | TYR | CB-CG-CD2 | -5.01 | 118.00 | 121.00 |
| 1 | A | 521 | THR | O-C-N | -5.00 | 114.69 | 122.70 |
| 1 | I | 384 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | N | 490 | TYR | CD1-CE1-CZ | -5.00 | 115.30 | 119.80 |
| 1 | K | 97 | ASP | CA-C-O | 5.00 | 130.61 | 120.10 |
| 1 | H | 120 | ASP | CB-CG-OD1 | 5.00 | 122.80 | 118.30 |

There are no chirality outliers.

All (185) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 110 | PHE | Sidechain |
| 1 | A | 135 | TYR | Sidechain |
| 1 | A | 162 | ARG | Sidechain |
| 1 | A | 201 | TYR | Sidechain |
| 1 | A | 224 | TYR | Sidechain |
| 1 | A | 240 | ARG | Sidechain |
| 1 | A | 265 | ARG | Sidechain |
| 1 | A | 360 | ARG | Sidechain |
| 1 | A | 399 | ARG | Sidechain |
| 1 | A | 430 | ARG | Sidechain |
| 1 | A | 525 | ARG | Sidechain |
| 1 | B | 123 | TYR | Sidechain |
| 1 | B | 135 | TYR | Sidechain |
| 1 | B | 178 | ARG | Sidechain |
| 1 | B | 196 | ARG | Sidechain |
| 1 | B | 224 | TYR | Sidechain |
| 1 | B | 240 | ARG | Sidechain |
| 1 | B | 321 | ARG | Sidechain |
| 1 | B | 353 | TYR | Sidechain |
| 1 | B | 399 | ARG | Sidechain |
| 1 | B | 432 | TYR | Sidechain |
| 1 | B | 447 | TYR | Sidechain |
| 1 | B | 474 | ARG | Sidechain |
| 1 | B | 490 | TYR | Sidechain |
| 1 | B | 50 | TYR | Sidechain |
| 1 | B | 53 | ARG | Sidechain |
| 1 | C | 333 | ARG | Sidechain |
| 1 | C | 353 | TYR | Sidechain |
| 1 | C | 389 | ARG | Sidechain |
| 1 | C | 399 | ARG | Sidechain |
| 1 | C | 474 | ARG | Sidechain |
| 1 | D | 162 | ARG | Sidechain |
| 1 | D | 275 | PHE | Sidechain |
| 1 | D | 311 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | D | 321 | ARG | Sidechain |
| 1 | D | 322 | ARG | Sidechain |
| 1 | D | 338 | ARG | Sidechain |
| 1 | D | 353 | TYR | Sidechain |
| 1 | D | 360 | ARG | Sidechain |
| 1 | D | 430 | ARG | Sidechain |
| 1 | D | 490 | TYR | Sidechain |
| 1 | D | 53 | ARG | Sidechain |
| 1 | E | 123 | TYR | Sidechain |
| 1 | E | 162 | ARG | Sidechain |
| 1 | E | 240 | ARG | Sidechain |
| 1 | E | 33 | ARG | Sidechain |
| 1 | E | 333 | ARG | Mainchain |
| 1 | E | 360 | ARG | Sidechain |
| 1 | E | 396 | ARG | Sidechain |
| 1 | E | 430 | ARG | Sidechain |
| 1 | E | 447 | TYR | Sidechain |
| 1 | E | 525 | ARG | Sidechain |
| 1 | F | 196 | ARG | Sidechain |
| 1 | F | 224 | TYR | Sidechain |
| 1 | F | 322 | ARG | Sidechain |
| 1 | F | 353 | TYR | Sidechain |
| 1 | F | 360 | ARG | Sidechain |
| 1 | F | 389 | ARG | Sidechain |
| 1 | F | 399 | ARG | Sidechain |
| 1 | F | 413 | ARG | Sidechain |
| 1 | F | 447 | TYR | Sidechain |
| 1 | F | 50 | TYR | Sidechain |
| 1 | G | 110 | PHE | Sidechain |
| 1 | G | 178 | ARG | Sidechain |
| 1 | G | 180 | TYR | Sidechain |
| 1 | G | 196 | ARG | Sidechain |
| 1 | G | 224 | TYR | Sidechain |
| 1 | G | 240 | ARG | Sidechain |
| 1 | G | 321 | ARG | Sidechain |
| 1 | G | 353 | TYR | Sidechain |
| 1 | G | 413 | ARG | Sidechain |
| 1 | G | 430 | ARG | Sidechain |
| 1 | G | 525 | ARG | Sidechain |
| 1 | H | 224 | TYR | Sidechain |
| 1 | H | 265 | ARG | Sidechain |
| 1 | H | 275 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | H | 311 | TYR | Sidechain |
| 1 | H | 333 | ARG | Sidechain |
| 1 | H | 360 | ARG | Sidechain |
| 1 | H | 389 | ARG | Sidechain |
| 1 | H | 474 | ARG | Sidechain |
| 1 | I | 162 | ARG | Sidechain |
| 1 | I | 180 | TYR | Sidechain |
| 1 | I | 311 | TYR | Sidechain |
| 1 | I | 321 | ARG | Sidechain |
| 1 | I | 322 | ARG | Sidechain |
| 1 | I | 430 | ARG | Sidechain |
| 1 | I | 50 | TYR | Sidechain |
| 1 | I | 525 | ARG | Sidechain |
| 1 | K | 127 | HIS | Sidechain |
| 1 | K | 135 | TYR | Sidechain |
| 1 | K | 224 | TYR | Sidechain |
| 1 | K | 234 | HIS | Sidechain |
| 1 | K | 311 | TYR | Sidechain |
| 1 | K | 322 | ARG | Sidechain |
| 1 | K | 360 | ARG | Sidechain |
| 1 | K | 399 | ARG | Sidechain |
| 1 | K | 447 | TYR | Sidechain |
| 1 | K | 464 | PHE | Sidechain |
| 1 | K | 474 | ARG | Sidechain |
| 1 | K | 53 | ARG | Sidechain |
| 1 | L | 180 | TYR | Sidechain |
| 1 | L | 240 | ARG | Sidechain |
| 1 | L | 265 | ARG | Sidechain |
| 1 | L | 322 | ARG | Sidechain |
| 1 | L | 474 | ARG | Sidechain |
| 1 | L | 485 | TYR | Sidechain |
| 1 | L | 490 | TYR | Sidechain |
| 1 | L | 525 | ARG | Sidechain |
| 1 | M | 110 | PHE | Sidechain |
| 1 | M | 309 | GLN | Mainchain |
| 1 | M | 311 | TYR | Sidechain |
| 1 | M | 384 | ARG | Sidechain |
| 1 | M | 389 | ARG | Sidechain |
| 1 | M | 399 | ARG | Sidechain |
| 1 | M | 430 | ARG | Sidechain |
| 1 | M | 447 | TYR | Sidechain |
| 1 | M | 474 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | M | 490 | TYR | Sidechain |
| 1 | N | 110 | PHE | Sidechain |
| 1 | N | 123 | TYR | Sidechain |
| 1 | N | 178 | ARG | Sidechain |
| 1 | N | 196 | ARG | Sidechain |
| 1 | N | 201 | TYR | Sidechain |
| 1 | N | 224 | TYR | Sidechain |
| 1 | N | 240 | ARG | Sidechain |
| 1 | N | 311 | TYR | Sidechain |
| 1 | N | 321 | ARG | Sidechain |
| 1 | N | 333 | ARG | Sidechain |
| 1 | N | 360 | ARG | Sidechain |
| 1 | N | 389 | ARG | Sidechain |
| 1 | N | 396 | ARG | Sidechain |
| 1 | N | 447 | TYR | Sidechain |
| 1 | N | 525 | ARG | Sidechain |
| 1 | O | 178 | ARG | Sidechain |
| 1 | O | 180 | TYR | Sidechain |
| 1 | O | 33 | ARG | Sidechain |
| 1 | O | 396 | ARG | Sidechain |
| 1 | O | 432 | TYR | Sidechain |
| 1 | O | 447 | TYR | Sidechain |
| 1 | O | 525 | ARG | Sidechain |
| 1 | P | 123 | TYR | Sidechain |
| 1 | P | 135 | TYR | Sidechain |
| 1 | P | 162 | ARG | Sidechain |
| 1 | P | 224 | TYR | Sidechain |
| 1 | P | 265 | ARG | Sidechain |
| 1 | P | 333 | ARG | Sidechain |
| 1 | P | 384 | ARG | Sidechain |
| 1 | P | 474 | ARG | Sidechain |
| 1 | P | 480 | GLU | Sidechain |
| 1 | Q | 123 | TYR | Sidechain |
| 1 | Q | 135 | TYR | Sidechain |
| 1 | Q | 162 | ARG | Sidechain |
| 1 | Q | 29 | LYS | Mainchain |
| 1 | Q | 33 | ARG | Sidechain |
| 1 | Q | 333 | ARG | Sidechain |
| 1 | Q | 353 | TYR | Sidechain |
| 1 | Q | 432 | TYR | Sidechain |
| 1 | Q | 447 | TYR | Sidechain |
| 1 | Q | 464 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | Q | 477 | HIS | Sidechain |
| 1 | Q | 490 | TYR | Sidechain |
| 1 | Q | 50 | TYR | Sidechain |
| 1 | Q | 525 | ARG | Sidechain |
| 1 | R | 135 | TYR | Sidechain |
| 1 | R | 162 | ARG | Sidechain |
| 1 | R | 201 | TYR | Sidechain |
| 1 | R | 240 | ARG | Sidechain |
| 1 | R | 265 | ARG | Sidechain |
| 1 | R | 333 | ARG | Sidechain |
| 1 | R | 338 | ARG | Sidechain |
| 1 | R | 389 | ARG | Sidechain |
| 1 | R | 399 | ARG | Sidechain |
| 1 | R | 432 | TYR | Sidechain |
| 1 | S | 135 | TYR | Sidechain |
| 1 | S | 162 | ARG | Sidechain |
| 1 | S | 178 | ARG | Sidechain |
| 1 | S | 224 | TYR | Sidechain |
| 1 | S | 311 | TYR | Sidechain |
| 1 | S | 389 | ARG | Sidechain |
| 1 | S | 399 | ARG | Sidechain |
| 1 | S | 432 | TYR | Sidechain |
| 1 | S | 474 | ARG | Sidechain |
| 1 | S | 50 | TYR | Sidechain |
| 1 | S | 53 | ARG | Sidechain |

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 | 3849 | 0 | 3995 | 14 | 0 |
| 1 | B | 3849 | 0 | 3995 | 17 | 0 |
| 1 | C | 3849 | 0 | 3995 | 17 | 0 |
| 1 | D | 3849 | 0 | 3995 | 14 | 0 |
| 1 | E | 3849 | 0 | 3995 | 6 | 0 |
| 1 | F | 3849 | 0 | 3995 | 14 | 0 |
| 1 | G | 3849 | 0 | 3995 | 19 | 0 |
| 1 | H | 3849 | 0 | 3995 | 20 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | I | 3849 | 0 | 3995 | 12 | 0 |
| 1 | K | 3849 | 0 | 3995 | 13 | 0 |
| 1 | L | 3849 | 0 | 3995 | 18 | 0 |
| 1 | M | 3849 | 0 | 3995 | 21 | 0 |
| 1 | N | 3849 | 0 | 3995 | 7 | 0 |
| 1 | O | 3849 | 0 | 3995 | 12 | 0 |
| 1 | P | 3849 | 0 | 3995 | 28 | 0 |
| 1 | Q | 3849 | 0 | 3995 | 13 | 0 |
| 1 | R | 3849 | 0 | 3995 | 9 | 0 |
| 1 | S | 3849 | 0 | 3995 | 17 | 0 |
| All | All | 69282 | 0 | 71910 | 259 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:415:ILE:HD12 | 1:G:421:VAL:HG21 | 1.72 | 0.71 |
| 1:D:89:LEU:HD12 | 1:D:519:ALA:HB1 | 1.73 | 0.71 |
| 1:G:246:ILE:HD12 | 1:G:246:ILE:H | 1.53 | 0.71 |
| 1:M:153:VAL:HG22 | 1:M:160:LEU:HD23 | 1.76 | 0.67 |
| 1:P:474:ARG:HE | 1:P:477:HIS:CE1 | 2.13 | 0.66 |
| 1:B:127:HIS:CD2 | 1:C:463:GLY:HA2 | 2.34 | 0.63 |
| 1:H:507:LEU:HD23 | 1:H:507:LEU:H | 1.64 | 0.63 |
| 1:F:246:ILE:HA | 1:F:297:VAL:HG13 | 1.82 | 0.62 |
| 1:G:191:GLN:HG2 | 1:G:379:ILE:HD13 | 1.82 | 0.61 |
| 1:S:167:THR:O | 1:S:167:THR:HG22 | 2.00 | 0.61 |
| 1:S:297:VAL:HG21 | 1:S:357:ILE:HD13 | 1.83 | 0.60 |
| 1:G:100:THR:HG21 | 1:G:508:VAL:HG13 | 1.84 | 0.59 |
| 1:K:244:ALA:HB2 | 1:K:357:ILE:HG22 | 1.84 | 0.58 |
| 1:R:246:ILE:HD12 | 1:R:246:ILE:H | 1.67 | 0.58 |
| 1:F:155:ILE:HG13 | 1:F:190:THR:HG22 | 1.86 | 0.57 |
| 1:G:486:GLY:O | 1:G:494:PRO:HA | 2.05 | 0.57 |
| 1:L:30:GLU:H | 1:L:30:GLU:CD | 2.08 | 0.57 |
| 1:A:164:ILE:HG21 | 1:A:408:VAL:HG21 | 1.87 | 0.57 |
| 1:I:246:ILE:HA | 1:I:297:VAL:HG13 | 1.87 | 0.56 |
| 1:C:423:ILE:HD13 | 1:C:473:LEU:HD13 | 1.87 | 0.56 |
| 1:M:220:THR:HG22 | 1:M:384:ARG:H | 1.70 | 0.56 |
| 1:Q:290:ILE:HA | 1:Q:346:ILE:HG21 | 1.88 | 0.56 |
| 1:D:442:LEU:H | 1:D:442:LEU:HD12 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:153:VAL:HG22 | 1:P:160:LEU:CD2 | 2.37 | 0.55 |
| 1:M:153:VAL:HG22 | 1:M:160:LEU:CD2 | 2.36 | 0.55 |
| 1:H:164:ILE:HG21 | 1:H:408:VAL:HG21 | 1.89 | 0.54 |
| 1:R:480:GLU:CD | 1:R:480:GLU:H | 2.11 | 0.54 |
| 1:L:423:ILE:HD13 | 1:L:473:LEU:HD13 | 1.90 | 0.54 |
| 1:S:430:ARG:HH21 | 1:S:452:GLU:CD | 2.12 | 0.53 |
| 1:A:290:ILE:HA | 1:A:346:ILE:HG21 | 1.90 | 0.53 |
| 1:L:297:VAL:HG21 | 1:L:357:ILE:HD13 | 1.90 | 0.53 |
| 1:M:452:GLU:CD | 1:M:474:ARG:HH22 | 2.11 | 0.53 |
| 1:E:246:ILE:HA | 1:E:297:VAL:HG13 | 1.89 | 0.53 |
| 1:L:474:ARG:HA | 1:L:477:HIS:CD2 | 2.43 | 0.52 |
| 1:O:425:ILE:HG22 | 1:O:451:LEU:HD13 | 1.92 | 0.52 |
| 1:P:153:VAL:HG22 | 1:P:160:LEU:HD23 | 1.90 | 0.52 |
| 1:Q:220:THR:HG22 | 1:Q:383:ILE:HA | 1.90 | 0.52 |
| 1:K:234:HIS:CD2 | 1:K:236:GLY:H | 2.28 | 0.52 |
| 1:H:477:HIS:O | 1:H:477:HIS:CG | 2.63 | 0.52 |
| 1:M:192:VAL:HG13 | 1:M:206:ASN:HB2 | 1.92 | 0.52 |
| 1:B:246:ILE:H | 1:B:246:ILE:HD12 | 1.74 | 0.52 |
| 1:K:127:HIS:CG | 1:L:463:GLY:HA2 | 2.45 | 0.52 |
| 1:I:246:ILE:HD12 | 1:I:246:ILE:H | 1.74 | 0.51 |
| 1:S:404:THR:O | 1:S:408:VAL:HG23 | 2.10 | 0.51 |
| 1:B:532:ALA:HB3 | 1:C:61:ASP:HA | 1.92 | 0.51 |
| 1:F:383:ILE:N | 1:F:383:ILE:HD12 | 2.26 | 0.51 |
| 1:I:244:ALA:HB2 | 1:I:357:ILE:HG22 | 1.93 | 0.51 |
| 1:R:238:PRO:HB2 | 1:R:241:LEU:HD21 | 1.93 | 0.51 |
| 1:B:283:ILE:HG23 | 1:B:308:ALA:HB2 | 1.93 | 0.50 |
| 1:E:421:VAL:O | 1:E:425:ILE:HG13 | 2.11 | 0.50 |
| 1:L:244:ALA:HB2 | 1:L:357:ILE:HG22 | 1.93 | 0.50 |
| 1:P:505:PRO:HB2 | 1:P:508:VAL:HG12 | 1.93 | 0.50 |
| 1:B:526:ILE:HD11 | 1:C:68:ILE:HD13 | 1.93 | 0.50 |
| 1:E:473:LEU:HD13 | 1:E:473:LEU:C | 2.31 | 0.50 |
| 1:I:312:LEU:HD22 | 1:I:317:VAL:HG11 | 1.93 | 0.50 |
| 1:G:312:LEU:HD22 | 1:G:317:VAL:HG11 | 1.94 | 0.49 |
| 1:S:383:ILE:CD1 | 1:S:395:GLU:HA | 2.42 | 0.49 |
| 1:G:220:THR:HG22 | 1:G:383:ILE:HA | 1.94 | 0.49 |
| 1:S:121:LEU:HB2 | 1:S:131:ILE:HD11 | 1.93 | 0.49 |
| 1:P:227:VAL:HG22 | 1:P:369:PHE:CD1 | 2.48 | 0.49 |
| 1:I:185:VAL:HG13 | 1:I:402:LEU:HA | 1.95 | 0.49 |
| 1:H:89:LEU:HD11 | 1:H:111:SER:HB3 | 1.95 | 0.49 |
| 1:P:213:ALA:HA | 1:P:391:VAL:HG11 | 1.93 | 0.49 |
| 1:O:249:ILE:HG22 | 1:O:251:ALA:H | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:430:ARG:HH21 | 1:A:452:GLU:CD | 2.16 | 0.49 |
| 1:E:498:TRP:CZ3 | 1:E:503:ILE:HG23 | 2.48 | 0.49 |
| 1:K:164:ILE:HG21 | 1:K:408:VAL:HG21 | 1.95 | 0.49 |
| 1:C:423:ILE:HD12 | 1:C:477:HIS:CD2 | 2.47 | 0.48 |
| 1:L:474:ARG:HG3 | 1:L:477:HIS:CE1 | 2.48 | 0.48 |
| 1:F:483:LYS:HE2 | 1:F:484:TRP:CE2 | 2.48 | 0.48 |
| 1:D:415:ILE:HB | 1:D:421:VAL:HG21 | 1.95 | 0.48 |
| 1:G:227:VAL:HG22 | 1:G:369:PHE:CD1 | 2.49 | 0.48 |
| 1:B:161:LEU:HD22 | 1:B:405:VAL:HG13 | 1.95 | 0.48 |
| 1:F:312:LEU:HD22 | 1:F:317:VAL:HG11 | 1.95 | 0.48 |
| 1:M:149:LEU:HD21 | 1:M:421:VAL:HG12 | 1.96 | 0.48 |
| 1:S:298:ILE:CG2 | 1:S:319:ALA:HB2 | 2.44 | 0.48 |
| 1:R:164:ILE:HG21 | 1:R:408:VAL:HG21 | 1.96 | 0.48 |
| 1:I:178:ARG:NE | 1:I:178:ARG:H | 2.12 | 0.48 |
| 1:R:455:VAL:O | 1:R:459:ILE:HG12 | 2.14 | 0.48 |
| 1:F:527:ASP:HB2 | 1:G:55:MET:HB3 | 1.95 | 0.47 |
| 1:P:268:ASP:HB2 | 1:P:271:GLN:HE21 | 1.79 | 0.47 |
| 1:D:129:THR:HG23 | 1:D:130:ILE:HD13 | 1.95 | 0.47 |
| 1:R:158:THR:HB | 1:R:186:VAL:HG11 | 1.95 | 0.47 |
| 1:P:255:VAL:HG12 | 1:P:279:GLU:HG3 | 1.96 | 0.47 |
| 1:B:459:ILE:HD13 | 1:B:469:LEU:HB2 | 1.96 | 0.47 |
| 1:O:226:ILE:HG13 | 1:O:334:ALA:CB | 2.45 | 0.47 |
| 1:P:248:LEU:H | 1:P:248:LEU:HD12 | 1.79 | 0.47 |
| 1:K:459:ILE:HG21 | 1:K:466:PRO:HA | 1.97 | 0.47 |
| 1:L:88:LEU:CD1 | 1:M:68:ILE:HD11 | 2.44 | 0.47 |
| 1:B:497:MET:HB3 | 1:B:502:VAL:HB | 1.97 | 0.47 |
| 1:K:253:LEU:HD11 | 1:K:298:ILE:HD11 | 1.96 | 0.47 |
| 1:B:248:LEU:H | 1:B:248:LEU:HD22 | 1.80 | 0.47 |
| 1:A:453:SER:O | 1:A:456:SER:HB2 | 2.15 | 0.47 |
| 1:P:387:LEU:HD23 | 1:P:389:ARG:H | 1.80 | 0.47 |
| 1:H:220:THR:HG22 | 1:H:384:ARG:H | 1.80 | 0.47 |
| 1:I:485:TYR:CE1 | 1:I:496:ASP:HB2 | 2.50 | 0.46 |
| 1:K:192:VAL:HG13 | 1:K:206:ASN:HD22 | 1.81 | 0.46 |
| 1:D:504:GLU:HB2 | 1:D:505:PRO:HD2 | 1.98 | 0.46 |
| 1:S:310:SER:O | 1:S:314:LYS:HE2 | 2.15 | 0.46 |
| 1:C:291:LEU:HD11 | 1:C:312:LEU:HD23 | 1.97 | 0.46 |
| 1:F:408:VAL:HG22 | 1:F:505:PRO:HG3 | 1.98 | 0.46 |
| 1:A:106:THR:HG23 | 1:A:454:LEU:HD21 | 1.98 | 0.46 |
| 1:N:404:THR:O | 1:N:408:VAL:HG23 | 2.15 | 0.46 |
| 1:A:225:GLY:HA3 | 1:A:371:GLU:HA | 1.98 | 0.46 |
| 1:K:340:VAL:HG21 | 1:K:346:ILE:HD13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:114:LEU:HD11 | 1:B:447:TYR:CD2 | 2.51 | 0.46 |
| 1:G:423:ILE:HG23 | 1:G:477:HIS:CD2 | 2.51 | 0.46 |
| 1:H:217:ILE:HD12 | 1:H:217:ILE:H | 1.81 | 0.46 |
| 1:O:226:ILE:HG13 | 1:O:334:ALA:HB2 | 1.98 | 0.46 |
| 1:N:477:HIS:O | 1:N:477:HIS:CD2 | 2.69 | 0.46 |
| 1:M:233:VAL:HG12 | 1:M:319:ALA:O | 2.16 | 0.45 |
| 1:L:248:LEU:H | 1:L:248:LEU:HD22 | 1.81 | 0.45 |
| 1:B:242:GLU:CD | 1:B:242:GLU:H | 2.19 | 0.45 |
| 1:C:246:ILE:HA | 1:C:297:VAL:HG13 | 1.97 | 0.45 |
| 1:I:469:LEU:HD13 | 1:I:487:ILE:HD11 | 1.98 | 0.45 |
| 1:P:465:ASP:HA | 1:P:466:PRO:HD2 | 1.86 | 0.45 |
| 1:N:248:LEU:HD12 | 1:N:248:LEU:H | 1.81 | 0.45 |
| 1:R:430:ARG:HH21 | 1:R:452:GLU:CD | 2.18 | 0.45 |
| 1:L:46:LEU:HD12 | 1:L:108:VAL:HG11 | 1.97 | 0.45 |
| 1:Q:204:LEU:HD13 | 1:Q:204:LEU:O | 2.17 | 0.45 |
| 1:F:299:ILE:HA | 1:F:320:VAL:HB | 1.99 | 0.45 |
| 1:L:458:LEU:HG | 1:L:489:LEU:HD11 | 1.98 | 0.45 |
| 1:A:38:ALA:O | 1:A:41:ALA:HB3 | 2.17 | 0.45 |
| 1:Q:415:ILE:O | 1:Q:503:ILE:HG23 | 2.16 | 0.45 |
| 1:S:252:SER:HB2 | 1:S:302:LYS:HD3 | 1.98 | 0.45 |
| 1:M:415:ILE:HD12 | 1:M:415:ILE:O | 2.16 | 0.45 |
| 1:Q:297:VAL:HG21 | 1:Q:357:ILE:HG21 | 1.98 | 0.45 |
| 1:Q:488:ASP:HB3 | 1:Q:491:ALA:HB3 | 1.99 | 0.45 |
| 1:C:477:HIS:O | 1:C:477:HIS:CG | 2.69 | 0.45 |
| 1:H:192:VAL:HG21 | 1:H:207:ILE:CG1 | 2.47 | 0.45 |
| 1:H:241:LEU:HD23 | 1:H:318:LEU:HB2 | 1.99 | 0.45 |
| 1:G:232:VAL:HG12 | 1:G:318:LEU:HD21 | 1.99 | 0.44 |
| 1:N:312:LEU:HD22 | 1:N:317:VAL:HG11 | 1.99 | 0.44 |
| 1:B:290:ILE:HG21 | 1:B:298:ILE:HD12 | 1.98 | 0.44 |
| 1:H:383:ILE:HD13 | 1:H:395:GLU:HA | 1.99 | 0.44 |
| 1:P:357:ILE:HD11 | 1:P:370:VAL:HG13 | 1.98 | 0.44 |
| 1:P:517:THR:HG22 | 1:P:517:THR:O | 2.18 | 0.44 |
| 1:M:459:ILE:HD13 | 1:M:469:LEU:HB2 | 2.00 | 0.44 |
| 1:O:430:ARG:HH21 | 1:O:452:GLU:CD | 2.21 | 0.44 |
| 1:P:149:LEU:HG | 1:P:483:LYS:HD2 | 2.00 | 0.44 |
| 1:O:250:ASP:OD1 | 1:O:302:LYS:NZ | 2.50 | 0.44 |
| 1:K:38:ALA:O | 1:K:41:ALA:HB3 | 2.17 | 0.44 |
| 1:F:459:ILE:O | 1:F:462:ALA:HB3 | 2.17 | 0.44 |
| 1:B:127:HIS:CD2 | 1:C:463:GLY:CA | 3.01 | 0.44 |
| 1:N:234:HIS:CD2 | 1:N:236:GLY:H | 2.36 | 0.44 |
| 1:Q:383:ILE:HD11 | 1:Q:398:LEU:HD13 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:153:VAL:CG2 | 1:P:160:LEU:HD23 | 2.48 | 0.44 |
| 1:Q:283:ILE:HD13 | 1:Q:286:LYS:HD2 | 2.00 | 0.44 |
| 1:G:290:ILE:HD11 | 1:G:343:ILE:HG22 | 1.99 | 0.44 |
| 1:P:98:GLU:HG2 | 1:P:508:VAL:HB | 2.00 | 0.44 |
| 1:B:340:VAL:HG21 | 1:B:346:ILE:HD12 | 2.00 | 0.44 |
| 1:K:423:ILE:HD12 | 1:K:477:HIS:CG | 2.52 | 0.44 |
| 1:M:522:LEU:HD11 | 1:N:68:ILE:HD13 | 1.99 | 0.44 |
| 1:O:425:ILE:HG22 | 1:O:451:LEU:CD1 | 2.47 | 0.43 |
| 1:E:141:VAL:HA | 1:E:144:GLN:HG2 | 2.00 | 0.43 |
| 1:O:244:ALA:O | 1:O:353:TYR:HA | 2.18 | 0.43 |
| 1:D:254:GLU:CD | 1:D:321:ARG:HH12 | 2.22 | 0.43 |
| 1:R:153:VAL:HG21 | 1:R:414:ALA:HB3 | 2.00 | 0.43 |
| 1:L:233:VAL:HG23 | 1:L:321:ARG:HG2 | 1.99 | 0.43 |
| 1:H:232:VAL:HG13 | 1:H:319:ALA:O | 2.17 | 0.43 |
| 1:M:335:THR:HB | 1:M:353:TYR:H | 1.83 | 0.43 |
| 1:A:164:ILE:HG23 | 1:A:505:PRO:HD3 | 2.01 | 0.43 |
| 1:H:164:ILE:HG13 | 1:H:164:ILE:H | 1.63 | 0.43 |
| 1:S:127:HIS:O | 1:S:130:ILE:HB | 2.19 | 0.43 |
| 1:G:246:ILE:H | 1:G:246:ILE:CD1 | 2.25 | 0.43 |
| 1:P:451:LEU:HD13 | 1:P:451:LEU:HA | 1.85 | 0.43 |
| 1:O:195:LEU:HD23 | 1:O:200:TRP:HA | 2.01 | 0.43 |
| 1:C:433:ALA:HB1 | 1:C:441:GLN:HG3 | 2.01 | 0.43 |
| 1:Q:188:ALA:O | 1:Q:192:VAL:HG23 | 2.19 | 0.43 |
| 1:C:526:ILE:HD12 | 1:D:58:MET:HB2 | 2.01 | 0.43 |
| 1:M:241:LEU:HD12 | 1:M:318:LEU:HB2 | 2.01 | 0.43 |
| 1:G:106:THR:HG23 | 1:G:454:LEU:HD21 | 2.01 | 0.43 |
| 1:H:244:ALA:HB2 | 1:H:357:ILE:HG22 | 2.00 | 0.43 |
| 1:D:99:GLU:O | 1:D:100:THR:HB | 2.19 | 0.43 |
| 1:L:88:LEU:HD11 | 1:M:68:ILE:HD11 | 1.99 | 0.43 |
| 1:H:297:VAL:HG11 | 1:H:357:ILE:HG21 | 2.01 | 0.43 |
| 1:K:425:ILE:O | 1:K:429:LEU:HD13 | 2.19 | 0.43 |
| 1:I:462:ALA:HB2 | 1:I:489:LEU:HD22 | 1.99 | 0.43 |
| 1:R:291:LEU:HD11 | 1:R:312:LEU:HD23 | 2.01 | 0.42 |
| 1:O:473:LEU:HD12 | 1:O:487:ILE:HG13 | 2.01 | 0.42 |
| 1:S:195:LEU:HD13 | 1:S:200:TRP:CE2 | 2.54 | 0.42 |
| 1:C:161:LEU:HA | 1:C:164:ILE:HG22 | 2.02 | 0.42 |
| 1:F:89:LEU:HD11 | 1:F:111:SER:OG | 2.19 | 0.42 |
| 1:F:527:ASP:HB2 | 1:G:55:MET:CB | 2.49 | 0.42 |
| 1:H:364:GLU:CD | 1:H:384:ARG:HH22 | 2.22 | 0.42 |
| 1:C:233:VAL:HG12 | 1:C:319:ALA:O | 2.20 | 0.42 |
| 1:B:39:VAL:HG21 | 1:B:523:VAL:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:287:VAL:HG13 | 1:Q:312:LEU:HD21 | 2.00 | 0.42 |
| 1:P:427:LYS:HE3 | 1:P:477:HIS:CE1 | 2.55 | 0.42 |
| 1:S:312:LEU:HD22 | 1:S:317:VAL:HG11 | 2.02 | 0.42 |
| 1:H:462:ALA:HB2 | 1:H:489:LEU:HD22 | 2.01 | 0.42 |
| 1:O:226:ILE:HD11 | 1:O:378:SER:HB3 | 2.00 | 0.42 |
| 1:M:226:ILE:HD11 | 1:M:378:SER:HB3 | 2.01 | 0.42 |
| 1:P:226:ILE:HD11 | 1:P:378:SER:HB3 | 2.01 | 0.42 |
| 1:A:100:THR:HG22 | 1:A:103:GLY:H | 1.84 | 0.42 |
| 1:K:383:ILE:HD13 | 1:K:383:ILE:HG21 | 1.92 | 0.42 |
| 1:L:185:VAL:HG13 | 1:L:402:LEU:HA | 2.01 | 0.42 |
| 1:O:222:LEU:HD21 | 1:O:379:ILE:HD12 | 2.01 | 0.42 |
| 1:B:340:VAL:HG21 | 1:B:346:ILE:CD1 | 2.49 | 0.42 |
| 1:H:226:ILE:HD13 | 1:H:226:ILE:HA | 1.88 | 0.42 |
| 1:A:381:ILE:HD12 | 1:A:402:LEU:HD11 | 2.01 | 0.42 |
| 1:D:193:ALA:HA | 1:D:201:TYR:O | 2.20 | 0.42 |
| 1:S:298:ILE:HG23 | 1:S:319:ALA:HB2 | 2.00 | 0.42 |
| 1:D:81:LEU:HD12 | 1:D:81:LEU:HA | 1.92 | 0.42 |
| 1:D:110:PHE:CD2 | 1:D:454:LEU:HD22 | 2.55 | 0.42 |
| 1:F:31:ALA:O | 1:F:34:ALA:HB3 | 2.20 | 0.42 |
| 1:A:173:ALA:HB3 | 1:A:393:GLU:HG2 | 2.00 | 0.42 |
| 1:C:505:PRO:HG2 | 1:C:508:VAL:HB | 2.02 | 0.42 |
| 1:S:282:LEU:O | 1:S:285:GLU:HB3 | 2.20 | 0.41 |
| 1:I:477:HIS:CG | 1:I:477:HIS:O | 2.73 | 0.41 |
| 1:M:415:ILE:C | 1:M:415:ILE:HD12 | 2.40 | 0.41 |
| 1:P:423:ILE:HD13 | 1:P:473:LEU:HD13 | 2.02 | 0.41 |
| 1:F:343:ILE:O | 1:F:346:ILE:HG22 | 2.20 | 0.41 |
| 1:G:160:LEU:HD21 | 1:G:498:TRP:CZ2 | 2.55 | 0.41 |
| 1:D:245:LYS:HB3 | 1:D:351:LEU:HD23 | 2.03 | 0.41 |
| 1:S:181:ILE:HG23 | 1:S:398:LEU:HD12 | 2.03 | 0.41 |
| 1:H:430:ARG:HG2 | 1:H:430:ARG:HH11 | 1.86 | 0.41 |
| 1:M:234:HIS:HA | 1:M:235:PRO:HD3 | 1.79 | 0.41 |
| 1:S:361:LYS:HA | 1:S:366:LYS:HA | 2.01 | 0.41 |
| 1:M:145:THR:O | 1:M:145:THR:HG22 | 2.19 | 0.41 |
| 1:A:312:LEU:HD13 | 1:A:319:ALA:HB2 | 2.02 | 0.41 |
| 1:M:312:LEU:HD13 | 1:M:319:ALA:HB2 | 2.02 | 0.41 |
| 1:M:232:VAL:HG12 | 1:M:318:LEU:HD21 | 2.03 | 0.41 |
| 1:C:144:GLN:O | 1:C:148:GLU:HG2 | 2.20 | 0.41 |
| 1:A:28:GLY:N | 1:A:30:GLU:OE1 | 2.53 | 0.41 |
| 1:P:473:LEU:HB2 | 1:P:487:ILE:HD11 | 2.02 | 0.41 |
| 1:I:430:ARG:HH21 | 1:I:452:GLU:CD | 2.24 | 0.41 |
| 1:L:226:ILE:HD11 | 1:L:378:SER:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:440:GLU:O | 1:D:443:ALA:HB3 | 2.21 | 0.41 |
| 1:K:167:THR:O | 1:K:167:THR:HG22 | 2.20 | 0.41 |
| 1:I:487:ILE:HG23 | 1:I:487:ILE:O | 2.20 | 0.41 |
| 1:P:290:ILE:HD11 | 1:P:343:ILE:HG22 | 2.03 | 0.41 |
| 1:G:469:LEU:HA | 1:G:469:LEU:HD13 | 1.88 | 0.41 |
| 1:D:51:GLY:HA3 | 1:D:458:LEU:HD12 | 2.02 | 0.41 |
| 1:L:143:LEU:CD2 | 1:L:510:MET:HG3 | 2.50 | 0.41 |
| 1:Q:39:VAL:HG11 | 1:Q:115:VAL:HG21 | 2.03 | 0.41 |
| 1:H:107:ALA:HA | 1:H:516:ALA:HB2 | 2.03 | 0.41 |
| 1:F:290:ILE:CG1 | 1:F:343:ILE:HG23 | 2.51 | 0.41 |
| 1:P:415:ILE:HD12 | 1:P:421:VAL:HG21 | 2.03 | 0.41 |
| 1:M:361:LYS:HA | 1:M:366:LYS:HA | 2.03 | 0.41 |
| 1:P:521:THR:HA | 1:P:524:LEU:HD12 | 2.02 | 0.41 |
| 1:P:529:VAL:HG22 | 1:Q:58:MET:HE2 | 2.02 | 0.41 |
| 1:G:46:LEU:HD21 | 1:G:76:LEU:HD13 | 2.03 | 0.41 |
| 1:N:299:ILE:HD13 | 1:N:299:ILE:HG21 | 1.88 | 0.41 |
| 1:B:222:LEU:HD23 | 1:B:223:VAL:N | 2.35 | 0.41 |
| 1:C:423:ILE:HD12 | 1:C:477:HIS:CG | 2.57 | 0.40 |
| 1:S:304:ILE:HG21 | 1:S:304:ILE:HD13 | 1.86 | 0.40 |
| 1:P:305:ASP:O | 1:P:309:GLN:HG3 | 2.21 | 0.40 |
| 1:H:161:LEU:HD11 | 1:H:409:ILE:HD11 | 2.03 | 0.40 |
| 1:L:249:ILE:O | 1:L:300:CYS:HA | 2.21 | 0.40 |
| 1:G:93:ALA:HB1 | 1:G:108:VAL:HG22 | 2.03 | 0.40 |
| 1:P:30:GLU:CD | 1:P:30:GLU:H | 2.25 | 0.40 |
| 1:L:331:LEU:HA | 1:L:331:LEU:HD12 | 1.89 | 0.40 |
| 1:A:304:ILE:H | 1:A:321:ARG:HD3 | 1.86 | 0.40 |
| 1:E:84:PRO:O | 1:E:88:LEU:HG | 2.21 | 0.40 |
| 1:H:246:ILE:HG13 | 1:H:246:ILE:H | 1.61 | 0.40 |
| 1:P:451:LEU:HD13 | 1:P:454:LEU:HD12 | 2.04 | 0.40 |
| 1:Q:329:GLU:O | 1:Q:332:ALA:HB3 | 2.21 | 0.40 |
| 1:C:346:ILE:HG13 | 1:C:350:ASP:HB2 | 2.04 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 503/553 (91%) | 455 (90%) | 40 (8%) | 8 (2%) | 12 | 56 |
| 1 | B | 503/553 (91%) | 453 (90%) | 42 (8%) | 8 (2%) | 12 | 56 |
| 1 | C | 503/553 (91%) | 458 (91%) | 42 (8%) | 3 (1%) | 30 | 74 |
| 1 | D | 503/553 (91%) | 451 (90%) | 47 (9%) | 5 (1%) | 19 | 65 |
| 1 | E | 503/553 (91%) | 451 (90%) | 49 (10%) | 3 (1%) | 30 | 74 |
| 1 | F | 503/553 (91%) | 456 (91%) | 41 (8%) | 6 (1%) | 16 | 61 |
| 1 | G | 503/553 (91%) | 444 (88%) | 50 (10%) | 9 (2%) | 11 | 53 |
| 1 | H | 503/553 (91%) | 450 (90%) | 47 (9%) | 6 (1%) | 16 | 61 |
| 1 | I | 503/553 (91%) | 457 (91%) | 41 (8%) | 5 (1%) | 19 | 65 |
| 1 | K | 503/553 (91%) | 452 (90%) | 45 (9%) | 6 (1%) | 16 | 61 |
| 1 | L | 503/553 (91%) | 454 (90%) | 44 (9%) | 5 (1%) | 19 | 65 |
| 1 | M | 503/553 (91%) | 458 (91%) | 42 (8%) | 3 (1%) | 30 | 74 |
| 1 | N | 503/553 (91%) | 455 (90%) | 41 (8%) | 7 (1%) | 14 | 58 |
| 1 | O | 503/553 (91%) | 449 (89%) | 46 (9%) | 8 (2%) | 12 | 56 |
| 1 | P | 503/553 (91%) | 456 (91%) | 41 (8%) | 6 (1%) | 16 | 61 |
| 1 | Q | 503/553 (91%) | 454 (90%) | 44 (9%) | 5 (1%) | 19 | 65 |
| 1 | R | 503/553 (91%) | 455 (90%) | 42 (8%) | 6 (1%) | 16 | 61 |
| 1 | S | 503/553 (91%) | 450 (90%) | 49 (10%) | 4 (1%) | 24 | 69 |
| All | All | 9054/9954 (91%) | 8158 (90%) | 793 (9%) | 103 (1%) | 23 | 63 |

All (103) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 387 | LEU |
| 1 | M | 387 | LEU |
| 1 | N | 387 | LEU |
| 1 | O | 264 | ILE |
| 1 | R | 387 | LEU |
| 1 | A | 30 | GLU |
| 1 | D | 30 | GLU |
| 1 | D | 100 | THR |
| 1 | E | 30 | GLU |
| 1 | F | 30 | GLU |
| 1 | G | 30 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 100 | THR |
| 1 | H | 95 | GLY |
| 1 | K | 30 | GLU |
| 1 | K | 386 | GLY |
| 1 | K | 387 | LEU |
| 1 | K | 438 | GLY |
| 1 | O | 30 | GLU |
| 1 | O | 240 | ARG |
| 1 | Q | 385 | GLY |
| 1 | S | 438 | GLY |
| 1 | A | 100 | THR |
| 1 | A | 385 | GLY |
| 1 | A | 387 | LEU |
| 1 | B | 30 | GLU |
| 1 | B | 385 | GLY |
| 1 | C | 30 | GLU |
| 1 | C | 438 | GLY |
| 1 | E | 438 | GLY |
| 1 | F | 438 | GLY |
| 1 | G | 387 | LEU |
| 1 | H | 30 | GLU |
| 1 | I | 30 | GLU |
| 1 | L | 30 | GLU |
| 1 | L | 385 | GLY |
| 1 | L | 438 | GLY |
| 1 | M | 30 | GLU |
| 1 | N | 30 | GLU |
| 1 | N | 149 | LEU |
| 1 | N | 258 | PRO |
| 1 | N | 385 | GLY |
| 1 | O | 305 | ASP |
| 1 | P | 30 | GLU |
| 1 | P | 259 | GLU |
| 1 | P | 385 | GLY |
| 1 | Q | 30 | GLU |
| 1 | Q | 387 | LEU |
| 1 | Q | 438 | GLY |
| 1 | S | 30 | GLU |
| 1 | B | 148 | GLU |
| 1 | B | 149 | LEU |
| 1 | B | 438 | GLY |
| 1 | D | 385 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 438 | GLY |
| 1 | E | 266 | ILE |
| 1 | F | 149 | LEU |
| 1 | G | 61 | ASP |
| 1 | H | 149 | LEU |
| 1 | I | 149 | LEU |
| 1 | I | 387 | LEU |
| 1 | L | 149 | LEU |
| 1 | M | 438 | GLY |
| 1 | O | 385 | GLY |
| 1 | O | 438 | GLY |
| 1 | O | 499 | GLN |
| 1 | P | 438 | GLY |
| 1 | R | 322 | ARG |
| 1 | R | 385 | GLY |
| 1 | A | 149 | LEU |
| 1 | A | 438 | GLY |
| 1 | B | 258 | PRO |
| 1 | B | 387 | LEU |
| 1 | C | 149 | LEU |
| 1 | D | 258 | PRO |
| 1 | F | 47 | LYS |
| 1 | G | 149 | LEU |
| 1 | G | 363 | GLY |
| 1 | H | 438 | GLY |
| 1 | I | 438 | GLY |
| 1 | K | 149 | LEU |
| 1 | L | 148 | GLU |
| 1 | N | 438 | GLY |
| 1 | O | 149 | LEU |
| 1 | P | 47 | LYS |
| 1 | P | 149 | LEU |
| 1 | Q | 149 | LEU |
| 1 | R | 30 | GLU |
| 1 | R | 149 | LEU |
| 1 | R | 438 | GLY |
| 1 | S | 373 | ALA |
| 1 | A | 363 | GLY |
| 1 | F | 259 | GLU |
| 1 | G | 438 | GLY |
| 1 | H | 148 | GLU |
| 1 | K | 499 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 149 | LEU |
| 1 | F | 174 | VAL |
| 1 | G | 266 | ILE |
| 1 | G | 385 | GLY |
| 1 | I | 385 | GLY |
| 1 | N | 376 | PRO |
| 1 | B | 215 | GLY |
| 1 | A | 434 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 410/447 (92%) | 396 (97%) | 14 (3%) | 44 | 75 |
| 1 | B | 410/447 (92%) | 393 (96%) | 17 (4%) | 37 | 71 |
| 1 | C | 410/447 (92%) | 397 (97%) | 13 (3%) | 46 | 76 |
| 1 | D | 410/447 (92%) | 394 (96%) | 16 (4%) | 39 | 72 |
| 1 | E | 410/447 (92%) | 402 (98%) | 8 (2%) | 63 | 85 |
| 1 | F | 410/447 (92%) | 396 (97%) | 14 (3%) | 44 | 75 |
| 1 | G | 410/447 (92%) | 400 (98%) | 10 (2%) | 57 | 82 |
| 1 | H | 410/447 (92%) | 402 (98%) | 8 (2%) | 63 | 85 |
| 1 | I | 410/447 (92%) | 399 (97%) | 11 (3%) | 52 | 79 |
| 1 | K | 410/447 (92%) | 403 (98%) | 7 (2%) | 68 | 87 |
| 1 | L | 410/447 (92%) | 395 (96%) | 15 (4%) | 41 | 73 |
| 1 | M | 410/447 (92%) | 399 (97%) | 11 (3%) | 52 | 79 |
| 1 | N | 410/447 (92%) | 395 (96%) | 15 (4%) | 41 | 73 |
| 1 | O | 410/447 (92%) | 391 (95%) | 19 (5%) | 33 | 68 |
| 1 | P | 410/447 (92%) | 401 (98%) | 9 (2%) | 60 | 83 |
| 1 | Q | 410/447 (92%) | 401 (98%) | 9 (2%) | 60 | 83 |
| 1 | R | 410/447 (92%) | 401 (98%) | 9 (2%) | 60 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | S | 410/447 (92%) | 394 (96%) | 16 (4%) | 39 | 72 |
| All | All | 7380/8046 (92%) | 7159 (97%) | 221 (3%) | 52 | 77 |

All (221) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 94 | LYS |
| 1 | A | 144 | GLN |
| 1 | A | 167 | THR |
| 1 | A | 269 | PRO |
| 1 | A | 297 | VAL |
| 1 | A | 301 | GLN |
| 1 | A | 305 | ASP |
| 1 | A | 343 | ILE |
| 1 | A | 367 | MET |
| 1 | A | 369 | PHE |
| 1 | A | 370 | VAL |
| 1 | A | 422 | GLU |
| 1 | A | 423 | ILE |
| 1 | A | 473 | LEU |
| 1 | B | 56 | ASP |
| 1 | B | 76 | LEU |
| 1 | B | 80 | ASP |
| 1 | B | 83 | HIS |
| 1 | B | 149 | LEU |
| 1 | B | 242 | GLU |
| 1 | B | 248 | LEU |
| 1 | B | 273 | GLN |
| 1 | B | 297 | VAL |
| 1 | B | 331 | LEU |
| 1 | B | 356 | LEU |
| 1 | B | 367 | MET |
| 1 | B | 392 | ASP |
| 1 | B | 398 | LEU |
| 1 | B | 473 | LEU |
| 1 | B | 477 | HIS |
| 1 | B | 509 | LYS |
| 1 | C | 76 | LEU |
| 1 | C | 89 | LEU |
| 1 | C | 128 | PRO |
| 1 | C | 164 | ILE |
| 1 | C | 167 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 241 | LEU |
| 1 | C | 288 | ASP |
| 1 | C | 301 | GLN |
| 1 | C | 367 | MET |
| 1 | C | 453 | SER |
| 1 | C | 473 | LEU |
| 1 | C | 509 | LYS |
| 1 | C | 522 | LEU |
| 1 | D | 82 | GLN |
| 1 | D | 139 | GLU |
| 1 | D | 144 | GLN |
| 1 | D | 152 | THR |
| 1 | D | 159 | ASP |
| 1 | D | 203 | ASP |
| 1 | D | 204 | LEU |
| 1 | D | 241 | LEU |
| 1 | D | 288 | ASP |
| 1 | D | 297 | VAL |
| 1 | D | 301 | GLN |
| 1 | D | 341 | SER |
| 1 | D | 365 | ASP |
| 1 | D | 453 | SER |
| 1 | D | 470 | LEU |
| 1 | D | 477 | HIS |
| 1 | E | 76 | LEU |
| 1 | E | 153 | VAL |
| 1 | E | 246 | ILE |
| 1 | E | 273 | GLN |
| 1 | E | 288 | ASP |
| 1 | E | 297 | VAL |
| 1 | E | 305 | ASP |
| 1 | E | 365 | ASP |
| 1 | F | 84 | PRO |
| 1 | F | 160 | LEU |
| 1 | F | 167 | THR |
| 1 | F | 169 | LEU |
| 1 | F | 210 | VAL |
| 1 | F | 211 | LYS |
| 1 | F | 297 | VAL |
| 1 | F | 301 | GLN |
| 1 | F | 367 | MET |
| 1 | F | 436 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 473 | LEU |
| 1 | F | 476 | THR |
| 1 | F | 477 | HIS |
| 1 | F | 485 | TYR |
| 1 | G | 61 | ASP |
| 1 | G | 198 | ASP |
| 1 | G | 211 | LYS |
| 1 | G | 231 | GLU |
| 1 | G | 232 | VAL |
| 1 | G | 246 | ILE |
| 1 | G | 254 | GLU |
| 1 | G | 297 | VAL |
| 1 | G | 301 | GLN |
| 1 | G | 351 | LEU |
| 1 | H | 100 | THR |
| 1 | H | 241 | LEU |
| 1 | H | 297 | VAL |
| 1 | H | 301 | GLN |
| 1 | H | 356 | LEU |
| 1 | H | 422 | GLU |
| 1 | H | 441 | GLN |
| 1 | H | 473 | LEU |
| 1 | I | 33 | ARG |
| 1 | I | 47 | LYS |
| 1 | I | 62 | SER |
| 1 | I | 123 | TYR |
| 1 | I | 127 | HIS |
| 1 | I | 178 | ARG |
| 1 | I | 238 | PRO |
| 1 | I | 297 | VAL |
| 1 | I | 429 | LEU |
| 1 | I | 480 | GLU |
| 1 | I | 484 | TRP |
| 1 | K | 59 | LEU |
| 1 | K | 97 | ASP |
| 1 | K | 100 | THR |
| 1 | K | 297 | VAL |
| 1 | K | 434 | PRO |
| 1 | K | 473 | LEU |
| 1 | K | 484 | TRP |
| 1 | L | 30 | GLU |
| 1 | L | 47 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 56 | ASP |
| 1 | L | 129 | THR |
| 1 | L | 144 | GLN |
| 1 | L | 248 | LEU |
| 1 | L | 288 | ASP |
| 1 | L | 297 | VAL |
| 1 | L | 301 | GLN |
| 1 | L | 331 | LEU |
| 1 | L | 356 | LEU |
| 1 | L | 367 | MET |
| 1 | L | 391 | VAL |
| 1 | L | 392 | ASP |
| 1 | L | 477 | HIS |
| 1 | M | 56 | ASP |
| 1 | M | 82 | GLN |
| 1 | M | 167 | THR |
| 1 | M | 263 | GLU |
| 1 | M | 297 | VAL |
| 1 | M | 298 | ILE |
| 1 | M | 301 | GLN |
| 1 | M | 329 | GLU |
| 1 | M | 356 | LEU |
| 1 | M | 376 | PRO |
| 1 | M | 379 | ILE |
| 1 | N | 30 | GLU |
| 1 | N | 66 | ILE |
| 1 | N | 76 | LEU |
| 1 | N | 99 | GLU |
| 1 | N | 139 | GLU |
| 1 | N | 167 | THR |
| 1 | N | 297 | VAL |
| 1 | N | 301 | GLN |
| 1 | N | 305 | ASP |
| 1 | N | 329 | GLU |
| 1 | N | 367 | MET |
| 1 | N | 453 | SER |
| 1 | N | 473 | LEU |
| 1 | N | 484 | TRP |
| 1 | N | 517 | THR |
| 1 | O | 30 | GLU |
| 1 | O | 63 | LEU |
| 1 | O | 77 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 144 | GLN |
| 1 | O | 222 | LEU |
| 1 | O | 231 | GLU |
| 1 | O | 242 | GLU |
| 1 | O | 283 | ILE |
| 1 | O | 297 | VAL |
| 1 | O | 305 | ASP |
| 1 | O | 312 | LEU |
| 1 | O | 326 | SER |
| 1 | O | 329 | GLU |
| 1 | O | 343 | ILE |
| 1 | O | 356 | LEU |
| 1 | O | 367 | MET |
| 1 | O | 473 | LEU |
| 1 | O | 484 | TRP |
| 1 | O | 487 | ILE |
| 1 | P | 167 | THR |
| 1 | P | 211 | LYS |
| 1 | P | 241 | LEU |
| 1 | P | 269 | PRO |
| 1 | P | 367 | MET |
| 1 | P | 451 | LEU |
| 1 | P | 473 | LEU |
| 1 | P | 477 | HIS |
| 1 | P | 484 | TRP |
| 1 | Q | 29 | LYS |
| 1 | Q | 74 | THR |
| 1 | Q | 167 | THR |
| 1 | Q | 204 | LEU |
| 1 | Q | 208 | GLN |
| 1 | Q | 210 | VAL |
| 1 | Q | 273 | GLN |
| 1 | Q | 398 | LEU |
| 1 | Q | 510 | MET |
| 1 | R | 42 | VAL |
| 1 | R | 168 | SER |
| 1 | R | 297 | VAL |
| 1 | R | 301 | GLN |
| 1 | R | 322 | ARG |
| 1 | R | 367 | MET |
| 1 | R | 376 | PRO |
| 1 | R | 453 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 473 | LEU |
| 1 | S | 33 | ARG |
| 1 | S | 43 | GLU |
| 1 | S | 82 | GLN |
| 1 | S | 84 | PRO |
| 1 | S | 144 | GLN |
| 1 | S | 231 | GLU |
| 1 | S | 258 | PRO |
| 1 | S | 283 | ILE |
| 1 | S | 288 | ASP |
| 1 | S | 297 | VAL |
| 1 | S | 301 | GLN |
| 1 | S | 333 | ARG |
| 1 | S | 366 | LYS |
| 1 | S | 473 | LEU |
| 1 | S | 528 | ASP |
| 1 | S | 530 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 91 | GLN |
| 1 | B | 127 | HIS |
| 1 | B | 147 | GLN |
| 1 | C | 70 | ASN |
| 1 | D | 96 | GLN |
| 1 | E | 127 | HIS |
| 1 | F | 82 | GLN |
| 1 | F | 127 | HIS |
| 1 | F | 221 | GLN |
| 1 | F | 267 | ASN |
| 1 | G | 441 | GLN |
| 1 | G | 477 | HIS |
| 1 | H | 441 | GLN |
| 1 | I | 83 | HIS |
| 1 | K | 127 | HIS |
| 1 | K | 144 | GLN |
| 1 | K | 151 | GLN |
| 1 | K | 206 | ASN |
| 1 | L | 218 | ASN |
| 1 | M | 83 | HIS |
| 1 | M | 221 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 234 | HIS |
| 1 | N | 482 | ASN |
| 1 | O | 441 | GLN |
| 1 | O | 477 | HIS |
| 1 | P | 127 | HIS |
| 1 | P | 271 | GLN |
| 1 | P | 441 | GLN |
| 1 | S | 144 | GLN |
| 1 | S | 234 | HIS |
| 1 | S | 479 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.