



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:43 AM UTC

PDB ID : 3J1F / pdb\_00003j1f  
EMDB ID : EMD-5396  
Title : Cryo-EM structure of 9-fold symmetric rATcpn-beta in ATP-binding 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 : 6.20 Å(reported)  
Based on initial model : 3KO1

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

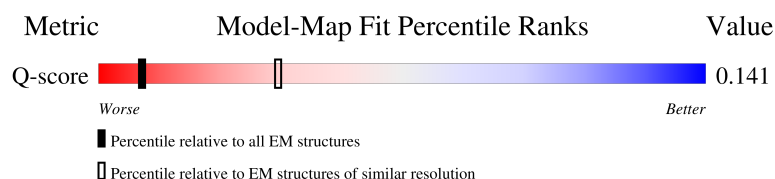
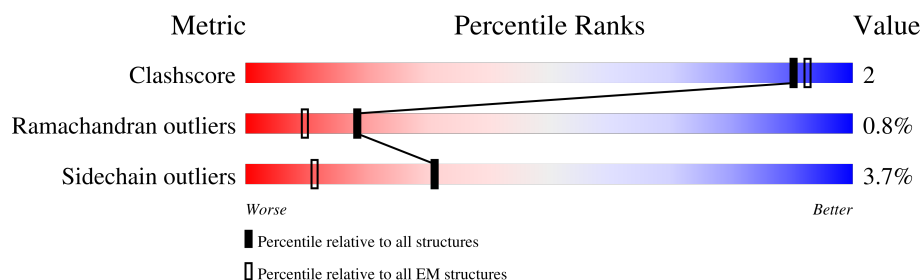
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 6.20 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.



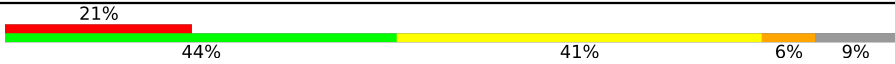
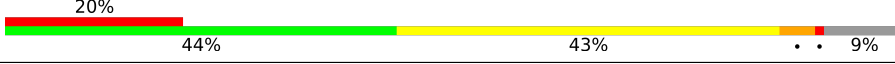
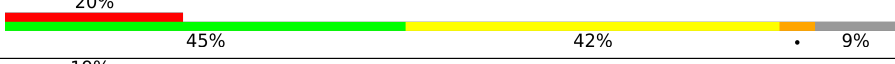
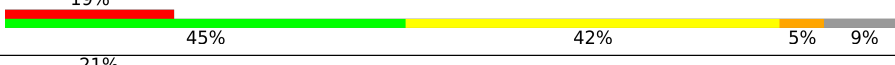
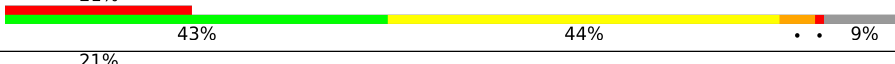
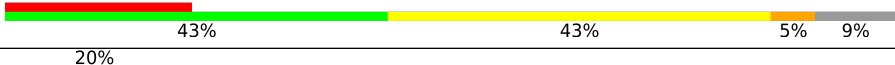
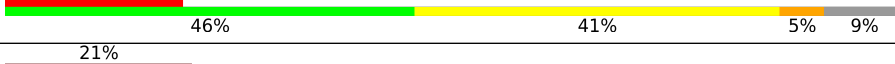
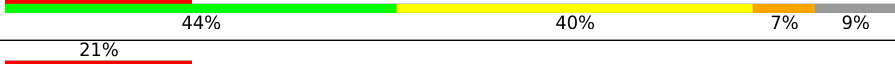
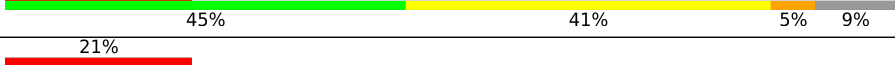
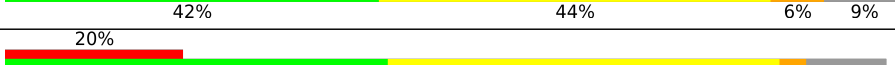
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 537 ( 5.70 - 6.70 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 553    | <div> <div>20%</div> <div>47%</div> <div>39%</div> <div>5%</div> <div>9%</div> </div> |
| 1   | B     | 553    | <div> <div>21%</div> <div>45%</div> <div>39%</div> <div>6%</div> <div>9%</div> </div> |
| 1   | C     | 553    | <div> <div>20%</div> <div>42%</div> <div>45%</div> <div>5%</div> <div>9%</div> </div> |
| 1   | D     | 553    | <div> <div>20%</div> <div>47%</div> <div>41%</div> <div>•</div> <div>9%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 553    |    |
| 1   | F     | 553    |    |
| 1   | G     | 553    |    |
| 1   | H     | 553    |    |
| 1   | I     | 553    |    |
| 1   | K     | 553    |    |
| 1   | L     | 553    |    |
| 1   | M     | 553    |    |
| 1   | N     | 553    |    |
| 1   | O     | 553    |    |
| 1   | P     | 553    |    |
| 1   | Q     | 553    |   |
| 1   | R     | 553    |  |
| 1   | S     | 553    |  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 69858 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.

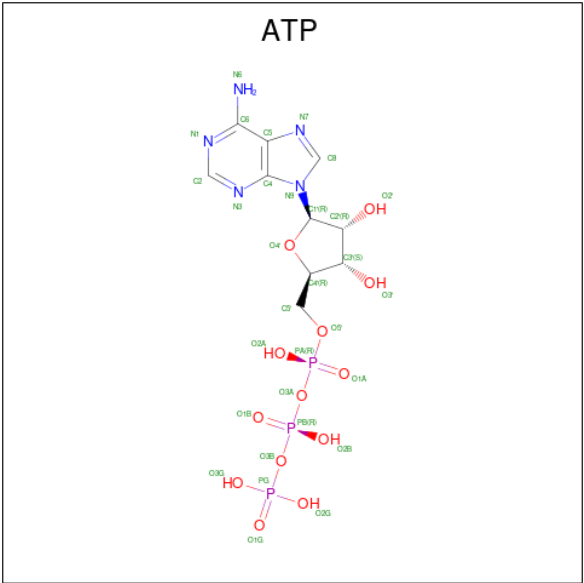
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 505      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3849  | 2423 | 658 | 757 | 11 |         | 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

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 2   | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | Q     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | R     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 2   | S     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | E     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | F     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | G     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | H     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | I     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | K     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 3   | L     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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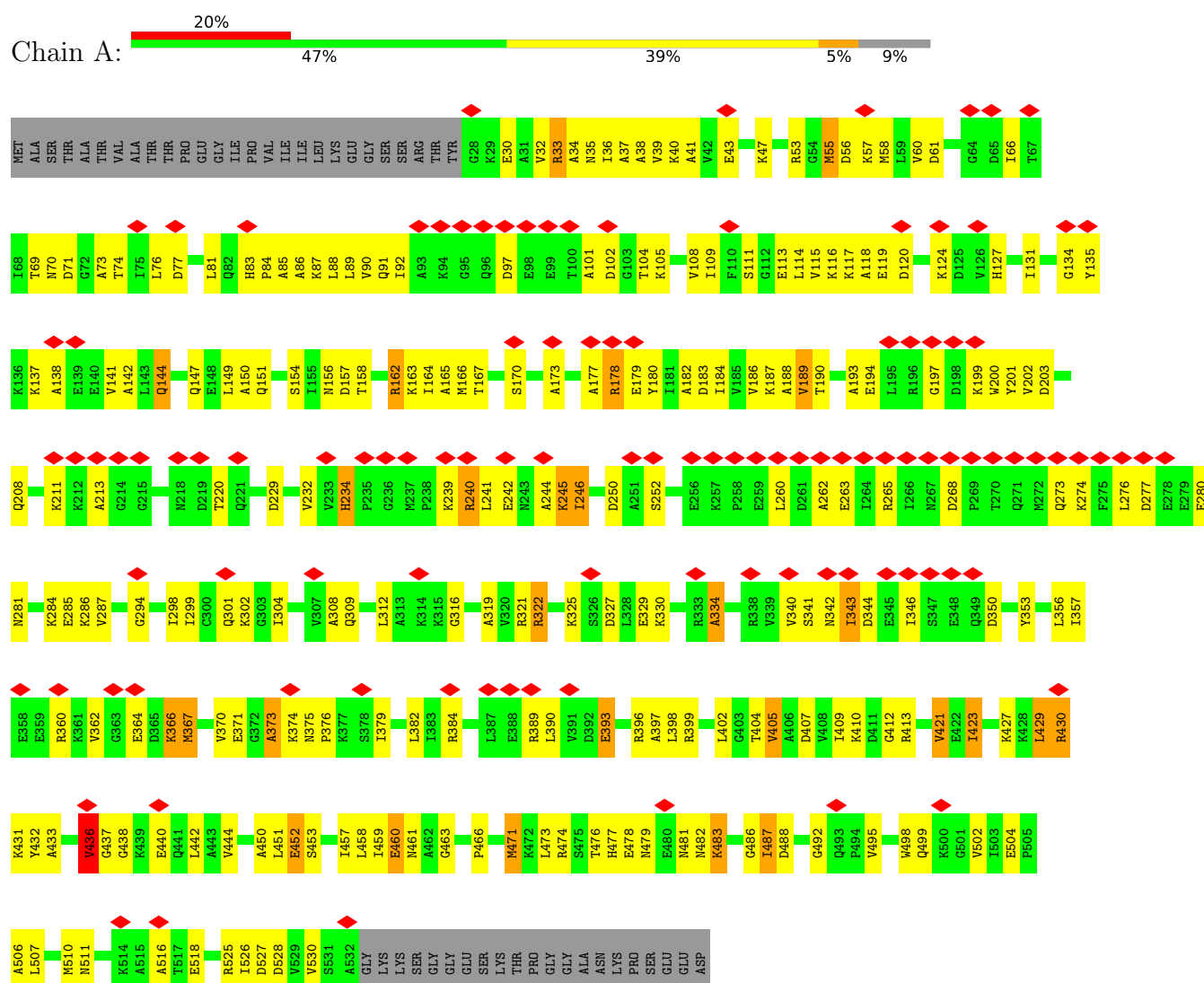
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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 3   | M     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | N     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | O     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | P     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | Q     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | R     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 3   | S     | 1        | Total<br>1 | Mg<br>1 | 0       |

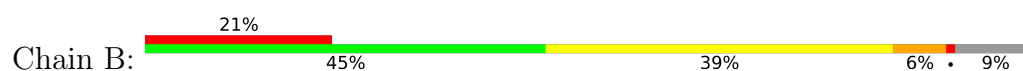
### 3 Residue-property plots

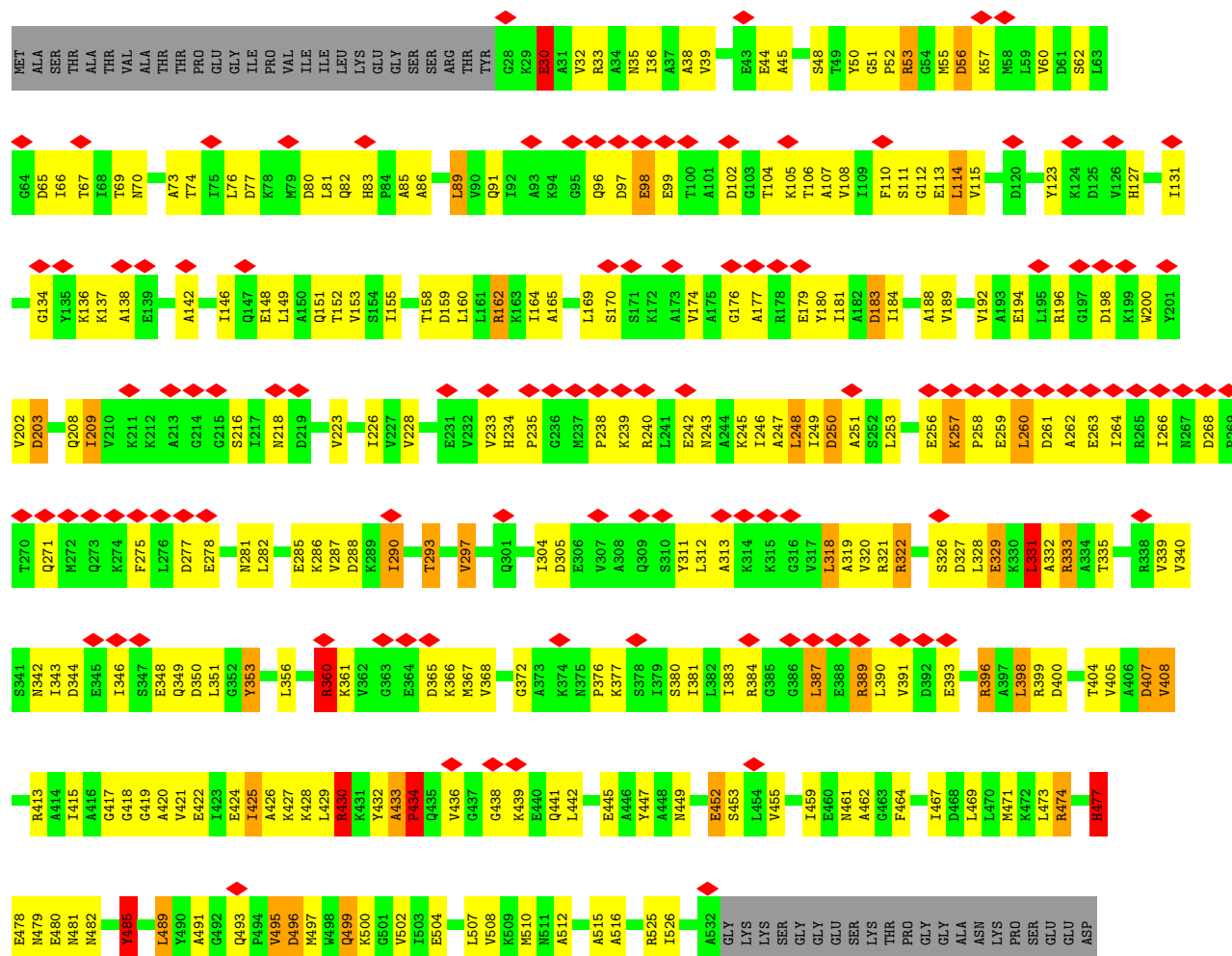
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Chaperonin beta subunit

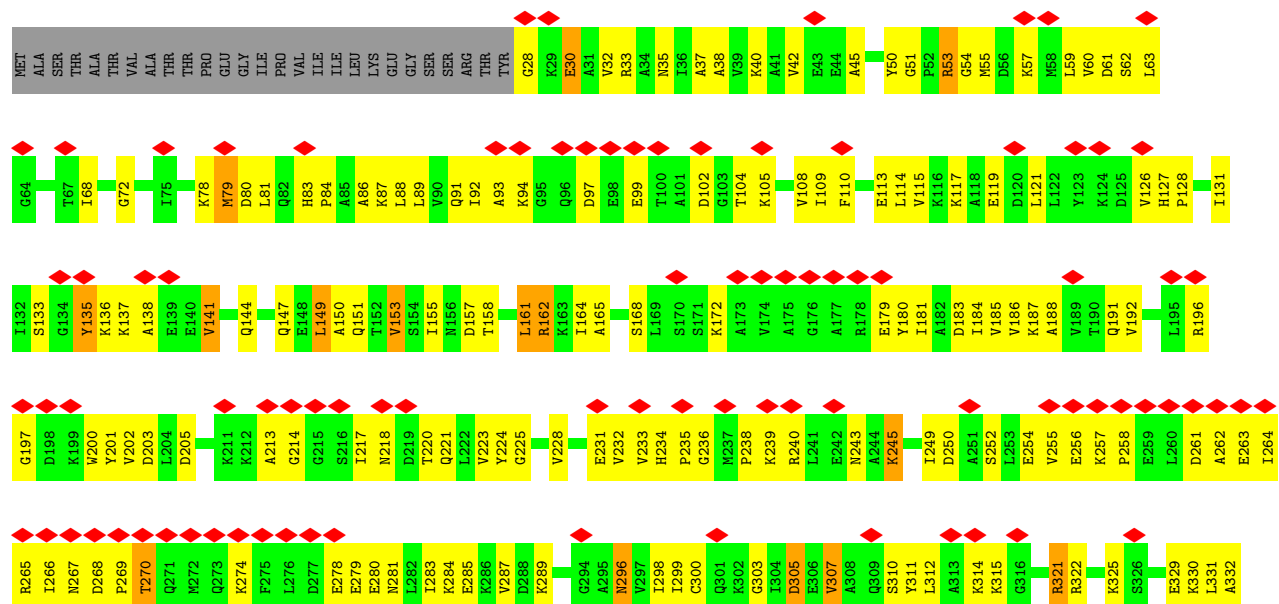


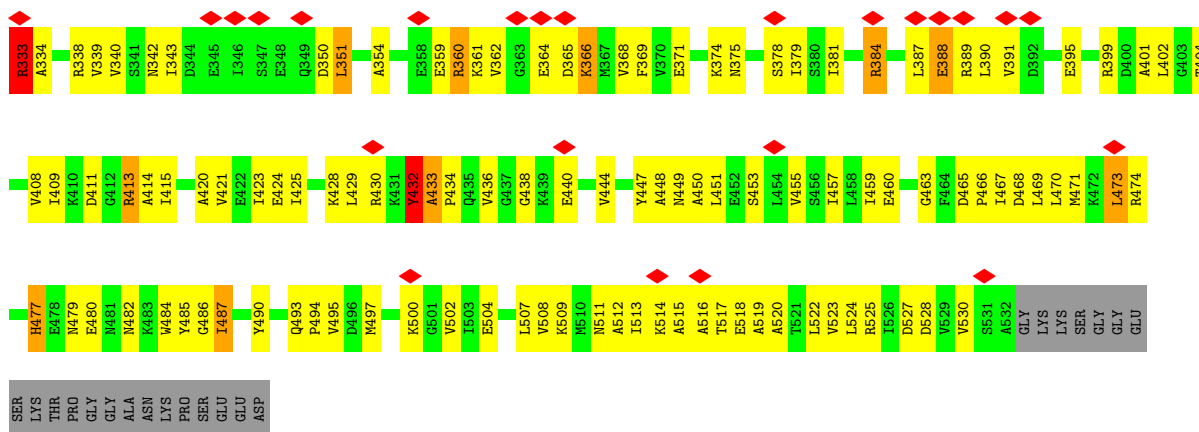
#### • Molecule 1: Chaperonin beta subunit



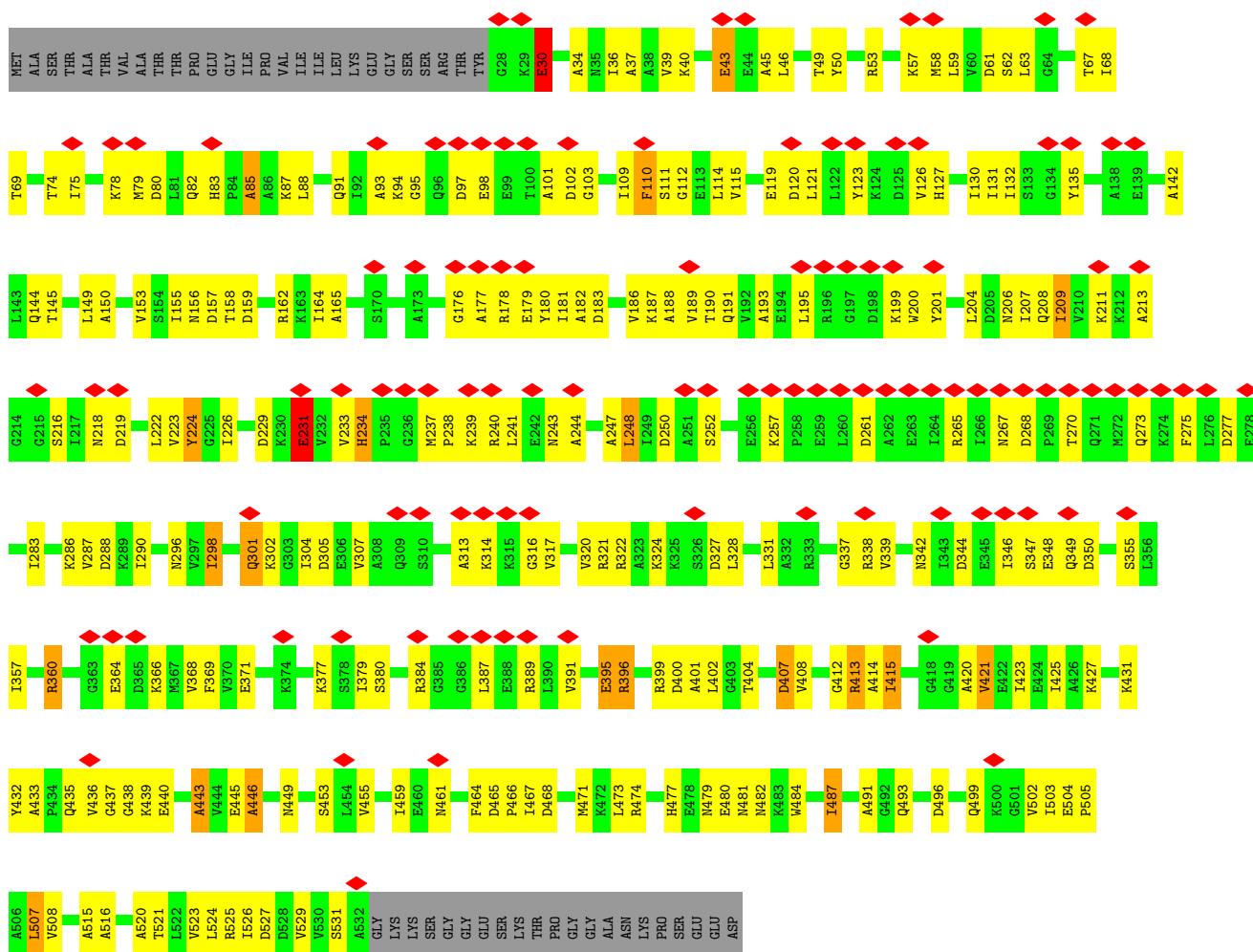


• Molecule 1: Chaperonin beta subunit



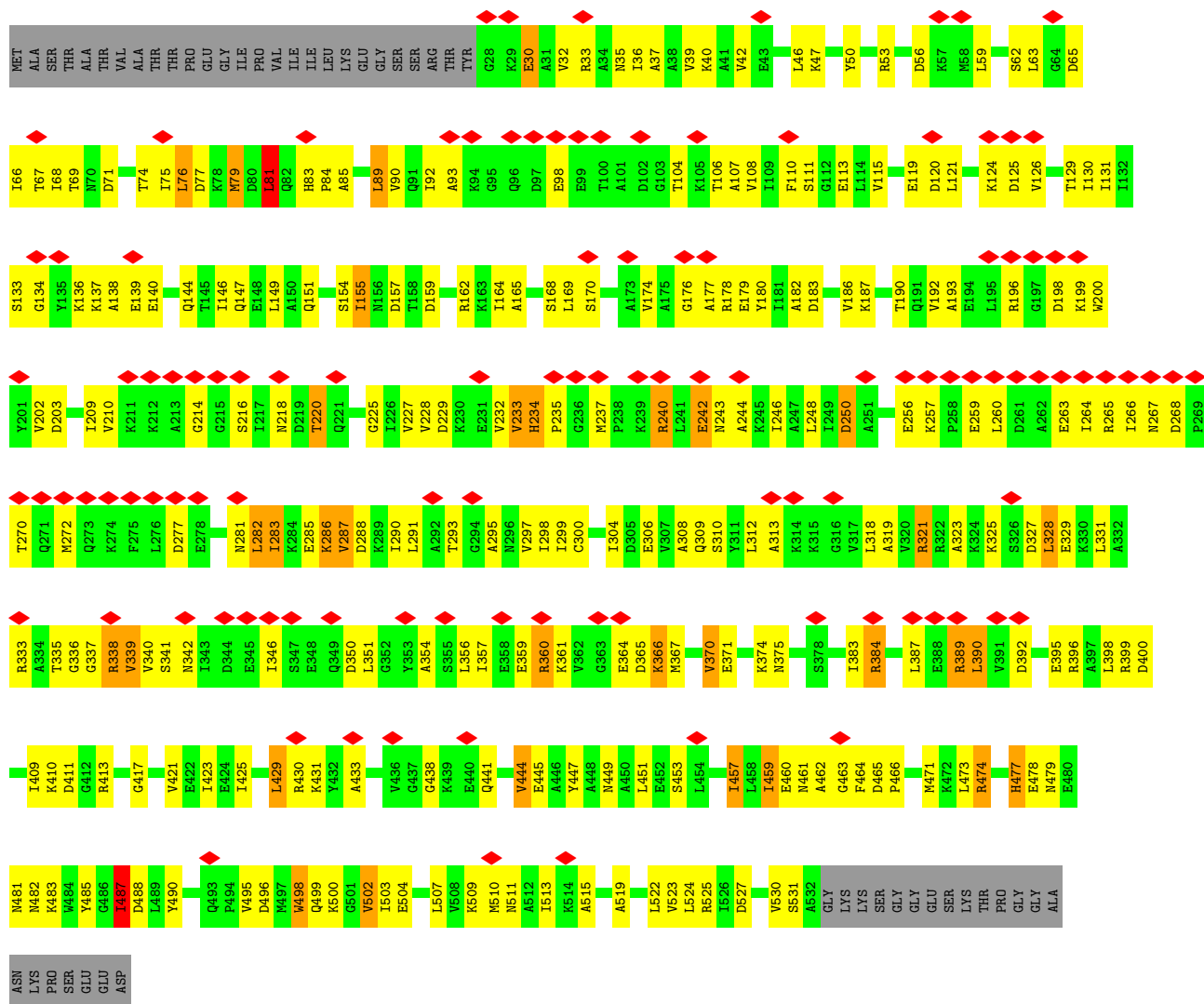


• Molecule 1: Chaperonin beta subunit

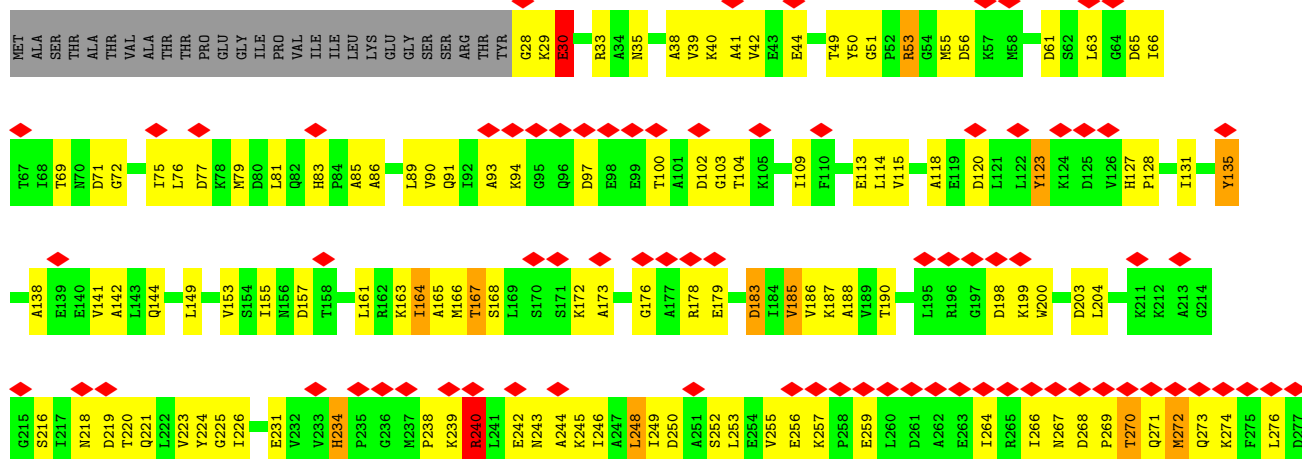


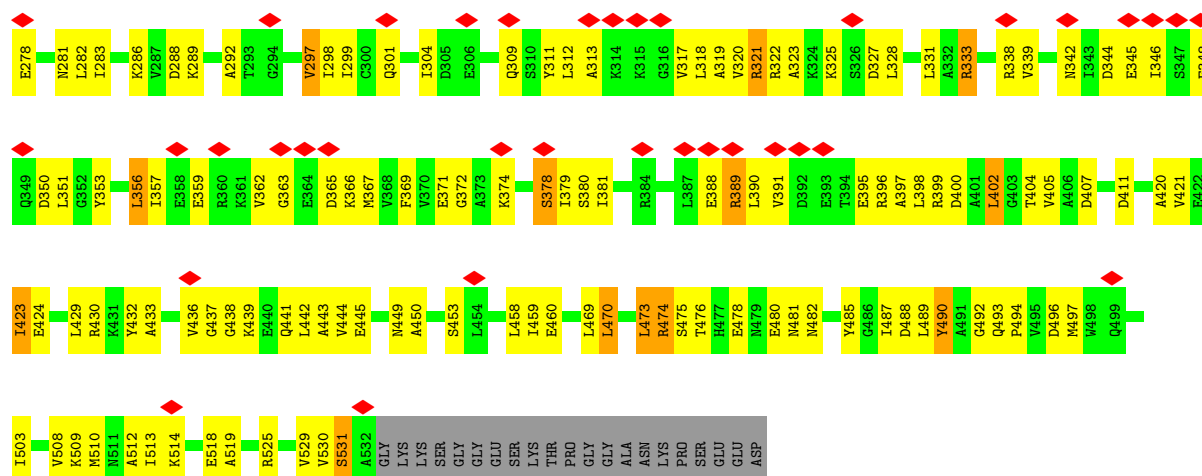
• Molecule 1: Chaperonin beta subunit



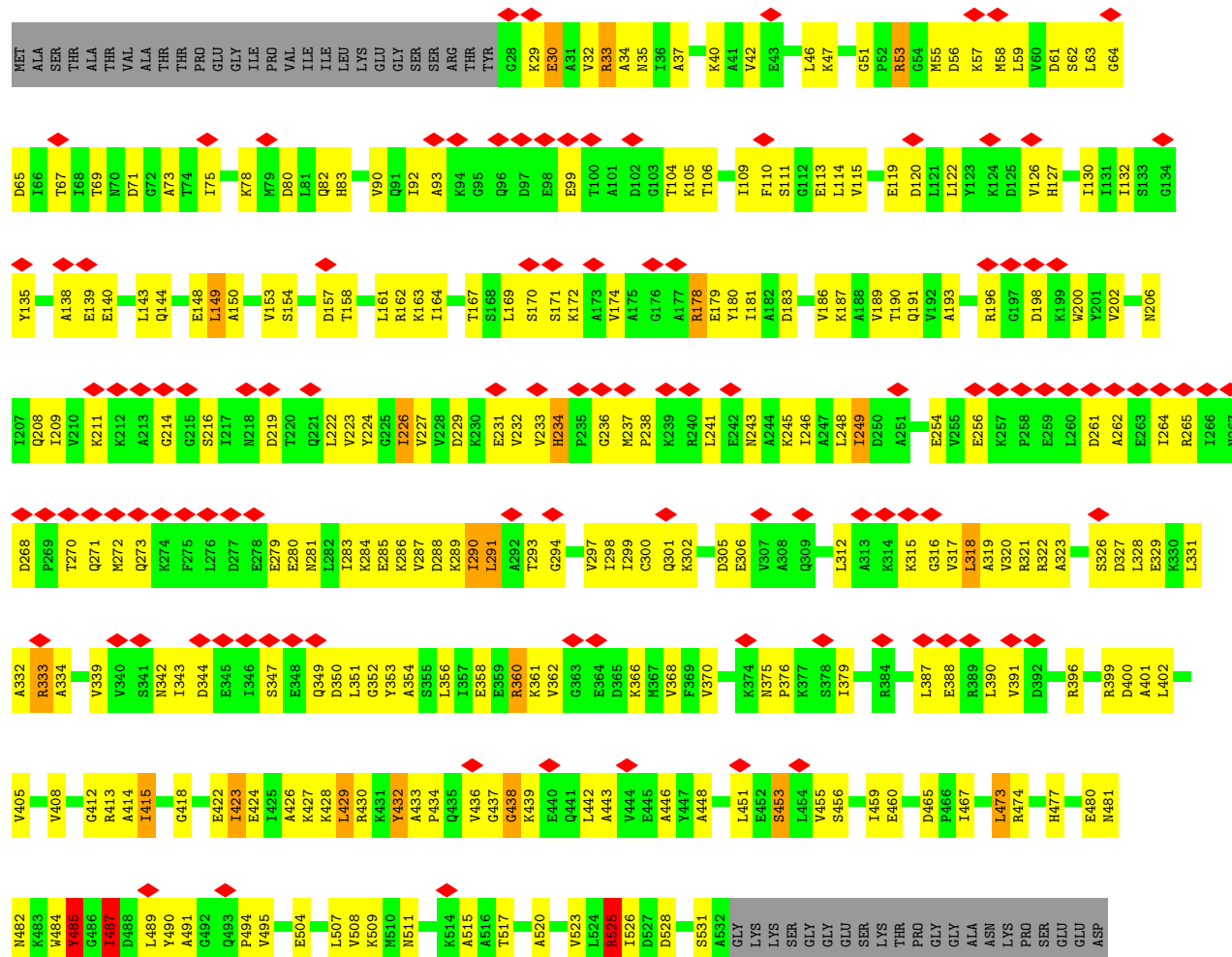
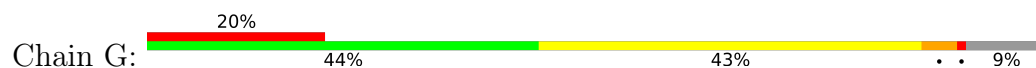


• Molecule 1: Chaperonin beta subunit

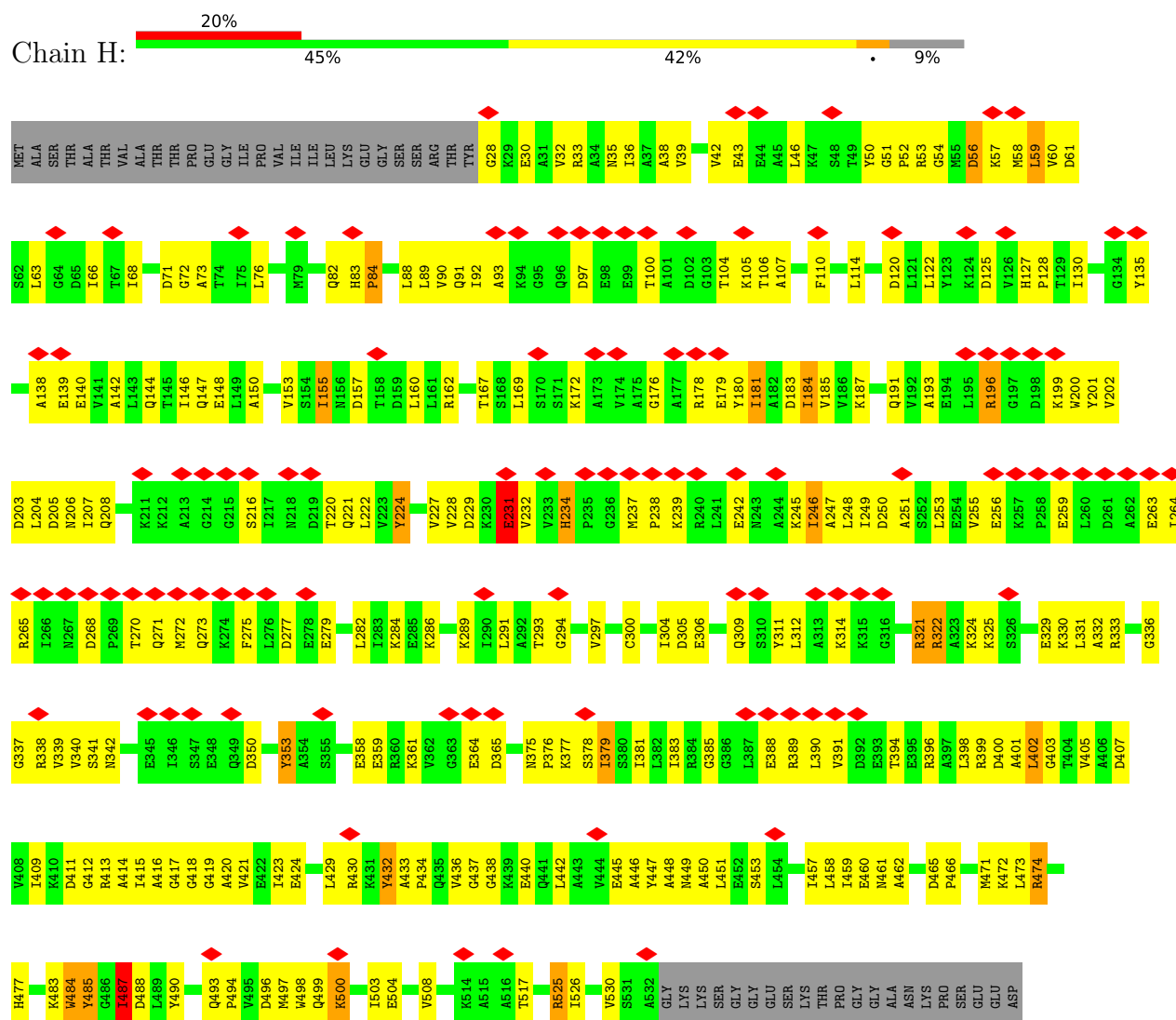




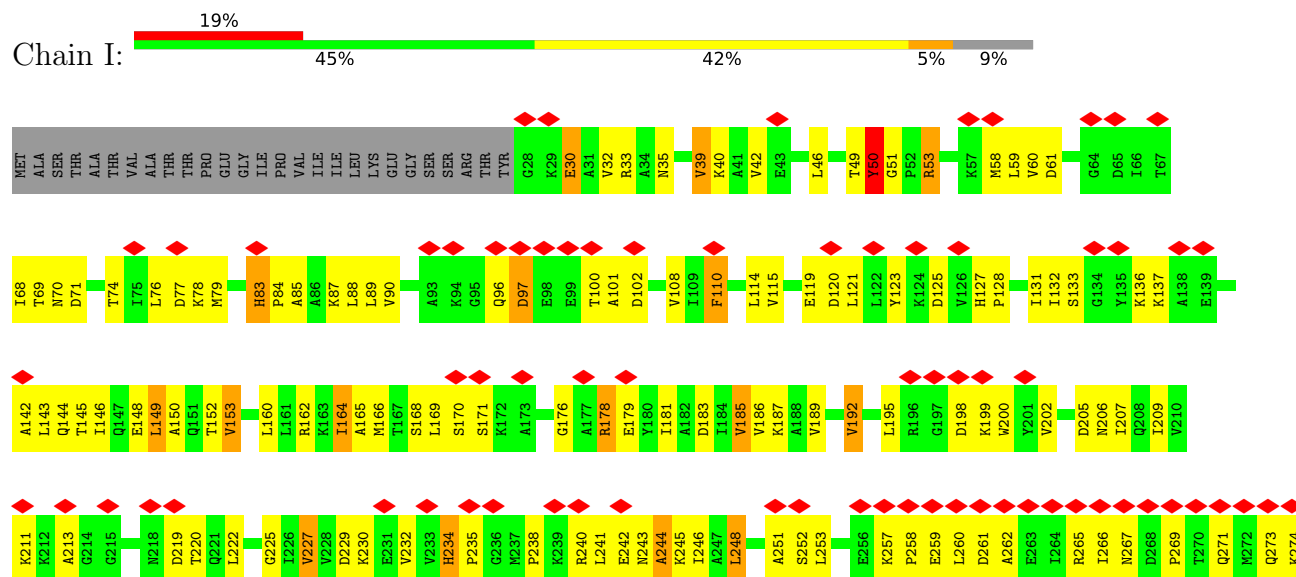
• Molecule 1: Chaperonin beta subunit

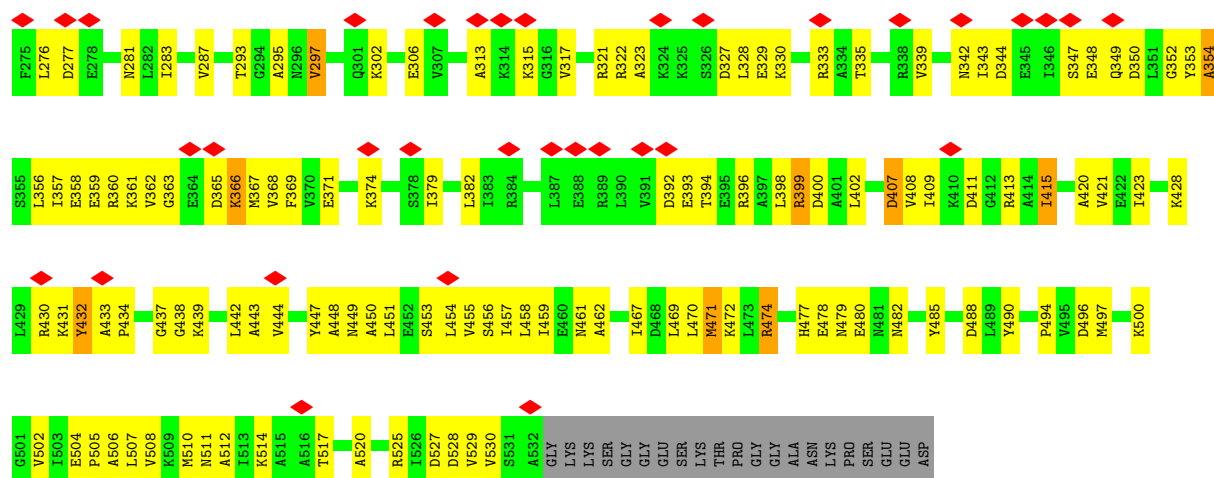


• Molecule 1: Chaperonin beta subunit

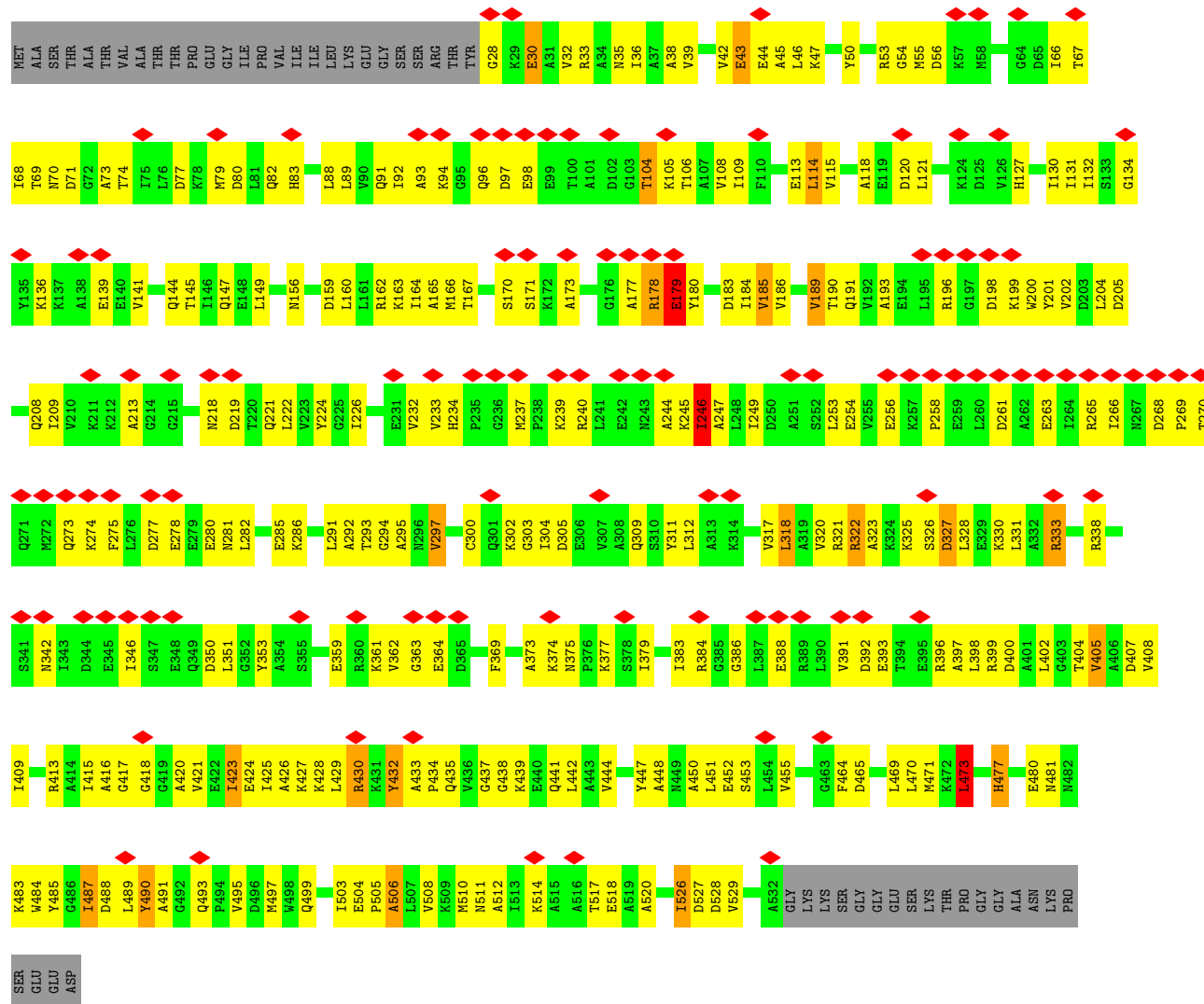
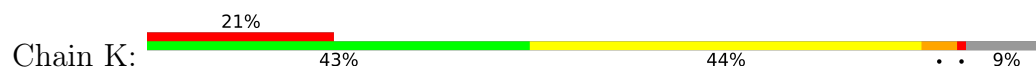


• Molecule 1: Chaperonin beta subunit

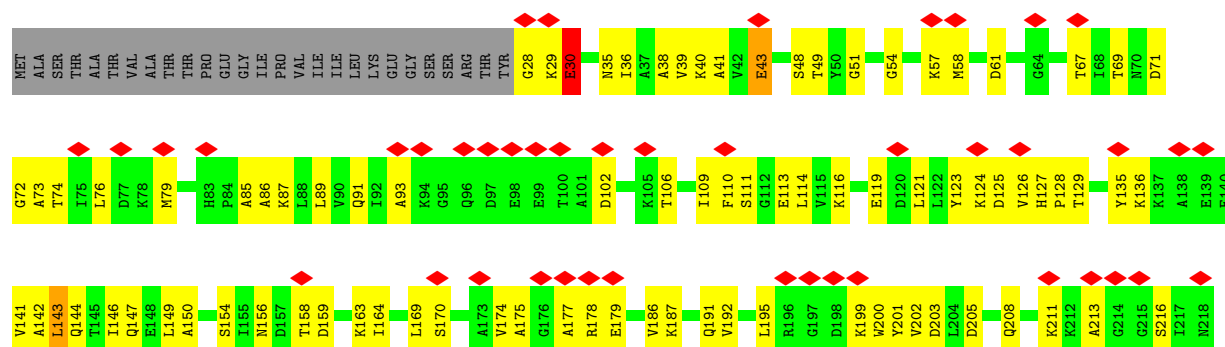


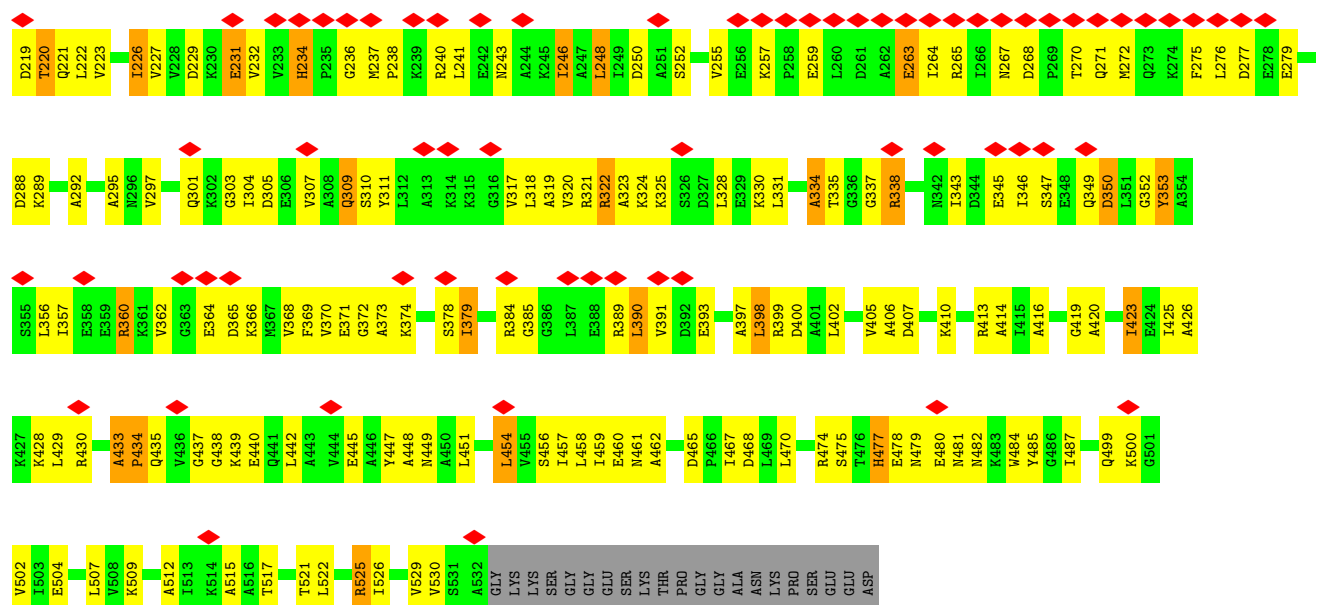


• Molecule 1: Chaperonin beta subunit

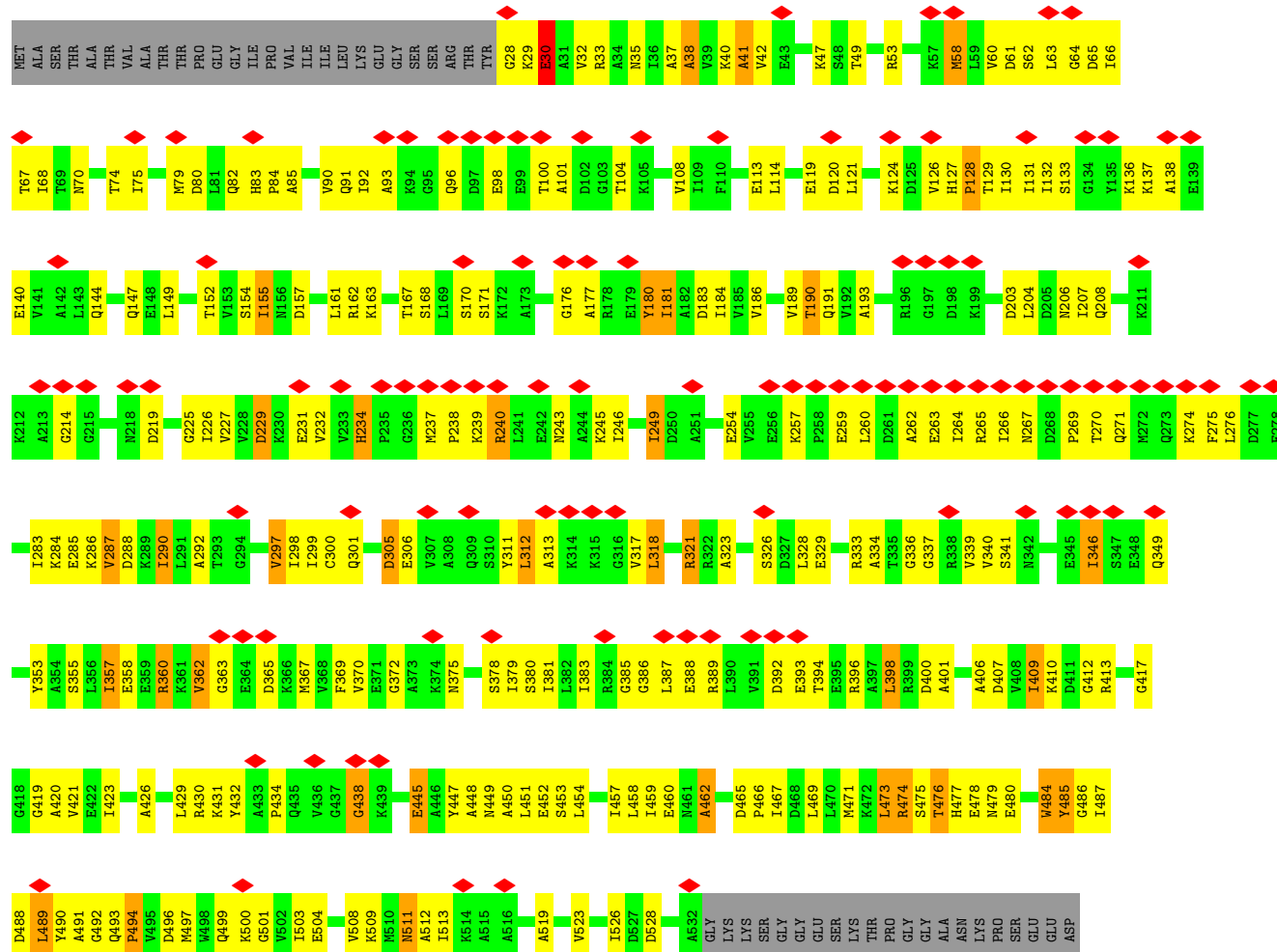


Chain L: 

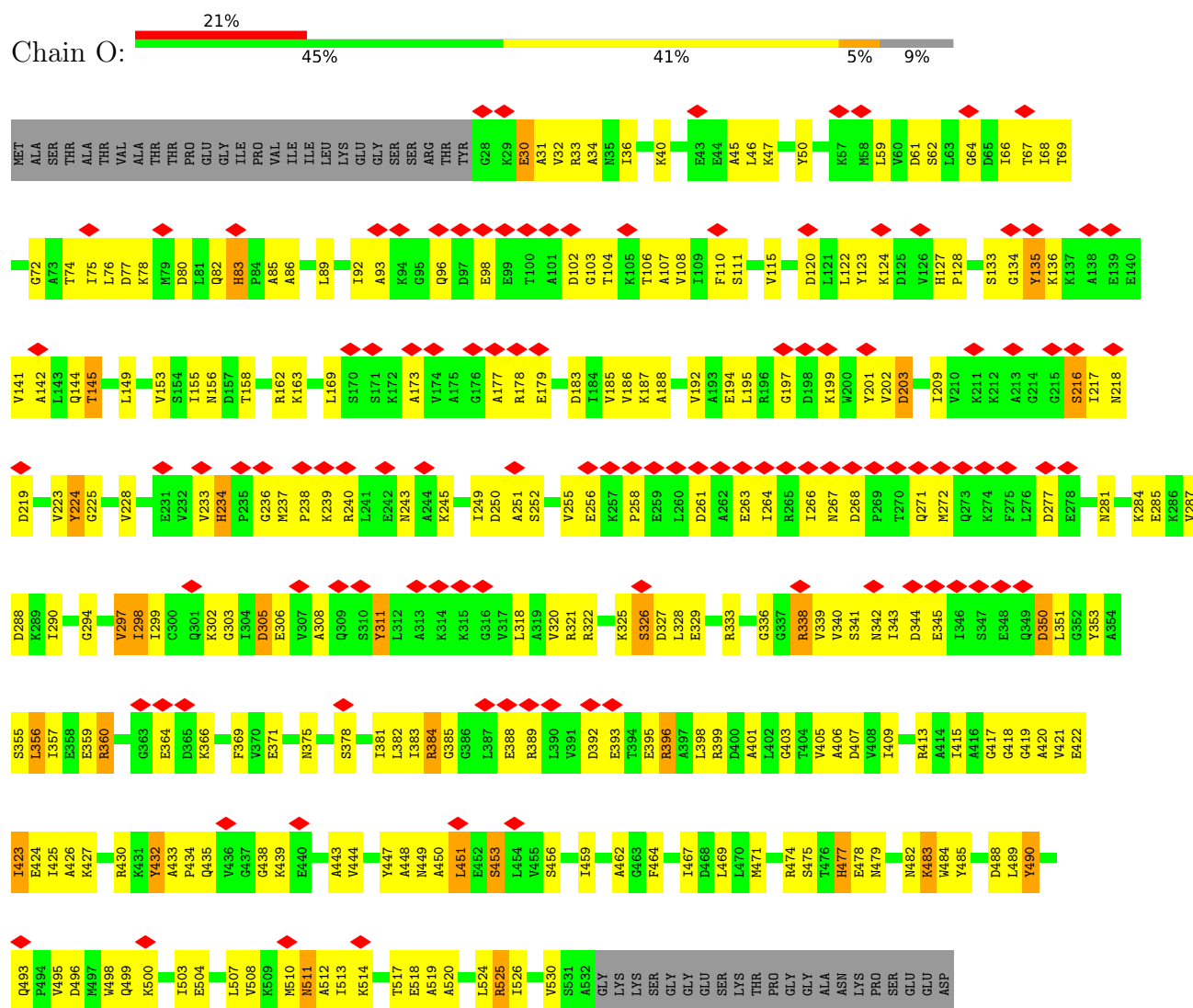




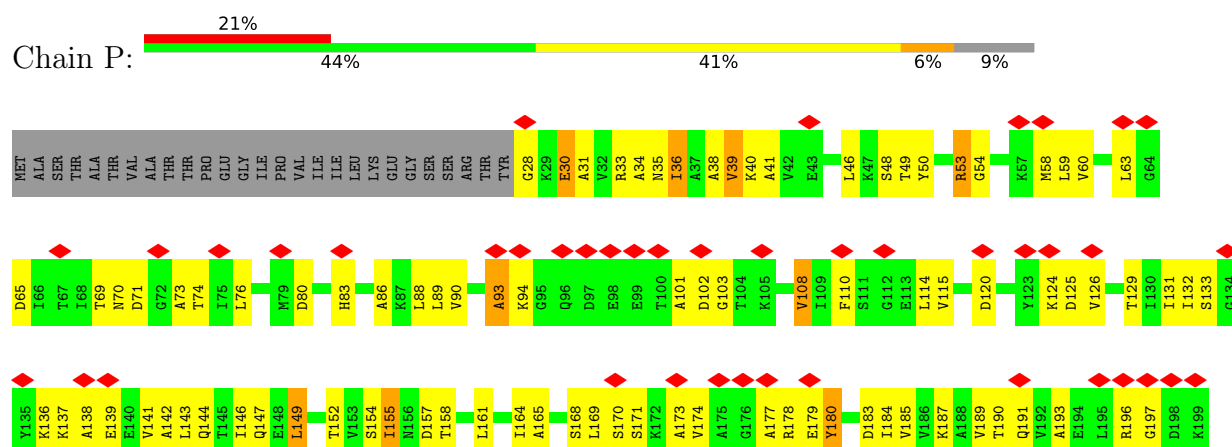
• Molecule 1: Chaperonin beta subunit

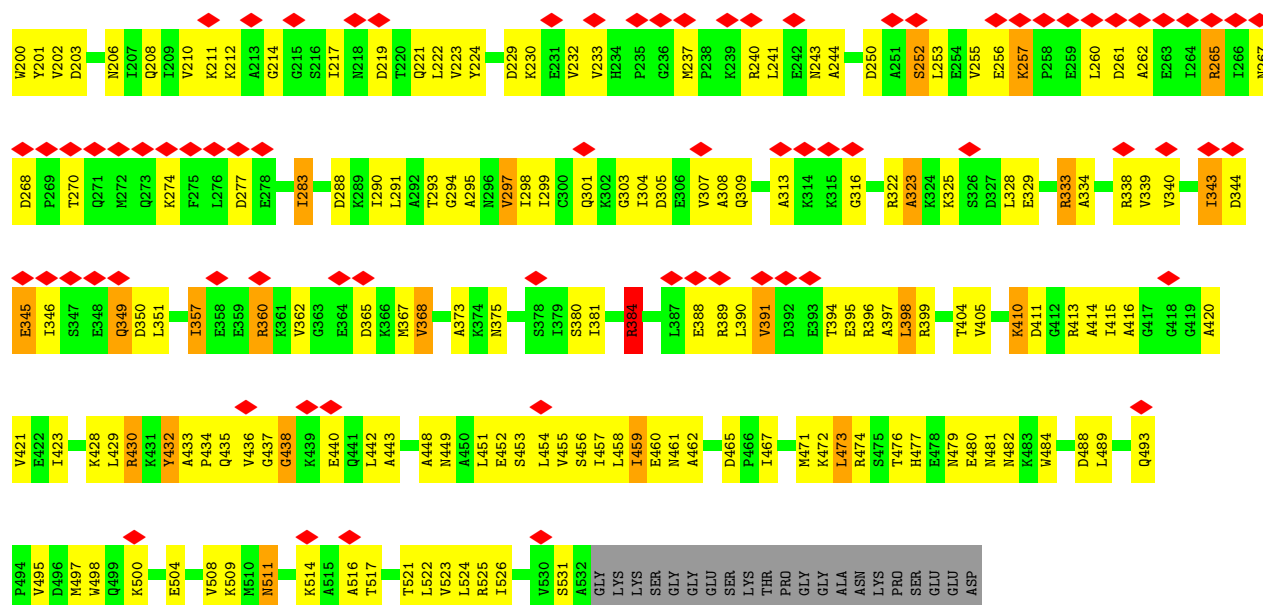


• Molecule 1: Chaperonin beta subunit

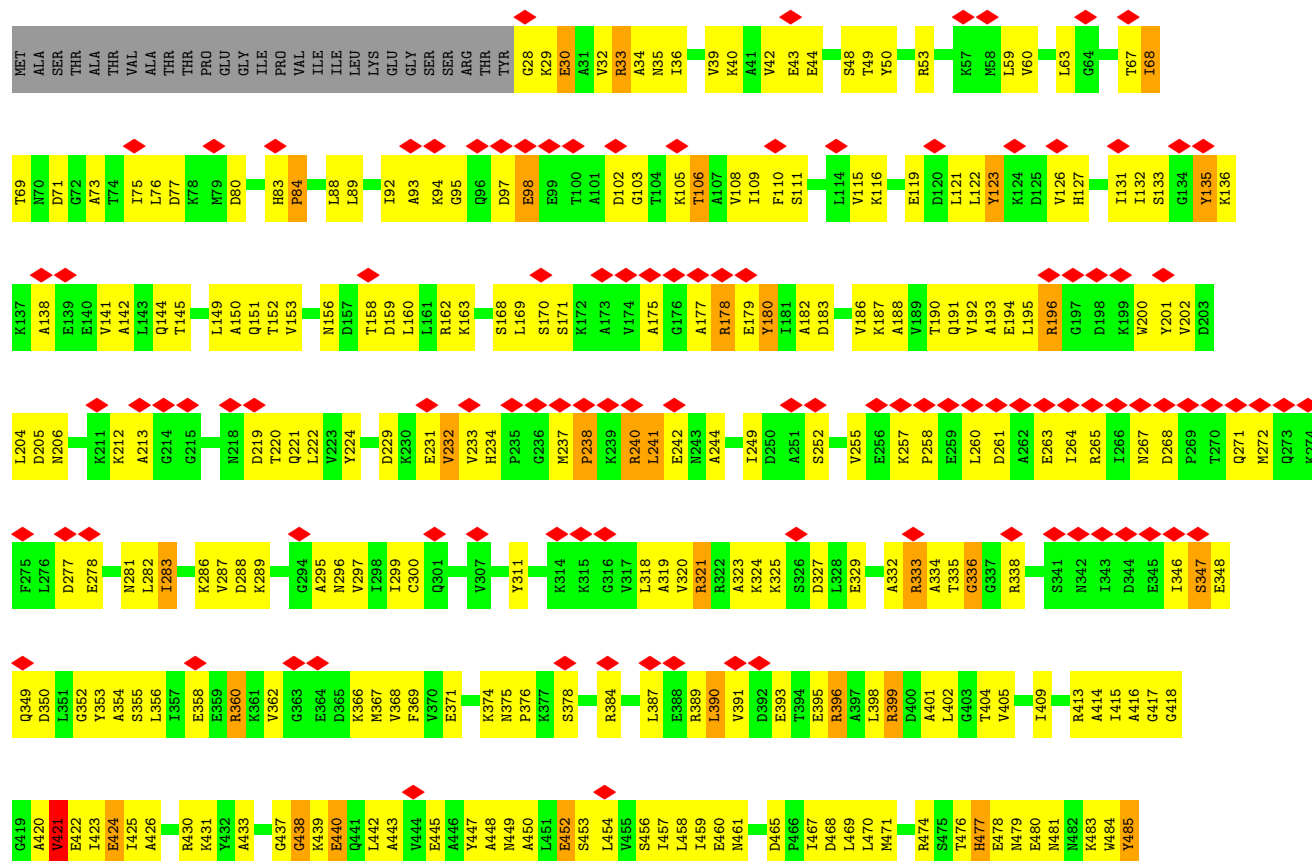


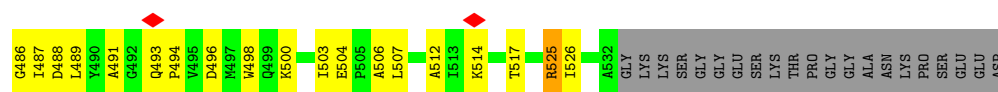
• Molecule 1: Chaperonin beta subunit



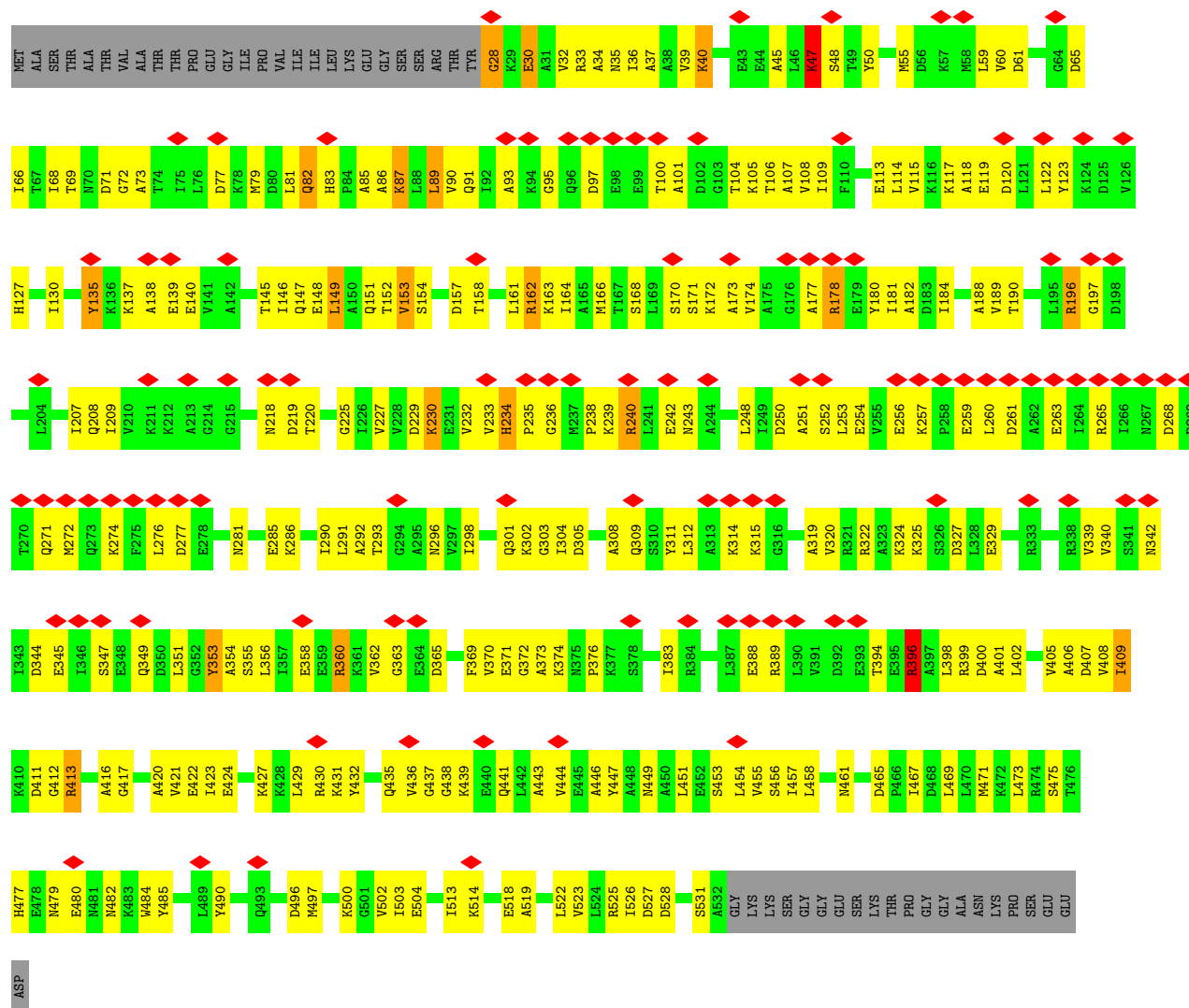
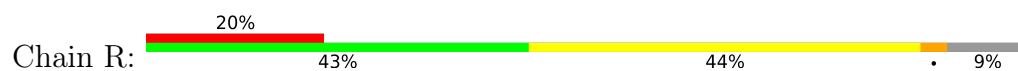


• Molecule 1: Chaperonin beta subunit

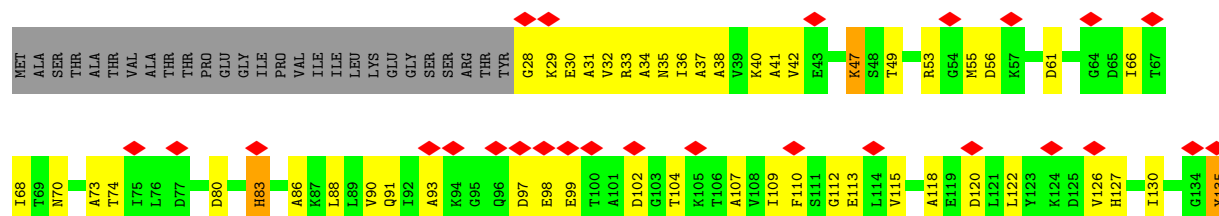




• Molecule 1: Chaperonin beta subunit



• Molecule 1: Chaperonin beta subunit



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| N511 | A512 | F513 | K514 | A515 | A516 | F517 | E518 | A519 | A520 | T521 | L522 | V523 |      | F526 | D527 | V529 | V530 | S531 | A532 | GLY  | LYS  | LYS  | SER  | GLY  | GLY  | GLU  | SER  | LYS  | THR  | PRO  | GLY  | GLY  | ALA  | ASN  | LYS  | PRO  | SER  | SER  | GLU  | GLU  | ASP  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| E424 | I425 | A426 | K427 | K428 | L429 | R430 |      | A433 | V436 | G437 | G438 | K439 |      | E440 | Q441 |      | V444 | Y447 |      | L451 | E452 | S453 | L454 | V455 | S456 | I457 | L458 | I459 | E460 | N461 |      | D468 | L469 | L470 | N471 |      | N481 | N482 | K483 | W484 |      | L489 | Y490 |      | Q493 | P494 | V495 | D496 |      | K500 | G501 | V502 | L503 | E504 |      | L507 | V508 |      |      |      |      |
| Q349 |      | G352 |      | S355 | L356 | I357 | E358 | E359 | R360 | K361 | V362 | G363 | E364 | D365 |      | V368 | F369 | V370 |      | K374 | N375 | P376 | K377 | S378 | I379 | S380 |      | R384 |      | L387 | E388 | R389 | L390 | V391 | D392 | E393 | T394 |      | R396 | A397 | L398 | R399 | D400 |      | V405 | A406 | D407 | V408 | I409 |      | R413 |      | A416 | G417 | G418 | A420 |      | I423 |      |      |      |
| M272 | Q273 | K274 | F275 | L276 | D277 | E278 |      | E279 | E280 | N281 |      | E285 | K286 | V287 |      | A292 | T293 | G294 |      | A296 | N296 | V297 | I298 | I299 | C300 | Q301 |      | D305 | E306 |      | Q309 | S310 | F311 | L312 | A313 | K314 | K315 | G316 |      | V320 | R321 | R322 | A323 | K324 | K325 | S326 | D327 |      | R333 |      | R338 | V339 | V340 | S341 | N342 | I343 | D344 | E345 | I346 | S347 | E348 |
| K211 | K212 | A213 | G214 | G215 | S216 | I217 | N218 | D219 | T220 | Q221 | L222 | V223 | Y224 | G225 | I226 |      | D229 | K230 |      | E231 | V232 | V233 | H234 | P235 | G236 | M237 | P238 | K239 | R240 | L241 | E242 | N243 | A244 | K245 | I246 | A247 | L248 | I249 | D250 | A251 | S252 | L253 | E254 | V255 | E256 | K257 | P258 | E259 | L260 | D261 | A262 | E263 | I264 | R265 | I266 | N267 | D268 | P269 | T270 | Q271 |      |
| A138 | E139 |      | A142 | L143 |      | I146 |      | L149 | A150 | Q151 | T152 | V153 | S154 | I155 | N156 | D157 | T158 |      | L161 | R162 | K163 |      | T167 | S168 | L169 | S170 | S171 | K172 | A173 | V174 | A175 | G176 | A177 | R178 | E179 | Y180 | I181 | D183 | I184 | V185 | V186 | K187 |      | V192 |      | L195 | R196 | G197 | D198 |      | Y201 |      | L204 |      | Q208 | I209 | V210 |      |      |      |      |

## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C9                       | Depositor |
| Number of particles used             | 28374                           | Depositor |
| Resolution determination method      | Not provided                    |           |
| 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 (4k x 4k)  | Depositor |
| Maximum map value                    | 17.418                          | Depositor |
| Minimum map value                    | -16.157                         | Depositor |
| Average map value                    | -0.139                          | Depositor |
| Map value standard deviation         | 1.599                           | Depositor |
| Recommended contour level            | 4                               | Depositor |
| Map size ( $\text{\AA}$ )            | 298.56, 298.56, 298.56          | wwPDB     |
| Map dimensions                       | 160, 160, 160                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.8659999, 1.8659999, 1.8659999 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                   | Bond angles |                   |
|-----|-------|--------------|-------------------|-------------|-------------------|
|     |       | RMSZ         | $\# Z  > 5$       | RMSZ        | $\# Z  > 5$       |
| 1   | A     | 2.14         | 110/3886 (2.8%)   | 2.49        | 256/5245 (4.9%)   |
| 1   | B     | 2.13         | 114/3886 (2.9%)   | 2.46        | 250/5245 (4.8%)   |
| 1   | C     | 2.19         | 125/3886 (3.2%)   | 2.48        | 279/5245 (5.3%)   |
| 1   | D     | 2.13         | 109/3886 (2.8%)   | 2.46        | 251/5245 (4.8%)   |
| 1   | E     | 2.14         | 119/3886 (3.1%)   | 2.44        | 261/5245 (5.0%)   |
| 1   | F     | 2.22         | 131/3886 (3.4%)   | 2.43        | 244/5245 (4.7%)   |
| 1   | G     | 2.15         | 118/3886 (3.0%)   | 2.46        | 253/5245 (4.8%)   |
| 1   | H     | 2.15         | 112/3886 (2.9%)   | 2.44        | 246/5245 (4.7%)   |
| 1   | I     | 2.21         | 125/3886 (3.2%)   | 2.45        | 240/5245 (4.6%)   |
| 1   | K     | 2.16         | 122/3886 (3.1%)   | 2.45        | 252/5245 (4.8%)   |
| 1   | L     | 2.12         | 96/3886 (2.5%)    | 2.55        | 294/5245 (5.6%)   |
| 1   | M     | 2.10         | 108/3886 (2.8%)   | 2.43        | 256/5245 (4.9%)   |
| 1   | N     | 2.16         | 120/3886 (3.1%)   | 2.47        | 269/5245 (5.1%)   |
| 1   | O     | 2.15         | 114/3886 (2.9%)   | 2.45        | 245/5245 (4.7%)   |
| 1   | P     | 2.11         | 108/3886 (2.8%)   | 2.50        | 268/5245 (5.1%)   |
| 1   | Q     | 2.14         | 95/3886 (2.4%)    | 2.51        | 297/5245 (5.7%)   |
| 1   | R     | 2.13         | 119/3886 (3.1%)   | 2.50        | 279/5245 (5.3%)   |
| 1   | S     | 2.14         | 107/3886 (2.8%)   | 2.46        | 254/5245 (4.8%)   |
| All | All   | 2.15         | 2052/69948 (2.9%) | 2.47        | 4694/94410 (5.0%) |

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                   | 9                   |
| 1   | B     | 0                   | 16                  |
| 1   | C     | 0                   | 15                  |
| 1   | D     | 0                   | 12                  |
| 1   | E     | 0                   | 7                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | F     | 0                   | 9                   |
| 1   | G     | 0                   | 14                  |
| 1   | H     | 0                   | 13                  |
| 1   | I     | 0                   | 12                  |
| 1   | K     | 0                   | 14                  |
| 1   | L     | 0                   | 13                  |
| 1   | M     | 0                   | 8                   |
| 1   | N     | 0                   | 6                   |
| 1   | O     | 0                   | 13                  |
| 1   | P     | 0                   | 10                  |
| 1   | Q     | 0                   | 17                  |
| 1   | R     | 0                   | 12                  |
| 1   | S     | 0                   | 7                   |
| All | All   | 0                   | 207                 |

All (2052) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 257 | LYS  | C-N     | 11.32  | 1.42        | 1.33     |
| 1   | K     | 234 | HIS  | CA-C    | -11.25 | 1.43        | 1.52     |
| 1   | D     | 95  | GLY  | CA-C    | -11.21 | 1.41        | 1.52     |
| 1   | H     | 504 | GLU  | N-CA    | -10.83 | 1.35        | 1.45     |
| 1   | C     | 502 | VAL  | CA-C    | 10.57  | 1.61        | 1.52     |
| 1   | L     | 234 | HIS  | ND1-CE1 | 10.27  | 1.42        | 1.32     |
| 1   | H     | 73  | ALA  | N-CA    | -10.08 | 1.34        | 1.46     |
| 1   | I     | 127 | HIS  | ND1-CE1 | 10.04  | 1.42        | 1.32     |
| 1   | O     | 287 | VAL  | CA-CB   | -9.98  | 1.42        | 1.54     |
| 1   | C     | 255 | VAL  | CA-C    | 9.97   | 1.65        | 1.52     |
| 1   | P     | 495 | VAL  | CA-C    | 9.95   | 1.63        | 1.52     |
| 1   | S     | 504 | GLU  | CA-C    | 9.87   | 1.62        | 1.52     |
| 1   | M     | 352 | GLY  | CA-C    | 9.87   | 1.62        | 1.52     |
| 1   | O     | 67  | THR  | CA-C    | -9.73  | 1.41        | 1.52     |
| 1   | D     | 199 | LYS  | CA-C    | -9.55  | 1.40        | 1.52     |
| 1   | D     | 414 | ALA  | CA-C    | 9.54   | 1.64        | 1.52     |
| 1   | G     | 352 | GLY  | CA-C    | -9.50  | 1.45        | 1.52     |
| 1   | M     | 346 | ILE  | CA-CB   | 9.49   | 1.64        | 1.54     |
| 1   | B     | 474 | ARG  | CD-NE   | 9.45   | 1.59        | 1.46     |
| 1   | K     | 74  | THR  | C-N     | 9.40   | 1.43        | 1.34     |
| 1   | S     | 384 | ARG  | CD-NE   | 9.31   | 1.59        | 1.46     |
| 1   | B     | 319 | ALA  | CA-C    | -9.28  | 1.41        | 1.52     |
| 1   | A     | 157 | ASP  | CA-CB   | 9.28   | 1.65        | 1.52     |
| 1   | A     | 81  | LEU  | CA-C    | -9.27  | 1.41        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 495 | VAL  | CA-C    | -9.21 | 1.43        | 1.52     |
| 1   | E     | 183 | ASP  | CA-C    | 9.17  | 1.64        | 1.52     |
| 1   | H     | 504 | GLU  | CA-C    | 9.16  | 1.61        | 1.52     |
| 1   | M     | 279 | GLU  | CA-C    | 9.16  | 1.65        | 1.52     |
| 1   | S     | 229 | ASP  | CA-CB   | 9.15  | 1.63        | 1.52     |
| 1   | E     | 329 | GLU  | CA-C    | 9.11  | 1.64        | 1.52     |
| 1   | H     | 284 | LYS  | CA-C    | 9.08  | 1.65        | 1.52     |
| 1   | N     | 126 | VAL  | CA-CB   | -9.01 | 1.43        | 1.54     |
| 1   | H     | 414 | ALA  | CA-C    | 8.99  | 1.63        | 1.52     |
| 1   | I     | 186 | VAL  | CA-CB   | -8.96 | 1.43        | 1.54     |
| 1   | B     | 114 | LEU  | CA-CB   | 8.94  | 1.67        | 1.53     |
| 1   | E     | 35  | ASN  | C-N     | 8.90  | 1.44        | 1.33     |
| 1   | I     | 148 | GLU  | CA-C    | 8.88  | 1.64        | 1.52     |
| 1   | G     | 361 | LYS  | CA-C    | 8.87  | 1.64        | 1.52     |
| 1   | B     | 194 | GLU  | CA-C    | 8.85  | 1.63        | 1.52     |
| 1   | C     | 92  | ILE  | CA-C    | 8.84  | 1.65        | 1.52     |
| 1   | O     | 484 | TRP  | N-CA    | -8.83 | 1.35        | 1.46     |
| 1   | B     | 134 | GLY  | CA-C    | 8.79  | 1.61        | 1.52     |
| 1   | O     | 89  | LEU  | CA-C    | -8.79 | 1.42        | 1.52     |
| 1   | S     | 507 | LEU  | C-N     | 8.76  | 1.44        | 1.33     |
| 1   | I     | 329 | GLU  | C-N     | 8.69  | 1.45        | 1.34     |
| 1   | S     | 300 | CYS  | CA-CB   | 8.67  | 1.66        | 1.53     |
| 1   | Q     | 83  | HIS  | ND1-CE1 | 8.66  | 1.41        | 1.32     |
| 1   | F     | 164 | ILE  | CA-C    | 8.66  | 1.63        | 1.52     |
| 1   | P     | 152 | THR  | CA-CB   | -8.64 | 1.42        | 1.53     |
| 1   | E     | 287 | VAL  | CA-CB   | -8.64 | 1.44        | 1.54     |
| 1   | Q     | 175 | ALA  | CA-C    | -8.63 | 1.40        | 1.52     |
| 1   | G     | 460 | GLU  | N-CA    | -8.61 | 1.36        | 1.46     |
| 1   | A     | 360 | ARG  | CD-NE   | 8.59  | 1.58        | 1.46     |
| 1   | P     | 93  | ALA  | CA-C    | -8.55 | 1.42        | 1.52     |
| 1   | K     | 261 | ASP  | CA-C    | 8.55  | 1.63        | 1.52     |
| 1   | S     | 437 | GLY  | CA-C    | -8.53 | 1.43        | 1.52     |
| 1   | Q     | 68  | ILE  | CA-CB   | -8.51 | 1.44        | 1.54     |
| 1   | N     | 494 | PRO  | N-CD    | -8.49 | 1.35        | 1.47     |
| 1   | G     | 196 | ARG  | CD-NE   | 8.49  | 1.58        | 1.46     |
| 1   | D     | 130 | ILE  | CA-CB   | -8.44 | 1.44        | 1.54     |
| 1   | E     | 140 | GLU  | N-CA    | -8.39 | 1.36        | 1.46     |
| 1   | A     | 39  | VAL  | CA-CB   | 8.39  | 1.63        | 1.54     |
| 1   | Q     | 169 | LEU  | CA-C    | -8.36 | 1.41        | 1.52     |
| 1   | C     | 105 | LYS  | N-CA    | -8.34 | 1.36        | 1.46     |
| 1   | E     | 293 | THR  | N-CA    | -8.34 | 1.35        | 1.46     |
| 1   | H     | 169 | LEU  | C-N     | 8.33  | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 127 | HIS  | ND1-CE1 | 8.31  | 1.40        | 1.32     |
| 1   | E     | 93  | ALA  | C-N     | 8.31  | 1.44        | 1.33     |
| 1   | C     | 93  | ALA  | N-CA    | 8.28  | 1.56        | 1.46     |
| 1   | N     | 41  | ALA  | C-N     | 8.28  | 1.44        | 1.33     |
| 1   | N     | 168 | SER  | CA-C    | 8.27  | 1.60        | 1.52     |
| 1   | P     | 484 | TRP  | N-CA    | -8.26 | 1.35        | 1.46     |
| 1   | F     | 449 | ASN  | C-N     | 8.25  | 1.44        | 1.33     |
| 1   | N     | 339 | VAL  | CA-CB   | -8.21 | 1.45        | 1.54     |
| 1   | Q     | 353 | TYR  | CA-C    | -8.20 | 1.42        | 1.52     |
| 1   | K     | 36  | ILE  | CA-CB   | -8.19 | 1.45        | 1.54     |
| 1   | A     | 444 | VAL  | CA-C    | 8.19  | 1.62        | 1.52     |
| 1   | I     | 246 | ILE  | CA-CB   | 8.19  | 1.62        | 1.54     |
| 1   | Q     | 442 | LEU  | CA-CB   | 8.19  | 1.66        | 1.53     |
| 1   | D     | 78  | LYS  | CA-C    | 8.18  | 1.64        | 1.52     |
| 1   | H     | 60  | VAL  | CA-CB   | 8.18  | 1.64        | 1.53     |
| 1   | N     | 497 | MET  | CA-C    | -8.17 | 1.42        | 1.52     |
| 1   | B     | 351 | LEU  | C-N     | 8.16  | 1.39        | 1.33     |
| 1   | R     | 479 | ASN  | CA-C    | -8.16 | 1.42        | 1.52     |
| 1   | P     | 308 | ALA  | C-N     | 8.15  | 1.44        | 1.33     |
| 1   | S     | 447 | TYR  | CA-CB   | 8.15  | 1.66        | 1.53     |
| 1   | N     | 246 | ILE  | CA-CB   | 8.12  | 1.62        | 1.54     |
| 1   | Q     | 450 | ALA  | CA-C    | 8.11  | 1.63        | 1.52     |
| 1   | F     | 508 | VAL  | CA-C    | 8.05  | 1.62        | 1.52     |
| 1   | M     | 178 | ARG  | C-N     | 8.05  | 1.44        | 1.33     |
| 1   | E     | 264 | ILE  | CA-C    | -8.04 | 1.44        | 1.53     |
| 1   | P     | 196 | ARG  | CA-C    | -8.04 | 1.42        | 1.53     |
| 1   | S     | 186 | VAL  | CA-CB   | -8.04 | 1.44        | 1.54     |
| 1   | H     | 242 | GLU  | CA-C    | 8.01  | 1.63        | 1.52     |
| 1   | H     | 342 | ASN  | CA-CB   | 8.01  | 1.63        | 1.53     |
| 1   | H     | 339 | VAL  | CA-C    | -7.99 | 1.43        | 1.52     |
| 1   | D     | 238 | PRO  | N-CA    | -7.97 | 1.37        | 1.47     |
| 1   | I     | 83  | HIS  | C-N     | -7.97 | 1.23        | 1.33     |
| 1   | S     | 127 | HIS  | ND1-CE1 | 7.97  | 1.40        | 1.32     |
| 1   | Q     | 194 | GLU  | CA-C    | 7.96  | 1.62        | 1.52     |
| 1   | K     | 497 | MET  | C-N     | 7.96  | 1.43        | 1.33     |
| 1   | D     | 94  | LYS  | CA-CB   | 7.94  | 1.65        | 1.53     |
| 1   | G     | 209 | ILE  | CA-CB   | 7.93  | 1.64        | 1.54     |
| 1   | D     | 423 | ILE  | CA-C    | 7.92  | 1.62        | 1.52     |
| 1   | E     | 256 | GLU  | CA-C    | -7.91 | 1.42        | 1.52     |
| 1   | R     | 502 | VAL  | CA-C    | 7.91  | 1.60        | 1.53     |
| 1   | O     | 255 | VAL  | CA-CB   | 7.90  | 1.63        | 1.54     |
| 1   | C     | 86  | ALA  | CA-C    | 7.89  | 1.63        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 517 | THR  | CA-CB | -7.88 | 1.41        | 1.53     |
| 1   | C     | 225 | GLY  | C-N   | 7.86  | 1.44        | 1.33     |
| 1   | F     | 223 | VAL  | CA-C  | -7.86 | 1.43        | 1.52     |
| 1   | C     | 508 | VAL  | CA-CB | -7.84 | 1.45        | 1.54     |
| 1   | A     | 530 | VAL  | CA-CB | -7.83 | 1.45        | 1.54     |
| 1   | I     | 266 | ILE  | CA-CB | 7.82  | 1.64        | 1.54     |
| 1   | B     | 115 | VAL  | CA-CB | -7.81 | 1.45        | 1.54     |
| 1   | B     | 342 | ASN  | CA-CB | 7.80  | 1.65        | 1.53     |
| 1   | F     | 166 | MET  | C-N   | 7.80  | 1.44        | 1.33     |
| 1   | F     | 320 | VAL  | C-O   | -7.79 | 1.16        | 1.24     |
| 1   | I     | 330 | LYS  | N-CA  | 7.78  | 1.56        | 1.46     |
| 1   | G     | 55  | MET  | C-N   | 7.78  | 1.44        | 1.33     |
| 1   | I     | 335 | THR  | CA-C  | -7.77 | 1.42        | 1.52     |
| 1   | C     | 187 | LYS  | CA-CB | 7.77  | 1.65        | 1.53     |
| 1   | I     | 265 | ARG  | NE-CZ | 7.77  | 1.41        | 1.33     |
| 1   | I     | 143 | LEU  | CA-C  | -7.76 | 1.43        | 1.52     |
| 1   | F     | 225 | GLY  | CA-C  | -7.73 | 1.41        | 1.52     |
| 1   | O     | 359 | GLU  | CA-C  | 7.72  | 1.61        | 1.52     |
| 1   | O     | 66  | ILE  | N-CA  | -7.71 | 1.37        | 1.46     |
| 1   | O     | 339 | VAL  | C-N   | 7.66  | 1.43        | 1.33     |
| 1   | Q     | 514 | LYS  | N-CA  | -7.66 | 1.37        | 1.46     |
| 1   | M     | 353 | TYR  | C-N   | 7.66  | 1.43        | 1.33     |
| 1   | Q     | 135 | TYR  | N-CA  | -7.66 | 1.37        | 1.46     |
| 1   | K     | 147 | GLN  | CA-CB | 7.65  | 1.65        | 1.53     |
| 1   | B     | 113 | GLU  | C-N   | 7.65  | 1.44        | 1.33     |
| 1   | A     | 460 | GLU  | N-CA  | 7.64  | 1.55        | 1.46     |
| 1   | A     | 440 | GLU  | CA-C  | 7.64  | 1.63        | 1.52     |
| 1   | S     | 436 | VAL  | C-N   | 7.63  | 1.41        | 1.32     |
| 1   | C     | 298 | ILE  | CA-CB | -7.63 | 1.44        | 1.54     |
| 1   | S     | 248 | LEU  | C-N   | 7.63  | 1.43        | 1.33     |
| 1   | N     | 504 | GLU  | CA-C  | 7.63  | 1.60        | 1.52     |
| 1   | D     | 433 | ALA  | CA-C  | 7.62  | 1.62        | 1.52     |
| 1   | N     | 460 | GLU  | CA-C  | 7.60  | 1.63        | 1.52     |
| 1   | Q     | 447 | TYR  | CA-C  | 7.59  | 1.62        | 1.52     |
| 1   | F     | 513 | ILE  | CA-CB | -7.59 | 1.45        | 1.54     |
| 1   | F     | 135 | TYR  | N-CA  | -7.59 | 1.37        | 1.46     |
| 1   | I     | 368 | VAL  | CA-C  | -7.58 | 1.43        | 1.52     |
| 1   | R     | 480 | GLU  | CA-C  | 7.58  | 1.63        | 1.52     |
| 1   | A     | 41  | ALA  | CA-CB | 7.58  | 1.65        | 1.53     |
| 1   | O     | 61  | ASP  | C-N   | 7.57  | 1.45        | 1.33     |
| 1   | C     | 518 | GLU  | CA-C  | -7.57 | 1.43        | 1.52     |
| 1   | B     | 281 | ASN  | CA-C  | -7.55 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 531 | SER  | CA-C    | -7.55 | 1.43        | 1.52     |
| 1   | M     | 426 | ALA  | C-N     | 7.54  | 1.43        | 1.33     |
| 1   | D     | 302 | LYS  | CA-CB   | 7.54  | 1.64        | 1.53     |
| 1   | E     | 390 | LEU  | CA-CB   | 7.53  | 1.65        | 1.53     |
| 1   | K     | 364 | GLU  | CA-CB   | 7.53  | 1.65        | 1.53     |
| 1   | P     | 237 | MET  | CA-C    | -7.50 | 1.44        | 1.53     |
| 1   | G     | 200 | TRP  | NE1-CE2 | 7.50  | 1.45        | 1.37     |
| 1   | N     | 526 | ILE  | CA-C    | -7.50 | 1.44        | 1.53     |
| 1   | S     | 180 | TYR  | N-CA    | 7.50  | 1.55        | 1.46     |
| 1   | F     | 503 | ILE  | C-N     | 7.49  | 1.41        | 1.33     |
| 1   | A     | 115 | VAL  | C-O     | 7.49  | 1.32        | 1.24     |
| 1   | F     | 493 | GLN  | CA-CB   | 7.48  | 1.65        | 1.53     |
| 1   | Q     | 28  | GLY  | N-CA    | 7.48  | 1.57        | 1.45     |
| 1   | C     | 141 | VAL  | C-N     | 7.48  | 1.43        | 1.33     |
| 1   | N     | 260 | LEU  | CA-C    | -7.47 | 1.43        | 1.52     |
| 1   | S     | 216 | SER  | C-N     | 7.46  | 1.42        | 1.34     |
| 1   | Q     | 110 | PHE  | C-N     | 7.46  | 1.43        | 1.33     |
| 1   | E     | 136 | LYS  | CA-CB   | 7.45  | 1.65        | 1.53     |
| 1   | B     | 177 | ALA  | CA-C    | 7.45  | 1.61        | 1.53     |
| 1   | P     | 465 | ASP  | CA-C    | 7.44  | 1.62        | 1.52     |
| 1   | K     | 240 | ARG  | CA-C    | -7.43 | 1.43        | 1.52     |
| 1   | N     | 226 | ILE  | C-N     | 7.43  | 1.42        | 1.33     |
| 1   | M     | 360 | ARG  | CD-NE   | 7.43  | 1.56        | 1.46     |
| 1   | O     | 513 | ILE  | CA-C    | 7.43  | 1.62        | 1.52     |
| 1   | F     | 224 | TYR  | CA-C    | -7.43 | 1.44        | 1.53     |
| 1   | O     | 228 | VAL  | CA-C    | 7.42  | 1.62        | 1.52     |
| 1   | H     | 429 | LEU  | CA-C    | -7.42 | 1.43        | 1.52     |
| 1   | L     | 64  | GLY  | C-N     | 7.42  | 1.43        | 1.33     |
| 1   | G     | 232 | VAL  | N-CA    | 7.41  | 1.55        | 1.46     |
| 1   | C     | 381 | ILE  | N-CA    | -7.41 | 1.37        | 1.46     |
| 1   | M     | 257 | LYS  | CA-CB   | 7.41  | 1.65        | 1.53     |
| 1   | L     | 458 | LEU  | CA-CB   | 7.40  | 1.64        | 1.53     |
| 1   | B     | 391 | VAL  | CA-CB   | -7.39 | 1.45        | 1.54     |
| 1   | C     | 162 | ARG  | CD-NE   | 7.38  | 1.56        | 1.46     |
| 1   | R     | 182 | ALA  | C-N     | 7.38  | 1.43        | 1.33     |
| 1   | O     | 435 | GLN  | C-N     | 7.37  | 1.43        | 1.33     |
| 1   | R     | 399 | ARG  | CD-NE   | 7.37  | 1.56        | 1.46     |
| 1   | L     | 147 | GLN  | CA-C    | 7.36  | 1.61        | 1.52     |
| 1   | H     | 216 | SER  | CA-C    | 7.35  | 1.62        | 1.52     |
| 1   | R     | 441 | GLN  | C-N     | 7.34  | 1.43        | 1.33     |
| 1   | R     | 39  | VAL  | C-N     | 7.34  | 1.43        | 1.33     |
| 1   | O     | 240 | ARG  | CD-NE   | 7.34  | 1.56        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | R     | 277 | ASP  | CA-C    | 7.33  | 1.61        | 1.52     |
| 1   | K     | 136 | LYS  | CA-CB   | 7.33  | 1.64        | 1.53     |
| 1   | I     | 33  | ARG  | CA-CB   | 7.31  | 1.64        | 1.53     |
| 1   | I     | 348 | GLU  | CA-C    | 7.31  | 1.62        | 1.52     |
| 1   | F     | 113 | GLU  | CA-C    | -7.31 | 1.43        | 1.52     |
| 1   | S     | 234 | HIS  | CA-C    | 7.30  | 1.60        | 1.52     |
| 1   | N     | 245 | LYS  | CA-C    | -7.30 | 1.44        | 1.53     |
| 1   | P     | 142 | ALA  | CA-C    | -7.30 | 1.42        | 1.52     |
| 1   | N     | 287 | VAL  | N-CA    | 7.29  | 1.55        | 1.46     |
| 1   | F     | 83  | HIS  | CE1-NE2 | 7.29  | 1.39        | 1.32     |
| 1   | F     | 496 | ASP  | CA-CB   | 7.29  | 1.62        | 1.53     |
| 1   | S     | 143 | LEU  | N-CA    | -7.29 | 1.37        | 1.46     |
| 1   | D     | 213 | ALA  | N-CA    | -7.28 | 1.36        | 1.45     |
| 1   | C     | 137 | LYS  | N-CA    | -7.28 | 1.37        | 1.46     |
| 1   | F     | 238 | PRO  | N-CA    | 7.28  | 1.56        | 1.47     |
| 1   | A     | 165 | ALA  | CA-C    | 7.27  | 1.61        | 1.52     |
| 1   | F     | 86  | ALA  | CA-C    | 7.27  | 1.62        | 1.52     |
| 1   | C     | 233 | VAL  | CA-CB   | -7.26 | 1.44        | 1.54     |
| 1   | K     | 399 | ARG  | CA-C    | -7.26 | 1.43        | 1.52     |
| 1   | K     | 145 | THR  | C-N     | 7.26  | 1.42        | 1.33     |
| 1   | F     | 35  | ASN  | C-N     | 7.25  | 1.42        | 1.33     |
| 1   | E     | 199 | LYS  | N-CA    | -7.24 | 1.36        | 1.45     |
| 1   | P     | 396 | ARG  | C-N     | -7.24 | 1.24        | 1.33     |
| 1   | E     | 151 | GLN  | CA-C    | 7.24  | 1.61        | 1.52     |
| 1   | O     | 82  | GLN  | CA-CB   | 7.24  | 1.64        | 1.53     |
| 1   | E     | 522 | LEU  | C-N     | 7.23  | 1.43        | 1.33     |
| 1   | P     | 381 | ILE  | CA-C    | 7.23  | 1.61        | 1.52     |
| 1   | H     | 337 | GLY  | CA-C    | 7.23  | 1.61        | 1.51     |
| 1   | K     | 130 | ILE  | C-N     | 7.22  | 1.42        | 1.34     |
| 1   | O     | 124 | LYS  | CA-C    | 7.22  | 1.62        | 1.52     |
| 1   | C     | 153 | VAL  | CA-CB   | 7.21  | 1.63        | 1.54     |
| 1   | I     | 283 | ILE  | C-N     | 7.21  | 1.43        | 1.34     |
| 1   | L     | 528 | ASP  | CA-C    | -7.20 | 1.43        | 1.52     |
| 1   | D     | 101 | ALA  | CA-CB   | 7.20  | 1.62        | 1.53     |
| 1   | S     | 280 | GLU  | CA-CB   | 7.20  | 1.65        | 1.53     |
| 1   | L     | 340 | VAL  | CA-CB   | 7.19  | 1.62        | 1.53     |
| 1   | Q     | 123 | TYR  | N-CA    | -7.19 | 1.37        | 1.46     |
| 1   | P     | 158 | THR  | CA-C    | -7.19 | 1.43        | 1.52     |
| 1   | Q     | 80  | ASP  | CA-C    | -7.19 | 1.44        | 1.52     |
| 1   | I     | 353 | TYR  | N-CA    | -7.18 | 1.37        | 1.45     |
| 1   | Q     | 234 | HIS  | CE1-NE2 | 7.18  | 1.39        | 1.32     |
| 1   | P     | 297 | VAL  | N-CA    | -7.17 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 270 | THR  | C-N     | 7.17  | 1.43        | 1.33     |
| 1   | N     | 154 | SER  | C-O     | -7.17 | 1.18        | 1.24     |
| 1   | D     | 183 | ASP  | CA-C    | 7.16  | 1.61        | 1.52     |
| 1   | I     | 127 | HIS  | C-N     | 7.15  | 1.42        | 1.33     |
| 1   | O     | 478 | GLU  | CA-C    | 7.15  | 1.61        | 1.52     |
| 1   | E     | 50  | TYR  | CA-C    | 7.14  | 1.62        | 1.52     |
| 1   | M     | 317 | VAL  | CA-C    | -7.14 | 1.44        | 1.53     |
| 1   | L     | 360 | ARG  | CD-NE   | 7.14  | 1.56        | 1.46     |
| 1   | D     | 186 | VAL  | N-CA    | -7.14 | 1.38        | 1.46     |
| 1   | C     | 497 | MET  | C-O     | -7.13 | 1.15        | 1.24     |
| 1   | O     | 267 | ASN  | N-CA    | -7.12 | 1.37        | 1.46     |
| 1   | O     | 499 | GLN  | CA-C    | 7.12  | 1.62        | 1.52     |
| 1   | H     | 322 | ARG  | CD-NE   | 7.12  | 1.56        | 1.46     |
| 1   | K     | 393 | GLU  | CA-C    | 7.12  | 1.62        | 1.52     |
| 1   | H     | 494 | PRO  | CA-CB   | -7.12 | 1.44        | 1.53     |
| 1   | D     | 431 | LYS  | N-CA    | -7.11 | 1.37        | 1.46     |
| 1   | E     | 496 | ASP  | N-CA    | -7.10 | 1.37        | 1.46     |
| 1   | D     | 286 | LYS  | CA-CB   | 7.10  | 1.64        | 1.53     |
| 1   | O     | 409 | ILE  | CA-C    | -7.10 | 1.44        | 1.52     |
| 1   | M     | 200 | TRP  | NE1-CE2 | 7.10  | 1.45        | 1.37     |
| 1   | I     | 120 | ASP  | CA-C    | 7.09  | 1.62        | 1.52     |
| 1   | R     | 45  | ALA  | C-N     | 7.08  | 1.43        | 1.33     |
| 1   | F     | 437 | GLY  | N-CA    | 7.08  | 1.51        | 1.45     |
| 1   | N     | 53  | ARG  | C-N     | 7.08  | 1.43        | 1.33     |
| 1   | Q     | 461 | ASN  | CA-C    | 7.06  | 1.62        | 1.52     |
| 1   | M     | 487 | ILE  | CA-C    | -7.06 | 1.43        | 1.52     |
| 1   | G     | 127 | HIS  | ND1-CE1 | 7.05  | 1.39        | 1.32     |
| 1   | N     | 396 | ARG  | CA-CB   | 7.05  | 1.64        | 1.53     |
| 1   | N     | 465 | ASP  | CA-C    | 7.05  | 1.60        | 1.52     |
| 1   | P     | 178 | ARG  | CD-NE   | 7.05  | 1.56        | 1.46     |
| 1   | E     | 444 | VAL  | C-N     | 7.04  | 1.43        | 1.33     |
| 1   | C     | 389 | ARG  | CA-CB   | 7.04  | 1.64        | 1.53     |
| 1   | L     | 527 | ASP  | CA-C    | 7.03  | 1.62        | 1.52     |
| 1   | G     | 55  | MET  | N-CA    | -7.03 | 1.37        | 1.45     |
| 1   | K     | 526 | ILE  | N-CA    | -7.03 | 1.37        | 1.46     |
| 1   | N     | 63  | LEU  | N-CA    | -7.03 | 1.36        | 1.46     |
| 1   | I     | 327 | ASP  | CA-C    | -7.02 | 1.43        | 1.52     |
| 1   | F     | 378 | SER  | CA-CB   | 7.02  | 1.61        | 1.53     |
| 1   | R     | 190 | THR  | CA-C    | 7.01  | 1.62        | 1.52     |
| 1   | G     | 279 | GLU  | N-CA    | 7.01  | 1.55        | 1.46     |
| 1   | G     | 332 | ALA  | CA-C    | -7.01 | 1.43        | 1.52     |
| 1   | B     | 396 | ARG  | CA-C    | 7.00  | 1.61        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | Q     | 333 | ARG  | NE-CZ   | 7.00  | 1.40        | 1.33     |
| 1   | I     | 131 | ILE  | C-N     | 7.00  | 1.42        | 1.33     |
| 1   | I     | 171 | SER  | C-N     | 7.00  | 1.42        | 1.33     |
| 1   | K     | 471 | MET  | N-CA    | -7.00 | 1.38        | 1.46     |
| 1   | I     | 257 | LYS  | C-N     | 7.00  | 1.40        | 1.33     |
| 1   | F     | 242 | GLU  | CA-CB   | 6.99  | 1.63        | 1.53     |
| 1   | O     | 504 | GLU  | N-CA    | 6.99  | 1.54        | 1.45     |
| 1   | H     | 383 | ILE  | CA-CB   | -6.99 | 1.45        | 1.54     |
| 1   | Q     | 150 | ALA  | CA-C    | 6.99  | 1.62        | 1.52     |
| 1   | K     | 70  | ASN  | C-N     | 6.98  | 1.43        | 1.33     |
| 1   | I     | 392 | ASP  | N-CA    | -6.98 | 1.38        | 1.46     |
| 1   | K     | 327 | ASP  | C-N     | 6.98  | 1.42        | 1.33     |
| 1   | O     | 333 | ARG  | NE-CZ   | 6.97  | 1.40        | 1.33     |
| 1   | R     | 304 | ILE  | N-CA    | 6.97  | 1.55        | 1.46     |
| 1   | C     | 453 | SER  | CA-CB   | 6.97  | 1.64        | 1.53     |
| 1   | N     | 301 | GLN  | N-CA    | -6.96 | 1.36        | 1.46     |
| 1   | D     | 164 | ILE  | CA-C    | 6.96  | 1.61        | 1.52     |
| 1   | N     | 284 | LYS  | C-N     | 6.96  | 1.43        | 1.33     |
| 1   | R     | 127 | HIS  | ND1-CE1 | 6.96  | 1.39        | 1.32     |
| 1   | S     | 268 | ASP  | CA-C    | 6.96  | 1.60        | 1.52     |
| 1   | A     | 273 | GLN  | C-N     | 6.96  | 1.43        | 1.33     |
| 1   | C     | 289 | LYS  | C-N     | 6.95  | 1.42        | 1.33     |
| 1   | H     | 277 | ASP  | CA-CB   | 6.95  | 1.64        | 1.53     |
| 1   | M     | 154 | SER  | CA-C    | -6.95 | 1.44        | 1.52     |
| 1   | F     | 248 | LEU  | CA-C    | 6.95  | 1.62        | 1.52     |
| 1   | H     | 130 | ILE  | CA-CB   | -6.95 | 1.46        | 1.54     |
| 1   | P     | 524 | LEU  | CA-C    | -6.94 | 1.43        | 1.52     |
| 1   | G     | 189 | VAL  | CA-CB   | 6.94  | 1.63        | 1.54     |
| 1   | D     | 287 | VAL  | CA-C    | 6.93  | 1.61        | 1.52     |
| 1   | Q     | 334 | ALA  | CA-C    | -6.92 | 1.43        | 1.52     |
| 1   | N     | 58  | MET  | CA-CB   | 6.92  | 1.64        | 1.53     |
| 1   | Q     | 268 | ASP  | CA-C    | 6.92  | 1.61        | 1.52     |
| 1   | A     | 37  | ALA  | C-N     | 6.91  | 1.42        | 1.33     |
| 1   | M     | 304 | ILE  | C-N     | 6.91  | 1.42        | 1.33     |
| 1   | S     | 142 | ALA  | N-CA    | 6.90  | 1.54        | 1.46     |
| 1   | I     | 442 | LEU  | C-N     | 6.90  | 1.42        | 1.33     |
| 1   | I     | 431 | LYS  | CA-C    | 6.90  | 1.62        | 1.52     |
| 1   | A     | 213 | ALA  | C-N     | 6.89  | 1.42        | 1.33     |
| 1   | E     | 318 | LEU  | C-N     | 6.89  | 1.43        | 1.33     |
| 1   | L     | 46  | LEU  | CA-C    | 6.89  | 1.61        | 1.52     |
| 1   | A     | 396 | ARG  | CA-CB   | 6.88  | 1.64        | 1.53     |
| 1   | R     | 374 | LYS  | CA-C    | -6.88 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 241 | LEU  | N-CA    | 6.88  | 1.54        | 1.46     |
| 1   | D     | 207 | ILE  | C-O     | -6.87 | 1.16        | 1.24     |
| 1   | C     | 243 | ASN  | N-CA    | -6.87 | 1.37        | 1.46     |
| 1   | G     | 178 | ARG  | CD-NE   | 6.87  | 1.55        | 1.46     |
| 1   | Q     | 526 | ILE  | C-N     | 6.87  | 1.42        | 1.33     |
| 1   | P     | 467 | ILE  | CA-CB   | -6.86 | 1.46        | 1.54     |
| 1   | B     | 356 | LEU  | N-CA    | -6.86 | 1.38        | 1.46     |
| 1   | K     | 361 | LYS  | C-N     | 6.86  | 1.41        | 1.33     |
| 1   | D     | 520 | ALA  | CA-C    | -6.86 | 1.43        | 1.52     |
| 1   | M     | 234 | HIS  | ND1-CE1 | 6.86  | 1.39        | 1.32     |
| 1   | M     | 208 | GLN  | N-CA    | -6.86 | 1.37        | 1.45     |
| 1   | I     | 96  | GLN  | N-CA    | 6.85  | 1.54        | 1.46     |
| 1   | M     | 223 | VAL  | CA-C    | -6.85 | 1.44        | 1.52     |
| 1   | G     | 430 | ARG  | CD-NE   | 6.85  | 1.55        | 1.46     |
| 1   | A     | 346 | ILE  | CA-C    | 6.84  | 1.60        | 1.52     |
| 1   | D     | 189 | VAL  | CA-CB   | -6.84 | 1.45        | 1.54     |
| 1   | S     | 483 | LYS  | CA-CB   | 6.84  | 1.64        | 1.53     |
| 1   | L     | 474 | ARG  | CD-NE   | 6.84  | 1.55        | 1.46     |
| 1   | L     | 178 | ARG  | CA-CB   | 6.83  | 1.64        | 1.53     |
| 1   | F     | 240 | ARG  | CD-NE   | 6.83  | 1.55        | 1.46     |
| 1   | I     | 97  | ASP  | CA-C    | -6.83 | 1.44        | 1.52     |
| 1   | R     | 469 | LEU  | CA-C    | -6.83 | 1.44        | 1.52     |
| 1   | D     | 265 | ARG  | CD-NE   | 6.83  | 1.55        | 1.46     |
| 1   | M     | 164 | ILE  | CA-C    | 6.82  | 1.61        | 1.52     |
| 1   | L     | 420 | ALA  | CA-C    | 6.82  | 1.61        | 1.52     |
| 1   | Q     | 220 | THR  | N-CA    | 6.82  | 1.54        | 1.46     |
| 1   | H     | 172 | LYS  | C-N     | 6.82  | 1.42        | 1.33     |
| 1   | N     | 83  | HIS  | ND1-CE1 | 6.82  | 1.39        | 1.32     |
| 1   | C     | 375 | ASN  | C-N     | 6.81  | 1.41        | 1.34     |
| 1   | I     | 371 | GLU  | CA-C    | -6.80 | 1.44        | 1.52     |
| 1   | A     | 516 | ALA  | C-N     | 6.80  | 1.43        | 1.34     |
| 1   | G     | 511 | ASN  | C-N     | 6.80  | 1.42        | 1.33     |
| 1   | L     | 184 | ILE  | CA-CB   | 6.80  | 1.62        | 1.54     |
| 1   | N     | 469 | LEU  | CA-C    | -6.80 | 1.44        | 1.52     |
| 1   | K     | 392 | ASP  | CA-CB   | 6.79  | 1.63        | 1.53     |
| 1   | P     | 36  | ILE  | CA-C    | -6.79 | 1.45        | 1.52     |
| 1   | A     | 286 | LYS  | CA-CB   | 6.78  | 1.63        | 1.53     |
| 1   | L     | 525 | ARG  | C-N     | 6.78  | 1.40        | 1.33     |
| 1   | E     | 361 | LYS  | CA-C    | -6.77 | 1.44        | 1.52     |
| 1   | Q     | 111 | SER  | CA-C    | -6.77 | 1.44        | 1.52     |
| 1   | R     | 81  | LEU  | CA-CB   | 6.77  | 1.61        | 1.53     |
| 1   | N     | 243 | ASN  | C-N     | 6.77  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | H     | 42  | VAL  | N-CA  | 6.76  | 1.54        | 1.46     |
| 1   | K     | 196 | ARG  | CD-NE | 6.76  | 1.55        | 1.46     |
| 1   | P     | 479 | ASN  | CA-C  | 6.76  | 1.61        | 1.52     |
| 1   | A     | 495 | VAL  | CA-C  | -6.76 | 1.45        | 1.52     |
| 1   | K     | 191 | GLN  | C-N   | 6.76  | 1.42        | 1.33     |
| 1   | M     | 345 | GLU  | C-N   | 6.76  | 1.42        | 1.33     |
| 1   | O     | 111 | SER  | C-N   | 6.76  | 1.43        | 1.33     |
| 1   | M     | 211 | LYS  | CA-C  | -6.75 | 1.44        | 1.52     |
| 1   | A     | 528 | ASP  | N-CA  | 6.74  | 1.54        | 1.45     |
| 1   | E     | 79  | MET  | C-N   | 6.74  | 1.43        | 1.34     |
| 1   | K     | 435 | GLN  | N-CA  | -6.74 | 1.37        | 1.46     |
| 1   | D     | 131 | ILE  | N-CA  | 6.73  | 1.54        | 1.46     |
| 1   | I     | 297 | VAL  | CA-C  | -6.73 | 1.44        | 1.52     |
| 1   | L     | 33  | ARG  | NE-CZ | 6.73  | 1.40        | 1.33     |
| 1   | G     | 53  | ARG  | NE-CZ | 6.72  | 1.40        | 1.33     |
| 1   | B     | 266 | ILE  | CA-C  | 6.72  | 1.60        | 1.52     |
| 1   | E     | 225 | GLY  | N-CA  | 6.72  | 1.53        | 1.45     |
| 1   | F     | 342 | ASN  | N-CA  | -6.72 | 1.38        | 1.46     |
| 1   | S     | 74  | THR  | C-N   | 6.72  | 1.41        | 1.34     |
| 1   | B     | 228 | VAL  | N-CA  | -6.71 | 1.38        | 1.46     |
| 1   | R     | 324 | LYS  | CA-CB | 6.71  | 1.62        | 1.53     |
| 1   | G     | 150 | ALA  | CA-C  | 6.71  | 1.61        | 1.52     |
| 1   | K     | 430 | ARG  | CD-NE | 6.71  | 1.55        | 1.46     |
| 1   | M     | 474 | ARG  | CD-NE | 6.71  | 1.55        | 1.46     |
| 1   | B     | 321 | ARG  | CA-C  | 6.70  | 1.60        | 1.52     |
| 1   | C     | 331 | LEU  | CA-C  | 6.70  | 1.61        | 1.52     |
| 1   | Q     | 423 | ILE  | N-CA  | 6.70  | 1.54        | 1.46     |
| 1   | K     | 71  | ASP  | N-CA  | -6.69 | 1.38        | 1.46     |
| 1   | G     | 525 | ARG  | CD-NE | 6.69  | 1.55        | 1.46     |
| 1   | G     | 232 | VAL  | C-N   | -6.68 | 1.25        | 1.33     |
| 1   | S     | 31  | ALA  | N-CA  | 6.68  | 1.54        | 1.46     |
| 1   | C     | 513 | ILE  | CA-C  | 6.68  | 1.60        | 1.52     |
| 1   | C     | 187 | LYS  | CA-C  | 6.68  | 1.61        | 1.52     |
| 1   | D     | 241 | LEU  | CA-C  | -6.68 | 1.44        | 1.52     |
| 1   | F     | 530 | VAL  | C-N   | 6.68  | 1.42        | 1.33     |
| 1   | Q     | 459 | ILE  | CA-C  | -6.67 | 1.44        | 1.52     |
| 1   | A     | 74  | THR  | C-N   | 6.67  | 1.41        | 1.34     |
| 1   | I     | 458 | LEU  | CA-C  | 6.67  | 1.61        | 1.52     |
| 1   | S     | 220 | THR  | CA-CB | -6.67 | 1.43        | 1.53     |
| 1   | I     | 265 | ARG  | CD-NE | 6.66  | 1.55        | 1.46     |
| 1   | Q     | 349 | GLN  | CA-C  | 6.66  | 1.61        | 1.52     |
| 1   | G     | 315 | LYS  | C-N   | 6.65  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 135 | TYR  | CA-C  | 6.65  | 1.61        | 1.52     |
| 1   | K     | 33  | ARG  | CD-NE | 6.65  | 1.55        | 1.46     |
| 1   | O     | 284 | LYS  | CA-C  | 6.65  | 1.61        | 1.52     |
| 1   | R     | 525 | ARG  | CD-NE | 6.65  | 1.55        | 1.46     |
| 1   | G     | 528 | ASP  | CA-C  | -6.65 | 1.44        | 1.52     |
| 1   | B     | 136 | LYS  | C-N   | 6.64  | 1.42        | 1.33     |
| 1   | F     | 168 | SER  | CA-C  | 6.64  | 1.59        | 1.52     |
| 1   | L     | 265 | ARG  | CD-NE | 6.64  | 1.55        | 1.46     |
| 1   | S     | 253 | LEU  | N-CA  | -6.64 | 1.39        | 1.46     |
| 1   | S     | 326 | SER  | CA-CB | 6.64  | 1.63        | 1.53     |
| 1   | L     | 234 | HIS  | CB-CG | 6.64  | 1.59        | 1.50     |
| 1   | O     | 328 | LEU  | C-N   | 6.64  | 1.42        | 1.33     |
| 1   | E     | 396 | ARG  | N-CA  | -6.63 | 1.38        | 1.46     |
| 1   | O     | 136 | LYS  | C-N   | 6.63  | 1.42        | 1.33     |
| 1   | C     | 504 | GLU  | CA-CB | 6.63  | 1.63        | 1.54     |
| 1   | D     | 157 | ASP  | CA-CB | 6.62  | 1.61        | 1.52     |
| 1   | M     | 467 | ILE  | CA-CB | -6.62 | 1.46        | 1.54     |
| 1   | E     | 182 | ALA  | CA-C  | -6.62 | 1.44        | 1.52     |
| 1   | O     | 268 | ASP  | C-N   | -6.62 | 1.25        | 1.34     |
| 1   | H     | 462 | ALA  | CA-C  | -6.62 | 1.43        | 1.52     |
| 1   | I     | 142 | ALA  | CA-C  | 6.62  | 1.61        | 1.52     |
| 1   | G     | 164 | ILE  | CA-C  | 6.62  | 1.61        | 1.52     |
| 1   | A     | 325 | LYS  | CA-C  | 6.61  | 1.61        | 1.52     |
| 1   | K     | 413 | ARG  | CD-NE | 6.61  | 1.55        | 1.46     |
| 1   | H     | 311 | TYR  | N-CA  | -6.60 | 1.38        | 1.46     |
| 1   | R     | 71  | ASP  | C-N   | 6.60  | 1.42        | 1.33     |
| 1   | A     | 294 | GLY  | CA-C  | -6.60 | 1.42        | 1.51     |
| 1   | H     | 114 | LEU  | C-N   | 6.59  | 1.42        | 1.33     |
| 1   | Q     | 378 | SER  | N-CA  | -6.59 | 1.38        | 1.46     |
| 1   | B     | 251 | ALA  | N-CA  | -6.59 | 1.37        | 1.46     |
| 1   | C     | 192 | VAL  | CA-C  | -6.59 | 1.44        | 1.52     |
| 1   | R     | 272 | MET  | CA-C  | -6.59 | 1.44        | 1.52     |
| 1   | B     | 304 | ILE  | C-N   | 6.58  | 1.42        | 1.33     |
| 1   | F     | 298 | ILE  | CA-C  | -6.58 | 1.44        | 1.52     |
| 1   | K     | 115 | VAL  | N-CA  | 6.58  | 1.54        | 1.46     |
| 1   | O     | 423 | ILE  | CA-C  | 6.58  | 1.61        | 1.52     |
| 1   | S     | 209 | ILE  | C-N   | 6.58  | 1.42        | 1.33     |
| 1   | G     | 248 | LEU  | CA-C  | -6.58 | 1.44        | 1.52     |
| 1   | G     | 418 | GLY  | C-N   | 6.58  | 1.43        | 1.33     |
| 1   | R     | 345 | GLU  | CA-CB | 6.58  | 1.63        | 1.53     |
| 1   | R     | 107 | ALA  | C-N   | 6.57  | 1.41        | 1.33     |
| 1   | R     | 421 | VAL  | CA-C  | 6.57  | 1.62        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | H     | 176 | GLY  | C-O   | -6.57 | 1.18        | 1.24     |
| 1   | M     | 429 | LEU  | CA-CB | 6.57  | 1.64        | 1.53     |
| 1   | H     | 227 | VAL  | CA-CB | 6.56  | 1.62        | 1.54     |
| 1   | B     | 436 | VAL  | N-CA  | -6.56 | 1.38        | 1.46     |
| 1   | B     | 489 | LEU  | CA-C  | 6.56  | 1.64        | 1.52     |
| 1   | M     | 362 | VAL  | CA-C  | 6.56  | 1.61        | 1.52     |
| 1   | N     | 317 | VAL  | N-CA  | 6.56  | 1.54        | 1.46     |
| 1   | I     | 248 | LEU  | CA-CB | 6.56  | 1.61        | 1.52     |
| 1   | C     | 469 | LEU  | CA-CB | 6.55  | 1.63        | 1.53     |
| 1   | H     | 38  | ALA  | CA-C  | 6.55  | 1.61        | 1.52     |
| 1   | I     | 470 | LEU  | CA-C  | 6.54  | 1.61        | 1.52     |
| 1   | Q     | 418 | GLY  | CA-C  | 6.54  | 1.58        | 1.51     |
| 1   | B     | 36  | ILE  | CA-C  | -6.54 | 1.45        | 1.52     |
| 1   | K     | 198 | ASP  | CA-C  | -6.54 | 1.44        | 1.52     |
| 1   | C     | 514 | LYS  | CA-C  | 6.54  | 1.61        | 1.52     |
| 1   | C     | 63  | LEU  | CA-CB | 6.53  | 1.63        | 1.53     |
| 1   | D     | 144 | GLN  | CA-C  | 6.53  | 1.61        | 1.52     |
| 1   | R     | 145 | THR  | C-N   | 6.53  | 1.41        | 1.33     |
| 1   | R     | 436 | VAL  | N-CA  | 6.53  | 1.54        | 1.46     |
| 1   | H     | 488 | ASP  | CA-C  | 6.51  | 1.61        | 1.52     |
| 1   | N     | 114 | LEU  | C-N   | 6.51  | 1.42        | 1.33     |
| 1   | H     | 419 | GLY  | CA-C  | -6.51 | 1.43        | 1.51     |
| 1   | N     | 447 | TYR  | CA-C  | -6.51 | 1.44        | 1.52     |
| 1   | O     | 86  | ALA  | C-N   | 6.51  | 1.42        | 1.33     |
| 1   | E     | 113 | GLU  | N-CA  | 6.51  | 1.54        | 1.46     |
| 1   | N     | 326 | SER  | CA-C  | -6.51 | 1.43        | 1.52     |
| 1   | R     | 358 | GLU  | N-CA  | -6.51 | 1.37        | 1.45     |
| 1   | D     | 371 | GLU  | C-N   | 6.50  | 1.39        | 1.33     |
| 1   | O     | 389 | ARG  | NE-CZ | 6.50  | 1.40        | 1.33     |
| 1   | G     | 349 | GLN  | C-N   | 6.50  | 1.43        | 1.34     |
| 1   | M     | 328 | LEU  | CA-C  | 6.50  | 1.61        | 1.52     |
| 1   | E     | 242 | GLU  | CA-CB | 6.50  | 1.63        | 1.53     |
| 1   | P     | 223 | VAL  | C-N   | 6.49  | 1.42        | 1.33     |
| 1   | S     | 517 | THR  | N-CA  | 6.49  | 1.54        | 1.46     |
| 1   | G     | 297 | VAL  | CA-C  | -6.49 | 1.44        | 1.52     |
| 1   | G     | 318 | LEU  | CA-CB | 6.49  | 1.62        | 1.53     |
| 1   | R     | 240 | ARG  | C-N   | 6.49  | 1.42        | 1.33     |
| 1   | R     | 349 | GLN  | C-N   | -6.49 | 1.23        | 1.33     |
| 1   | E     | 503 | ILE  | C-N   | 6.48  | 1.40        | 1.33     |
| 1   | N     | 346 | ILE  | CA-CB | 6.48  | 1.60        | 1.54     |
| 1   | P     | 54  | GLY  | CA-C  | -6.48 | 1.46        | 1.52     |
| 1   | M     | 113 | GLU  | CA-C  | -6.48 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 278 | GLU  | C-N    | 6.48  | 1.43        | 1.34     |
| 1   | O     | 378 | SER  | C-N    | 6.48  | 1.42        | 1.33     |
| 1   | P     | 179 | GLU  | C-N    | 6.47  | 1.42        | 1.33     |
| 1   | C     | 83  | HIS  | C-N    | 6.47  | 1.42        | 1.33     |
| 1   | K     | 234 | HIS  | C-N    | 6.47  | 1.42        | 1.33     |
| 1   | L     | 367 | MET  | CA-C   | -6.47 | 1.44        | 1.52     |
| 1   | Q     | 399 | ARG  | N-CA   | -6.47 | 1.38        | 1.46     |
| 1   | L     | 490 | TYR  | CZ-OH  | 6.47  | 1.51        | 1.38     |
| 1   | Q     | 424 | GLU  | N-CA   | 6.47  | 1.54        | 1.46     |
| 1   | N     | 132 | ILE  | C-N    | 6.47  | 1.42        | 1.33     |
| 1   | S     | 286 | LYS  | CA-CB  | 6.47  | 1.63        | 1.53     |
| 1   | C     | 240 | ARG  | CA-CB  | 6.46  | 1.64        | 1.53     |
| 1   | D     | 222 | LEU  | N-CA   | -6.46 | 1.38        | 1.46     |
| 1   | Q     | 59  | LEU  | N-CA   | -6.46 | 1.38        | 1.46     |
| 1   | O     | 163 | LYS  | CA-CB  | 6.46  | 1.63        | 1.53     |
| 1   | Q     | 332 | ALA  | C-O    | 6.46  | 1.32        | 1.24     |
| 1   | C     | 374 | LYS  | N-CA   | -6.46 | 1.38        | 1.46     |
| 1   | L     | 292 | ALA  | N-CA   | -6.45 | 1.37        | 1.46     |
| 1   | P     | 375 | ASN  | CA-C   | 6.45  | 1.61        | 1.52     |
| 1   | A     | 281 | ASN  | C-N    | 6.45  | 1.42        | 1.33     |
| 1   | I     | 497 | MET  | CA-C   | -6.45 | 1.44        | 1.52     |
| 1   | L     | 227 | VAL  | C-N    | -6.45 | 1.24        | 1.33     |
| 1   | S     | 66  | ILE  | CA-C   | 6.44  | 1.60        | 1.52     |
| 1   | B     | 110 | PHE  | CA-CB  | 6.44  | 1.63        | 1.53     |
| 1   | N     | 509 | LYS  | C-N    | 6.43  | 1.42        | 1.33     |
| 1   | B     | 45  | ALA  | N-CA   | -6.43 | 1.37        | 1.46     |
| 1   | C     | 525 | ARG  | N-CA   | -6.43 | 1.38        | 1.46     |
| 1   | N     | 186 | VAL  | CA-CB  | -6.42 | 1.46        | 1.54     |
| 1   | L     | 225 | GLY  | N-CA   | 6.42  | 1.51        | 1.45     |
| 1   | E     | 288 | ASP  | CA-C   | 6.42  | 1.61        | 1.52     |
| 1   | R     | 89  | LEU  | CA-C   | 6.42  | 1.60        | 1.52     |
| 1   | P     | 137 | LYS  | CA-CB  | 6.41  | 1.64        | 1.53     |
| 1   | P     | 189 | VAL  | CA-CB  | -6.41 | 1.46        | 1.54     |
| 1   | C     | 235 | PRO  | N-CD   | -6.41 | 1.38        | 1.47     |
| 1   | F     | 220 | THR  | C-N    | 6.40  | 1.41        | 1.33     |
| 1   | I     | 46  | LEU  | C-N    | 6.40  | 1.42        | 1.33     |
| 1   | C     | 60  | VAL  | C-N    | 6.40  | 1.42        | 1.33     |
| 1   | I     | 127 | HIS  | CG-CD2 | 6.40  | 1.42        | 1.35     |
| 1   | G     | 271 | GLN  | C-O    | -6.40 | 1.16        | 1.24     |
| 1   | A     | 57  | LYS  | CA-C   | -6.39 | 1.45        | 1.52     |
| 1   | E     | 339 | VAL  | CA-CB  | 6.39  | 1.61        | 1.53     |
| 1   | O     | 268 | ASP  | CA-CB  | 6.39  | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | P     | 508 | VAL  | C-O   | -6.39 | 1.17        | 1.24     |
| 1   | P     | 28  | GLY  | N-CA  | 6.39  | 1.55        | 1.45     |
| 1   | F     | 367 | MET  | N-CA  | -6.39 | 1.37        | 1.45     |
| 1   | R     | 322 | ARG  | CD-NE | 6.39  | 1.55        | 1.46     |
| 1   | O     | 285 | GLU  | CA-C  | -6.39 | 1.44        | 1.52     |
| 1   | F     | 459 | ILE  | C-N   | 6.38  | 1.41        | 1.33     |
| 1   | N     | 460 | GLU  | C-N   | -6.38 | 1.25        | 1.33     |
| 1   | N     | 513 | ILE  | C-N   | 6.37  | 1.42        | 1.33     |
| 1   | F     | 28  | GLY  | N-CA  | 6.37  | 1.55        | 1.45     |
| 1   | B     | 249 | ILE  | CA-C  | -6.37 | 1.46        | 1.52     |
| 1   | L     | 256 | GLU  | CA-C  | -6.36 | 1.45        | 1.52     |
| 1   | L     | 333 | ARG  | CD-NE | 6.36  | 1.55        | 1.46     |
| 1   | K     | 444 | VAL  | CA-CB | -6.36 | 1.46        | 1.54     |
| 1   | E     | 67  | THR  | CA-C  | -6.36 | 1.45        | 1.52     |
| 1   | E     | 523 | VAL  | C-N   | 6.35  | 1.42        | 1.34     |
| 1   | H     | 178 | ARG  | CD-NE | 6.35  | 1.55        | 1.46     |
| 1   | I     | 520 | ALA  | N-CA  | -6.35 | 1.38        | 1.46     |
| 1   | A     | 527 | ASP  | CA-C  | -6.35 | 1.44        | 1.53     |
| 1   | I     | 507 | LEU  | CA-C  | 6.35  | 1.61        | 1.52     |
| 1   | M     | 271 | GLN  | C-N   | 6.34  | 1.41        | 1.33     |
| 1   | O     | 405 | VAL  | CA-CB | -6.34 | 1.46        | 1.54     |
| 1   | C     | 240 | ARG  | CD-NE | 6.34  | 1.55        | 1.46     |
| 1   | E     | 313 | ALA  | CA-C  | -6.34 | 1.44        | 1.52     |
| 1   | K     | 33  | ARG  | N-CA  | 6.34  | 1.53        | 1.46     |
| 1   | I     | 277 | ASP  | N-CA  | 6.33  | 1.53        | 1.46     |
| 1   | L     | 334 | ALA  | C-N   | 6.33  | 1.42        | 1.33     |
| 1   | B     | 169 | LEU  | N-CA  | -6.33 | 1.38        | 1.46     |
| 1   | F     | 97  | ASP  | CA-CB | 6.33  | 1.63        | 1.53     |
| 1   | F     | 253 | LEU  | CA-CB | 6.33  | 1.61        | 1.53     |
| 1   | H     | 309 | GLN  | CA-CB | 6.33  | 1.63        | 1.53     |
| 1   | G     | 455 | VAL  | CA-C  | 6.33  | 1.61        | 1.52     |
| 1   | M     | 461 | ASN  | CA-CB | 6.33  | 1.64        | 1.53     |
| 1   | C     | 268 | ASP  | CA-C  | 6.32  | 1.60        | 1.52     |
| 1   | F     | 443 | ALA  | CA-C  | 6.32  | 1.60        | 1.52     |
| 1   | F     | 245 | LYS  | C-N   | 6.32  | 1.41        | 1.33     |
| 1   | B     | 372 | GLY  | CA-C  | 6.32  | 1.59        | 1.51     |
| 1   | E     | 429 | LEU  | CA-C  | -6.32 | 1.44        | 1.52     |
| 1   | A     | 138 | ALA  | CA-C  | -6.32 | 1.44        | 1.52     |
| 1   | P     | 267 | ASN  | CA-CB | 6.32  | 1.63        | 1.54     |
| 1   | Q     | 443 | ALA  | CA-C  | 6.32  | 1.60        | 1.52     |
| 1   | S     | 213 | ALA  | C-N   | -6.32 | 1.24        | 1.33     |
| 1   | Q     | 186 | VAL  | C-N   | 6.32  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | R     | 166 | MET  | N-CA    | -6.31 | 1.38        | 1.46     |
| 1   | S     | 238 | PRO  | CA-CB   | 6.31  | 1.61        | 1.53     |
| 1   | E     | 234 | HIS  | CG-CD2  | 6.31  | 1.42        | 1.35     |
| 1   | S     | 86  | ALA  | C-N     | 6.31  | 1.42        | 1.34     |
| 1   | C     | 365 | ASP  | CA-CB   | 6.30  | 1.62        | 1.53     |
| 1   | N     | 503 | ILE  | C-N     | 6.30  | 1.40        | 1.33     |
| 1   | E     | 359 | GLU  | N-CA    | -6.30 | 1.38        | 1.46     |
| 1   | N     | 480 | GLU  | CA-C    | 6.30  | 1.60        | 1.52     |
| 1   | K     | 473 | LEU  | CA-C    | 6.30  | 1.60        | 1.52     |
| 1   | D     | 366 | LYS  | CA-C    | 6.30  | 1.60        | 1.52     |
| 1   | A     | 390 | LEU  | C-N     | 6.29  | 1.41        | 1.33     |
| 1   | K     | 233 | VAL  | CA-C    | 6.29  | 1.61        | 1.52     |
| 1   | B     | 152 | THR  | CA-C    | -6.29 | 1.44        | 1.52     |
| 1   | E     | 477 | HIS  | CE1-NE2 | -6.29 | 1.26        | 1.32     |
| 1   | O     | 525 | ARG  | CA-C    | 6.29  | 1.61        | 1.52     |
| 1   | F     | 496 | ASP  | C-O     | -6.29 | 1.16        | 1.24     |
| 1   | S     | 324 | LYS  | N-CA    | -6.29 | 1.38        | 1.46     |
| 1   | E     | 92  | ILE  | C-N     | 6.29  | 1.41        | 1.33     |
| 1   | F     | 42  | VAL  | CA-CB   | 6.29  | 1.62        | 1.54     |
| 1   | B     | 56  | ASP  | C-O     | -6.28 | 1.16        | 1.24     |
| 1   | M     | 457 | ILE  | CA-CB   | 6.28  | 1.62        | 1.54     |
| 1   | A     | 322 | ARG  | C-N     | 6.28  | 1.42        | 1.33     |
| 1   | L     | 63  | LEU  | CA-CB   | 6.28  | 1.64        | 1.53     |
| 1   | G     | 171 | SER  | CA-C    | -6.28 | 1.44        | 1.52     |
| 1   | M     | 416 | ALA  | CA-CB   | 6.28  | 1.62        | 1.53     |
| 1   | A     | 451 | LEU  | CA-C    | -6.27 | 1.44        | 1.52     |
| 1   | L     | 526 | ILE  | CA-CB   | 6.27  | 1.60        | 1.53     |
| 1   | R     | 184 | ILE  | CA-C    | -6.27 | 1.45        | 1.52     |
| 1   | C     | 79  | MET  | CA-C    | -6.27 | 1.45        | 1.52     |
| 1   | G     | 427 | LYS  | N-CA    | 6.27  | 1.53        | 1.46     |
| 1   | H     | 122 | LEU  | CA-CB   | 6.27  | 1.63        | 1.53     |
| 1   | B     | 432 | TYR  | C-O     | 6.27  | 1.31        | 1.24     |
| 1   | G     | 423 | ILE  | CA-CB   | -6.27 | 1.45        | 1.54     |
| 1   | K     | 330 | LYS  | CA-CB   | 6.26  | 1.63        | 1.53     |
| 1   | P     | 477 | HIS  | N-CA    | -6.26 | 1.40        | 1.46     |
| 1   | A     | 154 | SER  | N-CA    | -6.26 | 1.37        | 1.45     |
| 1   | I     | 269 | PRO  | CA-CB   | -6.26 | 1.44        | 1.53     |
| 1   | R     | 119 | GLU  | N-CA    | -6.26 | 1.38        | 1.46     |
| 1   | R     | 122 | LEU  | N-CA    | 6.26  | 1.54        | 1.46     |
| 1   | E     | 130 | ILE  | N-CA    | -6.25 | 1.39        | 1.46     |
| 1   | M     | 231 | GLU  | CA-CB   | 6.25  | 1.64        | 1.53     |
| 1   | N     | 485 | TYR  | CA-CB   | 6.25  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 350 | ASP  | CA-C    | -6.25 | 1.44        | 1.52     |
| 1   | E     | 139 | GLU  | CA-C    | 6.25  | 1.60        | 1.52     |
| 1   | L     | 288 | ASP  | CA-C    | 6.25  | 1.60        | 1.52     |
| 1   | O     | 503 | ILE  | C-N     | 6.25  | 1.40        | 1.33     |
| 1   | H     | 54  | GLY  | CA-C    | -6.24 | 1.45        | 1.52     |
| 1   | D     | 421 | VAL  | CA-CB   | -6.24 | 1.45        | 1.54     |
| 1   | Q     | 35  | ASN  | CA-C    | 6.24  | 1.60        | 1.52     |
| 1   | M     | 301 | GLN  | C-N     | -6.23 | 1.27        | 1.33     |
| 1   | K     | 199 | LYS  | N-CA    | -6.23 | 1.38        | 1.46     |
| 1   | S     | 49  | THR  | C-N     | 6.23  | 1.41        | 1.33     |
| 1   | O     | 290 | ILE  | C-O     | -6.23 | 1.17        | 1.23     |
| 1   | K     | 204 | LEU  | CA-CB   | 6.23  | 1.63        | 1.53     |
| 1   | P     | 126 | VAL  | CA-CB   | -6.22 | 1.46        | 1.54     |
| 1   | I     | 100 | THR  | CA-C    | -6.22 | 1.45        | 1.52     |
| 1   | Q     | 423 | ILE  | C-N     | 6.22  | 1.41        | 1.33     |
| 1   | F     | 531 | SER  | C-N     | 6.21  | 1.42        | 1.33     |
| 1   | C     | 255 | VAL  | C-N     | 6.21  | 1.41        | 1.33     |
| 1   | S     | 436 | VAL  | N-CA    | 6.21  | 1.53        | 1.46     |
| 1   | K     | 510 | MET  | C-N     | 6.21  | 1.42        | 1.34     |
| 1   | O     | 127 | HIS  | CA-CB   | 6.21  | 1.62        | 1.53     |
| 1   | N     | 471 | MET  | N-CA    | -6.21 | 1.39        | 1.46     |
| 1   | D     | 142 | ALA  | CA-CB   | 6.21  | 1.63        | 1.53     |
| 1   | Q     | 459 | ILE  | N-CA    | 6.21  | 1.53        | 1.46     |
| 1   | R     | 106 | THR  | N-CA    | 6.20  | 1.53        | 1.46     |
| 1   | F     | 273 | GLN  | CA-CB   | -6.20 | 1.43        | 1.53     |
| 1   | A     | 184 | ILE  | CA-C    | -6.20 | 1.45        | 1.52     |
| 1   | P     | 203 | ASP  | CA-C    | 6.20  | 1.60        | 1.52     |
| 1   | L     | 160 | LEU  | CA-C    | -6.20 | 1.45        | 1.53     |
| 1   | I     | 394 | THR  | C-N     | 6.20  | 1.42        | 1.33     |
| 1   | D     | 320 | VAL  | CA-C    | 6.19  | 1.60        | 1.52     |
| 1   | A     | 330 | LYS  | C-O     | -6.19 | 1.16        | 1.24     |
| 1   | F     | 115 | VAL  | CA-CB   | -6.19 | 1.47        | 1.54     |
| 1   | H     | 88  | LEU  | CA-CB   | 6.19  | 1.63        | 1.53     |
| 1   | C     | 110 | PHE  | C-N     | 6.19  | 1.41        | 1.33     |
| 1   | F     | 474 | ARG  | C-N     | 6.19  | 1.42        | 1.33     |
| 1   | Q     | 105 | LYS  | CA-C    | 6.19  | 1.60        | 1.52     |
| 1   | A     | 179 | GLU  | C-N     | 6.18  | 1.41        | 1.33     |
| 1   | N     | 234 | HIS  | CD2-NE2 | 6.18  | 1.44        | 1.37     |
| 1   | D     | 446 | ALA  | CA-C    | -6.18 | 1.45        | 1.52     |
| 1   | E     | 474 | ARG  | C-N     | 6.18  | 1.42        | 1.33     |
| 1   | L     | 304 | ILE  | N-CA    | 6.18  | 1.53        | 1.46     |
| 1   | K     | 130 | ILE  | CA-C    | -6.18 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 32  | VAL  | C-N   | -6.18 | 1.26        | 1.33     |
| 1   | K     | 304 | ILE  | N-CA  | -6.18 | 1.39        | 1.46     |
| 1   | N     | 98  | GLU  | C-N   | -6.18 | 1.25        | 1.33     |
| 1   | G     | 388 | GLU  | N-CA  | 6.18  | 1.54        | 1.46     |
| 1   | R     | 77  | ASP  | N-CA  | -6.18 | 1.39        | 1.46     |
| 1   | M     | 400 | ASP  | CA-C  | -6.18 | 1.44        | 1.52     |
| 1   | F     | 450 | ALA  | CA-C  | 6.17  | 1.60        | 1.52     |
| 1   | P     | 161 | LEU  | CB-CG | 6.17  | 1.65        | 1.53     |
| 1   | I     | 58  | MET  | CA-C  | -6.17 | 1.45        | 1.52     |
| 1   | A     | 189 | VAL  | CA-C  | 6.17  | 1.60        | 1.52     |
| 1   | G     | 439 | LYS  | CA-CB | 6.17  | 1.63        | 1.53     |
| 1   | N     | 406 | ALA  | N-CA  | -6.17 | 1.38        | 1.46     |
| 1   | R     | 342 | ASN  | CA-CB | 6.17  | 1.63        | 1.53     |
| 1   | A     | 43  | GLU  | N-CA  | -6.17 | 1.39        | 1.46     |
| 1   | K     | 43  | GLU  | CA-CB | 6.17  | 1.62        | 1.53     |
| 1   | H     | 200 | TRP  | CA-C  | 6.17  | 1.60        | 1.52     |
| 1   | N     | 489 | LEU  | CA-C  | -6.17 | 1.44        | 1.52     |
| 1   | S     | 149 | LEU  | C-N   | 6.17  | 1.41        | 1.33     |
| 1   | M     | 338 | ARG  | CD-NE | 6.16  | 1.54        | 1.46     |
| 1   | N     | 274 | LYS  | N-CA  | 6.16  | 1.54        | 1.46     |
| 1   | D     | 316 | GLY  | CA-C  | -6.16 | 1.43        | 1.51     |
| 1   | P     | 101 | ALA  | C-N   | 6.16  | 1.42        | 1.33     |
| 1   | A     | 211 | LYS  | C-N   | 6.16  | 1.42        | 1.33     |
| 1   | I     | 181 | ILE  | CA-CB | 6.16  | 1.62        | 1.54     |
| 1   | I     | 269 | PRO  | N-CA  | 6.16  | 1.55        | 1.47     |
| 1   | K     | 434 | PRO  | CA-C  | 6.16  | 1.61        | 1.52     |
| 1   | H     | 415 | ILE  | N-CA  | -6.16 | 1.38        | 1.46     |
| 1   | O     | 103 | GLY  | C-N   | 6.16  | 1.42        | 1.33     |
| 1   | P     | 526 | ILE  | C-N   | 6.15  | 1.41        | 1.33     |
| 1   | D     | 195 | LEU  | CA-C  | 6.15  | 1.61        | 1.52     |
| 1   | I     | 461 | ASN  | CA-C  | 6.15  | 1.61        | 1.52     |
| 1   | A     | 208 | GLN  | C-N   | 6.15  | 1.41        | 1.33     |
| 1   | P     | 80  | ASP  | CA-CB | 6.15  | 1.61        | 1.52     |
| 1   | B     | 138 | ALA  | C-N   | 6.14  | 1.41        | 1.33     |
| 1   | F     | 219 | ASP  | C-N   | 6.14  | 1.41        | 1.33     |
| 1   | N     | 108 | VAL  | C-N   | 6.14  | 1.41        | 1.33     |
| 1   | R     | 71  | ASP  | N-CA  | -6.14 | 1.38        | 1.46     |
| 1   | A     | 308 | ALA  | CA-C  | 6.14  | 1.61        | 1.52     |
| 1   | B     | 526 | ILE  | N-CA  | -6.14 | 1.38        | 1.46     |
| 1   | E     | 342 | ASN  | N-CA  | -6.14 | 1.39        | 1.46     |
| 1   | L     | 477 | HIS  | C-N   | 6.14  | 1.42        | 1.33     |
| 1   | P     | 288 | ASP  | CA-C  | 6.14  | 1.61        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 234 | HIS  | ND1-CE1 | 6.13  | 1.38        | 1.32     |
| 1   | H     | 90  | VAL  | CA-C    | 6.13  | 1.60        | 1.52     |
| 1   | N     | 137 | LYS  | CA-C    | -6.13 | 1.44        | 1.52     |
| 1   | N     | 287 | VAL  | CA-CB   | 6.13  | 1.61        | 1.54     |
| 1   | P     | 219 | ASP  | C-O     | 6.13  | 1.32        | 1.24     |
| 1   | O     | 306 | GLU  | C-N     | 6.13  | 1.41        | 1.33     |
| 1   | R     | 82  | GLN  | CA-CB   | 6.12  | 1.62        | 1.53     |
| 1   | F     | 359 | GLU  | CA-C    | 6.12  | 1.59        | 1.52     |
| 1   | E     | 299 | ILE  | N-CA    | 6.12  | 1.53        | 1.46     |
| 1   | I     | 225 | GLY  | CA-C    | -6.12 | 1.43        | 1.51     |
| 1   | S     | 508 | VAL  | CA-CB   | -6.12 | 1.47        | 1.54     |
| 1   | A     | 55  | MET  | C-N     | 6.12  | 1.42        | 1.33     |
| 1   | B     | 51  | GLY  | N-CA    | 6.11  | 1.53        | 1.44     |
| 1   | E     | 398 | LEU  | CA-CB   | 6.11  | 1.63        | 1.53     |
| 1   | O     | 133 | SER  | CA-C    | -6.11 | 1.45        | 1.52     |
| 1   | P     | 232 | VAL  | CA-C    | -6.11 | 1.46        | 1.53     |
| 1   | B     | 250 | ASP  | CA-CB   | 6.11  | 1.62        | 1.53     |
| 1   | C     | 414 | ALA  | CA-C    | 6.11  | 1.59        | 1.52     |
| 1   | N     | 413 | ARG  | CD-NE   | 6.11  | 1.54        | 1.46     |
| 1   | L     | 223 | VAL  | CA-C    | 6.11  | 1.60        | 1.52     |
| 1   | C     | 220 | THR  | CA-C    | -6.11 | 1.44        | 1.52     |
| 1   | E     | 227 | VAL  | N-CA    | -6.11 | 1.38        | 1.46     |
| 1   | N     | 276 | LEU  | N-CA    | -6.11 | 1.38        | 1.46     |
| 1   | R     | 376 | PRO  | N-CD    | -6.11 | 1.39        | 1.47     |
| 1   | S     | 40  | LYS  | C-O     | -6.11 | 1.16        | 1.24     |
| 1   | F     | 405 | VAL  | CA-CB   | -6.10 | 1.46        | 1.54     |
| 1   | Q     | 438 | GLY  | N-CA    | 6.10  | 1.54        | 1.45     |
| 1   | A     | 38  | ALA  | CA-C    | 6.10  | 1.60        | 1.52     |
| 1   | C     | 343 | ILE  | CA-C    | 6.10  | 1.61        | 1.52     |
| 1   | D     | 93  | ALA  | CA-C    | -6.10 | 1.45        | 1.52     |
| 1   | S     | 352 | GLY  | N-CA    | 6.10  | 1.53        | 1.44     |
| 1   | C     | 484 | TRP  | CA-CB   | 6.10  | 1.61        | 1.53     |
| 1   | E     | 138 | ALA  | C-N     | 6.10  | 1.41        | 1.33     |
| 1   | I     | 504 | GLU  | CA-CB   | 6.10  | 1.61        | 1.53     |
| 1   | H     | 203 | ASP  | CA-C    | 6.09  | 1.59        | 1.53     |
| 1   | O     | 144 | GLN  | C-N     | 6.09  | 1.42        | 1.33     |
| 1   | Q     | 180 | TYR  | CA-C    | -6.09 | 1.45        | 1.52     |
| 1   | H     | 449 | ASN  | CA-C    | 6.09  | 1.60        | 1.52     |
| 1   | E     | 337 | GLY  | CA-C    | -6.08 | 1.45        | 1.52     |
| 1   | M     | 67  | THR  | N-CA    | -6.08 | 1.39        | 1.46     |
| 1   | A     | 334 | ALA  | CA-C    | -6.08 | 1.44        | 1.52     |
| 1   | O     | 518 | GLU  | N-CA    | 6.08  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 201 | TYR  | CA-C  | 6.08  | 1.60        | 1.52     |
| 1   | L     | 473 | LEU  | CA-CB | 6.08  | 1.63        | 1.53     |
| 1   | M     | 454 | LEU  | CA-CB | 6.08  | 1.62        | 1.53     |
| 1   | B     | 242 | GLU  | C-N   | 6.08  | 1.41        | 1.33     |
| 1   | F     | 33  | ARG  | NE-CZ | 6.08  | 1.39        | 1.33     |
| 1   | M     | 319 | ALA  | N-CA  | -6.07 | 1.38        | 1.45     |
| 1   | F     | 270 | THR  | CA-C  | 6.07  | 1.60        | 1.52     |
| 1   | D     | 401 | ALA  | CA-CB | 6.07  | 1.62        | 1.53     |
| 1   | E     | 272 | MET  | N-CA  | 6.07  | 1.53        | 1.46     |
| 1   | Q     | 63  | LEU  | CA-CB | 6.07  | 1.63        | 1.53     |
| 1   | F     | 272 | MET  | CA-C  | 6.07  | 1.60        | 1.52     |
| 1   | H     | 407 | ASP  | C-O   | -6.07 | 1.16        | 1.24     |
| 1   | K     | 363 | GLY  | C-N   | 6.07  | 1.41        | 1.33     |
| 1   | L     | 417 | GLY  | N-CA  | 6.07  | 1.51        | 1.45     |
| 1   | O     | 493 | GLN  | CA-CB | 6.06  | 1.63        | 1.53     |
| 1   | M     | 378 | SER  | C-O   | 6.06  | 1.31        | 1.24     |
| 1   | B     | 427 | LYS  | CA-C  | 6.06  | 1.60        | 1.52     |
| 1   | D     | 57  | LYS  | CA-C  | -6.06 | 1.45        | 1.52     |
| 1   | F     | 173 | ALA  | C-N   | 6.06  | 1.40        | 1.33     |
| 1   | B     | 478 | GLU  | CA-C  | 6.06  | 1.60        | 1.52     |
| 1   | H     | 61  | ASP  | CA-CB | 6.06  | 1.62        | 1.53     |
| 1   | P     | 297 | VAL  | C-N   | 6.06  | 1.41        | 1.33     |
| 1   | G     | 401 | ALA  | N-CA  | -6.06 | 1.39        | 1.46     |
| 1   | H     | 321 | ARG  | CD-NE | 6.06  | 1.54        | 1.46     |
| 1   | L     | 526 | ILE  | CA-C  | -6.05 | 1.46        | 1.53     |
| 1   | P     | 152 | THR  | N-CA  | -6.05 | 1.38        | 1.46     |
| 1   | S     | 211 | LYS  | N-CA  | -6.05 | 1.38        | 1.46     |
| 1   | C     | 203 | ASP  | CA-CB | 6.05  | 1.60        | 1.53     |
| 1   | E     | 115 | VAL  | CA-CB | -6.05 | 1.47        | 1.54     |
| 1   | S     | 177 | ALA  | CA-C  | 6.05  | 1.60        | 1.52     |
| 1   | A     | 436 | VAL  | C-N   | -6.05 | 1.26        | 1.32     |
| 1   | H     | 424 | GLU  | CA-C  | 6.05  | 1.60        | 1.52     |
| 1   | D     | 412 | GLY  | CA-C  | -6.05 | 1.43        | 1.51     |
| 1   | K     | 359 | GLU  | CA-C  | 6.04  | 1.59        | 1.52     |
| 1   | E     | 337 | GLY  | N-CA  | -6.04 | 1.39        | 1.44     |
| 1   | A     | 375 | ASN  | CA-C  | 6.04  | 1.59        | 1.52     |
| 1   | C     | 389 | ARG  | N-CA  | -6.04 | 1.38        | 1.46     |
| 1   | F     | 322 | ARG  | CD-NE | 6.04  | 1.54        | 1.46     |
| 1   | L     | 103 | GLY  | CA-C  | 6.03  | 1.60        | 1.51     |
| 1   | M     | 442 | LEU  | CA-CB | 6.03  | 1.62        | 1.53     |
| 1   | C     | 191 | GLN  | N-CA  | -6.03 | 1.39        | 1.46     |
| 1   | O     | 169 | LEU  | N-CA  | -6.03 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | R     | 257 | LYS  | C-N     | -6.03 | 1.28        | 1.34     |
| 1   | B     | 427 | LYS  | C-N     | 6.03  | 1.41        | 1.33     |
| 1   | K     | 53  | ARG  | CD-NE   | 6.03  | 1.54        | 1.46     |
| 1   | D     | 524 | LEU  | N-CA    | -6.02 | 1.38        | 1.46     |
| 1   | E     | 509 | LYS  | C-N     | 6.02  | 1.41        | 1.33     |
| 1   | R     | 55  | MET  | N-CA    | -6.02 | 1.38        | 1.46     |
| 1   | F     | 221 | GLN  | C-N     | 6.02  | 1.41        | 1.33     |
| 1   | K     | 274 | LYS  | C-N     | 6.02  | 1.42        | 1.33     |
| 1   | F     | 441 | GLN  | N-CA    | -6.02 | 1.39        | 1.46     |
| 1   | B     | 70  | ASN  | N-CA    | -6.01 | 1.41        | 1.46     |
| 1   | K     | 80  | ASP  | C-O     | 6.01  | 1.31        | 1.23     |
| 1   | K     | 163 | LYS  | N-CA    | -6.01 | 1.39        | 1.46     |
| 1   | L     | 168 | SER  | C-N     | 6.01  | 1.42        | 1.33     |
| 1   | M     | 449 | ASN  | C-N     | 6.01  | 1.41        | 1.33     |
| 1   | N     | 127 | HIS  | CA-CB   | 6.01  | 1.62        | 1.53     |
| 1   | A     | 183 | ASP  | C-N     | 6.01  | 1.41        | 1.33     |
| 1   | B     | 223 | VAL  | N-CA    | -6.01 | 1.39        | 1.46     |
| 1   | R     | 242 | GLU  | CA-CB   | 6.01  | 1.61        | 1.53     |
| 1   | C     | 270 | THR  | C-N     | 6.00  | 1.42        | 1.33     |
| 1   | F     | 183 | ASP  | N-CA    | 6.00  | 1.53        | 1.46     |
| 1   | F     | 178 | ARG  | C-O     | -6.00 | 1.16        | 1.24     |
| 1   | N     | 429 | LEU  | CA-C    | -6.00 | 1.45        | 1.52     |
| 1   | Q     | 53  | ARG  | CD-NE   | 6.00  | 1.54        | 1.46     |
| 1   | A     | 374 | LYS  | CA-CB   | 6.00  | 1.63        | 1.53     |
| 1   | B     | 253 | LEU  | CA-C    | 6.00  | 1.61        | 1.52     |
| 1   | K     | 130 | ILE  | N-CA    | -6.00 | 1.39        | 1.46     |
| 1   | D     | 247 | ALA  | CA-C    | -6.00 | 1.45        | 1.53     |
| 1   | G     | 504 | GLU  | C-O     | -6.00 | 1.17        | 1.24     |
| 1   | P     | 149 | LEU  | CA-C    | 6.00  | 1.60        | 1.52     |
| 1   | C     | 68  | ILE  | CA-CB   | -6.00 | 1.47        | 1.54     |
| 1   | E     | 216 | SER  | CA-CB   | 6.00  | 1.63        | 1.53     |
| 1   | O     | 216 | SER  | C-N     | 5.99  | 1.40        | 1.34     |
| 1   | D     | 507 | LEU  | CA-C    | -5.99 | 1.44        | 1.52     |
| 1   | R     | 101 | ALA  | CA-C    | 5.99  | 1.60        | 1.53     |
| 1   | R     | 149 | LEU  | N-CA    | -5.99 | 1.38        | 1.46     |
| 1   | F     | 89  | LEU  | C-N     | 5.99  | 1.41        | 1.34     |
| 1   | G     | 415 | ILE  | CA-CB   | -5.99 | 1.45        | 1.54     |
| 1   | L     | 210 | VAL  | N-CA    | 5.98  | 1.53        | 1.46     |
| 1   | N     | 501 | GLY  | CA-C    | -5.98 | 1.42        | 1.51     |
| 1   | K     | 408 | VAL  | CA-C    | -5.98 | 1.45        | 1.52     |
| 1   | N     | 70  | ASN  | N-CA    | -5.97 | 1.40        | 1.46     |
| 1   | O     | 477 | HIS  | CE1-NE2 | 5.97  | 1.38        | 1.32     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 412 | GLY  | C-N   | 5.97  | 1.42        | 1.33     |
| 1   | I     | 70  | ASN  | CA-C  | -5.97 | 1.45        | 1.52     |
| 1   | M     | 57  | LYS  | C-N   | 5.97  | 1.41        | 1.33     |
| 1   | M     | 216 | SER  | CA-CB | 5.97  | 1.62        | 1.53     |
| 1   | H     | 42  | VAL  | C-N   | 5.97  | 1.41        | 1.33     |
| 1   | G     | 227 | VAL  | CA-C  | -5.97 | 1.45        | 1.52     |
| 1   | C     | 147 | GLN  | CA-CB | 5.96  | 1.63        | 1.53     |
| 1   | L     | 32  | VAL  | CA-C  | 5.96  | 1.60        | 1.52     |
| 1   | G     | 427 | LYS  | CA-CB | 5.96  | 1.63        | 1.53     |
| 1   | M     | 72  | GLY  | CA-C  | -5.96 | 1.45        | 1.51     |
| 1   | A     | 240 | ARG  | CD-NE | 5.96  | 1.54        | 1.46     |
| 1   | A     | 466 | PRO  | C-N   | 5.96  | 1.41        | 1.33     |
| 1   | C     | 467 | ILE  | CA-C  | -5.96 | 1.45        | 1.52     |
| 1   | F     | 490 | TYR  | CA-C  | -5.96 | 1.45        | 1.52     |
| 1   | A     | 277 | ASP  | CA-C  | 5.95  | 1.60        | 1.52     |
| 1   | H     | 148 | GLU  | CA-C  | 5.95  | 1.60        | 1.52     |
| 1   | S     | 221 | GLN  | CA-C  | -5.95 | 1.45        | 1.52     |
| 1   | O     | 525 | ARG  | N-CA  | -5.95 | 1.38        | 1.46     |
| 1   | S     | 36  | ILE  | CA-CB | -5.95 | 1.47        | 1.54     |
| 1   | F     | 135 | TYR  | CA-CB | 5.95  | 1.62        | 1.53     |
| 1   | P     | 395 | GLU  | CA-C  | -5.95 | 1.45        | 1.52     |
| 1   | S     | 468 | ASP  | N-CA  | -5.95 | 1.39        | 1.46     |
| 1   | M     | 79  | MET  | CA-CB | 5.94  | 1.63        | 1.53     |
| 1   | G     | 291 | LEU  | CA-CB | 5.94  | 1.64        | 1.53     |
| 1   | H     | 304 | ILE  | C-N   | 5.94  | 1.41        | 1.33     |
| 1   | O     | 233 | VAL  | CA-CB | -5.94 | 1.46        | 1.54     |
| 1   | N     | 85  | ALA  | CA-CB | -5.94 | 1.44        | 1.53     |
| 1   | B     | 198 | ASP  | C-N   | 5.94  | 1.41        | 1.33     |
| 1   | G     | 424 | GLU  | CA-C  | 5.94  | 1.60        | 1.52     |
| 1   | R     | 416 | ALA  | N-CA  | -5.94 | 1.38        | 1.46     |
| 1   | D     | 337 | GLY  | N-CA  | 5.93  | 1.53        | 1.45     |
| 1   | O     | 395 | GLU  | CA-CB | 5.93  | 1.62        | 1.53     |
| 1   | R     | 411 | ASP  | CA-CB | 5.93  | 1.63        | 1.53     |
| 1   | B     | 183 | ASP  | C-N   | 5.93  | 1.41        | 1.33     |
| 1   | K     | 144 | GLN  | CA-C  | 5.93  | 1.60        | 1.52     |
| 1   | M     | 259 | GLU  | CA-CB | 5.93  | 1.62        | 1.53     |
| 1   | E     | 33  | ARG  | CA-C  | -5.92 | 1.45        | 1.52     |
| 1   | A     | 147 | GLN  | CA-C  | 5.92  | 1.60        | 1.52     |
| 1   | P     | 108 | VAL  | CA-CB | -5.92 | 1.47        | 1.54     |
| 1   | I     | 49  | THR  | CA-C  | -5.92 | 1.44        | 1.52     |
| 1   | B     | 516 | ALA  | N-CA  | -5.92 | 1.39        | 1.46     |
| 1   | N     | 398 | LEU  | CA-C  | 5.92  | 1.60        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | O     | 156 | ASN  | N-CA  | -5.91 | 1.39        | 1.46     |
| 1   | S     | 419 | GLY  | CA-C  | -5.91 | 1.43        | 1.51     |
| 1   | C     | 401 | ALA  | C-N   | 5.91  | 1.41        | 1.33     |
| 1   | R     | 177 | ALA  | N-CA  | 5.91  | 1.53        | 1.46     |
| 1   | K     | 177 | ALA  | CA-C  | -5.91 | 1.47        | 1.53     |
| 1   | Q     | 231 | GLU  | C-N   | 5.90  | 1.41        | 1.33     |
| 1   | D     | 314 | LYS  | C-N   | 5.90  | 1.42        | 1.33     |
| 1   | S     | 47  | LYS  | N-CA  | 5.90  | 1.53        | 1.46     |
| 1   | Q     | 300 | CYS  | CA-CB | 5.90  | 1.63        | 1.53     |
| 1   | D     | 78  | LYS  | CA-CB | 5.89  | 1.63        | 1.53     |
| 1   | G     | 289 | LYS  | N-CA  | 5.89  | 1.54        | 1.46     |
| 1   | O     | 76  | LEU  | CB-CG | 5.89  | 1.65        | 1.53     |
| 1   | K     | 193 | ALA  | N-CA  | 5.89  | 1.53        | 1.46     |
| 1   | L     | 429 | LEU  | N-CA  | -5.89 | 1.39        | 1.46     |
| 1   | S     | 102 | ASP  | CA-CB | 5.89  | 1.63        | 1.53     |
| 1   | I     | 61  | ASP  | N-CA  | -5.89 | 1.38        | 1.46     |
| 1   | N     | 499 | GLN  | CA-C  | 5.89  | 1.60        | 1.52     |
| 1   | P     | 102 | ASP  | CA-CB | 5.89  | 1.62        | 1.53     |
| 1   | R     | 130 | ILE  | N-CA  | -5.89 | 1.39        | 1.46     |
| 1   | G     | 56  | ASP  | C-O   | -5.89 | 1.16        | 1.23     |
| 1   | B     | 329 | GLU  | CA-CB | 5.89  | 1.62        | 1.53     |
| 1   | D     | 240 | ARG  | N-CA  | -5.89 | 1.38        | 1.45     |
| 1   | O     | 249 | ILE  | N-CA  | -5.89 | 1.39        | 1.46     |
| 1   | R     | 358 | GLU  | CA-C  | 5.89  | 1.59        | 1.52     |
| 1   | L     | 160 | LEU  | C-N   | 5.88  | 1.41        | 1.34     |
| 1   | Q     | 465 | ASP  | C-N   | -5.88 | 1.25        | 1.33     |
| 1   | R     | 239 | LYS  | C-O   | 5.88  | 1.30        | 1.24     |
| 1   | D     | 402 | LEU  | C-N   | 5.88  | 1.42        | 1.33     |
| 1   | G     | 484 | TRP  | CA-CB | 5.88  | 1.61        | 1.53     |
| 1   | M     | 456 | SER  | CA-CB | 5.88  | 1.62        | 1.53     |
| 1   | R     | 422 | GLU  | CA-C  | -5.88 | 1.44        | 1.52     |
| 1   | G     | 413 | ARG  | N-CA  | -5.88 | 1.38        | 1.46     |
| 1   | H     | 282 | LEU  | C-N   | 5.88  | 1.41        | 1.33     |
| 1   | K     | 66  | ILE  | C-O   | -5.87 | 1.17        | 1.24     |
| 1   | I     | 271 | GLN  | CA-CB | 5.87  | 1.62        | 1.53     |
| 1   | E     | 447 | TYR  | C-N   | 5.87  | 1.41        | 1.33     |
| 1   | D     | 529 | VAL  | N-CA  | -5.87 | 1.38        | 1.46     |
| 1   | D     | 437 | GLY  | C-O   | -5.86 | 1.16        | 1.23     |
| 1   | G     | 261 | ASP  | C-N   | 5.86  | 1.40        | 1.33     |
| 1   | L     | 106 | THR  | C-N   | 5.86  | 1.41        | 1.33     |
| 1   | Q     | 249 | ILE  | N-CA  | 5.86  | 1.53        | 1.46     |
| 1   | I     | 514 | LYS  | CA-C  | -5.86 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 195 | LEU  | N-CA    | -5.86 | 1.39        | 1.46     |
| 1   | H     | 300 | CYS  | CA-CB   | 5.86  | 1.63        | 1.53     |
| 1   | D     | 468 | ASP  | N-CA    | -5.86 | 1.39        | 1.46     |
| 1   | I     | 49  | THR  | N-CA    | -5.86 | 1.38        | 1.46     |
| 1   | N     | 445 | GLU  | C-N     | 5.86  | 1.41        | 1.33     |
| 1   | E     | 507 | LEU  | CA-C    | 5.86  | 1.60        | 1.52     |
| 1   | N     | 508 | VAL  | CA-CB   | 5.86  | 1.61        | 1.54     |
| 1   | O     | 104 | THR  | N-CA    | 5.85  | 1.53        | 1.46     |
| 1   | P     | 405 | VAL  | CA-C    | 5.85  | 1.60        | 1.52     |
| 1   | L     | 323 | ALA  | CA-C    | -5.85 | 1.45        | 1.52     |
| 1   | G     | 272 | MET  | C-N     | 5.85  | 1.41        | 1.33     |
| 1   | H     | 84  | PRO  | N-CD    | -5.85 | 1.39        | 1.47     |
| 1   | H     | 493 | GLN  | C-N     | 5.85  | 1.40        | 1.33     |
| 1   | K     | 469 | LEU  | CA-CB   | 5.85  | 1.62        | 1.53     |
| 1   | E     | 121 | LEU  | CA-CB   | 5.85  | 1.62        | 1.53     |
| 1   | G     | 291 | LEU  | N-CA    | -5.84 | 1.38        | 1.46     |
| 1   | H     | 286 | LYS  | C-N     | 5.84  | 1.41        | 1.33     |
| 1   | F     | 66  | ILE  | CA-CB   | 5.84  | 1.61        | 1.54     |
| 1   | K     | 160 | LEU  | CA-C    | -5.84 | 1.45        | 1.53     |
| 1   | L     | 255 | VAL  | CA-C    | 5.84  | 1.59        | 1.53     |
| 1   | O     | 225 | GLY  | N-CA    | 5.84  | 1.51        | 1.45     |
| 1   | P     | 461 | ASN  | CA-C    | -5.84 | 1.44        | 1.52     |
| 1   | H     | 484 | TRP  | C-N     | 5.84  | 1.41        | 1.33     |
| 1   | G     | 178 | ARG  | N-CA    | -5.83 | 1.38        | 1.46     |
| 1   | F     | 163 | LYS  | CA-C    | -5.83 | 1.46        | 1.53     |
| 1   | N     | 144 | GLN  | N-CA    | 5.83  | 1.53        | 1.46     |
| 1   | E     | 133 | SER  | C-N     | 5.83  | 1.41        | 1.33     |
| 1   | F     | 345 | GLU  | C-N     | 5.83  | 1.41        | 1.33     |
| 1   | I     | 497 | MET  | C-N     | 5.83  | 1.40        | 1.33     |
| 1   | Q     | 182 | ALA  | C-O     | -5.83 | 1.17        | 1.24     |
| 1   | A     | 197 | GLY  | N-CA    | 5.83  | 1.54        | 1.45     |
| 1   | M     | 385 | GLY  | N-CA    | 5.83  | 1.53        | 1.45     |
| 1   | H     | 127 | HIS  | CG-ND1  | 5.83  | 1.44        | 1.38     |
| 1   | S     | 285 | GLU  | CA-C    | -5.83 | 1.45        | 1.52     |
| 1   | G     | 190 | THR  | CA-C    | -5.82 | 1.44        | 1.52     |
| 1   | D     | 270 | THR  | C-N     | -5.82 | 1.26        | 1.33     |
| 1   | G     | 183 | ASP  | N-CA    | -5.82 | 1.39        | 1.46     |
| 1   | B     | 353 | TYR  | N-CA    | -5.82 | 1.39        | 1.46     |
| 1   | Q     | 498 | TRP  | NE1-CE2 | 5.82  | 1.43        | 1.37     |
| 1   | B     | 243 | ASN  | CA-CB   | 5.82  | 1.62        | 1.53     |
| 1   | G     | 40  | LYS  | CA-CB   | 5.82  | 1.62        | 1.53     |
| 1   | I     | 198 | ASP  | CA-C    | -5.82 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | K     | 131 | ILE  | CA-CB | -5.82 | 1.46        | 1.54     |
| 1   | K     | 254 | GLU  | CA-C  | 5.82  | 1.59        | 1.52     |
| 1   | E     | 310 | SER  | CA-C  | 5.81  | 1.60        | 1.52     |
| 1   | Q     | 191 | GLN  | CA-CB | 5.81  | 1.62        | 1.53     |
| 1   | B     | 361 | LYS  | CA-CB | 5.81  | 1.60        | 1.53     |
| 1   | N     | 147 | GLN  | CA-C  | 5.81  | 1.60        | 1.52     |
| 1   | Q     | 242 | GLU  | C-N   | 5.81  | 1.41        | 1.33     |
| 1   | D     | 399 | ARG  | CD-NE | 5.81  | 1.54        | 1.46     |
| 1   | M     | 384 | ARG  | CD-NE | 5.81  | 1.54        | 1.46     |
| 1   | B     | 106 | THR  | N-CA  | -5.81 | 1.39        | 1.46     |
| 1   | B     | 179 | GLU  | CA-C  | -5.81 | 1.45        | 1.52     |
| 1   | N     | 214 | GLY  | N-CA  | 5.81  | 1.51        | 1.45     |
| 1   | N     | 477 | HIS  | CA-CB | 5.81  | 1.62        | 1.53     |
| 1   | P     | 323 | ALA  | C-N   | 5.81  | 1.41        | 1.33     |
| 1   | D     | 130 | ILE  | C-N   | 5.81  | 1.41        | 1.34     |
| 1   | F     | 309 | GLN  | C-N   | 5.80  | 1.41        | 1.34     |
| 1   | B     | 97  | ASP  | N-CA  | -5.80 | 1.38        | 1.46     |
| 1   | C     | 128 | PRO  | CA-CB | 5.80  | 1.61        | 1.53     |
| 1   | P     | 399 | ARG  | CD-NE | 5.79  | 1.54        | 1.46     |
| 1   | N     | 328 | LEU  | CA-CB | 5.79  | 1.62        | 1.53     |
| 1   | C     | 147 | GLN  | N-CA  | -5.79 | 1.38        | 1.46     |
| 1   | B     | 188 | ALA  | CA-C  | 5.79  | 1.60        | 1.52     |
| 1   | G     | 256 | GLU  | N-CA  | -5.79 | 1.39        | 1.46     |
| 1   | B     | 96  | GLN  | N-CA  | -5.79 | 1.39        | 1.46     |
| 1   | I     | 434 | PRO  | CA-CB | 5.79  | 1.61        | 1.53     |
| 1   | N     | 334 | ALA  | C-O   | -5.79 | 1.16        | 1.23     |
| 1   | H     | 411 | ASP  | CA-CB | 5.79  | 1.63        | 1.53     |
| 1   | N     | 283 | ILE  | CA-CB | 5.79  | 1.61        | 1.54     |
| 1   | O     | 382 | LEU  | CA-CB | 5.78  | 1.62        | 1.53     |
| 1   | O     | 449 | ASN  | N-CA  | -5.78 | 1.39        | 1.46     |
| 1   | O     | 311 | TYR  | CA-CB | 5.78  | 1.62        | 1.53     |
| 1   | B     | 153 | VAL  | CA-CB | -5.78 | 1.47        | 1.54     |
| 1   | C     | 205 | ASP  | C-O   | -5.78 | 1.16        | 1.24     |
| 1   | O     | 256 | GLU  | CA-C  | -5.78 | 1.45        | 1.52     |
| 1   | F     | 518 | GLU  | C-O   | 5.78  | 1.30        | 1.24     |
| 1   | G     | 302 | LYS  | CA-CB | 5.78  | 1.63        | 1.53     |
| 1   | H     | 139 | GLU  | CA-C  | 5.78  | 1.60        | 1.52     |
| 1   | K     | 121 | LEU  | C-O   | -5.78 | 1.17        | 1.24     |
| 1   | R     | 135 | TYR  | C-N   | 5.78  | 1.41        | 1.33     |
| 1   | R     | 59  | LEU  | CB-CG | 5.77  | 1.65        | 1.53     |
| 1   | E     | 126 | VAL  | CA-CB | -5.77 | 1.47        | 1.54     |
| 1   | E     | 511 | ASN  | CA-CB | 5.77  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | R     | 163 | LYS  | N-CA    | -5.77 | 1.39        | 1.46     |
| 1   | O     | 40  | LYS  | CA-C    | 5.77  | 1.60        | 1.52     |
| 1   | Q     | 163 | LYS  | N-CA    | -5.77 | 1.39        | 1.46     |
| 1   | B     | 275 | PHE  | CA-CB   | 5.77  | 1.62        | 1.53     |
| 1   | M     | 397 | ALA  | C-O     | 5.77  | 1.30        | 1.24     |
| 1   | D     | 234 | HIS  | CE1-NE2 | 5.76  | 1.38        | 1.32     |
| 1   | B     | 137 | LYS  | N-CA    | 5.76  | 1.53        | 1.46     |
| 1   | S     | 226 | ILE  | CA-CB   | -5.76 | 1.47        | 1.54     |
| 1   | N     | 259 | GLU  | C-N     | 5.76  | 1.41        | 1.33     |
| 1   | C     | 459 | ILE  | N-CA    | 5.76  | 1.53        | 1.46     |
| 1   | H     | 440 | GLU  | CA-C    | 5.76  | 1.60        | 1.52     |
| 1   | I     | 459 | ILE  | CA-CB   | 5.76  | 1.61        | 1.54     |
| 1   | M     | 323 | ALA  | C-N     | 5.76  | 1.41        | 1.33     |
| 1   | G     | 214 | GLY  | CA-C    | 5.76  | 1.60        | 1.52     |
| 1   | G     | 306 | GLU  | N-CA    | 5.76  | 1.53        | 1.46     |
| 1   | F     | 482 | ASN  | CA-CB   | 5.75  | 1.61        | 1.53     |
| 1   | O     | 271 | GLN  | CA-C    | 5.75  | 1.60        | 1.52     |
| 1   | Q     | 333 | ARG  | CD-NE   | 5.75  | 1.54        | 1.46     |
| 1   | B     | 66  | ILE  | CA-CB   | -5.75 | 1.47        | 1.54     |
| 1   | G     | 467 | ILE  | CA-CB   | -5.75 | 1.47        | 1.54     |
| 1   | I     | 363 | GLY  | CA-C    | -5.75 | 1.43        | 1.52     |
| 1   | D     | 380 | SER  | CA-C    | -5.75 | 1.45        | 1.52     |
| 1   | D     | 421 | VAL  | C-N     | 5.75  | 1.41        | 1.33     |
| 1   | L     | 70  | ASN  | CA-C    | -5.75 | 1.45        | 1.52     |
| 1   | O     | 267 | ASN  | CA-CB   | 5.75  | 1.62        | 1.53     |
| 1   | Q     | 295 | ALA  | CA-CB   | 5.75  | 1.62        | 1.53     |
| 1   | C     | 127 | HIS  | CA-C    | -5.74 | 1.46        | 1.52     |
| 1   | F     | 510 | MET  | C-N     | 5.74  | 1.41        | 1.33     |
| 1   | K     | 234 | HIS  | ND1-CE1 | 5.74  | 1.38        | 1.32     |
| 1   | R     | 251 | ALA  | C-N     | 5.74  | 1.41        | 1.33     |
| 1   | G     | 254 | GLU  | C-N     | -5.74 | 1.27        | 1.33     |
| 1   | K     | 263 | GLU  | CA-CB   | 5.74  | 1.63        | 1.53     |
| 1   | F     | 475 | SER  | CA-CB   | 5.74  | 1.62        | 1.53     |
| 1   | G     | 322 | ARG  | CD-NE   | 5.74  | 1.54        | 1.46     |
| 1   | L     | 510 | MET  | CA-CB   | 5.74  | 1.62        | 1.53     |
| 1   | R     | 157 | ASP  | CA-CB   | 5.74  | 1.60        | 1.52     |
| 1   | H     | 193 | ALA  | CA-CB   | 5.73  | 1.62        | 1.53     |
| 1   | A     | 384 | ARG  | CD-NE   | 5.73  | 1.54        | 1.46     |
| 1   | E     | 513 | ILE  | CA-C    | 5.73  | 1.60        | 1.52     |
| 1   | K     | 300 | CYS  | C-N     | 5.73  | 1.42        | 1.33     |
| 1   | O     | 59  | LEU  | C-N     | 5.73  | 1.41        | 1.33     |
| 1   | B     | 262 | ALA  | CA-CB   | -5.73 | 1.43        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 526 | ILE  | CB-CG1 | 5.73  | 1.65        | 1.53     |
| 1   | K     | 205 | ASP  | N-CA   | 5.73  | 1.53        | 1.46     |
| 1   | F     | 402 | LEU  | CA-CB  | 5.73  | 1.62        | 1.53     |
| 1   | R     | 108 | VAL  | CA-CB  | 5.73  | 1.60        | 1.54     |
| 1   | F     | 163 | LYS  | CA-CB  | 5.72  | 1.62        | 1.53     |
| 1   | K     | 489 | LEU  | N-CA   | -5.72 | 1.38        | 1.46     |
| 1   | D     | 324 | LYS  | CA-C   | -5.72 | 1.45        | 1.52     |
| 1   | A     | 88  | LEU  | C-N    | 5.72  | 1.40        | 1.33     |
| 1   | K     | 28  | GLY  | N-CA   | 5.72  | 1.54        | 1.45     |
| 1   | C     | 453 | SER  | N-CA   | 5.72  | 1.53        | 1.46     |
| 1   | O     | 467 | ILE  | CA-CB  | -5.72 | 1.47        | 1.54     |
| 1   | B     | 313 | ALA  | CA-C   | 5.72  | 1.60        | 1.52     |
| 1   | Q     | 171 | SER  | CA-C   | -5.72 | 1.44        | 1.52     |
| 1   | R     | 477 | HIS  | CG-ND1 | -5.72 | 1.31        | 1.38     |
| 1   | Q     | 201 | TYR  | CA-C   | -5.71 | 1.45        | 1.52     |
| 1   | Q     | 241 | LEU  | CA-CB  | 5.71  | 1.62        | 1.53     |
| 1   | C     | 234 | HIS  | CA-C   | -5.71 | 1.45        | 1.52     |
| 1   | F     | 172 | LYS  | CA-CB  | 5.71  | 1.62        | 1.53     |
| 1   | L     | 65  | ASP  | CA-CB  | 5.71  | 1.62        | 1.53     |
| 1   | N     | 392 | ASP  | C-N    | 5.71  | 1.41        | 1.33     |
| 1   | O     | 353 | TYR  | CA-C   | -5.71 | 1.45        | 1.52     |
| 1   | O     | 389 | ARG  | CD-NE  | 5.71  | 1.54        | 1.46     |
| 1   | B     | 38  | ALA  | C-N    | 5.71  | 1.40        | 1.33     |
| 1   | L     | 459 | ILE  | CA-C   | 5.71  | 1.59        | 1.52     |
| 1   | S     | 120 | ASP  | CA-C   | 5.71  | 1.60        | 1.52     |
| 1   | F     | 339 | VAL  | CA-C   | -5.71 | 1.46        | 1.52     |
| 1   | S     | 496 | ASP  | CA-CB  | 5.71  | 1.60        | 1.53     |
| 1   | A     | 427 | LYS  | CA-C   | 5.70  | 1.60        | 1.52     |
| 1   | C     | 299 | ILE  | CA-CB  | 5.70  | 1.62        | 1.54     |
| 1   | A     | 242 | GLU  | CA-CB  | 5.70  | 1.61        | 1.53     |
| 1   | M     | 54  | GLY  | N-CA   | 5.70  | 1.52        | 1.45     |
| 1   | M     | 272 | MET  | CA-C   | 5.70  | 1.60        | 1.52     |
| 1   | E     | 523 | VAL  | CA-C   | -5.70 | 1.45        | 1.52     |
| 1   | I     | 199 | LYS  | C-N    | 5.70  | 1.41        | 1.33     |
| 1   | M     | 289 | LYS  | C-N    | 5.70  | 1.40        | 1.33     |
| 1   | O     | 385 | GLY  | CA-C   | -5.69 | 1.44        | 1.52     |
| 1   | K     | 127 | HIS  | N-CA   | 5.69  | 1.53        | 1.45     |
| 1   | G     | 119 | GLU  | CA-C   | 5.69  | 1.60        | 1.52     |
| 1   | A     | 399 | ARG  | CD-NE  | 5.68  | 1.54        | 1.46     |
| 1   | F     | 219 | ASP  | CA-CB  | 5.68  | 1.62        | 1.53     |
| 1   | O     | 519 | ALA  | C-N    | 5.68  | 1.40        | 1.33     |
| 1   | S     | 278 | GLU  | N-CA   | -5.68 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 234 | HIS  | ND1-CE1 | 5.68  | 1.38        | 1.32     |
| 1   | K     | 66  | ILE  | CA-CB   | 5.68  | 1.61        | 1.54     |
| 1   | A     | 177 | ALA  | CA-C    | 5.68  | 1.60        | 1.52     |
| 1   | L     | 214 | GLY  | CA-C    | -5.68 | 1.43        | 1.51     |
| 1   | Q     | 300 | CYS  | CA-C    | 5.68  | 1.60        | 1.52     |
| 1   | L     | 67  | THR  | CA-C    | -5.67 | 1.45        | 1.52     |
| 1   | D     | 238 | PRO  | CA-CB   | -5.67 | 1.46        | 1.53     |
| 1   | I     | 87  | LYS  | CA-C    | 5.67  | 1.60        | 1.52     |
| 1   | R     | 148 | GLU  | N-CA    | 5.67  | 1.53        | 1.46     |
| 1   | H     | 97  | ASP  | CA-C    | 5.67  | 1.60        | 1.52     |
| 1   | N     | 519 | ALA  | C-N     | 5.67  | 1.40        | 1.33     |
| 1   | R     | 351 | LEU  | CA-CB   | -5.67 | 1.44        | 1.53     |
| 1   | L     | 410 | LYS  | CA-C    | 5.67  | 1.60        | 1.52     |
| 1   | S     | 135 | TYR  | CG-CD2  | 5.67  | 1.51        | 1.39     |
| 1   | A     | 183 | ASP  | N-CA    | -5.66 | 1.39        | 1.46     |
| 1   | C     | 263 | GLU  | C-N     | 5.66  | 1.41        | 1.33     |
| 1   | G     | 294 | GLY  | N-CA    | 5.66  | 1.53        | 1.45     |
| 1   | I     | 145 | THR  | C-N     | 5.66  | 1.40        | 1.33     |
| 1   | S     | 192 | VAL  | C-N     | -5.66 | 1.25        | 1.33     |
| 1   | A     | 342 | ASN  | N-CA    | -5.66 | 1.39        | 1.46     |
| 1   | Q     | 517 | THR  | N-CA    | 5.66  | 1.53        | 1.46     |
| 1   | F     | 508 | VAL  | CA-CB   | -5.66 | 1.47        | 1.54     |
| 1   | M     | 410 | LYS  | C-N     | 5.66  | 1.41        | 1.33     |
| 1   | E     | 375 | ASN  | CA-CB   | 5.65  | 1.62        | 1.53     |
| 1   | C     | 42  | VAL  | C-O     | -5.65 | 1.17        | 1.24     |
| 1   | K     | 189 | VAL  | CA-CB   | 5.65  | 1.61        | 1.54     |
| 1   | P     | 525 | ARG  | N-CA    | -5.65 | 1.39        | 1.46     |
| 1   | Q     | 234 | HIS  | CA-CB   | 5.65  | 1.59        | 1.53     |
| 1   | H     | 430 | ARG  | CA-CB   | 5.65  | 1.62        | 1.53     |
| 1   | D     | 46  | LEU  | CA-C    | -5.65 | 1.45        | 1.52     |
| 1   | K     | 504 | GLU  | N-CA    | -5.65 | 1.40        | 1.45     |
| 1   | B     | 261 | ASP  | CA-C    | 5.64  | 1.60        | 1.52     |
| 1   | R     | 302 | LYS  | CA-CB   | 5.64  | 1.61        | 1.53     |
| 1   | B     | 400 | ASP  | CA-C    | 5.64  | 1.60        | 1.52     |
| 1   | P     | 373 | ALA  | CA-C    | -5.64 | 1.45        | 1.53     |
| 1   | A     | 134 | GLY  | CA-C    | 5.64  | 1.59        | 1.51     |
| 1   | L     | 334 | ALA  | N-CA    | -5.64 | 1.38        | 1.46     |
| 1   | H     | 231 | GLU  | N-CA    | 5.63  | 1.52        | 1.45     |
| 1   | I     | 449 | ASN  | CA-C    | 5.63  | 1.60        | 1.52     |
| 1   | M     | 79  | MET  | N-CA    | 5.63  | 1.52        | 1.45     |
| 1   | M     | 221 | GLN  | N-CA    | 5.63  | 1.52        | 1.45     |
| 1   | S     | 248 | LEU  | N-CA    | -5.63 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 89  | LEU  | CA-CB   | 5.63  | 1.62        | 1.53     |
| 1   | E     | 360 | ARG  | NE-CZ   | 5.63  | 1.39        | 1.33     |
| 1   | R     | 253 | LEU  | CA-CB   | 5.63  | 1.62        | 1.53     |
| 1   | B     | 189 | VAL  | N-CA    | -5.63 | 1.39        | 1.46     |
| 1   | C     | 245 | LYS  | C-N     | 5.63  | 1.40        | 1.33     |
| 1   | L     | 404 | THR  | N-CA    | -5.63 | 1.39        | 1.46     |
| 1   | L     | 530 | VAL  | C-O     | 5.63  | 1.30        | 1.24     |
| 1   | S     | 168 | SER  | CA-C    | -5.63 | 1.46        | 1.52     |
| 1   | S     | 196 | ARG  | C-N     | 5.63  | 1.41        | 1.33     |
| 1   | E     | 235 | PRO  | N-CA    | -5.62 | 1.40        | 1.47     |
| 1   | I     | 132 | ILE  | CA-C    | 5.62  | 1.59        | 1.52     |
| 1   | O     | 202 | VAL  | CA-CB   | 5.62  | 1.62        | 1.54     |
| 1   | R     | 396 | ARG  | CD-NE   | 5.62  | 1.54        | 1.46     |
| 1   | M     | 360 | ARG  | NE-CZ   | 5.62  | 1.39        | 1.33     |
| 1   | P     | 473 | LEU  | C-N     | 5.62  | 1.41        | 1.33     |
| 1   | E     | 192 | VAL  | N-CA    | 5.62  | 1.53        | 1.46     |
| 1   | O     | 102 | ASP  | N-CA    | -5.62 | 1.39        | 1.46     |
| 1   | E     | 366 | LYS  | CA-C    | -5.62 | 1.45        | 1.52     |
| 1   | K     | 170 | SER  | CA-C    | 5.62  | 1.60        | 1.52     |
| 1   | N     | 421 | VAL  | N-CA    | 5.62  | 1.53        | 1.46     |
| 1   | M     | 203 | ASP  | C-O     | -5.61 | 1.17        | 1.24     |
| 1   | H     | 423 | ILE  | CA-C    | 5.61  | 1.60        | 1.52     |
| 1   | L     | 229 | ASP  | CA-C    | -5.61 | 1.47        | 1.53     |
| 1   | Q     | 481 | ASN  | N-CA    | 5.61  | 1.53        | 1.46     |
| 1   | A     | 410 | LYS  | CA-CB   | 5.61  | 1.62        | 1.53     |
| 1   | L     | 454 | LEU  | N-CA    | 5.61  | 1.53        | 1.46     |
| 1   | S     | 459 | ILE  | C-N     | 5.60  | 1.40        | 1.33     |
| 1   | B     | 400 | ASP  | CA-CB   | 5.60  | 1.62        | 1.53     |
| 1   | B     | 428 | LYS  | N-CA    | -5.60 | 1.39        | 1.46     |
| 1   | G     | 144 | GLN  | CA-C    | 5.60  | 1.60        | 1.52     |
| 1   | P     | 197 | GLY  | CA-C    | -5.60 | 1.44        | 1.51     |
| 1   | Q     | 395 | GLU  | CA-C    | -5.60 | 1.45        | 1.52     |
| 1   | D     | 181 | ILE  | C-N     | 5.60  | 1.41        | 1.33     |
| 1   | O     | 128 | PRO  | C-N     | 5.60  | 1.41        | 1.34     |
| 1   | B     | 200 | TRP  | CD2-CE3 | -5.60 | 1.31        | 1.40     |
| 1   | E     | 71  | ASP  | CA-CB   | 5.60  | 1.61        | 1.53     |
| 1   | E     | 396 | ARG  | CD-NE   | -5.60 | 1.38        | 1.46     |
| 1   | F     | 508 | VAL  | N-CA    | -5.60 | 1.40        | 1.46     |
| 1   | I     | 321 | ARG  | C-O     | -5.60 | 1.17        | 1.23     |
| 1   | D     | 247 | ALA  | C-N     | 5.60  | 1.41        | 1.33     |
| 1   | H     | 228 | VAL  | CA-CB   | -5.60 | 1.47        | 1.54     |
| 1   | H     | 497 | MET  | C-N     | -5.59 | 1.27        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 32  | VAL  | CA-CB  | -5.59 | 1.46        | 1.54     |
| 1   | A     | 341 | SER  | CA-C   | -5.59 | 1.45        | 1.52     |
| 1   | C     | 213 | ALA  | N-CA   | 5.59  | 1.53        | 1.45     |
| 1   | L     | 350 | ASP  | N-CA   | 5.59  | 1.53        | 1.46     |
| 1   | H     | 403 | GLY  | CA-C   | -5.59 | 1.44        | 1.51     |
| 1   | P     | 338 | ARG  | CZ-NH2 | 5.59  | 1.40        | 1.33     |
| 1   | G     | 153 | VAL  | N-CA   | -5.58 | 1.39        | 1.46     |
| 1   | N     | 362 | VAL  | CA-CB  | -5.58 | 1.47        | 1.54     |
| 1   | P     | 334 | ALA  | CA-C   | -5.58 | 1.45        | 1.53     |
| 1   | C     | 225 | GLY  | CA-C   | -5.58 | 1.46        | 1.51     |
| 1   | L     | 35  | ASN  | CA-CB  | 5.58  | 1.62        | 1.53     |
| 1   | S     | 155 | ILE  | C-N    | -5.58 | 1.25        | 1.33     |
| 1   | C     | 471 | MET  | CA-CB  | 5.58  | 1.62        | 1.53     |
| 1   | D     | 277 | ASP  | CA-C   | 5.58  | 1.59        | 1.52     |
| 1   | G     | 376 | PRO  | CA-C   | 5.58  | 1.60        | 1.52     |
| 1   | Q     | 115 | VAL  | CA-CB  | -5.58 | 1.47        | 1.54     |
| 1   | S     | 68  | ILE  | CA-C   | -5.58 | 1.46        | 1.52     |
| 1   | A     | 486 | GLY  | C-N    | 5.58  | 1.40        | 1.33     |
| 1   | M     | 279 | GLU  | CA-CB  | 5.58  | 1.62        | 1.53     |
| 1   | O     | 459 | ILE  | CA-C   | -5.58 | 1.46        | 1.52     |
| 1   | O     | 475 | SER  | CA-C   | 5.58  | 1.60        | 1.53     |
| 1   | O     | 136 | LYS  | CA-CB  | 5.57  | 1.62        | 1.53     |
| 1   | I     | 297 | VAL  | N-CA   | 5.57  | 1.52        | 1.46     |
| 1   | F     | 200 | TRP  | C-N    | 5.57  | 1.41        | 1.33     |
| 1   | M     | 512 | ALA  | CA-C   | 5.57  | 1.59        | 1.52     |
| 1   | I     | 361 | LYS  | N-CA   | -5.57 | 1.39        | 1.46     |
| 1   | N     | 385 | GLY  | N-CA   | -5.57 | 1.37        | 1.45     |
| 1   | S     | 322 | ARG  | C-N    | 5.57  | 1.41        | 1.33     |
| 1   | G     | 428 | LYS  | N-CA   | -5.57 | 1.39        | 1.46     |
| 1   | K     | 139 | GLU  | C-N    | 5.57  | 1.40        | 1.33     |
| 1   | A     | 170 | SER  | N-CA   | 5.56  | 1.53        | 1.46     |
| 1   | S     | 453 | SER  | C-N    | 5.56  | 1.41        | 1.33     |
| 1   | A     | 409 | ILE  | CA-C   | -5.56 | 1.46        | 1.52     |
| 1   | I     | 454 | LEU  | C-N    | 5.56  | 1.40        | 1.33     |
| 1   | K     | 178 | ARG  | NE-CZ  | 5.56  | 1.39        | 1.33     |
| 1   | M     | 461 | ASN  | CB-CG  | 5.56  | 1.66        | 1.52     |
| 1   | S     | 242 | GLU  | CA-C   | -5.56 | 1.45        | 1.52     |
| 1   | F     | 322 | ARG  | CA-C   | 5.56  | 1.60        | 1.53     |
| 1   | R     | 527 | ASP  | N-CA   | -5.56 | 1.39        | 1.46     |
| 1   | L     | 479 | ASN  | CA-CB  | 5.56  | 1.61        | 1.53     |
| 1   | P     | 345 | GLU  | CA-C   | -5.56 | 1.45        | 1.52     |
| 1   | E     | 228 | VAL  | CA-CB  | -5.55 | 1.47        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | M     | 43  | GLU  | N-CA  | -5.55 | 1.39        | 1.46     |
| 1   | S     | 130 | ILE  | C-O   | -5.55 | 1.17        | 1.24     |
| 1   | P     | 304 | ILE  | CA-C  | 5.55  | 1.60        | 1.52     |
| 1   | A     | 85  | ALA  | CA-C  | 5.55  | 1.60        | 1.52     |
| 1   | K     | 429 | LEU  | C-N   | 5.55  | 1.41        | 1.33     |
| 1   | B     | 360 | ARG  | CA-C  | -5.55 | 1.45        | 1.52     |
| 1   | I     | 339 | VAL  | N-CA  | -5.55 | 1.39        | 1.46     |
| 1   | D     | 484 | TRP  | CA-CB | 5.54  | 1.60        | 1.53     |
| 1   | C     | 249 | ILE  | CA-CB | 5.54  | 1.60        | 1.53     |
| 1   | G     | 130 | ILE  | C-N   | 5.54  | 1.40        | 1.34     |
| 1   | R     | 115 | VAL  | C-N   | 5.54  | 1.40        | 1.33     |
| 1   | I     | 68  | ILE  | CA-C  | -5.54 | 1.46        | 1.52     |
| 1   | O     | 524 | LEU  | C-O   | 5.54  | 1.31        | 1.24     |
| 1   | H     | 144 | GLN  | CA-CB | 5.54  | 1.62        | 1.53     |
| 1   | K     | 427 | LYS  | C-N   | 5.54  | 1.41        | 1.34     |
| 1   | B     | 479 | ASN  | CA-CB | 5.54  | 1.63        | 1.53     |
| 1   | D     | 347 | SER  | CA-C  | -5.54 | 1.46        | 1.52     |
| 1   | K     | 338 | ARG  | NE-CZ | 5.53  | 1.39        | 1.33     |
| 1   | L     | 232 | VAL  | CA-CB | 5.53  | 1.60        | 1.54     |
| 1   | M     | 320 | VAL  | CA-CB | -5.53 | 1.47        | 1.54     |
| 1   | A     | 379 | ILE  | CA-CB | -5.53 | 1.46        | 1.54     |
| 1   | A     | 397 | ALA  | C-N   | 5.53  | 1.41        | 1.33     |
| 1   | C     | 191 | GLN  | CA-C  | 5.53  | 1.59        | 1.52     |
| 1   | H     | 208 | GLN  | C-N   | 5.53  | 1.40        | 1.33     |
| 1   | S     | 413 | ARG  | CD-NE | 5.53  | 1.53        | 1.46     |
| 1   | B     | 331 | LEU  | CA-C  | 5.53  | 1.60        | 1.52     |
| 1   | N     | 68  | ILE  | CA-CB | 5.53  | 1.60        | 1.54     |
| 1   | E     | 81  | LEU  | N-CA  | 5.53  | 1.53        | 1.46     |
| 1   | Q     | 484 | TRP  | C-N   | 5.53  | 1.41        | 1.33     |
| 1   | C     | 359 | GLU  | C-O   | -5.52 | 1.17        | 1.24     |
| 1   | D     | 127 | HIS  | CA-C  | 5.52  | 1.59        | 1.53     |
| 1   | C     | 269 | PRO  | N-CA  | -5.52 | 1.40        | 1.47     |
| 1   | I     | 432 | TYR  | CA-CB | 5.52  | 1.62        | 1.53     |
| 1   | O     | 209 | ILE  | CA-CB | -5.52 | 1.46        | 1.54     |
| 1   | D     | 366 | LYS  | C-O   | 5.52  | 1.30        | 1.24     |
| 1   | E     | 137 | LYS  | CA-CB | 5.52  | 1.61        | 1.53     |
| 1   | N     | 232 | VAL  | N-CA  | -5.52 | 1.40        | 1.46     |
| 1   | H     | 405 | VAL  | C-N   | 5.52  | 1.41        | 1.34     |
| 1   | R     | 376 | PRO  | C-O   | -5.52 | 1.17        | 1.24     |
| 1   | D     | 525 | ARG  | NE-CZ | 5.51  | 1.39        | 1.33     |
| 1   | D     | 531 | SER  | CA-CB | 5.51  | 1.60        | 1.53     |
| 1   | K     | 44  | GLU  | N-CA  | -5.51 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 435 | GLN  | CA-C    | -5.51 | 1.45        | 1.52     |
| 1   | P     | 50  | TYR  | CZ-OH   | 5.51  | 1.49        | 1.38     |
| 1   | C     | 51  | GLY  | C-N     | 5.51  | 1.39        | 1.33     |
| 1   | D     | 180 | TYR  | C-N     | 5.51  | 1.40        | 1.33     |
| 1   | Q     | 297 | VAL  | CA-C    | 5.51  | 1.59        | 1.52     |
| 1   | S     | 181 | ILE  | C-N     | 5.51  | 1.40        | 1.33     |
| 1   | P     | 125 | ASP  | CA-CB   | 5.51  | 1.62        | 1.53     |
| 1   | P     | 457 | ILE  | C-O     | -5.51 | 1.17        | 1.24     |
| 1   | F     | 144 | GLN  | C-N     | 5.50  | 1.41        | 1.33     |
| 1   | N     | 66  | ILE  | CA-C    | -5.50 | 1.45        | 1.52     |
| 1   | R     | 109 | ILE  | CA-CB   | -5.50 | 1.48        | 1.54     |
| 1   | P     | 290 | ILE  | C-N     | 5.50  | 1.41        | 1.33     |
| 1   | S     | 234 | HIS  | CE1-NE2 | -5.50 | 1.27        | 1.32     |
| 1   | M     | 125 | ASP  | CA-CB   | 5.50  | 1.61        | 1.53     |
| 1   | Q     | 103 | GLY  | C-N     | 5.50  | 1.41        | 1.33     |
| 1   | B     | 491 | ALA  | CA-CB   | 5.50  | 1.62        | 1.54     |
| 1   | M     | 252 | SER  | N-CA    | -5.50 | 1.39        | 1.45     |
| 1   | R     | 230 | LYS  | CA-C    | -5.50 | 1.45        | 1.52     |
| 1   | S     | 56  | ASP  | CA-C    | -5.50 | 1.45        | 1.52     |
| 1   | F     | 374 | LYS  | CA-C    | 5.50  | 1.59        | 1.52     |
| 1   | G     | 46  | LEU  | C-O     | -5.50 | 1.16        | 1.23     |
| 1   | S     | 408 | VAL  | CA-C    | 5.50  | 1.59        | 1.52     |
| 1   | S     | 530 | VAL  | CA-C    | -5.50 | 1.45        | 1.52     |
| 1   | E     | 56  | ASP  | CA-C    | 5.49  | 1.59        | 1.52     |
| 1   | O     | 294 | GLY  | CA-C    | -5.49 | 1.43        | 1.51     |
| 1   | N     | 84  | PRO  | N-CA    | -5.49 | 1.40        | 1.47     |
| 1   | R     | 371 | GLU  | N-CA    | -5.49 | 1.39        | 1.45     |
| 1   | K     | 398 | LEU  | N-CA    | -5.49 | 1.39        | 1.46     |
| 1   | L     | 432 | TYR  | CA-CB   | 5.49  | 1.62        | 1.53     |
| 1   | M     | 163 | LYS  | C-O     | -5.49 | 1.17        | 1.24     |
| 1   | M     | 321 | ARG  | CD-NE   | 5.49  | 1.53        | 1.46     |
| 1   | P     | 380 | SER  | N-CA    | -5.48 | 1.38        | 1.45     |
| 1   | Q     | 237 | MET  | CA-C    | 5.48  | 1.59        | 1.53     |
| 1   | C     | 487 | ILE  | C-N     | 5.48  | 1.41        | 1.33     |
| 1   | D     | 499 | GLN  | CA-CB   | 5.48  | 1.62        | 1.53     |
| 1   | I     | 261 | ASP  | N-CA    | -5.48 | 1.39        | 1.46     |
| 1   | P     | 240 | ARG  | C-O     | 5.48  | 1.29        | 1.23     |
| 1   | C     | 126 | VAL  | CA-CB   | -5.48 | 1.47        | 1.54     |
| 1   | D     | 45  | ALA  | CA-C    | -5.48 | 1.45        | 1.52     |
| 1   | F     | 272 | MET  | N-CA    | -5.48 | 1.40        | 1.46     |
| 1   | H     | 400 | ASP  | C-O     | -5.48 | 1.17        | 1.24     |
| 1   | I     | 192 | VAL  | CA-CB   | -5.48 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 341 | SER  | CA-C    | -5.48 | 1.45        | 1.52     |
| 1   | O     | 234 | HIS  | CB-CG   | 5.48  | 1.57        | 1.50     |
| 1   | A     | 114 | LEU  | CA-CB   | 5.47  | 1.61        | 1.53     |
| 1   | G     | 484 | TRP  | CA-C    | -5.47 | 1.45        | 1.52     |
| 1   | K     | 514 | LYS  | C-N     | 5.47  | 1.40        | 1.33     |
| 1   | B     | 114 | LEU  | CA-C    | -5.47 | 1.45        | 1.52     |
| 1   | I     | 219 | ASP  | N-CA    | -5.47 | 1.38        | 1.46     |
| 1   | K     | 423 | ILE  | N-CA    | 5.47  | 1.52        | 1.46     |
| 1   | R     | 497 | MET  | CA-CB   | 5.47  | 1.62        | 1.53     |
| 1   | A     | 390 | LEU  | C-O     | 5.47  | 1.30        | 1.24     |
| 1   | B     | 288 | ASP  | N-CA    | 5.47  | 1.53        | 1.46     |
| 1   | C     | 468 | ASP  | CA-C    | -5.47 | 1.45        | 1.52     |
| 1   | I     | 431 | LYS  | C-N     | 5.47  | 1.40        | 1.33     |
| 1   | I     | 432 | TYR  | CA-C    | -5.47 | 1.46        | 1.52     |
| 1   | K     | 222 | LEU  | CA-C    | -5.47 | 1.46        | 1.52     |
| 1   | E     | 84  | PRO  | C-N     | 5.46  | 1.40        | 1.33     |
| 1   | Q     | 108 | VAL  | CA-CB   | -5.46 | 1.47        | 1.54     |
| 1   | F     | 317 | VAL  | C-N     | 5.46  | 1.41        | 1.33     |
| 1   | P     | 200 | TRP  | CA-C    | 5.46  | 1.59        | 1.52     |
| 1   | F     | 109 | ILE  | C-N     | 5.46  | 1.41        | 1.33     |
| 1   | H     | 162 | ARG  | CA-CB   | 5.46  | 1.62        | 1.53     |
| 1   | H     | 221 | GLN  | N-CA    | -5.46 | 1.39        | 1.46     |
| 1   | K     | 265 | ARG  | NE-CZ   | 5.46  | 1.39        | 1.33     |
| 1   | K     | 383 | ILE  | CA-CB   | 5.46  | 1.61        | 1.54     |
| 1   | Q     | 504 | GLU  | CA-CB   | 5.46  | 1.62        | 1.54     |
| 1   | A     | 518 | GLU  | C-N     | 5.46  | 1.40        | 1.33     |
| 1   | L     | 442 | LEU  | CA-CB   | 5.46  | 1.62        | 1.53     |
| 1   | L     | 498 | TRP  | NE1-CE2 | 5.46  | 1.43        | 1.37     |
| 1   | Q     | 36  | ILE  | CA-CB   | -5.46 | 1.48        | 1.54     |
| 1   | E     | 374 | LYS  | CA-C    | -5.46 | 1.45        | 1.52     |
| 1   | G     | 75  | ILE  | CA-C    | 5.46  | 1.60        | 1.52     |
| 1   | I     | 432 | TYR  | N-CA    | -5.46 | 1.40        | 1.46     |
| 1   | E     | 350 | ASP  | C-N     | 5.45  | 1.40        | 1.33     |
| 1   | K     | 258 | PRO  | C-O     | -5.45 | 1.16        | 1.24     |
| 1   | C     | 342 | ASN  | N-CA    | 5.45  | 1.52        | 1.46     |
| 1   | S     | 91  | GLN  | CA-C    | 5.45  | 1.59        | 1.52     |
| 1   | C     | 201 | TYR  | C-N     | 5.45  | 1.40        | 1.33     |
| 1   | L     | 274 | LYS  | N-CA    | 5.45  | 1.53        | 1.46     |
| 1   | S     | 216 | SER  | CA-CB   | 5.45  | 1.63        | 1.53     |
| 1   | P     | 48  | SER  | C-N     | 5.44  | 1.42        | 1.33     |
| 1   | I     | 152 | THR  | CA-C    | -5.44 | 1.45        | 1.52     |
| 1   | I     | 450 | ALA  | N-CA    | -5.44 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | L     | 386 | GLY  | CA-C    | -5.44 | 1.45        | 1.52     |
| 1   | N     | 96  | GLN  | N-CA    | -5.44 | 1.39        | 1.46     |
| 1   | O     | 186 | VAL  | CA-CB   | -5.44 | 1.48        | 1.54     |
| 1   | P     | 256 | GLU  | N-CA    | 5.44  | 1.53        | 1.46     |
| 1   | C     | 321 | ARG  | NE-CZ   | 5.44  | 1.39        | 1.33     |
| 1   | C     | 258 | PRO  | N-CA    | -5.44 | 1.42        | 1.47     |
| 1   | N     | 263 | GLU  | C-N     | 5.44  | 1.40        | 1.33     |
| 1   | R     | 97  | ASP  | N-CA    | 5.44  | 1.52        | 1.46     |
| 1   | B     | 474 | ARG  | N-CA    | 5.44  | 1.53        | 1.46     |
| 1   | E     | 259 | GLU  | CA-C    | 5.44  | 1.60        | 1.52     |
| 1   | F     | 299 | ILE  | CA-C    | -5.44 | 1.46        | 1.52     |
| 1   | L     | 459 | ILE  | C-N     | 5.44  | 1.40        | 1.33     |
| 1   | B     | 162 | ARG  | CA-CB   | 5.43  | 1.62        | 1.53     |
| 1   | F     | 138 | ALA  | N-CA    | -5.43 | 1.39        | 1.46     |
| 1   | G     | 114 | LEU  | N-CA    | -5.43 | 1.39        | 1.46     |
| 1   | H     | 246 | ILE  | C-N     | 5.43  | 1.40        | 1.33     |
| 1   | I     | 449 | ASN  | CA-CB   | 5.43  | 1.61        | 1.53     |
| 1   | P     | 428 | LYS  | CA-CB   | -5.43 | 1.44        | 1.53     |
| 1   | S     | 38  | ALA  | CA-C    | -5.43 | 1.45        | 1.52     |
| 1   | Q     | 240 | ARG  | CA-CB   | 5.43  | 1.62        | 1.53     |
| 1   | L     | 50  | TYR  | CA-C    | 5.43  | 1.60        | 1.53     |
| 1   | R     | 429 | LEU  | CA-C    | -5.43 | 1.45        | 1.52     |
| 1   | K     | 312 | LEU  | N-CA    | -5.43 | 1.39        | 1.46     |
| 1   | R     | 50  | TYR  | C-N     | 5.43  | 1.41        | 1.33     |
| 1   | B     | 515 | ALA  | CA-C    | -5.43 | 1.46        | 1.52     |
| 1   | D     | 267 | ASN  | CA-C    | -5.43 | 1.45        | 1.52     |
| 1   | G     | 34  | ALA  | C-O     | -5.43 | 1.17        | 1.24     |
| 1   | K     | 297 | VAL  | N-CA    | -5.42 | 1.40        | 1.46     |
| 1   | P     | 165 | ALA  | CA-CB   | -5.42 | 1.44        | 1.53     |
| 1   | C     | 200 | TRP  | CD2-CE3 | 5.42  | 1.49        | 1.40     |
| 1   | K     | 293 | THR  | N-CA    | -5.42 | 1.38        | 1.46     |
| 1   | B     | 426 | ALA  | CA-C    | -5.42 | 1.47        | 1.53     |
| 1   | P     | 221 | GLN  | CA-C    | 5.42  | 1.59        | 1.52     |
| 1   | P     | 481 | ASN  | C-N     | 5.42  | 1.41        | 1.33     |
| 1   | Q     | 470 | LEU  | N-CA    | -5.42 | 1.39        | 1.46     |
| 1   | C     | 252 | SER  | CA-CB   | 5.42  | 1.62        | 1.53     |
| 1   | M     | 240 | ARG  | CD-NE   | 5.42  | 1.53        | 1.46     |
| 1   | H     | 106 | THR  | N-CA    | -5.42 | 1.40        | 1.46     |
| 1   | M     | 390 | LEU  | CA-CB   | 5.42  | 1.61        | 1.53     |
| 1   | Q     | 34  | ALA  | C-N     | 5.41  | 1.40        | 1.33     |
| 1   | S     | 346 | ILE  | C-N     | 5.41  | 1.40        | 1.33     |
| 1   | S     | 259 | GLU  | CA-CB   | 5.41  | 1.60        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 424 | GLU  | CA-CB   | 5.41  | 1.61        | 1.53     |
| 1   | H     | 83  | HIS  | CE1-NE2 | 5.41  | 1.38        | 1.32     |
| 1   | M     | 389 | ARG  | C-N     | 5.41  | 1.41        | 1.33     |
| 1   | P     | 53  | ARG  | CD-NE   | 5.41  | 1.53        | 1.46     |
| 1   | P     | 221 | GLN  | C-O     | 5.41  | 1.30        | 1.23     |
| 1   | H     | 402 | LEU  | N-CA    | 5.41  | 1.52        | 1.46     |
| 1   | M     | 414 | ALA  | CA-C    | 5.41  | 1.58        | 1.52     |
| 1   | O     | 325 | LYS  | C-N     | 5.41  | 1.41        | 1.34     |
| 1   | S     | 358 | GLU  | CA-C    | -5.41 | 1.46        | 1.52     |
| 1   | C     | 62  | SER  | CA-C    | -5.41 | 1.45        | 1.52     |
| 1   | G     | 105 | LYS  | CA-C    | -5.41 | 1.45        | 1.52     |
| 1   | Q     | 471 | MET  | N-CA    | 5.41  | 1.52        | 1.46     |
| 1   | R     | 225 | GLY  | N-CA    | 5.41  | 1.50        | 1.45     |
| 1   | D     | 464 | PHE  | N-CA    | 5.41  | 1.52        | 1.45     |
| 1   | S     | 338 | ARG  | CA-C    | -5.41 | 1.45        | 1.52     |
| 1   | F     | 509 | LYS  | C-N     | 5.40  | 1.41        | 1.33     |
| 1   | M     | 468 | ASP  | CA-C    | 5.40  | 1.59        | 1.52     |
| 1   | N     | 162 | ARG  | CD-NE   | 5.40  | 1.53        | 1.46     |
| 1   | S     | 393 | GLU  | C-N     | 5.40  | 1.41        | 1.34     |
| 1   | I     | 211 | LYS  | CA-C    | -5.40 | 1.46        | 1.52     |
| 1   | P     | 313 | ALA  | C-N     | 5.40  | 1.41        | 1.33     |
| 1   | B     | 36  | ILE  | CA-CB   | 5.40  | 1.60        | 1.54     |
| 1   | K     | 68  | ILE  | N-CA    | -5.40 | 1.39        | 1.46     |
| 1   | O     | 96  | GLN  | C-O     | 5.40  | 1.30        | 1.23     |
| 1   | P     | 440 | GLU  | N-CA    | 5.40  | 1.53        | 1.46     |
| 1   | F     | 531 | SER  | CA-CB   | 5.40  | 1.61        | 1.53     |
| 1   | H     | 255 | VAL  | CA-C    | 5.39  | 1.58        | 1.53     |
| 1   | H     | 340 | VAL  | N-CA    | -5.39 | 1.40        | 1.46     |
| 1   | M     | 135 | TYR  | CA-CB   | 5.39  | 1.61        | 1.53     |
| 1   | D     | 191 | GLN  | CA-C    | 5.39  | 1.59        | 1.52     |
| 1   | E     | 164 | ILE  | CB-CG1  | 5.39  | 1.64        | 1.53     |
| 1   | I     | 277 | ASP  | CA-C    | -5.39 | 1.46        | 1.52     |
| 1   | N     | 465 | ASP  | CA-CB   | 5.39  | 1.62        | 1.52     |
| 1   | Q     | 393 | GLU  | CA-C    | 5.39  | 1.60        | 1.52     |
| 1   | I     | 400 | ASP  | N-CA    | -5.39 | 1.40        | 1.46     |
| 1   | M     | 128 | PRO  | N-CD    | -5.39 | 1.40        | 1.47     |
| 1   | A     | 525 | ARG  | CD-NE   | 5.39  | 1.53        | 1.46     |
| 1   | C     | 375 | ASN  | C-O     | -5.39 | 1.17        | 1.24     |
| 1   | Q     | 138 | ALA  | C-N     | 5.39  | 1.40        | 1.33     |
| 1   | F     | 299 | ILE  | CA-CB   | -5.39 | 1.46        | 1.55     |
| 1   | K     | 73  | ALA  | N-CA    | -5.39 | 1.39        | 1.46     |
| 1   | G     | 262 | ALA  | C-N     | 5.39  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 172 | LYS  | CA-C  | -5.38 | 1.45        | 1.53     |
| 1   | I     | 525 | ARG  | C-N   | 5.38  | 1.39        | 1.33     |
| 1   | N     | 126 | VAL  | CA-C  | 5.38  | 1.59        | 1.52     |
| 1   | A     | 131 | ILE  | N-CA  | 5.38  | 1.53        | 1.46     |
| 1   | F     | 371 | GLU  | CA-CB | 5.38  | 1.62        | 1.53     |
| 1   | H     | 508 | VAL  | CA-C  | 5.38  | 1.59        | 1.52     |
| 1   | K     | 353 | TYR  | C-N   | 5.38  | 1.40        | 1.33     |
| 1   | L     | 28  | GLY  | N-CA  | 5.38  | 1.54        | 1.45     |
| 1   | B     | 434 | PRO  | N-CD  | -5.38 | 1.40        | 1.47     |
| 1   | R     | 232 | VAL  | CA-C  | 5.38  | 1.59        | 1.52     |
| 1   | F     | 478 | GLU  | CA-CB | 5.38  | 1.62        | 1.53     |
| 1   | B     | 467 | ILE  | CA-CB | -5.38 | 1.48        | 1.54     |
| 1   | K     | 512 | ALA  | N-CA  | -5.38 | 1.40        | 1.46     |
| 1   | L     | 260 | LEU  | CA-CB | 5.38  | 1.61        | 1.53     |
| 1   | N     | 154 | SER  | C-N   | 5.38  | 1.40        | 1.33     |
| 1   | F     | 81  | LEU  | CA-CB | 5.38  | 1.64        | 1.53     |
| 1   | O     | 68  | ILE  | C-N   | 5.38  | 1.40        | 1.33     |
| 1   | Q     | 478 | GLU  | CA-C  | -5.38 | 1.45        | 1.52     |
| 1   | M     | 40  | LYS  | CA-CB | 5.38  | 1.61        | 1.53     |
| 1   | R     | 100 | THR  | CA-C  | -5.38 | 1.45        | 1.52     |
| 1   | D     | 216 | SER  | C-N   | 5.37  | 1.39        | 1.34     |
| 1   | P     | 224 | TYR  | N-CA  | -5.37 | 1.40        | 1.46     |
| 1   | B     | 320 | VAL  | C-N   | 5.37  | 1.40        | 1.33     |
| 1   | K     | 134 | GLY  | CA-C  | -5.37 | 1.44        | 1.51     |
| 1   | S     | 316 | GLY  | CA-C  | -5.37 | 1.44        | 1.51     |
| 1   | B     | 242 | GLU  | CA-C  | 5.37  | 1.59        | 1.52     |
| 1   | B     | 107 | ALA  | C-N   | 5.37  | 1.40        | 1.33     |
| 1   | K     | 46  | LEU  | C-N   | 5.37  | 1.41        | 1.33     |
| 1   | A     | 498 | TRP  | C-O   | -5.37 | 1.17        | 1.24     |
| 1   | F     | 93  | ALA  | N-CA  | -5.37 | 1.40        | 1.46     |
| 1   | I     | 505 | PRO  | CA-C  | 5.37  | 1.60        | 1.52     |
| 1   | N     | 108 | VAL  | CA-C  | 5.37  | 1.59        | 1.52     |
| 1   | R     | 48  | SER  | CA-CB | 5.37  | 1.61        | 1.53     |
| 1   | G     | 525 | ARG  | C-N   | 5.36  | 1.39        | 1.33     |
| 1   | H     | 294 | GLY  | CA-C  | 5.36  | 1.59        | 1.51     |
| 1   | O     | 357 | ILE  | C-O   | 5.36  | 1.30        | 1.24     |
| 1   | R     | 113 | GLU  | N-CA  | -5.36 | 1.39        | 1.46     |
| 1   | G     | 327 | ASP  | C-N   | 5.36  | 1.41        | 1.33     |
| 1   | P     | 293 | THR  | CA-C  | -5.36 | 1.45        | 1.52     |
| 1   | G     | 154 | SER  | CA-CB | 5.36  | 1.61        | 1.53     |
| 1   | N     | 180 | TYR  | C-N   | -5.36 | 1.27        | 1.33     |
| 1   | P     | 368 | VAL  | C-O   | -5.36 | 1.17        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 217 | ILE  | C-N     | 5.36  | 1.41        | 1.33     |
| 1   | P     | 350 | ASP  | C-N     | 5.36  | 1.40        | 1.33     |
| 1   | P     | 471 | MET  | N-CA    | 5.36  | 1.52        | 1.46     |
| 1   | N     | 138 | ALA  | CA-C    | -5.36 | 1.45        | 1.52     |
| 1   | E     | 277 | ASP  | C-N     | 5.35  | 1.41        | 1.33     |
| 1   | P     | 183 | ASP  | N-CA    | -5.35 | 1.40        | 1.46     |
| 1   | R     | 274 | LYS  | C-N     | 5.35  | 1.40        | 1.33     |
| 1   | F     | 85  | ALA  | C-O     | -5.35 | 1.18        | 1.24     |
| 1   | L     | 227 | VAL  | C-O     | -5.35 | 1.18        | 1.24     |
| 1   | N     | 489 | LEU  | C-N     | 5.35  | 1.41        | 1.33     |
| 1   | N     | 528 | ASP  | C-N     | -5.35 | 1.26        | 1.33     |
| 1   | B     | 469 | LEU  | C-O     | -5.35 | 1.17        | 1.24     |
| 1   | H     | 59  | LEU  | CA-C    | -5.35 | 1.46        | 1.52     |
| 1   | I     | 514 | LYS  | C-N     | 5.35  | 1.40        | 1.33     |
| 1   | L     | 183 | ASP  | CA-CB   | 5.35  | 1.61        | 1.53     |
| 1   | M     | 458 | LEU  | N-CA    | -5.35 | 1.40        | 1.46     |
| 1   | O     | 351 | LEU  | C-N     | 5.35  | 1.36        | 1.33     |
| 1   | B     | 399 | ARG  | CD-NE   | 5.35  | 1.53        | 1.46     |
| 1   | D     | 527 | ASP  | CA-C    | -5.35 | 1.46        | 1.52     |
| 1   | O     | 451 | LEU  | CA-C    | 5.35  | 1.59        | 1.52     |
| 1   | R     | 85  | ALA  | N-CA    | -5.34 | 1.40        | 1.46     |
| 1   | B     | 155 | ILE  | CA-C    | -5.34 | 1.45        | 1.52     |
| 1   | F     | 51  | GLY  | C-N     | -5.34 | 1.27        | 1.34     |
| 1   | G     | 495 | VAL  | CA-C    | -5.34 | 1.47        | 1.52     |
| 1   | E     | 268 | ASP  | CA-C    | 5.34  | 1.58        | 1.52     |
| 1   | N     | 234 | HIS  | N-CA    | 5.34  | 1.52        | 1.46     |
| 1   | N     | 333 | ARG  | CD-NE   | 5.34  | 1.53        | 1.46     |
| 1   | H     | 200 | TRP  | CA-CB   | 5.34  | 1.62        | 1.53     |
| 1   | O     | 490 | TYR  | CA-CB   | 5.34  | 1.61        | 1.53     |
| 1   | S     | 399 | ARG  | C-N     | 5.34  | 1.41        | 1.33     |
| 1   | E     | 83  | HIS  | CE1-NE2 | 5.34  | 1.37        | 1.32     |
| 1   | K     | 318 | LEU  | N-CA    | 5.34  | 1.53        | 1.46     |
| 1   | C     | 411 | ASP  | N-CA    | -5.33 | 1.39        | 1.46     |
| 1   | E     | 155 | ILE  | C-N     | 5.33  | 1.41        | 1.33     |
| 1   | O     | 107 | ALA  | C-N     | 5.33  | 1.40        | 1.33     |
| 1   | D     | 400 | ASP  | N-CA    | -5.33 | 1.40        | 1.46     |
| 1   | Q     | 43  | GLU  | CA-CB   | 5.33  | 1.61        | 1.53     |
| 1   | E     | 209 | ILE  | C-O     | -5.33 | 1.18        | 1.24     |
| 1   | E     | 462 | ALA  | CA-CB   | 5.33  | 1.62        | 1.53     |
| 1   | K     | 452 | GLU  | N-CA    | -5.33 | 1.39        | 1.46     |
| 1   | S     | 98  | GLU  | CA-C    | -5.33 | 1.46        | 1.53     |
| 1   | L     | 472 | LYS  | N-CA    | 5.32  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | N     | 449 | ASN  | CA-C  | -5.32 | 1.45        | 1.52     |
| 1   | A     | 479 | ASN  | CA-CB | 5.32  | 1.62        | 1.53     |
| 1   | C     | 256 | GLU  | CA-CB | 5.32  | 1.61        | 1.53     |
| 1   | F     | 333 | ARG  | CA-C  | 5.32  | 1.60        | 1.52     |
| 1   | F     | 398 | LEU  | C-N   | 5.32  | 1.40        | 1.33     |
| 1   | E     | 290 | ILE  | C-N   | 5.32  | 1.41        | 1.33     |
| 1   | M     | 393 | GLU  | C-N   | 5.32  | 1.41        | 1.34     |
| 1   | D     | 466 | PRO  | CA-C  | -5.32 | 1.44        | 1.52     |
| 1   | S     | 424 | GLU  | N-CA  | 5.32  | 1.52        | 1.46     |
| 1   | A     | 407 | ASP  | C-N   | 5.32  | 1.40        | 1.33     |
| 1   | I     | 176 | GLY  | C-N   | 5.32  | 1.41        | 1.33     |
| 1   | P     | 430 | ARG  | N-CA  | -5.32 | 1.40        | 1.46     |
| 1   | B     | 256 | GLU  | CA-CB | 5.31  | 1.63        | 1.53     |
| 1   | D     | 121 | LEU  | CA-CB | 5.31  | 1.61        | 1.53     |
| 1   | F     | 271 | GLN  | N-CA  | -5.31 | 1.39        | 1.46     |
| 1   | G     | 34  | ALA  | N-CA  | -5.31 | 1.40        | 1.46     |
| 1   | S     | 416 | ALA  | CA-C  | 5.31  | 1.59        | 1.52     |
| 1   | S     | 444 | VAL  | N-CA  | -5.31 | 1.40        | 1.46     |
| 1   | C     | 440 | GLU  | N-CA  | 5.31  | 1.53        | 1.46     |
| 1   | F     | 97  | ASP  | C-O   | 5.31  | 1.31        | 1.24     |
| 1   | R     | 320 | VAL  | C-O   | -5.31 | 1.18        | 1.24     |
| 1   | R     | 443 | ALA  | C-O   | -5.31 | 1.18        | 1.24     |
| 1   | L     | 152 | THR  | C-N   | 5.31  | 1.40        | 1.33     |
| 1   | S     | 154 | SER  | CA-C  | 5.31  | 1.59        | 1.52     |
| 1   | F     | 444 | VAL  | CA-CB | -5.30 | 1.48        | 1.54     |
| 1   | G     | 104 | THR  | CA-C  | -5.30 | 1.46        | 1.52     |
| 1   | G     | 211 | LYS  | C-N   | 5.30  | 1.40        | 1.33     |
| 1   | M     | 109 | ILE  | CA-CB | 5.30  | 1.59        | 1.54     |
| 1   | P     | 522 | LEU  | N-CA  | -5.30 | 1.39        | 1.46     |
| 1   | R     | 355 | SER  | N-CA  | -5.30 | 1.39        | 1.46     |
| 1   | A     | 60  | VAL  | CA-CB | -5.30 | 1.47        | 1.53     |
| 1   | A     | 111 | SER  | CA-CB | 5.30  | 1.61        | 1.53     |
| 1   | B     | 485 | TYR  | CA-C  | -5.30 | 1.45        | 1.52     |
| 1   | G     | 196 | ARG  | CA-C  | 5.30  | 1.58        | 1.52     |
| 1   | R     | 354 | ALA  | CA-CB | 5.30  | 1.62        | 1.53     |
| 1   | B     | 365 | ASP  | CA-CB | 5.30  | 1.62        | 1.53     |
| 1   | E     | 413 | ARG  | CD-NE | 5.30  | 1.53        | 1.46     |
| 1   | Q     | 391 | VAL  | C-N   | 5.30  | 1.40        | 1.33     |
| 1   | A     | 117 | LYS  | N-CA  | -5.30 | 1.39        | 1.46     |
| 1   | F     | 203 | ASP  | C-N   | 5.30  | 1.41        | 1.34     |
| 1   | H     | 196 | ARG  | CA-C  | 5.30  | 1.58        | 1.52     |
| 1   | K     | 265 | ARG  | CD-NE | 5.30  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | N     | 128 | PRO  | CA-CB  | -5.30 | 1.46        | 1.53     |
| 1   | P     | 430 | ARG  | CZ-NH2 | -5.30 | 1.26        | 1.33     |
| 1   | P     | 443 | ALA  | C-N    | 5.30  | 1.40        | 1.33     |
| 1   | L     | 390 | LEU  | CA-C   | -5.30 | 1.45        | 1.52     |
| 1   | E     | 297 | VAL  | C-N    | -5.30 | 1.26        | 1.33     |
| 1   | O     | 479 | ASN  | CA-CB  | 5.30  | 1.61        | 1.53     |
| 1   | R     | 271 | GLN  | CA-C   | 5.30  | 1.59        | 1.52     |
| 1   | I     | 358 | GLU  | C-N    | 5.29  | 1.40        | 1.33     |
| 1   | D     | 360 | ARG  | CD-NE  | 5.29  | 1.53        | 1.46     |
| 1   | K     | 141 | VAL  | C-N    | 5.29  | 1.40        | 1.33     |
| 1   | R     | 148 | GLU  | CA-C   | 5.29  | 1.59        | 1.52     |
| 1   | A     | 164 | ILE  | N-CA   | 5.29  | 1.52        | 1.46     |
| 1   | B     | 48  | SER  | CA-CB  | 5.29  | 1.61        | 1.53     |
| 1   | D     | 516 | ALA  | C-N    | 5.29  | 1.41        | 1.34     |
| 1   | Q     | 348 | GLU  | C-O    | -5.29 | 1.18        | 1.24     |
| 1   | R     | 173 | ALA  | CA-C   | -5.29 | 1.46        | 1.52     |
| 1   | C     | 217 | ILE  | CA-CB  | -5.29 | 1.47        | 1.54     |
| 1   | E     | 210 | VAL  | CA-C   | 5.29  | 1.58        | 1.52     |
| 1   | F     | 50  | TYR  | N-CA   | -5.29 | 1.39        | 1.46     |
| 1   | F     | 266 | ILE  | C-O    | -5.29 | 1.18        | 1.24     |
| 1   | G     | 80  | ASP  | CA-C   | -5.29 | 1.46        | 1.52     |
| 1   | M     | 368 | VAL  | CA-C   | -5.29 | 1.46        | 1.52     |
| 1   | N     | 458 | LEU  | C-N    | 5.29  | 1.40        | 1.33     |
| 1   | I     | 352 | GLY  | C-O    | -5.28 | 1.18        | 1.23     |
| 1   | R     | 407 | ASP  | N-CA   | -5.28 | 1.39        | 1.46     |
| 1   | I     | 478 | GLU  | C-N    | 5.28  | 1.40        | 1.33     |
| 1   | O     | 435 | GLN  | N-CA   | -5.28 | 1.39        | 1.46     |
| 1   | S     | 529 | VAL  | CA-C   | -5.28 | 1.46        | 1.52     |
| 1   | A     | 367 | MET  | N-CA   | -5.28 | 1.39        | 1.45     |
| 1   | K     | 487 | ILE  | CA-C   | 5.28  | 1.59        | 1.52     |
| 1   | F     | 404 | THR  | N-CA   | -5.28 | 1.40        | 1.46     |
| 1   | I     | 149 | LEU  | CA-C   | 5.28  | 1.59        | 1.52     |
| 1   | N     | 318 | LEU  | C-N    | 5.28  | 1.41        | 1.33     |
| 1   | R     | 209 | ILE  | CA-C   | -5.28 | 1.45        | 1.52     |
| 1   | B     | 353 | TYR  | CA-CB  | 5.27  | 1.60        | 1.53     |
| 1   | D     | 94  | LYS  | C-N    | 5.27  | 1.40        | 1.33     |
| 1   | D     | 493 | GLN  | C-N    | -5.27 | 1.27        | 1.33     |
| 1   | B     | 478 | GLU  | CA-CB  | 5.27  | 1.62        | 1.53     |
| 1   | A     | 340 | VAL  | CA-CB  | -5.27 | 1.48        | 1.54     |
| 1   | C     | 261 | ASP  | N-CA   | 5.27  | 1.52        | 1.46     |
| 1   | P     | 333 | ARG  | CD-NE  | 5.27  | 1.53        | 1.46     |
| 1   | S     | 234 | HIS  | C-N    | -5.27 | 1.28        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 228 | VAL  | CA-C   | 5.27  | 1.59        | 1.52     |
| 1   | I     | 327 | ASP  | N-CA   | 5.27  | 1.53        | 1.46     |
| 1   | N     | 285 | GLU  | CA-CB  | 5.27  | 1.61        | 1.53     |
| 1   | N     | 467 | ILE  | CA-C   | -5.27 | 1.46        | 1.52     |
| 1   | D     | 119 | GLU  | CA-CB  | 5.27  | 1.61        | 1.53     |
| 1   | K     | 105 | LYS  | CA-C   | -5.27 | 1.46        | 1.52     |
| 1   | K     | 386 | GLY  | CA-C   | -5.27 | 1.46        | 1.51     |
| 1   | K     | 488 | ASP  | C-N    | 5.27  | 1.41        | 1.33     |
| 1   | Q     | 123 | TYR  | CA-C   | 5.26  | 1.59        | 1.52     |
| 1   | R     | 457 | ILE  | CB-CG1 | 5.26  | 1.64        | 1.53     |
| 1   | H     | 180 | TYR  | CA-CB  | 5.26  | 1.61        | 1.53     |
| 1   | H     | 311 | TYR  | CA-C   | 5.26  | 1.59        | 1.52     |
| 1   | P     | 430 | ARG  | CA-C   | -5.26 | 1.46        | 1.52     |
| 1   | E     | 530 | VAL  | N-CA   | 5.26  | 1.52        | 1.46     |
| 1   | G     | 285 | GLU  | CA-CB  | 5.26  | 1.61        | 1.53     |
| 1   | H     | 239 | LYS  | CA-CB  | 5.26  | 1.62        | 1.53     |
| 1   | K     | 114 | LEU  | CA-CB  | -5.26 | 1.45        | 1.53     |
| 1   | L     | 404 | THR  | CA-C   | 5.26  | 1.59        | 1.52     |
| 1   | A     | 499 | GLN  | C-N    | 5.26  | 1.44        | 1.34     |
| 1   | R     | 503 | ILE  | N-CA   | -5.26 | 1.40        | 1.46     |
| 1   | A     | 453 | SER  | N-CA   | 5.26  | 1.52        | 1.46     |
| 1   | F     | 510 | MET  | CA-CB  | 5.26  | 1.62        | 1.53     |
| 1   | K     | 441 | GLN  | C-O    | -5.26 | 1.18        | 1.24     |
| 1   | N     | 386 | GLY  | C-N    | 5.26  | 1.40        | 1.33     |
| 1   | F     | 231 | GLU  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | H     | 57  | LYS  | CA-CB  | 5.25  | 1.61        | 1.53     |
| 1   | M     | 482 | ASN  | CA-CB  | -5.25 | 1.46        | 1.53     |
| 1   | S     | 361 | LYS  | N-CA   | -5.25 | 1.40        | 1.46     |
| 1   | S     | 436 | VAL  | CA-CB  | -5.25 | 1.48        | 1.54     |
| 1   | C     | 411 | ASP  | CA-C   | 5.25  | 1.59        | 1.52     |
| 1   | E     | 32  | VAL  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | P     | 132 | ILE  | CA-CB  | -5.25 | 1.48        | 1.54     |
| 1   | I     | 137 | LYS  | N-CA   | -5.25 | 1.40        | 1.46     |
| 1   | L     | 91  | GLN  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | M     | 430 | ARG  | CA-CB  | 5.25  | 1.61        | 1.53     |
| 1   | S     | 362 | VAL  | C-N    | 5.25  | 1.41        | 1.33     |
| 1   | A     | 492 | GLY  | N-CA   | 5.25  | 1.52        | 1.45     |
| 1   | H     | 413 | ARG  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | F     | 141 | VAL  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | H     | 500 | LYS  | C-N    | 5.25  | 1.40        | 1.33     |
| 1   | G     | 150 | ALA  | C-N    | 5.24  | 1.40        | 1.33     |
| 1   | P     | 294 | GLY  | N-CA   | 5.24  | 1.52        | 1.45     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 460 | GLU  | C-N   | 5.24  | 1.41        | 1.33     |
| 1   | K     | 256 | GLU  | N-CA  | -5.24 | 1.40        | 1.46     |
| 1   | L     | 428 | LYS  | CA-C  | 5.24  | 1.59        | 1.52     |
| 1   | O     | 495 | VAL  | CA-CB | -5.24 | 1.47        | 1.54     |
| 1   | C     | 300 | CYS  | C-N   | 5.24  | 1.41        | 1.33     |
| 1   | D     | 112 | GLY  | C-N   | 5.24  | 1.41        | 1.33     |
| 1   | D     | 237 | MET  | CA-CB | 5.24  | 1.61        | 1.52     |
| 1   | G     | 482 | ASN  | N-CA  | -5.24 | 1.39        | 1.46     |
| 1   | M     | 521 | THR  | C-N   | 5.24  | 1.41        | 1.33     |
| 1   | N     | 63  | LEU  | CA-CB | 5.24  | 1.63        | 1.53     |
| 1   | O     | 188 | ALA  | CA-C  | 5.24  | 1.59        | 1.52     |
| 1   | E     | 259 | GLU  | N-CA  | 5.24  | 1.52        | 1.46     |
| 1   | I     | 455 | VAL  | CA-C  | 5.24  | 1.60        | 1.52     |
| 1   | A     | 507 | LEU  | C-N   | 5.23  | 1.40        | 1.33     |
| 1   | B     | 77  | ASP  | CA-CB | 5.23  | 1.61        | 1.53     |
| 1   | C     | 279 | GLU  | CA-C  | -5.23 | 1.46        | 1.52     |
| 1   | E     | 193 | ALA  | C-N   | 5.23  | 1.40        | 1.33     |
| 1   | P     | 80  | ASP  | C-N   | -5.23 | 1.26        | 1.33     |
| 1   | A     | 285 | GLU  | CA-CB | 5.23  | 1.61        | 1.53     |
| 1   | H     | 248 | LEU  | CA-C  | -5.23 | 1.46        | 1.53     |
| 1   | F     | 325 | LYS  | N-CA  | 5.23  | 1.52        | 1.46     |
| 1   | S     | 481 | ASN  | C-N   | 5.23  | 1.40        | 1.33     |
| 1   | O     | 308 | ALA  | N-CA  | -5.22 | 1.39        | 1.46     |
| 1   | O     | 383 | ILE  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | R     | 47  | LYS  | CA-C  | 5.22  | 1.59        | 1.52     |
| 1   | R     | 369 | PHE  | C-N   | 5.22  | 1.40        | 1.33     |
| 1   | D     | 224 | TYR  | CA-CB | 5.22  | 1.59        | 1.52     |
| 1   | D     | 420 | ALA  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | E     | 515 | ALA  | CA-C  | -5.22 | 1.46        | 1.52     |
| 1   | D     | 505 | PRO  | CA-C  | 5.22  | 1.59        | 1.52     |
| 1   | B     | 367 | MET  | N-CA  | -5.22 | 1.39        | 1.45     |
| 1   | E     | 306 | GLU  | C-N   | 5.22  | 1.40        | 1.33     |
| 1   | I     | 411 | ASP  | C-N   | 5.22  | 1.39        | 1.32     |
| 1   | S     | 256 | GLU  | N-CA  | -5.22 | 1.39        | 1.46     |
| 1   | O     | 467 | ILE  | C-N   | 5.22  | 1.40        | 1.33     |
| 1   | S     | 376 | PRO  | C-N   | -5.22 | 1.27        | 1.33     |
| 1   | D     | 304 | ILE  | C-O   | -5.22 | 1.18        | 1.24     |
| 1   | L     | 51  | GLY  | N-CA  | 5.22  | 1.51        | 1.44     |
| 1   | N     | 232 | VAL  | C-N   | -5.22 | 1.27        | 1.34     |
| 1   | E     | 266 | ILE  | N-CA  | 5.21  | 1.52        | 1.46     |
| 1   | M     | 201 | TYR  | C-N   | 5.21  | 1.39        | 1.33     |
| 1   | N     | 100 | THR  | N-CA  | 5.21  | 1.52        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | N     | 511 | ASN  | CA-CB   | 5.21  | 1.61        | 1.53     |
| 1   | O     | 342 | ASN  | CA-C    | -5.21 | 1.46        | 1.52     |
| 1   | P     | 455 | VAL  | C-N     | 5.21  | 1.40        | 1.33     |
| 1   | C     | 390 | LEU  | C-N     | 5.21  | 1.40        | 1.33     |
| 1   | E     | 502 | VAL  | N-CA    | -5.21 | 1.39        | 1.47     |
| 1   | E     | 519 | ALA  | C-O     | -5.21 | 1.18        | 1.24     |
| 1   | G     | 347 | SER  | C-N     | 5.21  | 1.41        | 1.33     |
| 1   | L     | 411 | ASP  | N-CA    | -5.21 | 1.39        | 1.46     |
| 1   | M     | 369 | PHE  | CA-C    | -5.21 | 1.46        | 1.52     |
| 1   | M     | 462 | ALA  | CA-C    | -5.21 | 1.45        | 1.52     |
| 1   | N     | 349 | GLN  | N-CA    | -5.21 | 1.39        | 1.46     |
| 1   | P     | 40  | LYS  | C-O     | -5.21 | 1.18        | 1.24     |
| 1   | M     | 91  | GLN  | N-CA    | 5.21  | 1.52        | 1.46     |
| 1   | O     | 308 | ALA  | CA-CB   | 5.21  | 1.62        | 1.53     |
| 1   | A     | 199 | LYS  | C-O     | -5.21 | 1.18        | 1.23     |
| 1   | H     | 332 | ALA  | N-CA    | -5.21 | 1.39        | 1.46     |
| 1   | K     | 79  | MET  | C-O     | 5.21  | 1.30        | 1.23     |
| 1   | P     | 133 | SER  | N-CA    | 5.21  | 1.52        | 1.46     |
| 1   | P     | 454 | LEU  | C-O     | -5.21 | 1.18        | 1.24     |
| 1   | F     | 69  | THR  | CA-C    | 5.21  | 1.58        | 1.52     |
| 1   | P     | 451 | LEU  | C-O     | -5.21 | 1.18        | 1.24     |
| 1   | R     | 235 | PRO  | N-CD    | -5.21 | 1.40        | 1.47     |
| 1   | C     | 188 | ALA  | CA-C    | 5.21  | 1.59        | 1.52     |
| 1   | H     | 247 | ALA  | CA-CB   | 5.20  | 1.61        | 1.53     |
| 1   | H     | 359 | GLU  | CA-C    | 5.20  | 1.58        | 1.52     |
| 1   | M     | 48  | SER  | CA-CB   | 5.20  | 1.62        | 1.53     |
| 1   | R     | 105 | LYS  | N-CA    | -5.20 | 1.40        | 1.46     |
| 1   | F     | 91  | GLN  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | G     | 305 | ASP  | CA-C    | -5.20 | 1.46        | 1.53     |
| 1   | L     | 282 | LEU  | CA-C    | -5.20 | 1.46        | 1.52     |
| 1   | L     | 328 | LEU  | C-N     | 5.20  | 1.40        | 1.33     |
| 1   | M     | 277 | ASP  | N-CA    | -5.20 | 1.40        | 1.46     |
| 1   | H     | 314 | LYS  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | M     | 477 | HIS  | ND1-CE1 | 5.20  | 1.37        | 1.32     |
| 1   | N     | 239 | LYS  | CA-C    | 5.20  | 1.59        | 1.52     |
| 1   | S     | 502 | VAL  | CA-C    | 5.20  | 1.57        | 1.52     |
| 1   | C     | 265 | ARG  | CD-NE   | 5.19  | 1.53        | 1.46     |
| 1   | E     | 433 | ALA  | N-CA    | 5.19  | 1.53        | 1.46     |
| 1   | I     | 474 | ARG  | NE-CZ   | 5.19  | 1.38        | 1.33     |
| 1   | I     | 169 | LEU  | CA-CB   | 5.19  | 1.61        | 1.53     |
| 1   | Q     | 168 | SER  | C-O     | -5.19 | 1.16        | 1.23     |
| 1   | I     | 227 | VAL  | CA-CB   | -5.19 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 488 | ASP  | CA-CB   | 5.19  | 1.62        | 1.53     |
| 1   | E     | 76  | LEU  | C-N     | 5.19  | 1.40        | 1.33     |
| 1   | F     | 497 | MET  | CA-C    | 5.19  | 1.59        | 1.52     |
| 1   | H     | 66  | ILE  | CA-CB   | -5.19 | 1.48        | 1.54     |
| 1   | E     | 325 | LYS  | N-CA    | 5.19  | 1.52        | 1.46     |
| 1   | H     | 66  | ILE  | CB-CG1  | 5.19  | 1.63        | 1.53     |
| 1   | I     | 274 | LYS  | CA-C    | -5.19 | 1.45        | 1.52     |
| 1   | M     | 158 | THR  | CA-CB   | 5.19  | 1.62        | 1.53     |
| 1   | E     | 364 | GLU  | C-N     | 5.19  | 1.40        | 1.33     |
| 1   | K     | 405 | VAL  | C-N     | 5.19  | 1.41        | 1.34     |
| 1   | D     | 145 | THR  | N-CA    | 5.18  | 1.53        | 1.46     |
| 1   | G     | 465 | ASP  | CA-C    | 5.18  | 1.59        | 1.52     |
| 1   | H     | 147 | GLN  | N-CA    | 5.18  | 1.52        | 1.46     |
| 1   | O     | 127 | HIS  | CG-CD2  | 5.18  | 1.41        | 1.35     |
| 1   | S     | 325 | LYS  | CA-CB   | 5.18  | 1.62        | 1.53     |
| 1   | A     | 211 | LYS  | N-CA    | 5.18  | 1.52        | 1.46     |
| 1   | G     | 202 | VAL  | C-N     | 5.18  | 1.41        | 1.33     |
| 1   | G     | 436 | VAL  | CA-C    | 5.18  | 1.59        | 1.52     |
| 1   | H     | 50  | TYR  | CA-CB   | 5.18  | 1.61        | 1.53     |
| 1   | I     | 252 | SER  | CA-C    | -5.18 | 1.46        | 1.52     |
| 1   | L     | 50  | TYR  | C-N     | 5.18  | 1.41        | 1.33     |
| 1   | B     | 318 | LEU  | CA-CB   | 5.18  | 1.60        | 1.53     |
| 1   | D     | 508 | VAL  | N-CA    | -5.18 | 1.40        | 1.46     |
| 1   | H     | 477 | HIS  | ND1-CE1 | 5.18  | 1.37        | 1.32     |
| 1   | P     | 509 | LYS  | CA-CB   | 5.18  | 1.62        | 1.53     |
| 1   | I     | 287 | VAL  | CA-CB   | -5.18 | 1.48        | 1.54     |
| 1   | K     | 253 | LEU  | CA-CB   | 5.18  | 1.61        | 1.53     |
| 1   | L     | 378 | SER  | C-N     | 5.18  | 1.40        | 1.33     |
| 1   | M     | 129 | THR  | CA-C    | -5.18 | 1.45        | 1.52     |
| 1   | I     | 232 | VAL  | CA-C    | -5.18 | 1.45        | 1.53     |
| 1   | F     | 353 | TYR  | C-N     | 5.17  | 1.40        | 1.33     |
| 1   | G     | 92  | ILE  | C-N     | 5.17  | 1.40        | 1.33     |
| 1   | I     | 362 | VAL  | CA-CB   | -5.17 | 1.47        | 1.54     |
| 1   | K     | 94  | LYS  | N-CA    | 5.17  | 1.52        | 1.46     |
| 1   | P     | 102 | ASP  | C-N     | 5.17  | 1.41        | 1.33     |
| 1   | Q     | 350 | ASP  | C-N     | 5.17  | 1.40        | 1.33     |
| 1   | B     | 114 | LEU  | C-O     | -5.17 | 1.18        | 1.24     |
| 1   | R     | 454 | LEU  | N-CA    | -5.17 | 1.40        | 1.46     |
| 1   | H     | 146 | ILE  | C-N     | 5.17  | 1.40        | 1.33     |
| 1   | H     | 333 | ARG  | NE-CZ   | 5.17  | 1.38        | 1.33     |
| 1   | L     | 34  | ALA  | CA-C    | -5.17 | 1.46        | 1.52     |
| 1   | L     | 487 | ILE  | CA-C    | -5.17 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 148 | GLU  | C-N    | 5.17  | 1.41        | 1.33     |
| 1   | B     | 52  | PRO  | C-N    | 5.17  | 1.42        | 1.34     |
| 1   | M     | 338 | ARG  | C-N    | -5.17 | 1.27        | 1.33     |
| 1   | C     | 420 | ALA  | C-N    | 5.17  | 1.40        | 1.33     |
| 1   | K     | 497 | MET  | N-CA   | -5.17 | 1.40        | 1.46     |
| 1   | N     | 271 | GLN  | C-N    | 5.17  | 1.40        | 1.33     |
| 1   | F     | 311 | TYR  | CA-C   | 5.17  | 1.59        | 1.52     |
| 1   | I     | 258 | PRO  | N-CA   | -5.17 | 1.41        | 1.47     |
| 1   | C     | 332 | ALA  | CA-C   | 5.16  | 1.59        | 1.52     |
| 1   | K     | 426 | ALA  | CA-CB  | 5.16  | 1.60        | 1.53     |
| 1   | M     | 199 | LYS  | CA-C   | -5.16 | 1.46        | 1.52     |
| 1   | B     | 165 | ALA  | CA-C   | 5.16  | 1.59        | 1.52     |
| 1   | A     | 463 | GLY  | CA-C   | 5.16  | 1.59        | 1.51     |
| 1   | C     | 168 | SER  | N-CA   | 5.16  | 1.52        | 1.46     |
| 1   | G     | 507 | LEU  | CA-C   | -5.16 | 1.45        | 1.52     |
| 1   | M     | 343 | ILE  | N-CA   | -5.16 | 1.40        | 1.46     |
| 1   | O     | 93  | ALA  | C-N    | 5.16  | 1.40        | 1.33     |
| 1   | B     | 160 | LEU  | N-CA   | -5.16 | 1.39        | 1.46     |
| 1   | C     | 413 | ARG  | CZ-NH1 | -5.16 | 1.25        | 1.32     |
| 1   | O     | 224 | TYR  | CA-C   | 5.16  | 1.60        | 1.53     |
| 1   | O     | 418 | GLY  | N-CA   | 5.16  | 1.52        | 1.45     |
| 1   | R     | 190 | THR  | C-N    | 5.16  | 1.41        | 1.33     |
| 1   | R     | 301 | GLN  | CA-CB  | 5.16  | 1.61        | 1.53     |
| 1   | G     | 334 | ALA  | CA-C   | -5.16 | 1.45        | 1.52     |
| 1   | L     | 229 | ASP  | CA-CB  | 5.16  | 1.59        | 1.52     |
| 1   | N     | 333 | ARG  | NE-CZ  | 5.16  | 1.38        | 1.33     |
| 1   | R     | 180 | TYR  | CA-CB  | 5.16  | 1.61        | 1.53     |
| 1   | B     | 389 | ARG  | CA-CB  | 5.15  | 1.61        | 1.53     |
| 1   | H     | 63  | LEU  | C-N    | -5.15 | 1.26        | 1.33     |
| 1   | K     | 166 | MET  | C-N    | 5.15  | 1.40        | 1.33     |
| 1   | C     | 232 | VAL  | CA-C   | 5.15  | 1.59        | 1.52     |
| 1   | O     | 366 | LYS  | N-CA   | -5.15 | 1.39        | 1.46     |
| 1   | O     | 526 | ILE  | CA-C   | 5.15  | 1.58        | 1.52     |
| 1   | H     | 440 | GLU  | N-CA   | -5.15 | 1.39        | 1.46     |
| 1   | N     | 438 | GLY  | CA-C   | 5.15  | 1.59        | 1.51     |
| 1   | R     | 207 | ILE  | C-N    | 5.15  | 1.40        | 1.33     |
| 1   | H     | 494 | PRO  | N-CA   | -5.15 | 1.41        | 1.47     |
| 1   | R     | 37  | ALA  | C-N    | 5.15  | 1.40        | 1.33     |
| 1   | S     | 389 | ARG  | CD-NE  | 5.15  | 1.53        | 1.46     |
| 1   | B     | 44  | GLU  | C-N    | 5.15  | 1.41        | 1.33     |
| 1   | G     | 190 | THR  | N-CA   | 5.15  | 1.52        | 1.46     |
| 1   | G     | 163 | LYS  | C-N    | 5.14  | 1.40        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 508 | VAL  | CA-C  | -5.14 | 1.46        | 1.52     |
| 1   | S     | 41  | ALA  | CA-CB | 5.14  | 1.61        | 1.53     |
| 1   | D     | 74  | THR  | C-N   | 5.14  | 1.39        | 1.34     |
| 1   | D     | 421 | VAL  | CA-C  | 5.14  | 1.60        | 1.52     |
| 1   | R     | 181 | ILE  | CA-C  | 5.14  | 1.59        | 1.52     |
| 1   | E     | 283 | ILE  | CA-CB | -5.14 | 1.47        | 1.54     |
| 1   | A     | 252 | SER  | N-CA  | 5.14  | 1.52        | 1.46     |
| 1   | G     | 485 | TYR  | N-CA  | -5.14 | 1.39        | 1.46     |
| 1   | I     | 121 | LEU  | C-N   | 5.14  | 1.40        | 1.34     |
| 1   | P     | 472 | LYS  | C-O   | -5.14 | 1.17        | 1.24     |
| 1   | H     | 36  | ILE  | CA-CB | 5.14  | 1.59        | 1.54     |
| 1   | H     | 249 | ILE  | CA-CB | 5.14  | 1.59        | 1.53     |
| 1   | C     | 37  | ALA  | CA-C  | 5.14  | 1.59        | 1.52     |
| 1   | C     | 72  | GLY  | CA-C  | 5.14  | 1.59        | 1.51     |
| 1   | C     | 432 | TYR  | CA-C  | -5.14 | 1.46        | 1.52     |
| 1   | D     | 162 | ARG  | CD-NE | 5.14  | 1.53        | 1.46     |
| 1   | E     | 84  | PRO  | N-CD  | -5.14 | 1.40        | 1.47     |
| 1   | A     | 187 | LYS  | N-CA  | -5.13 | 1.40        | 1.46     |
| 1   | E     | 36  | ILE  | CA-C  | -5.13 | 1.47        | 1.52     |
| 1   | E     | 202 | VAL  | N-CA  | 5.13  | 1.52        | 1.46     |
| 1   | F     | 39  | VAL  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | F     | 256 | GLU  | CA-CB | 5.13  | 1.59        | 1.53     |
| 1   | G     | 448 | ALA  | N-CA  | 5.13  | 1.52        | 1.46     |
| 1   | P     | 41  | ALA  | CA-CB | 5.13  | 1.61        | 1.53     |
| 1   | Q     | 119 | GLU  | N-CA  | -5.13 | 1.40        | 1.46     |
| 1   | D     | 455 | VAL  | C-N   | -5.13 | 1.27        | 1.33     |
| 1   | E     | 180 | TYR  | N-CA  | 5.13  | 1.52        | 1.46     |
| 1   | Q     | 136 | LYS  | N-CA  | -5.13 | 1.40        | 1.46     |
| 1   | K     | 106 | THR  | CA-CB | 5.13  | 1.61        | 1.53     |
| 1   | S     | 163 | LYS  | C-N   | 5.13  | 1.40        | 1.33     |
| 1   | D     | 283 | ILE  | C-N   | 5.13  | 1.40        | 1.34     |
| 1   | M     | 187 | LYS  | CA-C  | 5.13  | 1.59        | 1.52     |
| 1   | C     | 138 | ALA  | N-CA  | -5.13 | 1.40        | 1.46     |
| 1   | E     | 504 | GLU  | N-CA  | -5.13 | 1.41        | 1.45     |
| 1   | G     | 424 | GLU  | CA-CB | 5.13  | 1.61        | 1.53     |
| 1   | R     | 28  | GLY  | N-CA  | 5.13  | 1.53        | 1.45     |
| 1   | S     | 520 | ALA  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | B     | 233 | VAL  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | I     | 51  | GLY  | C-N   | 5.13  | 1.38        | 1.33     |
| 1   | A     | 274 | LYS  | CA-C  | 5.12  | 1.60        | 1.52     |
| 1   | G     | 399 | ARG  | NE-CZ | 5.12  | 1.38        | 1.33     |
| 1   | R     | 475 | SER  | CA-CB | 5.12  | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 280 | GLU  | C-N    | 5.12  | 1.41        | 1.33     |
| 1   | D     | 395 | GLU  | C-N    | 5.12  | 1.40        | 1.33     |
| 1   | F     | 397 | ALA  | C-N    | 5.12  | 1.40        | 1.33     |
| 1   | K     | 162 | ARG  | CA-CB  | -5.12 | 1.45        | 1.53     |
| 1   | K     | 326 | SER  | CA-CB  | 5.12  | 1.62        | 1.53     |
| 1   | O     | 498 | TRP  | CA-CB  | 5.12  | 1.61        | 1.53     |
| 1   | E     | 392 | ASP  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | I     | 101 | ALA  | CA-C   | 5.12  | 1.59        | 1.52     |
| 1   | R     | 518 | GLU  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | F     | 223 | VAL  | CA-CB  | 5.12  | 1.60        | 1.54     |
| 1   | M     | 364 | GLU  | C-O    | -5.12 | 1.17        | 1.24     |
| 1   | P     | 41  | ALA  | C-N    | 5.12  | 1.40        | 1.33     |
| 1   | Q     | 422 | GLU  | C-O    | -5.12 | 1.18        | 1.24     |
| 1   | F     | 164 | ILE  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | F     | 299 | ILE  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | H     | 33  | ARG  | CA-C   | 5.12  | 1.59        | 1.52     |
| 1   | L     | 334 | ALA  | CA-CB  | 5.12  | 1.61        | 1.53     |
| 1   | F     | 188 | ALA  | CA-CB  | 5.12  | 1.61        | 1.53     |
| 1   | F     | 218 | ASN  | N-CA   | 5.12  | 1.53        | 1.46     |
| 1   | I     | 143 | LEU  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | R     | 274 | LYS  | CA-CB  | 5.12  | 1.62        | 1.53     |
| 1   | R     | 469 | LEU  | CA-CB  | 5.12  | 1.61        | 1.53     |
| 1   | B     | 181 | ILE  | CA-CB  | -5.11 | 1.48        | 1.54     |
| 1   | D     | 68  | ILE  | CA-C   | 5.11  | 1.58        | 1.52     |
| 1   | G     | 480 | GLU  | CA-C   | 5.11  | 1.60        | 1.52     |
| 1   | H     | 457 | ILE  | CA-C   | -5.11 | 1.46        | 1.52     |
| 1   | K     | 426 | ALA  | C-O    | -5.11 | 1.18        | 1.23     |
| 1   | R     | 243 | ASN  | CA-CB  | 5.11  | 1.61        | 1.53     |
| 1   | D     | 200 | TRP  | CA-CB  | 5.11  | 1.59        | 1.52     |
| 1   | I     | 213 | ALA  | CA-CB  | 5.11  | 1.62        | 1.53     |
| 1   | I     | 443 | ALA  | CA-CB  | 5.11  | 1.61        | 1.53     |
| 1   | L     | 272 | MET  | C-O    | -5.11 | 1.18        | 1.24     |
| 1   | M     | 116 | LYS  | CA-CB  | -5.11 | 1.45        | 1.53     |
| 1   | O     | 297 | VAL  | N-CA   | -5.11 | 1.40        | 1.46     |
| 1   | A     | 131 | ILE  | CB-CG1 | 5.11  | 1.63        | 1.53     |
| 1   | M     | 125 | ASP  | N-CA   | -5.11 | 1.39        | 1.46     |
| 1   | N     | 434 | PRO  | C-O    | -5.11 | 1.17        | 1.24     |
| 1   | C     | 87  | LYS  | C-O    | -5.11 | 1.17        | 1.24     |
| 1   | D     | 155 | ILE  | N-CA   | -5.11 | 1.39        | 1.46     |
| 1   | D     | 366 | LYS  | N-CA   | -5.11 | 1.39        | 1.46     |
| 1   | G     | 208 | GLN  | C-N    | -5.11 | 1.27        | 1.33     |
| 1   | N     | 126 | VAL  | C-N    | 5.11  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | R     | 286 | LYS  | C-O    | 5.11  | 1.30        | 1.24     |
| 1   | Q     | 71  | ASP  | CA-CB  | -5.10 | 1.46        | 1.53     |
| 1   | I     | 114 | LEU  | CA-C   | 5.10  | 1.59        | 1.52     |
| 1   | P     | 362 | VAL  | CA-CB  | -5.10 | 1.47        | 1.53     |
| 1   | E     | 283 | ILE  | CA-C   | -5.10 | 1.46        | 1.52     |
| 1   | F     | 482 | ASN  | N-CA   | -5.10 | 1.40        | 1.46     |
| 1   | I     | 511 | ASN  | CA-CB  | 5.10  | 1.61        | 1.53     |
| 1   | N     | 357 | ILE  | CA-CB  | -5.10 | 1.48        | 1.54     |
| 1   | E     | 430 | ARG  | CD-NE  | 5.10  | 1.53        | 1.46     |
| 1   | I     | 437 | GLY  | CA-C   | -5.10 | 1.46        | 1.52     |
| 1   | O     | 375 | ASN  | CA-C   | 5.10  | 1.58        | 1.52     |
| 1   | Q     | 212 | LYS  | C-N    | 5.10  | 1.40        | 1.33     |
| 1   | R     | 162 | ARG  | CD-NE  | 5.10  | 1.53        | 1.46     |
| 1   | B     | 73  | ALA  | CA-CB  | 5.10  | 1.61        | 1.53     |
| 1   | C     | 33  | ARG  | CD-NE  | 5.10  | 1.53        | 1.46     |
| 1   | L     | 278 | GLU  | CA-C   | -5.10 | 1.45        | 1.52     |
| 1   | B     | 251 | ALA  | CA-CB  | 5.09  | 1.62        | 1.53     |
| 1   | C     | 311 | TYR  | N-CA   | -5.09 | 1.40        | 1.46     |
| 1   | D     | 491 | ALA  | CA-C   | -5.09 | 1.45        | 1.52     |
| 1   | Q     | 190 | THR  | CA-CB  | -5.09 | 1.44        | 1.53     |
| 1   | E     | 527 | ASP  | CA-CB  | 5.09  | 1.61        | 1.53     |
| 1   | F     | 103 | GLY  | CA-C   | -5.09 | 1.44        | 1.51     |
| 1   | F     | 405 | VAL  | CA-C   | -5.09 | 1.46        | 1.52     |
| 1   | I     | 146 | ILE  | C-N    | 5.09  | 1.40        | 1.33     |
| 1   | L     | 249 | ILE  | N-CA   | -5.09 | 1.40        | 1.46     |
| 1   | S     | 37  | ALA  | CA-C   | 5.09  | 1.59        | 1.52     |
| 1   | E     | 300 | CYS  | CA-CB  | 5.09  | 1.61        | 1.53     |
| 1   | H     | 376 | PRO  | CA-CB  | 5.09  | 1.60        | 1.53     |
| 1   | I     | 252 | SER  | N-CA   | 5.09  | 1.52        | 1.46     |
| 1   | S     | 126 | VAL  | CA-CB  | 5.09  | 1.60        | 1.54     |
| 1   | D     | 110 | PHE  | CG-CD2 | 5.09  | 1.49        | 1.38     |
| 1   | I     | 451 | LEU  | C-N    | 5.09  | 1.40        | 1.33     |
| 1   | Q     | 417 | GLY  | C-N    | 5.09  | 1.38        | 1.33     |
| 1   | B     | 342 | ASN  | C-O    | -5.09 | 1.17        | 1.24     |
| 1   | C     | 250 | ASP  | N-CA   | -5.09 | 1.40        | 1.46     |
| 1   | D     | 75  | ILE  | CA-CB  | -5.09 | 1.47        | 1.54     |
| 1   | A     | 302 | LYS  | C-N    | 5.08  | 1.39        | 1.33     |
| 1   | K     | 292 | ALA  | N-CA   | -5.08 | 1.39        | 1.46     |
| 1   | L     | 474 | ARG  | CA-C   | 5.08  | 1.59        | 1.52     |
| 1   | M     | 234 | HIS  | CB-CG  | 5.08  | 1.57        | 1.50     |
| 1   | S     | 248 | LEU  | CA-CB  | 5.08  | 1.62        | 1.53     |
| 1   | H     | 484 | TRP  | CA-CB  | 5.08  | 1.60        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 448 | ALA  | C-N    | 5.08  | 1.40        | 1.33     |
| 1   | N     | 454 | LEU  | CA-C   | 5.08  | 1.59        | 1.52     |
| 1   | E     | 478 | GLU  | C-N    | 5.08  | 1.40        | 1.33     |
| 1   | N     | 129 | THR  | N-CA   | 5.08  | 1.52        | 1.46     |
| 1   | N     | 412 | GLY  | CA-C   | -5.08 | 1.44        | 1.51     |
| 1   | K     | 113 | GLU  | CD-OE1 | 5.08  | 1.34        | 1.25     |
| 1   | K     | 221 | GLN  | CA-C   | 5.08  | 1.58        | 1.52     |
| 1   | P     | 46  | LEU  | C-N    | 5.08  | 1.40        | 1.33     |
| 1   | P     | 480 | GLU  | C-N    | 5.08  | 1.41        | 1.33     |
| 1   | C     | 57  | LYS  | C-N    | 5.07  | 1.40        | 1.33     |
| 1   | G     | 71  | ASP  | C-N    | 5.07  | 1.41        | 1.33     |
| 1   | L     | 230 | LYS  | CA-CB  | 5.07  | 1.62        | 1.53     |
| 1   | N     | 298 | ILE  | C-O    | -5.07 | 1.18        | 1.24     |
| 1   | P     | 58  | MET  | C-N    | 5.07  | 1.40        | 1.33     |
| 1   | R     | 196 | ARG  | CD-NE  | 5.07  | 1.53        | 1.46     |
| 1   | D     | 158 | THR  | N-CA   | -5.07 | 1.39        | 1.46     |
| 1   | E     | 165 | ALA  | N-CA   | -5.07 | 1.40        | 1.46     |
| 1   | F     | 512 | ALA  | N-CA   | 5.07  | 1.52        | 1.46     |
| 1   | O     | 447 | TYR  | C-O    | -5.07 | 1.18        | 1.24     |
| 1   | A     | 312 | LEU  | CA-CB  | 5.07  | 1.61        | 1.53     |
| 1   | F     | 44  | GLU  | C-N    | 5.07  | 1.41        | 1.33     |
| 1   | G     | 375 | ASN  | CA-C   | 5.07  | 1.59        | 1.52     |
| 1   | M     | 102 | ASP  | C-N    | 5.07  | 1.40        | 1.33     |
| 1   | B     | 258 | PRO  | N-CA   | -5.07 | 1.41        | 1.47     |
| 1   | F     | 85  | ALA  | CA-CB  | 5.07  | 1.61        | 1.53     |
| 1   | F     | 304 | ILE  | CA-C   | -5.07 | 1.46        | 1.52     |
| 1   | M     | 86  | ALA  | C-N    | 5.07  | 1.40        | 1.33     |
| 1   | R     | 412 | GLY  | CA-C   | -5.07 | 1.44        | 1.51     |
| 1   | A     | 89  | LEU  | CA-CB  | 5.06  | 1.61        | 1.53     |
| 1   | C     | 457 | ILE  | CA-CB  | 5.06  | 1.60        | 1.54     |
| 1   | E     | 524 | LEU  | C-O    | -5.06 | 1.17        | 1.24     |
| 1   | G     | 132 | ILE  | CA-CB  | 5.06  | 1.60        | 1.54     |
| 1   | O     | 464 | PHE  | CA-CB  | 5.06  | 1.60        | 1.53     |
| 1   | P     | 435 | GLN  | N-CA   | -5.06 | 1.39        | 1.46     |
| 1   | B     | 305 | ASP  | CA-CB  | 5.06  | 1.61        | 1.53     |
| 1   | H     | 333 | ARG  | CA-CB  | 5.06  | 1.61        | 1.53     |
| 1   | I     | 69  | THR  | CA-C   | -5.06 | 1.46        | 1.52     |
| 1   | C     | 469 | LEU  | N-CA   | 5.05  | 1.52        | 1.46     |
| 1   | M     | 226 | ILE  | C-O    | 5.05  | 1.31        | 1.24     |
| 1   | Q     | 260 | LEU  | N-CA   | 5.05  | 1.52        | 1.46     |
| 1   | E     | 308 | ALA  | C-O    | -5.05 | 1.17        | 1.24     |
| 1   | C     | 117 | LYS  | CA-CB  | 5.05  | 1.61        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 176 | GLY  | N-CA    | 5.05  | 1.52        | 1.45     |
| 1   | H     | 282 | LEU  | CB-CG   | 5.05  | 1.63        | 1.53     |
| 1   | M     | 175 | ALA  | CA-C    | -5.05 | 1.45        | 1.52     |
| 1   | Q     | 362 | VAL  | CA-CB   | 5.05  | 1.60        | 1.53     |
| 1   | R     | 83  | HIS  | CE1-NE2 | 5.05  | 1.37        | 1.32     |
| 1   | A     | 180 | TYR  | CA-C    | -5.05 | 1.46        | 1.52     |
| 1   | G     | 280 | GLU  | CA-C    | 5.05  | 1.59        | 1.52     |
| 1   | B     | 208 | GLN  | CA-C    | -5.05 | 1.46        | 1.52     |
| 1   | E     | 104 | THR  | CA-CB   | -5.05 | 1.45        | 1.53     |
| 1   | N     | 410 | LYS  | CA-C    | 5.05  | 1.59        | 1.52     |
| 1   | P     | 329 | GLU  | C-N     | 5.05  | 1.40        | 1.34     |
| 1   | E     | 159 | ASP  | C-N     | 5.05  | 1.40        | 1.33     |
| 1   | S     | 153 | VAL  | C-N     | 5.05  | 1.40        | 1.33     |
| 1   | C     | 479 | ASN  | N-CA    | -5.04 | 1.39        | 1.45     |
| 1   | B     | 164 | ILE  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | C     | 258 | PRO  | C-N     | 5.04  | 1.40        | 1.33     |
| 1   | I     | 195 | LEU  | CB-CG   | 5.04  | 1.63        | 1.53     |
| 1   | M     | 263 | GLU  | N-CA    | 5.04  | 1.52        | 1.45     |
| 1   | N     | 234 | HIS  | ND1-CE1 | 5.04  | 1.37        | 1.32     |
| 1   | O     | 47  | LYS  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | I     | 459 | ILE  | N-CA    | 5.04  | 1.52        | 1.46     |
| 1   | P     | 430 | ARG  | CD-NE   | 5.04  | 1.53        | 1.46     |
| 1   | R     | 347 | SER  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | S     | 223 | VAL  | CA-C    | 5.04  | 1.58        | 1.52     |
| 1   | F     | 120 | ASP  | CA-CB   | 5.04  | 1.61        | 1.53     |
| 1   | I     | 505 | PRO  | N-CA    | -5.04 | 1.40        | 1.47     |
| 1   | P     | 415 | ILE  | C-N     | 5.04  | 1.40        | 1.33     |
| 1   | A     | 56  | ASP  | N-CA    | -5.04 | 1.40        | 1.45     |
| 1   | C     | 522 | LEU  | C-O     | -5.04 | 1.18        | 1.24     |
| 1   | K     | 491 | ALA  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | R     | 373 | ALA  | C-N     | 5.04  | 1.40        | 1.33     |
| 1   | C     | 436 | VAL  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | G     | 226 | ILE  | CB-CG1  | 5.04  | 1.63        | 1.53     |
| 1   | O     | 381 | ILE  | CA-CB   | -5.04 | 1.48        | 1.54     |
| 1   | A     | 402 | LEU  | CA-CB   | 5.03  | 1.61        | 1.53     |
| 1   | E     | 233 | VAL  | CA-C    | 5.03  | 1.59        | 1.52     |
| 1   | I     | 240 | ARG  | CD-NE   | 5.03  | 1.53        | 1.46     |
| 1   | N     | 263 | GLU  | CA-C    | 5.03  | 1.59        | 1.52     |
| 1   | L     | 491 | ALA  | CA-C    | -5.03 | 1.46        | 1.52     |
| 1   | Q     | 422 | GLU  | C-N     | 5.03  | 1.40        | 1.34     |
| 1   | A     | 321 | ARG  | CA-CB   | 5.03  | 1.62        | 1.53     |
| 1   | F     | 323 | ALA  | C-N     | -5.03 | 1.26        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 414 | ALA  | C-O     | -5.03 | 1.18        | 1.23     |
| 1   | N     | 157 | ASP  | N-CA    | 5.03  | 1.52        | 1.46     |
| 1   | S     | 426 | ALA  | C-O     | -5.03 | 1.18        | 1.23     |
| 1   | C     | 530 | VAL  | C-O     | -5.03 | 1.18        | 1.24     |
| 1   | M     | 324 | LYS  | CA-CB   | 5.03  | 1.61        | 1.53     |
| 1   | O     | 224 | TYR  | C-N     | 5.03  | 1.38        | 1.33     |
| 1   | P     | 36  | ILE  | CA-CB   | 5.03  | 1.59        | 1.54     |
| 1   | M     | 509 | LYS  | CA-CB   | 5.03  | 1.61        | 1.53     |
| 1   | A     | 442 | LEU  | N-CA    | -5.02 | 1.40        | 1.46     |
| 1   | E     | 282 | LEU  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | K     | 71  | ASP  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | D     | 328 | LEU  | CA-CB   | 5.02  | 1.61        | 1.53     |
| 1   | R     | 292 | ALA  | N-CA    | -5.02 | 1.39        | 1.46     |
| 1   | K     | 149 | LEU  | CA-C    | -5.02 | 1.46        | 1.52     |
| 1   | K     | 489 | LEU  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | C     | 181 | ILE  | CA-C    | -5.02 | 1.46        | 1.52     |
| 1   | G     | 223 | VAL  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | G     | 366 | LYS  | CA-C    | -5.02 | 1.46        | 1.52     |
| 1   | H     | 498 | TRP  | CD1-NE1 | 5.02  | 1.48        | 1.37     |
| 1   | I     | 96  | GLN  | CA-C    | 5.02  | 1.58        | 1.52     |
| 1   | N     | 432 | TYR  | CA-CB   | 5.02  | 1.61        | 1.53     |
| 1   | R     | 356 | LEU  | CA-C    | 5.02  | 1.58        | 1.52     |
| 1   | N     | 140 | GLU  | C-N     | 5.02  | 1.40        | 1.33     |
| 1   | N     | 493 | GLN  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | Q     | 356 | LEU  | C-N     | 5.02  | 1.40        | 1.33     |
| 1   | R     | 118 | ALA  | CA-C    | -5.02 | 1.45        | 1.52     |
| 1   | K     | 465 | ASP  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | P     | 174 | VAL  | CA-C    | 5.02  | 1.59        | 1.52     |
| 1   | G     | 306 | GLU  | C-N     | 5.01  | 1.40        | 1.33     |
| 1   | Q     | 238 | PRO  | CA-CB   | 5.01  | 1.60        | 1.53     |
| 1   | A     | 379 | ILE  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | N     | 260 | LEU  | C-N     | 5.01  | 1.40        | 1.33     |
| 1   | B     | 240 | ARG  | CD-NE   | 5.01  | 1.53        | 1.46     |
| 1   | I     | 186 | VAL  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | B     | 234 | HIS  | CD2-NE2 | -5.01 | 1.32        | 1.37     |
| 1   | K     | 473 | LEU  | C-N     | 5.01  | 1.40        | 1.33     |
| 1   | L     | 127 | HIS  | CA-C    | 5.01  | 1.59        | 1.53     |
| 1   | L     | 434 | PRO  | CA-C    | 5.01  | 1.59        | 1.52     |
| 1   | S     | 99  | GLU  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | A     | 504 | GLU  | CA-C    | 5.01  | 1.57        | 1.52     |
| 1   | C     | 329 | GLU  | CA-C    | 5.01  | 1.59        | 1.52     |
| 1   | D     | 307 | VAL  | C-O     | -5.01 | 1.17        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 363 | GLY  | C-N   | -5.01 | 1.26        | 1.33     |
| 1   | L     | 446 | ALA  | CA-C  | -5.01 | 1.46        | 1.52     |
| 1   | S     | 380 | SER  | C-O   | -5.01 | 1.17        | 1.23     |
| 1   | A     | 150 | ALA  | C-N   | 5.00  | 1.40        | 1.33     |
| 1   | M     | 468 | ASP  | N-CA  | -5.00 | 1.40        | 1.46     |
| 1   | F     | 89  | LEU  | CA-C  | -5.00 | 1.46        | 1.52     |
| 1   | G     | 290 | ILE  | CA-C  | -5.00 | 1.46        | 1.52     |
| 1   | S     | 356 | LEU  | N-CA  | 5.00  | 1.52        | 1.46     |
| 1   | E     | 199 | LYS  | C-O   | -5.00 | 1.17        | 1.23     |
| 1   | F     | 359 | GLU  | CA-CB | 5.00  | 1.62        | 1.53     |
| 1   | G     | 284 | LYS  | CA-CB | 5.00  | 1.61        | 1.53     |
| 1   | R     | 522 | LEU  | CA-C  | -5.00 | 1.46        | 1.52     |

All (4694) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | I     | 302 | LYS  | CA-C-N    | 15.09  | 134.68      | 120.34   |
| 1   | I     | 302 | LYS  | C-N-CA    | 15.09  | 134.68      | 120.34   |
| 1   | G     | 196 | ARG  | NE-CZ-NH1 | -13.69 | 107.81      | 121.50   |
| 1   | A     | 156 | ASN  | CA-CB-CG  | -12.75 | 99.85       | 112.60   |
| 1   | E     | 327 | ASP  | CA-CB-CG  | -12.04 | 100.56      | 112.60   |
| 1   | L     | 483 | LYS  | N-CA-C    | 11.72  | 125.51      | 111.33   |
| 1   | Q     | 178 | ARG  | NE-CZ-NH2 | 11.64  | 129.67      | 119.20   |
| 1   | S     | 257 | LYS  | CA-C-O    | -11.58 | 109.98      | 119.71   |
| 1   | B     | 351 | LEU  | CA-C-N    | 11.50  | 132.66      | 121.62   |
| 1   | B     | 351 | LEU  | C-N-CA    | 11.50  | 132.66      | 121.62   |
| 1   | Q     | 98  | GLU  | CA-C-N    | 11.23  | 135.70      | 120.54   |
| 1   | Q     | 98  | GLU  | C-N-CA    | 11.23  | 135.70      | 120.54   |
| 1   | O     | 255 | VAL  | O-C-N     | -11.15 | 110.52      | 122.67   |
| 1   | N     | 155 | ILE  | N-CA-C    | 11.06  | 121.89      | 110.72   |
| 1   | P     | 325 | LYS  | CA-C-N    | 11.00  | 135.45      | 120.38   |
| 1   | P     | 325 | LYS  | C-N-CA    | 11.00  | 135.45      | 120.38   |
| 1   | O     | 520 | ALA  | O-C-N     | -11.00 | 110.31      | 122.08   |
| 1   | I     | 234 | HIS  | CA-CB-CG  | 10.90  | 124.70      | 113.80   |
| 1   | H     | 253 | LEU  | N-CA-C    | -10.74 | 98.44       | 112.41   |
| 1   | H     | 413 | ARG  | NE-CZ-NH2 | 10.74  | 128.87      | 119.20   |
| 1   | N     | 360 | ARG  | NE-CZ-NH2 | 10.74  | 128.86      | 119.20   |
| 1   | C     | 42  | VAL  | N-CA-C    | 10.67  | 121.51      | 110.62   |
| 1   | P     | 93  | ALA  | N-CA-C    | 10.56  | 122.75      | 111.03   |
| 1   | O     | 424 | GLU  | O-C-N     | -10.32 | 111.44      | 122.07   |
| 1   | A     | 344 | ASP  | CA-CB-CG  | -10.29 | 102.31      | 112.60   |
| 1   | L     | 411 | ASP  | CA-CB-CG  | -10.26 | 102.34      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 453 | SER  | N-CA-C     | 10.22 | 123.69      | 111.33   |
| 1   | D     | 257 | LYS  | CA-C-N     | 10.17 | 129.83      | 119.56   |
| 1   | D     | 257 | LYS  | C-N-CA     | 10.17 | 129.83      | 119.56   |
| 1   | N     | 504 | GLU  | N-CA-C     | 10.15 | 120.02      | 108.25   |
| 1   | C     | 399 | ARG  | NE-CZ-NH2  | 10.13 | 128.31      | 119.20   |
| 1   | O     | 483 | LYS  | N-CA-C     | 10.08 | 125.45      | 112.34   |
| 1   | L     | 274 | LYS  | N-CA-C     | 10.07 | 125.44      | 112.34   |
| 1   | E     | 360 | ARG  | NE-CZ-NH2  | 10.02 | 128.22      | 119.20   |
| 1   | C     | 279 | GLU  | O-C-N      | -9.99 | 111.53      | 122.12   |
| 1   | R     | 164 | ILE  | CA-C-N     | 9.98  | 134.02      | 120.44   |
| 1   | R     | 164 | ILE  | C-N-CA     | 9.98  | 134.02      | 120.44   |
| 1   | A     | 183 | ASP  | CA-CB-CG   | -9.97 | 102.63      | 112.60   |
| 1   | P     | 250 | ASP  | CA-CB-CG   | 9.96  | 122.56      | 112.60   |
| 1   | R     | 250 | ASP  | CA-CB-CG   | 9.95  | 122.55      | 112.60   |
| 1   | F     | 481 | ASN  | CA-CB-CG   | -9.82 | 102.78      | 112.60   |
| 1   | H     | 433 | ALA  | CA-C-N     | 9.82  | 132.11      | 119.84   |
| 1   | H     | 433 | ALA  | C-N-CA     | 9.82  | 132.11      | 119.84   |
| 1   | O     | 355 | SER  | N-CA-C     | 9.82  | 121.98      | 111.28   |
| 1   | G     | 196 | ARG  | NE-CZ-NH2  | 9.79  | 128.01      | 119.20   |
| 1   | Q     | 175 | ALA  | CA-C-N     | 9.78  | 129.31      | 119.92   |
| 1   | Q     | 175 | ALA  | C-N-CA     | 9.78  | 129.31      | 119.92   |
| 1   | D     | 425 | ILE  | O-C-N      | -9.76 | 112.01      | 121.87   |
| 1   | K     | 32  | VAL  | N-CA-C     | 9.75  | 121.74      | 110.62   |
| 1   | D     | 339 | VAL  | N-CA-C     | 9.73  | 121.47      | 109.30   |
| 1   | S     | 32  | VAL  | N-CA-C     | 9.71  | 121.69      | 110.62   |
| 1   | O     | 197 | GLY  | CA-C-N     | 9.70  | 136.71      | 122.74   |
| 1   | O     | 197 | GLY  | C-N-CA     | 9.70  | 136.71      | 122.74   |
| 1   | P     | 171 | SER  | N-CA-C     | -9.69 | 100.96      | 113.17   |
| 1   | A     | 376 | PRO  | CA-C-N     | 9.65  | 133.99      | 120.29   |
| 1   | A     | 376 | PRO  | C-N-CA     | 9.65  | 133.99      | 120.29   |
| 1   | B     | 512 | ALA  | CA-C-N     | 9.63  | 132.70      | 120.56   |
| 1   | B     | 512 | ALA  | C-N-CA     | 9.63  | 132.70      | 120.56   |
| 1   | D     | 91  | GLN  | N-CA-C     | 9.63  | 121.78      | 111.28   |
| 1   | H     | 365 | ASP  | CA-C-O     | 9.63  | 130.91      | 120.32   |
| 1   | F     | 402 | LEU  | CA-C-N     | 9.61  | 130.85      | 119.99   |
| 1   | F     | 402 | LEU  | C-N-CA     | 9.61  | 130.85      | 119.99   |
| 1   | P     | 391 | VAL  | CA-C-N     | 9.58  | 132.90      | 120.44   |
| 1   | P     | 391 | VAL  | C-N-CA     | 9.58  | 132.90      | 120.44   |
| 1   | B     | 151 | GLN  | OE1-CD-NE2 | -9.57 | 113.03      | 122.60   |
| 1   | C     | 339 | VAL  | CA-C-O     | 9.56  | 131.75      | 120.85   |
| 1   | H     | 268 | ASP  | O-C-N      | -9.54 | 113.50      | 121.23   |
| 1   | S     | 174 | VAL  | N-CA-CB    | 9.54  | 121.41      | 110.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 373 | ALA  | N-CA-C     | 9.52  | 123.40      | 110.55   |
| 1   | G     | 51  | GLY  | CA-C-N     | 9.50  | 129.25      | 119.56   |
| 1   | G     | 51  | GLY  | C-N-CA     | 9.50  | 129.25      | 119.56   |
| 1   | G     | 283 | ILE  | CB-CA-C    | -9.49 | 99.12       | 112.22   |
| 1   | H     | 71  | ASP  | CA-CB-CG   | 9.48  | 122.08      | 112.60   |
| 1   | P     | 146 | ILE  | CA-C-O     | 9.46  | 130.96      | 120.46   |
| 1   | L     | 33  | ARG  | NE-CZ-NH1  | 9.45  | 130.95      | 121.50   |
| 1   | Q     | 188 | ALA  | O-C-N      | -9.43 | 112.12      | 122.12   |
| 1   | S     | 360 | ARG  | NE-CZ-NH2  | 9.43  | 127.69      | 119.20   |
| 1   | C     | 360 | ARG  | NE-CZ-NH2  | 9.41  | 127.67      | 119.20   |
| 1   | D     | 465 | ASP  | CA-C-N     | 9.41  | 129.03      | 119.24   |
| 1   | D     | 465 | ASP  | C-N-CA     | 9.41  | 129.03      | 119.24   |
| 1   | B     | 286 | LYS  | O-C-N      | -9.39 | 112.33      | 122.09   |
| 1   | F     | 381 | ILE  | O-C-N      | -9.38 | 113.05      | 123.18   |
| 1   | C     | 104 | THR  | N-CA-C     | 9.36  | 121.56      | 111.36   |
| 1   | E     | 488 | ASP  | CA-CB-CG   | -9.35 | 103.25      | 112.60   |
| 1   | M     | 250 | ASP  | CA-CB-CG   | 9.34  | 121.94      | 112.60   |
| 1   | B     | 504 | GLU  | CA-C-N     | 9.33  | 131.50      | 119.84   |
| 1   | B     | 504 | GLU  | C-N-CA     | 9.33  | 131.50      | 119.84   |
| 1   | L     | 219 | ASP  | N-CA-CB    | -9.33 | 97.68       | 110.56   |
| 1   | O     | 102 | ASP  | O-C-N      | -9.32 | 112.85      | 123.48   |
| 1   | K     | 423 | ILE  | O-C-N      | -9.32 | 112.75      | 121.89   |
| 1   | E     | 83  | HIS  | CA-C-N     | 9.31  | 128.92      | 119.24   |
| 1   | E     | 83  | HIS  | C-N-CA     | 9.31  | 128.92      | 119.24   |
| 1   | M     | 141 | VAL  | N-CA-C     | 9.29  | 120.12      | 110.36   |
| 1   | M     | 71  | ASP  | CA-C-N     | 9.29  | 130.49      | 119.99   |
| 1   | M     | 71  | ASP  | C-N-CA     | 9.29  | 130.49      | 119.99   |
| 1   | E     | 125 | ASP  | CA-CB-CG   | -9.29 | 103.31      | 112.60   |
| 1   | F     | 400 | ASP  | N-CA-C     | 9.28  | 121.00      | 111.07   |
| 1   | I     | 474 | ARG  | N-CA-C     | 9.26  | 123.98      | 112.87   |
| 1   | N     | 392 | ASP  | O-C-N      | -9.23 | 112.56      | 122.07   |
| 1   | B     | 420 | ALA  | N-CA-C     | 9.22  | 122.27      | 111.02   |
| 1   | M     | 265 | ARG  | NE-CZ-NH2  | 9.21  | 127.49      | 119.20   |
| 1   | G     | 427 | LYS  | CA-C-N     | 9.19  | 132.59      | 120.28   |
| 1   | G     | 427 | LYS  | C-N-CA     | 9.19  | 132.59      | 120.28   |
| 1   | H     | 150 | ALA  | N-CA-C     | 9.17  | 123.44      | 110.50   |
| 1   | O     | 77  | ASP  | CA-CB-CG   | 9.17  | 121.77      | 112.60   |
| 1   | A     | 85  | ALA  | CA-C-N     | 9.17  | 132.36      | 120.44   |
| 1   | A     | 85  | ALA  | C-N-CA     | 9.17  | 132.36      | 120.44   |
| 1   | Q     | 488 | ASP  | CA-CB-CG   | -9.12 | 103.48      | 112.60   |
| 1   | N     | 144 | GLN  | OE1-CD-NE2 | -9.10 | 113.50      | 122.60   |
| 1   | E     | 481 | ASN  | CA-CB-CG   | -9.08 | 103.52      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 218 | ASN  | CA-CB-CG  | -9.07 | 103.53      | 112.60   |
| 1   | R     | 479 | ASN  | CA-CB-CG  | -9.06 | 103.54      | 112.60   |
| 1   | B     | 179 | GLU  | CA-C-N    | 9.06  | 132.61      | 120.65   |
| 1   | B     | 179 | GLU  | C-N-CA    | 9.06  | 132.61      | 120.65   |
| 1   | P     | 514 | LYS  | CA-C-N    | 9.04  | 132.58      | 120.65   |
| 1   | P     | 514 | LYS  | C-N-CA    | 9.04  | 132.58      | 120.65   |
| 1   | D     | 413 | ARG  | NE-CZ-NH1 | -9.04 | 112.46      | 121.50   |
| 1   | P     | 50  | TYR  | CA-C-O    | 9.04  | 131.09      | 120.70   |
| 1   | P     | 260 | LEU  | N-CA-C    | 9.02  | 121.12      | 111.28   |
| 1   | G     | 181 | ILE  | CA-C-O    | -9.01 | 111.30      | 120.85   |
| 1   | P     | 71  | ASP  | CA-CB-CG  | 8.98  | 121.58      | 112.60   |
| 1   | F     | 525 | ARG  | CA-C-O    | 8.98  | 130.29      | 119.97   |
| 1   | M     | 405 | VAL  | N-CA-C    | 8.97  | 119.77      | 110.62   |
| 1   | E     | 104 | THR  | N-CA-C    | 8.96  | 121.12      | 111.36   |
| 1   | M     | 465 | ASP  | CA-CB-CG  | 8.93  | 121.53      | 112.60   |
| 1   | A     | 327 | ASP  | CA-CB-CG  | -8.93 | 103.67      | 112.60   |
| 1   | S     | 33  | ARG  | CA-C-N    | 8.92  | 132.58      | 120.54   |
| 1   | S     | 33  | ARG  | C-N-CA    | 8.92  | 132.58      | 120.54   |
| 1   | M     | 357 | ILE  | O-C-N     | -8.91 | 114.06      | 123.14   |
| 1   | L     | 203 | ASP  | CA-C-N    | 8.90  | 133.09      | 120.28   |
| 1   | L     | 203 | ASP  | C-N-CA    | 8.90  | 133.09      | 120.28   |
| 1   | R     | 490 | TYR  | N-CA-C    | -8.89 | 102.23      | 113.43   |
| 1   | G     | 261 | ASP  | CA-CB-CG  | 8.88  | 121.48      | 112.60   |
| 1   | K     | 423 | ILE  | N-CA-CB   | 8.84  | 121.52      | 110.47   |
| 1   | M     | 479 | ASN  | CA-CB-CG  | -8.83 | 103.77      | 112.60   |
| 1   | I     | 185 | VAL  | N-CA-C    | 8.82  | 120.68      | 110.62   |
| 1   | P     | 344 | ASP  | CA-CB-CG  | 8.79  | 121.39      | 112.60   |
| 1   | F     | 490 | TYR  | N-CA-C    | -8.79 | 102.36      | 113.43   |
| 1   | S     | 35  | ASN  | CA-C-N    | 8.78  | 131.93      | 120.60   |
| 1   | S     | 35  | ASN  | C-N-CA    | 8.78  | 131.93      | 120.60   |
| 1   | H     | 413 | ARG  | NE-CZ-NH1 | -8.77 | 112.73      | 121.50   |
| 1   | M     | 413 | ARG  | NE-CZ-NH2 | 8.77  | 127.09      | 119.20   |
| 1   | M     | 57  | LYS  | CA-C-O    | 8.77  | 131.07      | 121.16   |
| 1   | A     | 477 | HIS  | CA-CB-CG  | 8.77  | 122.57      | 113.80   |
| 1   | E     | 471 | MET  | CG-SD-CE  | -8.76 | 81.62       | 100.90   |
| 1   | H     | 61  | ASP  | CA-C-O    | 8.75  | 131.92      | 122.03   |
| 1   | H     | 365 | ASP  | CA-CB-CG  | 8.74  | 121.34      | 112.60   |
| 1   | D     | 436 | VAL  | N-CA-C    | 8.74  | 118.81      | 110.42   |
| 1   | M     | 232 | VAL  | N-CA-C    | 8.74  | 121.42      | 109.80   |
| 1   | R     | 281 | ASN  | CA-C-N    | 8.72  | 132.67      | 120.29   |
| 1   | R     | 281 | ASN  | C-N-CA    | 8.72  | 132.67      | 120.29   |
| 1   | E     | 69  | THR  | CA-C-N    | 8.72  | 133.60      | 120.17   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 69  | THR  | C-N-CA     | 8.72  | 133.60      | 120.17   |
| 1   | I     | 245 | LYS  | CA-C-N     | 8.71  | 132.51      | 120.49   |
| 1   | I     | 245 | LYS  | C-N-CA     | 8.71  | 132.51      | 120.49   |
| 1   | K     | 118 | ALA  | CA-C-N     | 8.71  | 131.95      | 120.28   |
| 1   | K     | 118 | ALA  | C-N-CA     | 8.71  | 131.95      | 120.28   |
| 1   | F     | 118 | ALA  | CA-C-N     | 8.67  | 131.90      | 120.28   |
| 1   | F     | 118 | ALA  | C-N-CA     | 8.67  | 131.90      | 120.28   |
| 1   | Q     | 479 | ASN  | CA-C-N     | 8.67  | 133.04      | 120.38   |
| 1   | Q     | 479 | ASN  | C-N-CA     | 8.67  | 133.04      | 120.38   |
| 1   | M     | 250 | ASP  | CA-C-N     | 8.67  | 133.02      | 120.71   |
| 1   | M     | 250 | ASP  | C-N-CA     | 8.67  | 133.02      | 120.71   |
| 1   | I     | 83  | HIS  | CB-CA-C    | -8.66 | 100.19      | 110.15   |
| 1   | G     | 264 | ILE  | O-C-N      | -8.66 | 113.84      | 122.67   |
| 1   | B     | 184 | ILE  | CA-C-N     | 8.66  | 131.77      | 120.60   |
| 1   | B     | 184 | ILE  | C-N-CA     | 8.66  | 131.77      | 120.60   |
| 1   | O     | 209 | ILE  | O-C-N      | -8.65 | 114.64      | 123.03   |
| 1   | B     | 159 | ASP  | CA-CB-CG   | -8.65 | 103.95      | 112.60   |
| 1   | N     | 276 | LEU  | CA-C-N     | 8.64  | 132.19      | 120.44   |
| 1   | N     | 276 | LEU  | C-N-CA     | 8.64  | 132.19      | 120.44   |
| 1   | R     | 513 | ILE  | N-CA-C     | 8.63  | 119.42      | 110.62   |
| 1   | F     | 430 | ARG  | NE-CZ-NH1  | 8.63  | 130.13      | 121.50   |
| 1   | Q     | 39  | VAL  | N-CA-C     | 8.62  | 118.66      | 110.30   |
| 1   | N     | 375 | ASN  | CA-C-O     | -8.62 | 113.69      | 119.29   |
| 1   | D     | 265 | ARG  | NE-CZ-NH2  | 8.62  | 126.95      | 119.20   |
| 1   | K     | 83  | HIS  | CG-CD2-NE2 | 8.62  | 115.81      | 107.20   |
| 1   | G     | 494 | PRO  | CA-C-O     | -8.61 | 112.02      | 121.23   |
| 1   | A     | 201 | TYR  | CA-C-N     | 8.60  | 134.18      | 123.17   |
| 1   | A     | 201 | TYR  | C-N-CA     | 8.60  | 134.18      | 123.17   |
| 1   | I     | 60  | VAL  | CA-C-N     | 8.60  | 133.74      | 120.75   |
| 1   | I     | 60  | VAL  | C-N-CA     | 8.60  | 133.74      | 120.75   |
| 1   | K     | 200 | TRP  | N-CA-C     | 8.60  | 122.70      | 110.23   |
| 1   | B     | 461 | ASN  | CA-CB-CG   | -8.59 | 104.01      | 112.60   |
| 1   | G     | 408 | VAL  | CA-C-N     | 8.59  | 131.55      | 120.56   |
| 1   | G     | 408 | VAL  | C-N-CA     | 8.59  | 131.55      | 120.56   |
| 1   | G     | 399 | ARG  | CA-C-O     | -8.58 | 111.81      | 120.82   |
| 1   | I     | 411 | ASP  | CA-CB-CG   | -8.56 | 104.04      | 112.60   |
| 1   | M     | 267 | ASN  | CA-CB-CG   | -8.55 | 104.05      | 112.60   |
| 1   | R     | 79  | MET  | N-CA-CB    | -8.53 | 96.72       | 110.63   |
| 1   | C     | 399 | ARG  | NE-CZ-NH1  | -8.51 | 112.99      | 121.50   |
| 1   | C     | 374 | LYS  | N-CA-C     | 8.49  | 121.61      | 111.33   |
| 1   | Q     | 409 | ILE  | CA-C-N     | 8.49  | 132.78      | 120.38   |
| 1   | Q     | 409 | ILE  | C-N-CA     | 8.49  | 132.78      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 461 | ASN  | CA-CB-CG   | 8.48  | 121.08      | 112.60   |
| 1   | H     | 178 | ARG  | NE-CZ-NH2  | 8.47  | 126.83      | 119.20   |
| 1   | L     | 421 | VAL  | CA-C-N     | 8.47  | 131.83      | 120.65   |
| 1   | L     | 421 | VAL  | C-N-CA     | 8.47  | 131.83      | 120.65   |
| 1   | G     | 73  | ALA  | N-CA-C     | 8.46  | 121.34      | 111.02   |
| 1   | B     | 327 | ASP  | CA-CB-CG   | -8.46 | 104.14      | 112.60   |
| 1   | C     | 269 | PRO  | CA-C-N     | 8.46  | 131.61      | 120.28   |
| 1   | C     | 269 | PRO  | C-N-CA     | 8.46  | 131.61      | 120.28   |
| 1   | M     | 399 | ARG  | NE-CZ-NH2  | 8.46  | 126.81      | 119.20   |
| 1   | D     | 349 | GLN  | OE1-CD-NE2 | 8.45  | 131.05      | 122.60   |
| 1   | E     | 265 | ARG  | NE-CZ-NH2  | 8.44  | 126.80      | 119.20   |
| 1   | S     | 352 | GLY  | O-C-N      | -8.43 | 118.04      | 123.35   |
| 1   | P     | 410 | LYS  | CA-C-O     | 8.42  | 129.62      | 120.10   |
| 1   | L     | 490 | TYR  | N-CA-C     | -8.42 | 105.02      | 114.62   |
| 1   | H     | 465 | ASP  | CA-C-O     | -8.40 | 112.99      | 119.46   |
| 1   | P     | 349 | GLN  | OE1-CD-NE2 | -8.40 | 114.20      | 122.60   |
| 1   | D     | 391 | VAL  | CA-C-N     | 8.40  | 131.36      | 120.44   |
| 1   | D     | 391 | VAL  | C-N-CA     | 8.40  | 131.36      | 120.44   |
| 1   | O     | 169 | LEU  | N-CA-C     | 8.39  | 120.51      | 111.36   |
| 1   | E     | 411 | ASP  | CA-CB-CG   | -8.38 | 104.22      | 112.60   |
| 1   | S     | 511 | ASN  | CA-CB-CG   | 8.38  | 120.97      | 112.60   |
| 1   | P     | 124 | LYS  | CA-C-N     | 8.37  | 134.79      | 122.74   |
| 1   | P     | 124 | LYS  | C-N-CA     | 8.37  | 134.79      | 122.74   |
| 1   | Q     | 127 | HIS  | CA-CB-CG   | -8.37 | 105.43      | 113.80   |
| 1   | D     | 156 | ASN  | CA-CB-CG   | -8.37 | 104.23      | 112.60   |
| 1   | P     | 267 | ASN  | CA-C-N     | 8.36  | 133.24      | 121.61   |
| 1   | P     | 267 | ASN  | C-N-CA     | 8.36  | 133.24      | 121.61   |
| 1   | O     | 350 | ASP  | CA-C-O     | 8.35  | 129.04      | 119.27   |
| 1   | Q     | 354 | ALA  | O-C-N      | -8.35 | 114.48      | 123.42   |
| 1   | G     | 113 | GLU  | CA-C-O     | 8.34  | 129.26      | 120.42   |
| 1   | A     | 71  | ASP  | CA-CB-CG   | 8.33  | 120.93      | 112.60   |
| 1   | R     | 232 | VAL  | N-CA-CB    | 8.31  | 119.78      | 110.72   |
| 1   | O     | 298 | ILE  | O-C-N      | -8.30 | 112.20      | 122.57   |
| 1   | A     | 70  | ASN  | CA-CB-CG   | 8.30  | 120.90      | 112.60   |
| 1   | K     | 421 | VAL  | CA-C-N     | 8.30  | 131.60      | 120.65   |
| 1   | K     | 421 | VAL  | C-N-CA     | 8.30  | 131.60      | 120.65   |
| 1   | N     | 262 | ALA  | O-C-N      | -8.29 | 113.80      | 123.25   |
| 1   | H     | 325 | LYS  | CA-C-N     | 8.29  | 132.48      | 120.38   |
| 1   | H     | 325 | LYS  | C-N-CA     | 8.29  | 132.48      | 120.38   |
| 1   | G     | 343 | ILE  | CA-C-O     | 8.29  | 129.67      | 120.64   |
| 1   | Q     | 375 | ASN  | CA-C-N     | 8.29  | 128.77      | 119.32   |
| 1   | Q     | 375 | ASN  | C-N-CA     | 8.29  | 128.77      | 119.32   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 418 | GLY  | O-C-N     | -8.28 | 115.03      | 122.57   |
| 1   | M     | 317 | VAL  | N-CA-C    | 8.28  | 119.57      | 110.21   |
| 1   | O     | 252 | SER  | N-CA-C    | 8.27  | 121.91      | 109.25   |
| 1   | N     | 245 | LYS  | CA-C-N    | 8.27  | 131.58      | 120.50   |
| 1   | N     | 245 | LYS  | C-N-CA    | 8.27  | 131.58      | 120.50   |
| 1   | E     | 35  | ASN  | CA-CB-CG  | -8.26 | 104.34      | 112.60   |
| 1   | L     | 171 | SER  | CA-C-O    | 8.26  | 129.23      | 119.56   |
| 1   | N     | 181 | ILE  | CA-C-O    | -8.25 | 112.10      | 120.85   |
| 1   | R     | 127 | HIS  | CA-C-N    | 8.25  | 127.98      | 119.56   |
| 1   | R     | 127 | HIS  | C-N-CA    | 8.25  | 127.98      | 119.56   |
| 1   | R     | 340 | VAL  | O-C-N     | -8.24 | 113.60      | 122.83   |
| 1   | P     | 389 | ARG  | N-CA-C    | -8.24 | 103.74      | 113.88   |
| 1   | L     | 295 | ALA  | CA-C-O    | 8.24  | 130.28      | 121.55   |
| 1   | B     | 499 | GLN  | CA-C-N    | 8.23  | 132.85      | 120.17   |
| 1   | B     | 499 | GLN  | C-N-CA    | 8.23  | 132.85      | 120.17   |
| 1   | L     | 482 | ASN  | N-CA-CB   | 8.23  | 122.34      | 110.65   |
| 1   | E     | 459 | ILE  | N-CA-C    | 8.23  | 118.32      | 110.42   |
| 1   | K     | 511 | ASN  | CA-C-N    | 8.21  | 131.12      | 120.44   |
| 1   | K     | 511 | ASN  | C-N-CA    | 8.21  | 131.12      | 120.44   |
| 1   | G     | 224 | TYR  | CA-C-N    | 8.20  | 133.50      | 120.55   |
| 1   | G     | 224 | TYR  | C-N-CA    | 8.20  | 133.50      | 120.55   |
| 1   | F     | 390 | LEU  | N-CA-C    | 8.19  | 120.21      | 111.28   |
| 1   | M     | 126 | VAL  | N-CA-C    | -8.19 | 98.07       | 109.21   |
| 1   | D     | 407 | ASP  | CA-CB-CG  | -8.19 | 104.41      | 112.60   |
| 1   | G     | 504 | GLU  | N-CA-C    | 8.19  | 121.50      | 108.23   |
| 1   | O     | 356 | LEU  | O-C-N     | -8.19 | 114.08      | 123.42   |
| 1   | O     | 413 | ARG  | NE-CZ-NH1 | -8.18 | 113.32      | 121.50   |
| 1   | A     | 246 | ILE  | N-CA-C    | 8.18  | 121.41      | 109.63   |
| 1   | F     | 249 | ILE  | N-CA-C    | 8.18  | 119.31      | 106.88   |
| 1   | H     | 52  | PRO  | CA-C-O    | -8.17 | 111.50      | 121.31   |
| 1   | A     | 144 | GLN  | N-CA-C    | 8.17  | 121.10      | 111.71   |
| 1   | F     | 400 | ASP  | O-C-N     | -8.17 | 113.66      | 122.07   |
| 1   | Q     | 324 | LYS  | N-CA-C    | 8.16  | 122.24      | 110.24   |
| 1   | P     | 477 | HIS  | CA-C-O    | 8.16  | 128.00      | 119.51   |
| 1   | R     | 413 | ARG  | NE-CZ-NH2 | 8.16  | 126.54      | 119.20   |
| 1   | Q     | 44  | GLU  | N-CA-C    | 8.15  | 122.65      | 112.87   |
| 1   | S     | 196 | ARG  | NE-CZ-NH2 | 8.15  | 126.54      | 119.20   |
| 1   | N     | 480 | GLU  | N-CA-C    | 8.14  | 120.16      | 111.28   |
| 1   | G     | 193 | ALA  | N-CA-C    | 8.14  | 121.71      | 110.24   |
| 1   | C     | 285 | GLU  | CA-C-N    | 8.13  | 131.01      | 120.44   |
| 1   | C     | 285 | GLU  | C-N-CA    | 8.13  | 131.01      | 120.44   |
| 1   | F     | 288 | ASP  | CA-CB-CG  | 8.13  | 120.73      | 112.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 101 | ALA  | N-CA-C      | -8.12 | 102.41      | 113.30   |
| 1   | A     | 375 | ASN  | CA-CB-CG    | -8.11 | 104.49      | 112.60   |
| 1   | D     | 396 | ARG  | NE-CZ-NH1   | 8.11  | 129.60      | 121.50   |
| 1   | H     | 350 | ASP  | CA-CB-CG    | -8.10 | 104.50      | 112.60   |
| 1   | B     | 277 | ASP  | N-CA-C      | -8.09 | 102.40      | 111.14   |
| 1   | G     | 208 | GLN  | O-C-N       | -8.09 | 113.80      | 123.10   |
| 1   | L     | 282 | LEU  | CA-C-O      | 8.09  | 128.99      | 120.42   |
| 1   | K     | 184 | ILE  | CA-C-O      | -8.08 | 113.00      | 121.41   |
| 1   | P     | 170 | SER  | N-CA-C      | 8.08  | 122.24      | 112.38   |
| 1   | R     | 197 | GLY  | CA-C-N      | 8.08  | 134.37      | 122.74   |
| 1   | R     | 197 | GLY  | C-N-CA      | 8.08  | 134.37      | 122.74   |
| 1   | P     | 39  | VAL  | CA-C-N      | 8.07  | 131.44      | 120.38   |
| 1   | P     | 39  | VAL  | C-N-CA      | 8.07  | 131.44      | 120.38   |
| 1   | I     | 120 | ASP  | CA-CB-CG    | 8.05  | 120.65      | 112.60   |
| 1   | K     | 322 | ARG  | O-C-N       | -8.04 | 112.93      | 122.58   |
| 1   | K     | 83  | HIS  | CE1-NE2-CD2 | -8.04 | 100.96      | 109.00   |
| 1   | A     | 144 | GLN  | O-C-N       | 8.03  | 131.62      | 122.22   |
| 1   | E     | 511 | ASN  | CA-C-N      | 8.03  | 131.38      | 120.54   |
| 1   | E     | 511 | ASN  | C-N-CA      | 8.03  | 131.38      | 120.54   |
| 1   | G     | 428 | LYS  | N-CA-C      | 8.03  | 120.04      | 111.28   |
| 1   | O     | 111 | SER  | N-CA-CB     | 8.03  | 121.63      | 109.91   |
| 1   | C     | 450 | ALA  | CA-C-N      | 8.02  | 131.68      | 120.29   |
| 1   | C     | 450 | ALA  | C-N-CA      | 8.02  | 131.68      | 120.29   |
| 1   | D     | 176 | GLY  | CA-C-O      | 8.02  | 130.56      | 121.90   |
| 1   | Q     | 33  | ARG  | CA-C-N      | 8.02  | 131.94      | 120.79   |
| 1   | Q     | 33  | ARG  | C-N-CA      | 8.02  | 131.94      | 120.79   |
| 1   | Q     | 479 | ASN  | OD1-CG-ND2  | -8.02 | 114.58      | 122.60   |
| 1   | D     | 223 | VAL  | N-CA-C      | 8.02  | 119.39      | 108.17   |
| 1   | S     | 245 | LYS  | CA-C-N      | 8.02  | 131.25      | 120.50   |
| 1   | S     | 245 | LYS  | C-N-CA      | 8.02  | 131.25      | 120.50   |
| 1   | S     | 458 | LEU  | CA-C-O      | 8.02  | 129.24      | 120.82   |
| 1   | K     | 511 | ASN  | OD1-CG-ND2  | -8.01 | 114.59      | 122.60   |
| 1   | D     | 455 | VAL  | CA-C-N      | 8.00  | 130.84      | 120.44   |
| 1   | D     | 455 | VAL  | C-N-CA      | 8.00  | 130.84      | 120.44   |
| 1   | K     | 346 | ILE  | N-CA-C      | 8.00  | 120.17      | 109.37   |
| 1   | N     | 346 | ILE  | N-CA-C      | 8.00  | 121.15      | 109.63   |
| 1   | G     | 287 | VAL  | O-C-N       | -7.99 | 114.08      | 121.91   |
| 1   | O     | 511 | ASN  | CA-CB-CG    | 7.99  | 120.59      | 112.60   |
| 1   | R     | 243 | ASN  | OD1-CG-ND2  | -7.99 | 114.61      | 122.60   |
| 1   | G     | 491 | ALA  | N-CA-C      | 7.99  | 124.11      | 113.72   |
| 1   | F     | 351 | LEU  | N-CA-C      | 7.98  | 121.75      | 110.50   |
| 1   | L     | 275 | PHE  | CA-CB-CG    | -7.98 | 105.82      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | I     | 271 | GLN  | CA-C-N      | 7.97  | 131.18      | 120.65   |
| 1   | I     | 271 | GLN  | C-N-CA      | 7.97  | 131.18      | 120.65   |
| 1   | D     | 467 | ILE  | CA-C-N      | 7.97  | 131.87      | 120.79   |
| 1   | D     | 467 | ILE  | C-N-CA      | 7.97  | 131.87      | 120.79   |
| 1   | A     | 265 | ARG  | NE-CZ-NH1   | -7.96 | 113.54      | 121.50   |
| 1   | B     | 439 | LYS  | N-CA-C      | 7.96  | 119.73      | 111.14   |
| 1   | A     | 178 | ARG  | N-CA-C      | 7.95  | 122.25      | 112.23   |
| 1   | G     | 342 | ASN  | CA-CB-CG    | -7.95 | 104.65      | 112.60   |
| 1   | I     | 477 | HIS  | CE1-NE2-CD2 | -7.95 | 101.05      | 109.00   |
| 1   | I     | 125 | ASP  | CA-CB-CG    | -7.95 | 104.65      | 112.60   |
| 1   | O     | 336 | GLY  | CA-C-N      | 7.94  | 133.02      | 121.67   |
| 1   | O     | 336 | GLY  | C-N-CA      | 7.94  | 133.02      | 121.67   |
| 1   | P     | 350 | ASP  | CA-CB-CG    | -7.93 | 104.67      | 112.60   |
| 1   | I     | 520 | ALA  | N-CA-C      | 7.93  | 120.62      | 111.11   |
| 1   | R     | 424 | GLU  | CB-CG-CD    | 7.93  | 126.08      | 112.60   |
| 1   | M     | 337 | GLY  | O-C-N       | -7.92 | 116.53      | 122.71   |
| 1   | H     | 61  | ASP  | O-C-N       | -7.92 | 113.34      | 122.68   |
| 1   | M     | 474 | ARG  | NE-CZ-NH2   | 7.92  | 126.32      | 119.20   |
| 1   | P     | 76  | LEU  | CA-C-O      | 7.91  | 129.35      | 119.78   |
| 1   | S     | 493 | GLN  | CA-C-N      | 7.91  | 128.37      | 119.83   |
| 1   | S     | 493 | GLN  | C-N-CA      | 7.91  | 128.37      | 119.83   |
| 1   | F     | 389 | ARG  | N-CA-C      | -7.91 | 104.15      | 113.88   |
| 1   | G     | 126 | VAL  | O-C-N       | -7.91 | 115.08      | 123.14   |
| 1   | L     | 309 | GLN  | N-CA-C      | -7.90 | 101.77      | 111.40   |
| 1   | S     | 115 | VAL  | N-CA-CB     | 7.90  | 119.79      | 110.55   |
| 1   | I     | 423 | ILE  | CA-C-N      | 7.89  | 131.17      | 120.44   |
| 1   | I     | 423 | ILE  | C-N-CA      | 7.89  | 131.17      | 120.44   |
| 1   | M     | 420 | ALA  | O-C-N       | -7.89 | 113.64      | 122.08   |
| 1   | H     | 125 | ASP  | O-C-N       | -7.87 | 112.13      | 122.59   |
| 1   | O     | 326 | SER  | N-CA-C      | 7.87  | 121.82      | 111.75   |
| 1   | I     | 323 | ALA  | CA-C-N      | 7.86  | 131.96      | 120.95   |
| 1   | I     | 323 | ALA  | C-N-CA      | 7.86  | 131.96      | 120.95   |
| 1   | K     | 82  | GLN  | OE1-CD-NE2  | -7.86 | 114.74      | 122.60   |
| 1   | R     | 296 | ASN  | OD1-CG-ND2  | -7.86 | 114.74      | 122.60   |
| 1   | C     | 234 | HIS  | CA-CB-CG    | 7.86  | 121.66      | 113.80   |
| 1   | E     | 474 | ARG  | NE-CZ-NH2   | 7.86  | 126.27      | 119.20   |
| 1   | H     | 68  | ILE  | N-CA-CB     | 7.86  | 120.42      | 110.99   |
| 1   | O     | 64  | GLY  | CA-C-O      | 7.84  | 127.85      | 119.06   |
| 1   | Q     | 426 | ALA  | CA-C-N      | 7.84  | 132.58      | 120.82   |
| 1   | Q     | 426 | ALA  | C-N-CA      | 7.84  | 132.58      | 120.82   |
| 1   | K     | 442 | LEU  | CA-C-O      | 7.83  | 129.09      | 120.63   |
| 1   | Q     | 138 | ALA  | CA-C-N      | 7.83  | 130.62      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Q     | 138 | ALA  | C-N-CA     | 7.83  | 130.62      | 120.44   |
| 1   | P     | 141 | VAL  | CB-CA-C    | -7.83 | 101.86      | 111.88   |
| 1   | D     | 415 | ILE  | CA-C-O     | -7.82 | 113.38      | 121.67   |
| 1   | K     | 506 | ALA  | N-CA-C     | 7.82  | 122.67      | 113.20   |
| 1   | F     | 362 | VAL  | CA-C-O     | 7.82  | 127.97      | 120.31   |
| 1   | S     | 230 | LYS  | CA-C-O     | -7.82 | 112.23      | 120.99   |
| 1   | O     | 298 | ILE  | CA-CB-CG1  | 7.82  | 123.69      | 110.40   |
| 1   | F     | 313 | ALA  | CA-C-N     | 7.82  | 132.19      | 120.31   |
| 1   | F     | 313 | ALA  | C-N-CA     | 7.82  | 132.19      | 120.31   |
| 1   | O     | 82  | GLN  | OE1-CD-NE2 | -7.80 | 114.80      | 122.60   |
| 1   | D     | 413 | ARG  | NE-CZ-NH2  | 7.80  | 126.22      | 119.20   |
| 1   | R     | 429 | LEU  | N-CA-CB    | 7.80  | 121.67      | 110.13   |
| 1   | E     | 177 | ALA  | O-C-N      | -7.79 | 113.51      | 122.86   |
| 1   | E     | 374 | LYS  | N-CA-C     | 7.79  | 120.76      | 111.33   |
| 1   | L     | 230 | LYS  | CA-C-O     | -7.79 | 113.13      | 121.38   |
| 1   | B     | 218 | ASN  | CA-CB-CG   | -7.79 | 104.81      | 112.60   |
| 1   | O     | 179 | GLU  | CA-C-N     | 7.79  | 130.56      | 120.44   |
| 1   | O     | 179 | GLU  | C-N-CA     | 7.79  | 130.56      | 120.44   |
| 1   | C     | 369 | PHE  | CA-CB-CG   | -7.78 | 106.02      | 113.80   |
| 1   | P     | 453 | SER  | CA-C-N     | 7.77  | 130.55      | 120.44   |
| 1   | P     | 453 | SER  | C-N-CA     | 7.77  | 130.55      | 120.44   |
| 1   | F     | 388 | GLU  | N-CA-C     | 7.77  | 122.44      | 112.34   |
| 1   | B     | 281 | ASN  | CA-C-N     | 7.77  | 130.69      | 120.28   |
| 1   | B     | 281 | ASN  | C-N-CA     | 7.77  | 130.69      | 120.28   |
| 1   | G     | 448 | ALA  | CA-C-N     | 7.77  | 131.02      | 120.38   |
| 1   | G     | 448 | ALA  | C-N-CA     | 7.77  | 131.02      | 120.38   |
| 1   | Q     | 193 | ALA  | N-CA-C     | 7.76  | 121.67      | 110.10   |
| 1   | Q     | 491 | ALA  | CA-C-O     | 7.76  | 128.65      | 120.42   |
| 1   | G     | 446 | ALA  | CA-C-O     | -7.76 | 112.86      | 121.00   |
| 1   | D     | 482 | ASN  | CA-C-N     | 7.75  | 136.34      | 121.54   |
| 1   | D     | 482 | ASN  | C-N-CA     | 7.75  | 136.34      | 121.54   |
| 1   | S     | 368 | VAL  | CB-CA-C    | 7.75  | 121.91      | 110.98   |
| 1   | P     | 152 | THR  | CB-CA-C    | -7.75 | 98.89       | 110.67   |
| 1   | K     | 277 | ASP  | CA-CB-CG   | 7.74  | 120.34      | 112.60   |
| 1   | L     | 290 | ILE  | N-CA-C     | -7.74 | 104.25      | 111.45   |
| 1   | S     | 514 | LYS  | O-C-N      | -7.74 | 113.91      | 122.12   |
| 1   | G     | 37  | ALA  | CA-C-N     | 7.74  | 130.99      | 120.54   |
| 1   | G     | 37  | ALA  | C-N-CA     | 7.74  | 130.99      | 120.54   |
| 1   | Q     | 496 | ASP  | CA-C-O     | 7.73  | 129.34      | 120.60   |
| 1   | P     | 147 | GLN  | OE1-CD-NE2 | -7.73 | 114.87      | 122.60   |
| 1   | B     | 228 | VAL  | O-C-N      | -7.72 | 113.52      | 122.94   |
| 1   | P     | 429 | LEU  | CA-C-N     | 7.72  | 130.62      | 120.28   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 429 | LEU  | C-N-CA    | 7.72  | 130.62      | 120.28   |
| 1   | R     | 219 | ASP  | CA-CB-CG  | 7.72  | 120.32      | 112.60   |
| 1   | G     | 35  | ASN  | CA-C-N    | 7.72  | 130.88      | 120.77   |
| 1   | G     | 35  | ASN  | C-N-CA    | 7.72  | 130.88      | 120.77   |
| 1   | I     | 512 | ALA  | O-C-N     | 7.72  | 130.02      | 122.07   |
| 1   | O     | 142 | ALA  | CA-C-N    | 7.72  | 131.12      | 120.63   |
| 1   | O     | 142 | ALA  | C-N-CA    | 7.72  | 131.12      | 120.63   |
| 1   | A     | 350 | ASP  | N-CA-C    | -7.71 | 103.69      | 113.72   |
| 1   | S     | 172 | LYS  | CA-C-N    | 7.71  | 131.65      | 120.38   |
| 1   | S     | 172 | LYS  | C-N-CA    | 7.71  | 131.65      | 120.38   |
| 1   | Q     | 179 | GLU  | CA-C-N    | 7.71  | 130.47      | 120.44   |
| 1   | Q     | 179 | GLU  | C-N-CA    | 7.71  | 130.47      | 120.44   |
| 1   | B     | 415 | ILE  | CB-CA-C   | -7.71 | 100.63      | 111.19   |
| 1   | L     | 270 | THR  | O-C-N     | -7.71 | 113.95      | 122.12   |
| 1   | Q     | 352 | GLY  | O-C-N     | -7.71 | 115.64      | 123.35   |
| 1   | A     | 105 | LYS  | CA-C-N    | 7.70  | 131.10      | 120.63   |
| 1   | A     | 105 | LYS  | C-N-CA    | 7.70  | 131.10      | 120.63   |
| 1   | P     | 63  | LEU  | CA-C-O    | 7.70  | 128.94      | 119.78   |
| 1   | D     | 316 | GLY  | CA-C-N    | 7.70  | 132.51      | 120.34   |
| 1   | D     | 316 | GLY  | C-N-CA    | 7.70  | 132.51      | 120.34   |
| 1   | N     | 266 | ILE  | O-C-N     | -7.70 | 114.82      | 122.67   |
| 1   | B     | 335 | THR  | CA-CB-OG1 | 7.70  | 121.14      | 109.60   |
| 1   | D     | 145 | THR  | O-C-N     | -7.69 | 112.12      | 122.43   |
| 1   | B     | 196 | ARG  | NE-CZ-NH2 | 7.69  | 126.12      | 119.20   |
| 1   | C     | 214 | GLY  | CA-C-N    | 7.68  | 128.53      | 121.31   |
| 1   | C     | 214 | GLY  | C-N-CA    | 7.68  | 128.53      | 121.31   |
| 1   | I     | 322 | ARG  | N-CA-C    | 7.68  | 122.11      | 111.74   |
| 1   | S     | 93  | ALA  | CA-C-N    | 7.68  | 130.79      | 120.65   |
| 1   | S     | 93  | ALA  | C-N-CA    | 7.68  | 130.79      | 120.65   |
| 1   | D     | 396 | ARG  | NE-CZ-NH2 | -7.68 | 112.29      | 119.20   |
| 1   | F     | 190 | THR  | O-C-N     | -7.68 | 113.45      | 122.20   |
| 1   | L     | 338 | ARG  | NE-CZ-NH2 | -7.67 | 112.29      | 119.20   |
| 1   | R     | 308 | ALA  | N-CA-C    | 7.67  | 121.90      | 112.54   |
| 1   | G     | 211 | LYS  | CA-C-N    | 7.67  | 133.58      | 122.77   |
| 1   | G     | 211 | LYS  | C-N-CA    | 7.67  | 133.58      | 122.77   |
| 1   | G     | 329 | GLU  | O-C-N     | -7.66 | 114.18      | 122.07   |
| 1   | P     | 169 | LEU  | O-C-N     | -7.66 | 112.85      | 122.27   |
| 1   | P     | 458 | LEU  | N-CA-C    | 7.66  | 119.27      | 111.07   |
| 1   | O     | 141 | VAL  | CA-C-N    | 7.66  | 130.87      | 120.38   |
| 1   | O     | 141 | VAL  | C-N-CA    | 7.66  | 130.87      | 120.38   |
| 1   | O     | 345 | GLU  | CA-C-O    | 7.66  | 127.68      | 119.03   |
| 1   | G     | 453 | SER  | CA-C-N    | 7.65  | 130.87      | 120.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 453 | SER  | C-N-CA      | 7.65  | 130.87      | 120.54   |
| 1   | S     | 173 | ALA  | CA-C-N      | 7.65  | 132.66      | 121.18   |
| 1   | S     | 173 | ALA  | C-N-CA      | 7.65  | 132.66      | 121.18   |
| 1   | N     | 387 | LEU  | CA-C-N      | 7.65  | 131.55      | 120.38   |
| 1   | N     | 387 | LEU  | C-N-CA      | 7.65  | 131.55      | 120.38   |
| 1   | M     | 28  | GLY  | CA-C-N      | 7.65  | 131.55      | 120.38   |
| 1   | M     | 28  | GLY  | C-N-CA      | 7.65  | 131.55      | 120.38   |
| 1   | F     | 267 | ASN  | CA-CB-CG    | 7.65  | 120.25      | 112.60   |
| 1   | C     | 99  | GLU  | N-CA-C      | 7.65  | 119.25      | 111.07   |
| 1   | A     | 66  | ILE  | O-C-N       | -7.63 | 115.36      | 123.14   |
| 1   | H     | 361 | LYS  | O-C-N       | -7.62 | 114.35      | 123.27   |
| 1   | Q     | 229 | ASP  | O-C-N       | -7.61 | 112.46      | 122.59   |
| 1   | O     | 450 | ALA  | CA-C-N      | 7.61  | 131.10      | 120.29   |
| 1   | O     | 450 | ALA  | C-N-CA      | 7.61  | 131.10      | 120.29   |
| 1   | B     | 408 | VAL  | O-C-N       | 7.61  | 129.25      | 121.87   |
| 1   | Q     | 234 | HIS  | CE1-NE2-CD2 | -7.60 | 101.40      | 109.00   |
| 1   | G     | 443 | ALA  | O-C-N       | -7.60 | 113.88      | 122.09   |
| 1   | F     | 270 | THR  | N-CA-C      | 7.60  | 119.56      | 111.28   |
| 1   | O     | 421 | VAL  | CA-C-N      | 7.60  | 130.68      | 120.65   |
| 1   | O     | 421 | VAL  | C-N-CA      | 7.60  | 130.68      | 120.65   |
| 1   | Q     | 366 | LYS  | CA-C-O      | 7.60  | 128.76      | 120.71   |
| 1   | B     | 376 | PRO  | CA-C-N      | 7.59  | 131.85      | 120.31   |
| 1   | B     | 376 | PRO  | C-N-CA      | 7.59  | 131.85      | 120.31   |
| 1   | H     | 91  | GLN  | OE1-CD-NE2  | -7.59 | 115.01      | 122.60   |
| 1   | G     | 127 | HIS  | CA-C-O      | -7.59 | 112.49      | 120.23   |
| 1   | A     | 87  | LYS  | CA-C-N      | 7.58  | 131.06      | 120.29   |
| 1   | A     | 87  | LYS  | C-N-CA      | 7.58  | 131.06      | 120.29   |
| 1   | O     | 83  | HIS  | CE1-NE2-CD2 | -7.58 | 101.42      | 109.00   |
| 1   | M     | 192 | VAL  | CA-CB-CG2   | -7.58 | 97.52       | 110.40   |
| 1   | L     | 61  | ASP  | CA-C-N      | 7.57  | 130.43      | 120.28   |
| 1   | L     | 61  | ASP  | C-N-CA      | 7.57  | 130.43      | 120.28   |
| 1   | G     | 482 | ASN  | CA-CB-CG    | -7.57 | 105.03      | 112.60   |
| 1   | E     | 260 | LEU  | N-CA-C      | 7.56  | 119.16      | 111.07   |
| 1   | A     | 83  | HIS  | CA-C-N      | 7.56  | 126.83      | 118.97   |
| 1   | A     | 83  | HIS  | C-N-CA      | 7.56  | 126.83      | 118.97   |
| 1   | C     | 517 | THR  | CA-C-N      | 7.56  | 130.26      | 120.44   |
| 1   | C     | 517 | THR  | C-N-CA      | 7.56  | 130.26      | 120.44   |
| 1   | C     | 436 | VAL  | O-C-N       | -7.55 | 114.54      | 121.87   |
| 1   | G     | 227 | VAL  | CA-C-O      | 7.55  | 127.71      | 120.31   |
| 1   | K     | 55  | MET  | O-C-N       | -7.55 | 114.35      | 123.19   |
| 1   | B     | 502 | VAL  | CA-C-N      | 7.55  | 135.03      | 122.57   |
| 1   | B     | 502 | VAL  | C-N-CA      | 7.55  | 135.03      | 122.57   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | Q     | 232 | VAL  | N-CA-CB   | 7.55  | 121.91      | 110.13   |
| 1   | E     | 387 | LEU  | CA-C-N    | 7.55  | 131.40      | 120.38   |
| 1   | E     | 387 | LEU  | C-N-CA    | 7.55  | 131.40      | 120.38   |
| 1   | O     | 98  | GLU  | CB-CG-CD  | 7.55  | 125.43      | 112.60   |
| 1   | B     | 268 | ASP  | N-CA-C    | 7.54  | 119.72      | 109.24   |
| 1   | L     | 520 | ALA  | O-C-N     | -7.54 | 114.25      | 122.09   |
| 1   | A     | 440 | GLU  | CA-C-N    | 7.54  | 130.25      | 120.44   |
| 1   | A     | 440 | GLU  | C-N-CA    | 7.54  | 130.25      | 120.44   |
| 1   | K     | 54  | GLY  | N-CA-C    | 7.54  | 124.05      | 112.51   |
| 1   | P     | 488 | ASP  | CA-CB-CG  | 7.54  | 120.14      | 112.60   |
| 1   | L     | 192 | VAL  | CA-C-N    | 7.53  | 131.82      | 121.05   |
| 1   | L     | 192 | VAL  | C-N-CA    | 7.53  | 131.82      | 121.05   |
| 1   | Q     | 457 | ILE  | CA-C-N    | 7.53  | 130.23      | 120.44   |
| 1   | Q     | 457 | ILE  | C-N-CA    | 7.53  | 130.23      | 120.44   |
| 1   | M     | 29  | LYS  | N-CA-C    | 7.53  | 121.39      | 111.75   |
| 1   | Q     | 431 | LYS  | CA-C-N    | 7.53  | 130.68      | 120.44   |
| 1   | Q     | 431 | LYS  | C-N-CA    | 7.53  | 130.68      | 120.44   |
| 1   | G     | 299 | ILE  | N-CA-C    | -7.53 | 97.26       | 108.85   |
| 1   | E     | 186 | VAL  | O-C-N     | -7.51 | 114.55      | 121.91   |
| 1   | F     | 71  | ASP  | N-CA-C    | 7.51  | 120.63      | 109.59   |
| 1   | R     | 409 | ILE  | CA-C-O    | 7.51  | 128.81      | 120.85   |
| 1   | K     | 441 | GLN  | CA-C-N    | 7.51  | 130.66      | 120.38   |
| 1   | K     | 441 | GLN  | C-N-CA    | 7.51  | 130.66      | 120.38   |
| 1   | N     | 488 | ASP  | CA-CB-CG  | 7.51  | 120.11      | 112.60   |
| 1   | A     | 163 | LYS  | N-CA-C    | -7.50 | 101.56      | 111.24   |
| 1   | O     | 329 | GLU  | N-CA-C    | 7.50  | 119.10      | 111.07   |
| 1   | R     | 65  | ASP  | CA-CB-CG  | -7.50 | 105.10      | 112.60   |
| 1   | K     | 420 | ALA  | N-CA-C    | 7.50  | 120.17      | 111.02   |
| 1   | Q     | 474 | ARG  | NE-CZ-NH2 | 7.50  | 125.95      | 119.20   |
| 1   | B     | 113 | GLU  | O-C-N     | -7.49 | 113.61      | 122.15   |
| 1   | P     | 108 | VAL  | N-CA-C    | 7.49  | 117.57      | 110.53   |
| 1   | C     | 228 | VAL  | O-C-N     | -7.48 | 113.49      | 122.77   |
| 1   | Q     | 206 | ASN  | CA-CB-CG  | 7.48  | 120.08      | 112.60   |
| 1   | B     | 268 | ASP  | CA-C-O    | -7.47 | 113.79      | 119.32   |
| 1   | Q     | 29  | LYS  | CA-C-N    | 7.47  | 135.81      | 121.54   |
| 1   | Q     | 29  | LYS  | C-N-CA    | 7.47  | 135.81      | 121.54   |
| 1   | S     | 298 | ILE  | O-C-N     | -7.47 | 114.44      | 123.03   |
| 1   | G     | 179 | GLU  | CA-C-N    | 7.47  | 130.15      | 120.44   |
| 1   | G     | 179 | GLU  | C-N-CA    | 7.47  | 130.15      | 120.44   |
| 1   | A     | 452 | GLU  | O-C-N     | -7.46 | 113.64      | 122.15   |
| 1   | F     | 90  | VAL  | O-C-N     | -7.46 | 114.33      | 121.87   |
| 1   | C     | 84  | PRO  | CA-C-N    | 7.46  | 130.61      | 120.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 84  | PRO  | C-N-CA     | 7.46  | 130.61      | 120.54   |
| 1   | Q     | 135 | TYR  | CB-CG-CD1  | -7.46 | 109.61      | 120.80   |
| 1   | G     | 350 | ASP  | CA-CB-CG   | -7.46 | 105.14      | 112.60   |
| 1   | K     | 179 | GLU  | CA-C-N     | 7.46  | 130.13      | 120.44   |
| 1   | K     | 179 | GLU  | C-N-CA     | 7.46  | 130.13      | 120.44   |
| 1   | N     | 83  | HIS  | CA-C-N     | 7.45  | 126.99      | 119.24   |
| 1   | N     | 83  | HIS  | C-N-CA     | 7.45  | 126.99      | 119.24   |
| 1   | Q     | 323 | ALA  | O-C-N      | -7.45 | 114.85      | 123.27   |
| 1   | O     | 366 | LYS  | N-CA-C     | -7.45 | 96.76       | 108.90   |
| 1   | Q     | 456 | SER  | CA-C-N     | 7.44  | 131.03      | 120.53   |
| 1   | Q     | 456 | SER  | C-N-CA     | 7.44  | 131.03      | 120.53   |
| 1   | E     | 37  | ALA  | CA-C-N     | 7.44  | 130.59      | 120.54   |
| 1   | E     | 37  | ALA  | C-N-CA     | 7.44  | 130.59      | 120.54   |
| 1   | E     | 39  | VAL  | CA-C-N     | 7.44  | 130.57      | 120.38   |
| 1   | E     | 39  | VAL  | C-N-CA     | 7.44  | 130.57      | 120.38   |
| 1   | G     | 358 | GLU  | CA-C-O     | -7.43 | 113.50      | 121.45   |
| 1   | N     | 133 | SER  | CA-C-N     | 7.43  | 128.19      | 119.94   |
| 1   | N     | 133 | SER  | C-N-CA     | 7.43  | 128.19      | 119.94   |
| 1   | L     | 385 | GLY  | CA-C-N     | -7.43 | 114.67      | 122.69   |
| 1   | L     | 385 | GLY  | C-N-CA     | -7.43 | 114.67      | 122.69   |
| 1   | K     | 450 | ALA  | CA-C-N     | 7.42  | 130.83      | 120.29   |
| 1   | K     | 450 | ALA  | C-N-CA     | 7.42  | 130.83      | 120.29   |
| 1   | P     | 295 | ALA  | N-CA-C     | 7.42  | 120.99      | 110.23   |
| 1   | P     | 338 | ARG  | NH1-CZ-NH2 | -7.42 | 109.65      | 119.30   |
| 1   | O     | 80  | ASP  | CA-CB-CG   | -7.42 | 105.18      | 112.60   |
| 1   | C     | 322 | ARG  | N-CA-C     | 7.41  | 121.38      | 111.30   |
| 1   | I     | 85  | ALA  | N-CA-C     | 7.40  | 120.00      | 111.11   |
| 1   | C     | 165 | ALA  | CA-C-N     | 7.40  | 130.20      | 120.28   |
| 1   | C     | 165 | ALA  | C-N-CA     | 7.40  | 130.20      | 120.28   |
| 1   | H     | 229 | ASP  | CA-CB-CG   | 7.40  | 120.00      | 112.60   |
| 1   | B     | 245 | LYS  | CA-C-N     | 7.40  | 130.70      | 120.49   |
| 1   | B     | 245 | LYS  | C-N-CA     | 7.40  | 130.70      | 120.49   |
| 1   | D     | 83  | HIS  | O-C-N      | -7.40 | 114.88      | 121.31   |
| 1   | I     | 321 | ARG  | NE-CZ-NH1  | 7.40  | 128.90      | 121.50   |
| 1   | M     | 264 | ILE  | N-CA-C     | 7.39  | 118.56      | 110.21   |
| 1   | D     | 431 | LYS  | N-CA-C     | 7.39  | 120.21      | 111.71   |
| 1   | G     | 57  | LYS  | CA-C-O     | 7.39  | 128.54      | 120.71   |
| 1   | D     | 37  | ALA  | CA-C-N     | 7.38  | 130.50      | 120.54   |
| 1   | D     | 37  | ALA  | C-N-CA     | 7.38  | 130.50      | 120.54   |
| 1   | P     | 265 | ARG  | NE-CZ-NH2  | 7.38  | 125.84      | 119.20   |
| 1   | Q     | 300 | CYS  | N-CA-C     | 7.38  | 119.26      | 108.86   |
| 1   | A     | 245 | LYS  | CA-C-N     | 7.37  | 130.38      | 120.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 245 | LYS  | C-N-CA     | 7.37  | 130.38      | 120.50   |
| 1   | E     | 65  | ASP  | N-CA-CB    | -7.37 | 98.72       | 111.55   |
| 1   | H     | 208 | GLN  | OE1-CD-NE2 | -7.37 | 115.23      | 122.60   |
| 1   | L     | 110 | PHE  | N-CA-C     | 7.37  | 120.24      | 111.33   |
| 1   | B     | 449 | ASN  | CA-CB-CG   | -7.36 | 105.24      | 112.60   |
| 1   | D     | 36  | ILE  | O-C-N      | 7.36  | 129.30      | 121.94   |
| 1   | K     | 420 | ALA  | CA-C-O     | 7.36  | 129.17      | 121.07   |
| 1   | K     | 83  | HIS  | CB-CA-C    | -7.36 | 101.69      | 110.15   |
| 1   | E     | 232 | VAL  | N-CA-C     | 7.35  | 118.52      | 110.21   |
| 1   | I     | 245 | LYS  | N-CA-CB    | 7.35  | 121.90      | 110.21   |
| 1   | L     | 144 | GLN  | CA-C-O     | 7.35  | 128.39      | 119.49   |
| 1   | Q     | 144 | GLN  | N-CA-C     | 7.35  | 120.16      | 111.71   |
| 1   | F     | 244 | ALA  | N-CA-C     | 7.34  | 119.79      | 110.24   |
| 1   | N     | 93  | ALA  | N-CA-C     | 7.34  | 119.18      | 111.03   |
| 1   | K     | 426 | ALA  | CA-C-N     | 7.34  | 132.87      | 121.19   |
| 1   | K     | 426 | ALA  | C-N-CA     | 7.34  | 132.87      | 121.19   |
| 1   | A     | 66  | ILE  | CA-C-O     | 7.34  | 129.09      | 120.72   |
| 1   | O     | 209 | ILE  | CA-C-O     | 7.34  | 127.50      | 120.31   |
| 1   | I     | 462 | ALA  | CA-C-O     | 7.34  | 127.86      | 119.27   |
| 1   | A     | 170 | SER  | N-CA-C     | 7.34  | 121.33      | 112.38   |
| 1   | S     | 281 | ASN  | CA-C-N     | 7.33  | 130.70      | 120.29   |
| 1   | S     | 281 | ASN  | C-N-CA     | 7.33  | 130.70      | 120.29   |
| 1   | M     | 389 | ARG  | N-CA-C     | -7.33 | 104.31      | 113.55   |
| 1   | D     | 350 | ASP  | CA-CB-CG   | -7.33 | 105.27      | 112.60   |
| 1   | K     | 218 | ASN  | OD1-CG-ND2 | -7.33 | 115.27      | 122.60   |
| 1   | H     | 525 | ARG  | NE-CZ-NH2  | 7.33  | 125.80      | 119.20   |
| 1   | M     | 276 | LEU  | CA-C-N     | 7.32  | 130.40      | 120.44   |
| 1   | M     | 276 | LEU  | C-N-CA     | 7.32  | 130.40      | 120.44   |
| 1   | I     | 230 | LYS  | CA-C-N     | 7.32  | 134.29      | 120.97   |
| 1   | I     | 230 | LYS  | C-N-CA     | 7.32  | 134.29      | 120.97   |
| 1   | I     | 407 | ASP  | CA-CB-CG   | -7.31 | 105.29      | 112.60   |
| 1   | M     | 402 | LEU  | O-C-N      | 7.31  | 129.60      | 122.07   |
| 1   | D     | 479 | ASN  | CA-CB-CG   | -7.31 | 105.29      | 112.60   |
| 1   | R     | 162 | ARG  | N-CA-C     | 7.30  | 120.11      | 111.71   |
| 1   | D     | 526 | ILE  | CB-CA-C    | -7.30 | 103.39      | 111.35   |
| 1   | O     | 115 | VAL  | N-CA-C     | 7.30  | 118.07      | 110.62   |
| 1   | O     | 59  | LEU  | CA-C-O     | 7.30  | 127.98      | 120.24   |
| 1   | A     | 499 | GLN  | CA-C-N     | 7.29  | 131.41      | 120.17   |
| 1   | A     | 499 | GLN  | C-N-CA     | 7.29  | 131.41      | 120.17   |
| 1   | H     | 43  | GLU  | CA-C-O     | 7.29  | 128.48      | 120.82   |
| 1   | K     | 294 | GLY  | CA-C-N     | 7.29  | 131.54      | 120.82   |
| 1   | K     | 294 | GLY  | C-N-CA     | 7.29  | 131.54      | 120.82   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | R     | 127 | HIS  | CA-CB-CG  | -7.29 | 106.51      | 113.80   |
| 1   | A     | 97  | ASP  | CA-CB-CG  | -7.28 | 105.32      | 112.60   |
| 1   | B     | 234 | HIS  | CA-C-N    | 7.28  | 126.98      | 119.56   |
| 1   | B     | 234 | HIS  | C-N-CA    | 7.28  | 126.98      | 119.56   |
| 1   | H     | 187 | LYS  | CA-C-N    | 7.28  | 130.03      | 120.28   |
| 1   | H     | 187 | LYS  | C-N-CA    | 7.28  | 130.03      | 120.28   |
| 1   | N     | 130 | ILE  | N-CA-C    | -7.28 | 103.69      | 110.53   |
| 1   | Q     | 159 | ASP  | CA-CB-CG  | -7.28 | 105.32      | 112.60   |
| 1   | L     | 404 | THR  | O-C-N     | -7.28 | 114.58      | 122.07   |
| 1   | N     | 420 | ALA  | N-CA-C    | 7.27  | 119.89      | 111.02   |
| 1   | N     | 161 | LEU  | CA-C-N    | 7.27  | 130.75      | 120.28   |
| 1   | N     | 161 | LEU  | C-N-CA    | 7.27  | 130.75      | 120.28   |
| 1   | G     | 111 | SER  | N-CA-CB   | 7.27  | 120.52      | 109.91   |
| 1   | K     | 83  | HIS  | CA-C-N    | 7.27  | 126.80      | 119.24   |
| 1   | K     | 83  | HIS  | C-N-CA    | 7.27  | 126.80      | 119.24   |
| 1   | B     | 507 | LEU  | CA-C-N    | 7.26  | 129.71      | 120.56   |
| 1   | B     | 507 | LEU  | C-N-CA    | 7.26  | 129.71      | 120.56   |
| 1   | N     | 65  | ASP  | N-CA-CB   | 7.26  | 121.23      | 109.69   |
| 1   | Q     | 329 | GLU  | CA-C-N    | 7.26  | 132.22      | 120.60   |
| 1   | Q     | 329 | GLU  | C-N-CA    | 7.26  | 132.22      | 120.60   |
| 1   | A     | 479 | ASN  | N-CA-CB   | 7.26  | 120.71      | 110.04   |
| 1   | O     | 459 | ILE  | N-CA-CB   | -7.26 | 102.06      | 110.55   |
| 1   | H     | 526 | ILE  | CB-CA-C   | -7.25 | 102.59      | 111.08   |
| 1   | F     | 436 | VAL  | O-C-N     | -7.25 | 114.84      | 121.87   |
| 1   | E     | 357 | ILE  | CA-C-O    | -7.25 | 112.20      | 121.40   |
| 1   | F     | 487 | ILE  | N-CA-CB   | 7.24  | 121.03      | 111.90   |
| 1   | G     | 245 | LYS  | CA-C-N    | 7.24  | 130.21      | 120.50   |
| 1   | G     | 245 | LYS  | C-N-CA    | 7.24  | 130.21      | 120.50   |
| 1   | O     | 155 | ILE  | CA-C-N    | 7.24  | 130.58      | 120.29   |
| 1   | O     | 155 | ILE  | C-N-CA    | 7.24  | 130.58      | 120.29   |
| 1   | S     | 326 | SER  | N-CA-C    | 7.23  | 120.08      | 111.33   |
| 1   | R     | 93  | ALA  | N-CA-C    | 7.23  | 118.85      | 110.97   |
| 1   | B     | 459 | ILE  | CA-C-N    | 7.23  | 132.68      | 121.19   |
| 1   | B     | 459 | ILE  | C-N-CA    | 7.23  | 132.68      | 121.19   |
| 1   | R     | 329 | GLU  | CA-C-N    | 7.23  | 130.69      | 120.28   |
| 1   | R     | 329 | GLU  | C-N-CA    | 7.23  | 130.69      | 120.28   |
| 1   | S     | 152 | THR  | N-CA-C    | 7.23  | 119.56      | 109.15   |
| 1   | H     | 93  | ALA  | CA-C-N    | 7.22  | 130.18      | 120.65   |
| 1   | H     | 93  | ALA  | C-N-CA    | 7.22  | 130.18      | 120.65   |
| 1   | I     | 350 | ASP  | CA-CB-CG  | -7.22 | 105.38      | 112.60   |
| 1   | O     | 82  | GLN  | N-CA-C    | 7.22  | 119.15      | 111.28   |
| 1   | C     | 477 | HIS  | CB-CG-CD2 | -7.22 | 121.81      | 131.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | P     | 482 | ASN  | CA-C-N     | 7.21  | 130.26      | 120.38   |
| 1   | P     | 482 | ASN  | C-N-CA     | 7.21  | 130.26      | 120.38   |
| 1   | A     | 499 | GLN  | OE1-CD-NE2 | -7.21 | 115.39      | 122.60   |
| 1   | K     | 420 | ALA  | O-C-N      | -7.21 | 114.36      | 122.08   |
| 1   | F     | 362 | VAL  | O-C-N      | -7.21 | 116.03      | 123.03   |
| 1   | A     | 37  | ALA  | CA-C-N     | 7.21  | 130.27      | 120.54   |
| 1   | A     | 37  | ALA  | C-N-CA     | 7.21  | 130.27      | 120.54   |
| 1   | L     | 145 | THR  | O-C-N      | -7.21 | 112.51      | 122.46   |
| 1   | L     | 473 | LEU  | CA-C-O     | -7.21 | 111.30      | 120.31   |
| 1   | N     | 417 | GLY  | CA-C-N     | 7.21  | 130.99      | 120.11   |
| 1   | N     | 417 | GLY  | C-N-CA     | 7.21  | 130.99      | 120.11   |
| 1   | M     | 330 | LYS  | N-CA-C     | 7.20  | 121.17      | 112.38   |
| 1   | O     | 500 | LYS  | N-CA-C     | -7.20 | 101.62      | 113.50   |
| 1   | A     | 158 | THR  | CA-CB-OG1  | 7.20  | 120.40      | 109.60   |
| 1   | N     | 260 | LEU  | O-C-N      | -7.20 | 114.49      | 122.12   |
| 1   | B     | 407 | ASP  | CA-C-N     | 7.20  | 130.32      | 120.46   |
| 1   | B     | 407 | ASP  | C-N-CA     | 7.20  | 130.32      | 120.46   |
| 1   | M     | 515 | ALA  | CA-C-N     | 7.20  | 130.26      | 120.54   |
| 1   | M     | 515 | ALA  | C-N-CA     | 7.20  | 130.26      | 120.54   |
| 1   | H     | 391 | VAL  | CA-C-N     | 7.20  | 129.93      | 120.28   |
| 1   | H     | 391 | VAL  | C-N-CA     | 7.20  | 129.93      | 120.28   |
| 1   | I     | 500 | LYS  | CA-C-O     | 7.20  | 126.64      | 119.08   |
| 1   | A     | 260 | LEU  | N-CA-C     | 7.20  | 119.75      | 111.11   |
| 1   | L     | 127 | HIS  | CA-C-N     | 7.20  | 127.20      | 119.28   |
| 1   | L     | 127 | HIS  | C-N-CA     | 7.20  | 127.20      | 119.28   |
| 1   | A     | 104 | THR  | N-CA-C     | 7.19  | 119.20      | 111.36   |
| 1   | Q     | 224 | TYR  | CA-CB-CG   | -7.19 | 100.95      | 113.90   |
| 1   | A     | 232 | VAL  | CB-CA-C    | -7.19 | 103.68      | 111.59   |
| 1   | D     | 377 | LYS  | CA-C-O     | 7.19  | 128.37      | 120.82   |
| 1   | I     | 83  | HIS  | CA-C-N     | 7.19  | 126.72      | 119.24   |
| 1   | I     | 83  | HIS  | C-N-CA     | 7.19  | 126.72      | 119.24   |
| 1   | B     | 285 | GLU  | CA-C-N     | 7.19  | 130.25      | 120.54   |
| 1   | B     | 285 | GLU  | C-N-CA     | 7.19  | 130.25      | 120.54   |
| 1   | O     | 178 | ARG  | NE-CZ-NH2  | 7.19  | 125.67      | 119.20   |
| 1   | G     | 178 | ARG  | NE-CZ-NH2  | 7.18  | 125.67      | 119.20   |
| 1   | I     | 433 | ALA  | CA-C-O     | -7.18 | 110.32      | 120.16   |
| 1   | S     | 305 | ASP  | CA-CB-CG   | -7.18 | 105.42      | 112.60   |
| 1   | H     | 471 | MET  | O-C-N      | 7.18  | 129.47      | 122.07   |
| 1   | N     | 120 | ASP  | N-CA-CB    | -7.18 | 99.16       | 110.22   |
| 1   | P     | 373 | ALA  | CA-C-N     | 7.18  | 129.90      | 120.28   |
| 1   | P     | 373 | ALA  | C-N-CA     | 7.18  | 129.90      | 120.28   |
| 1   | H     | 100 | THR  | N-CA-CB    | 7.17  | 122.22      | 110.17   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 78  | LYS  | CA-C-N    | 7.17  | 131.06      | 120.87   |
| 1   | I     | 78  | LYS  | C-N-CA    | 7.17  | 131.06      | 120.87   |
| 1   | A     | 488 | ASP  | CA-CB-CG  | -7.17 | 105.43      | 112.60   |
| 1   | L     | 124 | LYS  | CA-C-N    | 7.17  | 132.90      | 122.36   |
| 1   | L     | 124 | LYS  | C-N-CA    | 7.17  | 132.90      | 122.36   |
| 1   | S     | 407 | ASP  | CA-CB-CG  | -7.17 | 105.43      | 112.60   |
| 1   | P     | 244 | ALA  | N-CA-C    | 7.17  | 119.47      | 109.15   |
| 1   | Q     | 103 | GLY  | N-CA-C    | -7.16 | 105.43      | 115.32   |
| 1   | N     | 423 | ILE  | N-CA-C    | 7.16  | 121.05      | 111.17   |
| 1   | E     | 227 | VAL  | CA-C-N    | 7.16  | 131.45      | 122.43   |
| 1   | E     | 227 | VAL  | C-N-CA    | 7.16  | 131.45      | 122.43   |
| 1   | Q     | 439 | LYS  | CA-C-N    | 7.16  | 130.83      | 120.38   |
| 1   | Q     | 439 | LYS  | C-N-CA    | 7.16  | 130.83      | 120.38   |
| 1   | B     | 417 | GLY  | CA-C-O    | -7.16 | 114.74      | 122.47   |
| 1   | N     | 234 | HIS  | CA-C-N    | 7.16  | 126.77      | 119.19   |
| 1   | N     | 234 | HIS  | C-N-CA    | 7.16  | 126.77      | 119.19   |
| 1   | A     | 413 | ARG  | NE-CZ-NH2 | 7.15  | 125.64      | 119.20   |
| 1   | O     | 111 | SER  | N-CA-C    | -7.15 | 103.17      | 110.97   |
| 1   | H     | 28  | GLY  | CA-C-N    | 7.15  | 130.82      | 120.38   |
| 1   | H     | 28  | GLY  | C-N-CA    | 7.15  | 130.82      | 120.38   |
| 1   | G     | 333 | ARG  | NE-CZ-NH1 | 7.15  | 128.65      | 121.50   |
| 1   | A     | 502 | VAL  | O-C-N     | -7.15 | 113.64      | 122.57   |
| 1   | B     | 293 | THR  | N-CA-C    | -7.15 | 104.71      | 113.50   |
| 1   | D     | 307 | VAL  | CA-CB-CG1 | 7.15  | 122.55      | 110.40   |
| 1   | N     | 372 | GLY  | CA-C-N    | 7.14  | 131.54      | 120.75   |
| 1   | N     | 372 | GLY  | C-N-CA    | 7.14  | 131.54      | 120.75   |
| 1   | Q     | 358 | GLU  | N-CA-C    | 7.14  | 118.60      | 108.74   |
| 1   | E     | 268 | ASP  | O-C-N     | -7.14 | 114.48      | 121.19   |
| 1   | I     | 205 | ASP  | CA-CB-CG  | 7.14  | 119.74      | 112.60   |
| 1   | G     | 433 | ALA  | CA-C-N    | 7.13  | 128.76      | 119.84   |
| 1   | G     | 433 | ALA  | C-N-CA    | 7.13  | 128.76      | 119.84   |
| 1   | G     | 161 | LEU  | CA-C-N    | 7.13  | 130.79      | 120.38   |
| 1   | G     | 161 | LEU  | C-N-CA    | 7.13  | 130.79      | 120.38   |
| 1   | D     | 219 | ASP  | N-CA-CB   | -7.13 | 100.72      | 110.56   |
| 1   | C     | 121 | LEU  | CA-C-N    | 7.12  | 130.41      | 120.29   |
| 1   | C     | 121 | LEU  | C-N-CA    | 7.12  | 130.41      | 120.29   |
| 1   | C     | 223 | VAL  | O-C-N     | -7.12 | 115.70      | 123.18   |
| 1   | B     | 350 | ASP  | CA-C-O    | 7.12  | 127.26      | 119.15   |
| 1   | H     | 517 | THR  | O-C-N     | -7.12 | 114.58      | 122.12   |
| 1   | R     | 85  | ALA  | N-CA-C    | 7.11  | 119.70      | 111.02   |
| 1   | N     | 90  | VAL  | O-C-N     | -7.11 | 114.69      | 121.87   |
| 1   | S     | 32  | VAL  | CB-CA-C   | -7.11 | 102.73      | 112.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 431 | LYS  | CA-C-N      | 7.11  | 130.10      | 120.44   |
| 1   | A     | 431 | LYS  | C-N-CA      | 7.11  | 130.10      | 120.44   |
| 1   | H     | 389 | ARG  | N-CA-CB     | 7.11  | 120.04      | 110.59   |
| 1   | F     | 179 | GLU  | CA-C-N      | 7.10  | 129.68      | 120.44   |
| 1   | F     | 179 | GLU  | C-N-CA      | 7.10  | 129.68      | 120.44   |
| 1   | L     | 184 | ILE  | N-CA-C      | 7.10  | 117.24      | 110.42   |
| 1   | F     | 525 | ARG  | N-CA-C      | 7.10  | 120.06      | 111.82   |
| 1   | O     | 479 | ASN  | CA-CB-CG    | -7.10 | 105.50      | 112.60   |
| 1   | K     | 518 | GLU  | CA-C-N      | 7.10  | 129.67      | 120.44   |
| 1   | K     | 518 | GLU  | C-N-CA      | 7.10  | 129.67      | 120.44   |
| 1   | P     | 351 | LEU  | N-CA-C      | 7.10  | 119.73      | 110.43   |
| 1   | F     | 299 | ILE  | CA-CB-CG1   | 7.09  | 122.46      | 110.40   |
| 1   | P     | 120 | ASP  | N-CA-CB     | -7.09 | 99.28       | 110.28   |
| 1   | D     | 449 | ASN  | CA-CB-CG    | -7.09 | 105.51      | 112.60   |
| 1   | L     | 301 | GLN  | OE1-CD-NE2  | -7.09 | 115.51      | 122.60   |
| 1   | L     | 110 | PHE  | CA-C-N      | 7.08  | 130.10      | 120.54   |
| 1   | L     | 110 | PHE  | C-N-CA      | 7.08  | 130.10      | 120.54   |
| 1   | H     | 82  | GLN  | OE1-CD-NE2  | 7.08  | 129.68      | 122.60   |
| 1   | N     | 431 | LYS  | O-C-N       | -7.08 | 113.56      | 122.27   |
| 1   | H     | 249 | ILE  | N-CA-C      | 7.08  | 118.05      | 107.51   |
| 1   | C     | 33  | ARG  | CA-C-N      | 7.07  | 130.09      | 120.54   |
| 1   | C     | 33  | ARG  | C-N-CA      | 7.07  | 130.09      | 120.54   |
| 1   | H     | 83  | HIS  | CE1-NE2-CD2 | -7.07 | 101.93      | 109.00   |
| 1   | I     | 166 | MET  | O-C-N       | -7.07 | 114.09      | 122.15   |
| 1   | B     | 35  | ASN  | CA-CB-CG    | -7.07 | 105.53      | 112.60   |
| 1   | I     | 420 | ALA  | N-CA-C      | 7.07  | 119.65      | 111.02   |
| 1   | Q     | 471 | MET  | CA-C-N      | 7.07  | 130.46      | 120.28   |
| 1   | Q     | 471 | MET  | C-N-CA      | 7.07  | 130.46      | 120.28   |
| 1   | K     | 268 | ASP  | CA-CB-CG    | -7.07 | 105.53      | 112.60   |
| 1   | F     | 530 | VAL  | O-C-N       | -7.07 | 115.54      | 123.10   |
| 1   | I     | 153 | VAL  | N-CA-C      | 7.07  | 118.06      | 108.17   |
| 1   | Q     | 355 | SER  | N-CA-CB     | 7.07  | 120.62      | 110.16   |
| 1   | B     | 85  | ALA  | CA-C-N      | 7.07  | 129.63      | 120.44   |
| 1   | B     | 85  | ALA  | C-N-CA      | 7.07  | 129.63      | 120.44   |
| 1   | I     | 257 | LYS  | CA-C-N      | 7.07  | 128.29      | 120.45   |
| 1   | I     | 257 | LYS  | C-N-CA      | 7.07  | 128.29      | 120.45   |
| 1   | F     | 234 | HIS  | CB-CG-CD2   | -7.06 | 122.02      | 131.20   |
| 1   | A     | 482 | ASN  | CA-C-N      | 7.06  | 129.74      | 120.28   |
| 1   | A     | 482 | ASN  | C-N-CA      | 7.06  | 129.74      | 120.28   |
| 1   | F     | 240 | ARG  | NE-CZ-NH1   | 7.06  | 128.56      | 121.50   |
| 1   | B     | 174 | VAL  | N-CA-C      | 7.06  | 118.55      | 109.30   |
| 1   | B     | 433 | ALA  | CA-C-O      | -7.06 | 110.49      | 120.16   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Q     | 40  | LYS  | CA-C-N     | 7.06  | 129.62      | 120.44   |
| 1   | Q     | 40  | LYS  | C-N-CA     | 7.06  | 129.62      | 120.44   |
| 1   | G     | 520 | ALA  | N-CA-C     | 7.06  | 119.63      | 111.02   |
| 1   | F     | 400 | ASP  | CA-C-O     | 7.06  | 128.23      | 120.82   |
| 1   | Q     | 494 | PRO  | CA-C-O     | -7.05 | 113.69      | 121.23   |
| 1   | D     | 346 | ILE  | N-CA-CB    | 7.05  | 118.98      | 110.31   |
| 1   | D     | 250 | ASP  | CA-C-N     | 7.05  | 130.84      | 120.90   |
| 1   | D     | 250 | ASP  | C-N-CA     | 7.05  | 130.84      | 120.90   |
| 1   | Q     | 366 | LYS  | O-C-N      | -7.05 | 114.26      | 123.21   |
| 1   | A     | 162 | ARG  | NE-CZ-NH1  | 7.04  | 128.54      | 121.50   |
| 1   | P     | 250 | ASP  | CA-C-N     | 7.04  | 131.39      | 120.75   |
| 1   | P     | 250 | ASP  | C-N-CA     | 7.04  | 131.39      | 120.75   |
| 1   | N     | 206 | ASN  | OD1-CG-ND2 | -7.04 | 115.56      | 122.60   |
| 1   | Q     | 288 | ASP  | CA-CB-CG   | -7.04 | 105.56      | 112.60   |
| 1   | Q     | 352 | GLY  | CA-C-O     | 7.04  | 127.37      | 121.18   |
| 1   | M     | 114 | LEU  | CA-C-N     | 7.04  | 129.42      | 120.56   |
| 1   | M     | 114 | LEU  | C-N-CA     | 7.04  | 129.42      | 120.56   |
| 1   | H     | 416 | ALA  | CB-CA-C    | -7.03 | 98.64       | 109.89   |
| 1   | C     | 61  | ASP  | CA-C-N     | 7.03  | 129.70      | 120.28   |
| 1   | C     | 61  | ASP  | C-N-CA     | 7.03  | 129.70      | 120.28   |
| 1   | E     | 176 | GLY  | CA-C-N     | 7.03  | 132.81      | 122.82   |
| 1   | E     | 176 | GLY  | C-N-CA     | 7.03  | 132.81      | 122.82   |
| 1   | H     | 220 | THR  | O-C-N      | -7.03 | 114.57      | 122.86   |
| 1   | A     | 319 | ALA  | CA-C-N     | 7.02  | 132.75      | 123.06   |
| 1   | A     | 319 | ALA  | C-N-CA     | 7.02  | 132.75      | 123.06   |
| 1   | Q     | 329 | GLU  | O-C-N      | -7.02 | 114.84      | 122.07   |
| 1   | A     | 516 | ALA  | CA-C-O     | -7.02 | 113.39      | 120.90   |
| 1   | C     | 183 | ASP  | CA-CB-CG   | 7.02  | 119.62      | 112.60   |
| 1   | L     | 379 | ILE  | CA-C-O     | -7.02 | 114.51      | 121.67   |
| 1   | A     | 76  | LEU  | N-CA-C     | -7.01 | 104.85      | 113.41   |
| 1   | C     | 266 | ILE  | CB-CA-C    | 7.01  | 119.61      | 110.91   |
| 1   | D     | 94  | LYS  | CA-C-N     | 7.01  | 127.00      | 120.34   |
| 1   | D     | 94  | LYS  | C-N-CA     | 7.01  | 127.00      | 120.34   |
| 1   | K     | 204 | LEU  | CA-C-O     | -7.01 | 112.18      | 120.10   |
| 1   | P     | 129 | THR  | CA-C-O     | 7.01  | 128.02      | 120.10   |
| 1   | P     | 365 | ASP  | CA-CB-CG   | -7.01 | 105.59      | 112.60   |
| 1   | B     | 55  | MET  | CA-C-N     | 7.01  | 134.92      | 121.54   |
| 1   | B     | 55  | MET  | C-N-CA     | 7.01  | 134.92      | 121.54   |
| 1   | C     | 371 | GLU  | O-C-N      | -7.01 | 115.04      | 122.96   |
| 1   | M     | 57  | LYS  | O-C-N      | -7.01 | 114.33      | 123.16   |
| 1   | I     | 392 | ASP  | CA-C-O     | 7.00  | 128.18      | 120.82   |
| 1   | S     | 482 | ASN  | CA-C-N     | 7.00  | 130.37      | 120.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | S     | 482 | ASN  | C-N-CA      | 7.00  | 130.37      | 120.28   |
| 1   | R     | 32  | VAL  | N-CA-C      | 7.00  | 120.83      | 111.17   |
| 1   | A     | 477 | HIS  | CE1-NE2-CD2 | -7.00 | 102.00      | 109.00   |
| 1   | H     | 83  | HIS  | CA-CB-CG    | -7.00 | 106.80      | 113.80   |
| 1   | M     | 440 | GLU  | CA-C-N      | 7.00  | 129.54      | 120.44   |
| 1   | M     | 440 | GLU  | C-N-CA      | 7.00  | 129.54      | 120.44   |
| 1   | P     | 303 | GLY  | N-CA-C      | 7.00  | 120.03      | 112.33   |
| 1   | B     | 474 | ARG  | NE-CZ-NH2   | 7.00  | 125.50      | 119.20   |
| 1   | B     | 53  | ARG  | NE-CZ-NH2   | -6.99 | 112.91      | 119.20   |
| 1   | R     | 127 | HIS  | CE1-NE2-CD2 | -6.99 | 102.01      | 109.00   |
| 1   | N     | 237 | MET  | O-C-N       | -6.99 | 113.60      | 121.43   |
| 1   | G     | 169 | LEU  | O-C-N       | -6.99 | 112.97      | 122.33   |
| 1   | S     | 521 | THR  | CA-C-N      | 6.99  | 130.21      | 120.29   |
| 1   | S     | 521 | THR  | C-N-CA      | 6.99  | 130.21      | 120.29   |
| 1   | I     | 399 | ARG  | CA-C-N      | 6.99  | 129.52      | 120.44   |
| 1   | I     | 399 | ARG  | C-N-CA      | 6.99  | 129.52      | 120.44   |
| 1   | N     | 229 | ASP  | CA-CB-CG    | 6.99  | 119.59      | 112.60   |
| 1   | P     | 171 | SER  | O-C-N       | -6.99 | 113.61      | 122.34   |
| 1   | A     | 138 | ALA  | CA-C-N      | 6.97  | 129.50      | 120.44   |
| 1   | A     | 138 | ALA  | C-N-CA      | 6.97  | 129.50      | 120.44   |
| 1   | P     | 489 | LEU  | N-CA-C      | 6.97  | 119.76      | 111.33   |
| 1   | S     | 405 | VAL  | O-C-N       | -6.97 | 115.11      | 121.87   |
| 1   | R     | 309 | GLN  | N-CA-C      | -6.97 | 103.61      | 111.14   |
| 1   | S     | 518 | GLU  | O-C-N       | 6.97  | 129.28      | 122.03   |
| 1   | A     | 200 | TRP  | N-CA-C      | 6.96  | 120.33      | 110.23   |
| 1   | N     | 161 | LEU  | N-CA-CB     | -6.96 | 99.50       | 110.22   |
| 1   | O     | 245 | LYS  | CA-C-N      | 6.96  | 130.10      | 120.49   |
| 1   | O     | 245 | LYS  | C-N-CA      | 6.96  | 130.10      | 120.49   |
| 1   | Q     | 457 | ILE  | O-C-N       | -6.96 | 115.06      | 121.89   |
| 1   | O     | 433 | ALA  | CA-C-N      | 6.96  | 128.54      | 119.84   |
| 1   | O     | 433 | ALA  | C-N-CA      | 6.96  | 128.54      | 119.84   |
| 1   | P     | 268 | ASP  | N-CA-C      | 6.96  | 118.92      | 109.24   |
| 1   | C     | 200 | TRP  | CB-CG-CD2   | -6.96 | 117.06      | 126.80   |
| 1   | K     | 56  | ASP  | CA-CB-CG    | -6.96 | 105.64      | 112.60   |
| 1   | M     | 310 | SER  | CA-C-N      | 6.96  | 132.33      | 120.71   |
| 1   | M     | 310 | SER  | C-N-CA      | 6.96  | 132.33      | 120.71   |
| 1   | R     | 115 | VAL  | CA-CB-CG2   | -6.96 | 98.57       | 110.40   |
| 1   | M     | 170 | SER  | N-CA-C      | 6.96  | 121.38      | 112.34   |
| 1   | H     | 442 | LEU  | N-CA-C      | 6.96  | 118.86      | 111.28   |
| 1   | L     | 391 | VAL  | CA-C-N      | 6.96  | 129.93      | 120.54   |
| 1   | L     | 391 | VAL  | C-N-CA      | 6.96  | 129.93      | 120.54   |
| 1   | K     | 80  | ASP  | N-CA-C      | -6.95 | 98.28       | 109.96   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | O     | 110 | PHE  | CA-C-N      | 6.95  | 129.83      | 120.65   |
| 1   | O     | 110 | PHE  | C-N-CA      | 6.95  | 129.83      | 120.65   |
| 1   | E     | 336 | GLY  | CA-C-N      | 6.95  | 128.62      | 122.43   |
| 1   | E     | 336 | GLY  | C-N-CA      | 6.95  | 128.62      | 122.43   |
| 1   | E     | 354 | ALA  | N-CA-C      | -6.95 | 98.45       | 109.23   |
| 1   | Q     | 48  | SER  | N-CA-CB     | 6.95  | 122.66      | 110.42   |
| 1   | B     | 326 | SER  | N-CA-C      | 6.95  | 120.65      | 111.75   |
| 1   | B     | 510 | MET  | N-CA-C      | -6.95 | 104.80      | 113.55   |
| 1   | G     | 328 | LEU  | CA-C-N      | 6.95  | 129.47      | 120.44   |
| 1   | G     | 328 | LEU  | C-N-CA      | 6.95  | 129.47      | 120.44   |
| 1   | I     | 61  | ASP  | O-C-N       | -6.95 | 114.27      | 122.81   |
| 1   | Q     | 162 | ARG  | N-CA-C      | 6.95  | 119.70      | 111.71   |
| 1   | H     | 76  | LEU  | N-CA-C      | -6.94 | 105.34      | 113.88   |
| 1   | L     | 499 | GLN  | O-C-N       | -6.94 | 113.36      | 122.59   |
| 1   | R     | 227 | VAL  | CA-C-N      | 6.93  | 132.01      | 122.93   |
| 1   | R     | 227 | VAL  | C-N-CA      | 6.93  | 132.01      | 122.93   |
| 1   | O     | 266 | ILE  | CA-C-N      | 6.93  | 133.04      | 122.37   |
| 1   | O     | 266 | ILE  | C-N-CA      | 6.93  | 133.04      | 122.37   |
| 1   | K     | 369 | PHE  | CA-CB-CG    | -6.93 | 106.87      | 113.80   |
| 1   | O     | 74  | THR  | CA-C-N      | 6.93  | 132.14      | 120.64   |
| 1   | O     | 74  | THR  | C-N-CA      | 6.93  | 132.14      | 120.64   |
| 1   | B     | 477 | HIS  | CE1-NE2-CD2 | -6.92 | 102.08      | 109.00   |
| 1   | E     | 399 | ARG  | CD-NE-CZ    | -6.92 | 114.70      | 124.40   |
| 1   | L     | 106 | THR  | CB-CA-C     | -6.92 | 100.22      | 110.95   |
| 1   | C     | 102 | ASP  | CA-C-O      | -6.92 | 113.82      | 121.23   |
| 1   | K     | 505 | PRO  | O-C-N       | -6.92 | 113.30      | 122.64   |
| 1   | N     | 400 | ASP  | CA-C-N      | 6.92  | 129.44      | 120.44   |
| 1   | N     | 400 | ASP  | C-N-CA      | 6.92  | 129.44      | 120.44   |
| 1   | D     | 234 | HIS  | CE1-NE2-CD2 | -6.92 | 102.08      | 109.00   |
| 1   | G     | 438 | GLY  | O-C-N       | -6.92 | 113.70      | 122.70   |
| 1   | S     | 90  | VAL  | CA-CB-CG1   | -6.92 | 98.64       | 110.40   |
| 1   | Q     | 131 | ILE  | CA-C-N      | 6.92  | 129.42      | 120.56   |
| 1   | Q     | 131 | ILE  | C-N-CA      | 6.92  | 129.42      | 120.56   |
| 1   | B     | 81  | LEU  | N-CA-CB     | 6.92  | 120.40      | 110.16   |
| 1   | K     | 97  | ASP  | CA-CB-CG    | 6.92  | 119.52      | 112.60   |
| 1   | C     | 110 | PHE  | CA-C-O      | -6.92 | 113.22      | 120.55   |
| 1   | Q     | 232 | VAL  | O-C-N       | -6.92 | 115.07      | 122.61   |
| 1   | Q     | 287 | VAL  | O-C-N       | -6.92 | 115.13      | 121.91   |
| 1   | B     | 74  | THR  | N-CA-C      | 6.91  | 119.69      | 111.33   |
| 1   | G     | 206 | ASN  | CA-CB-CG    | -6.91 | 105.69      | 112.60   |
| 1   | O     | 439 | LYS  | CA-C-N      | 6.91  | 130.47      | 120.38   |
| 1   | O     | 439 | LYS  | C-N-CA      | 6.91  | 130.47      | 120.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 32  | VAL  | N-CA-C   | 6.91  | 120.70      | 111.17   |
| 1   | G     | 434 | PRO  | N-CA-CB  | 6.91  | 110.50      | 103.25   |
| 1   | H     | 76  | LEU  | CA-C-O   | 6.91  | 127.05      | 119.24   |
| 1   | N     | 238 | PRO  | CA-C-N   | 6.90  | 129.53      | 120.28   |
| 1   | N     | 238 | PRO  | C-N-CA   | 6.90  | 129.53      | 120.28   |
| 1   | N     | 299 | ILE  | O-C-N    | -6.90 | 115.73      | 123.18   |
| 1   | P     | 83  | HIS  | CA-C-N   | 6.90  | 126.42      | 119.24   |
| 1   | P     | 83  | HIS  | C-N-CA   | 6.90  | 126.42      | 119.24   |
| 1   | E     | 157 | ASP  | CA-CB-CG | 6.90  | 119.50      | 112.60   |
| 1   | L     | 168 | SER  | N-CA-C   | -6.90 | 103.76      | 112.93   |
| 1   | Q     | 281 | ASN  | CA-CB-CG | -6.90 | 105.70      | 112.60   |
| 1   | G     | 456 | SER  | N-CA-CB  | 6.89  | 120.01      | 110.01   |
| 1   | H     | 58  | MET  | O-C-N    | -6.89 | 114.45      | 123.21   |
| 1   | K     | 173 | ALA  | CA-C-O   | 6.89  | 127.93      | 119.11   |
| 1   | F     | 405 | VAL  | CA-C-N   | 6.89  | 129.51      | 120.28   |
| 1   | F     | 405 | VAL  | C-N-CA   | 6.89  | 129.51      | 120.28   |
| 1   | M     | 179 | GLU  | CA-C-N   | 6.89  | 129.40      | 120.44   |
| 1   | M     | 179 | GLU  | C-N-CA   | 6.89  | 129.40      | 120.44   |
| 1   | E     | 354 | ALA  | CA-C-O   | 6.89  | 129.05      | 121.06   |
| 1   | H     | 53  | ARG  | CA-C-N   | 6.89  | 127.95      | 120.44   |
| 1   | H     | 53  | ARG  | C-N-CA   | 6.89  | 127.95      | 120.44   |
| 1   | N     | 429 | LEU  | CA-C-N   | 6.89  | 129.39      | 120.44   |
| 1   | N     | 429 | LEU  | C-N-CA   | 6.89  | 129.39      | 120.44   |
| 1   | C     | 520 | ALA  | N-CA-C   | 6.89  | 119.37      | 111.11   |
| 1   | S     | 138 | ALA  | CA-C-N   | 6.89  | 129.39      | 120.44   |
| 1   | S     | 138 | ALA  | C-N-CA   | 6.89  | 129.39      | 120.44   |
| 1   | O     | 526 | ILE  | O-C-N    | -6.88 | 114.75      | 122.66   |
| 1   | G     | 64  | GLY  | CA-C-N   | 6.88  | 131.56      | 121.31   |
| 1   | G     | 64  | GLY  | C-N-CA   | 6.88  | 131.56      | 121.31   |
| 1   | S     | 426 | ALA  | CA-C-N   | 6.88  | 132.12      | 121.19   |
| 1   | S     | 426 | ALA  | C-N-CA   | 6.88  | 132.12      | 121.19   |
| 1   | I     | 243 | ASN  | CA-C-N   | 6.88  | 131.69      | 121.72   |
| 1   | I     | 243 | ASN  | C-N-CA   | 6.88  | 131.69      | 121.72   |
| 1   | D     | 126 | VAL  | O-C-N    | -6.87 | 115.18      | 122.81   |
| 1   | M     | 136 | LYS  | N-CA-C   | 6.87  | 118.46      | 110.97   |
| 1   | O     | 264 | ILE  | O-C-N    | -6.87 | 115.54      | 122.62   |
| 1   | F     | 478 | GLU  | CA-C-N   | 6.87  | 130.50      | 120.82   |
| 1   | F     | 478 | GLU  | C-N-CA   | 6.87  | 130.50      | 120.82   |
| 1   | E     | 325 | LYS  | CA-CB-CG | 6.87  | 127.83      | 114.10   |
| 1   | C     | 254 | GLU  | CA-C-O   | -6.86 | 113.29      | 120.70   |
| 1   | D     | 468 | ASP  | O-C-N    | -6.86 | 114.74      | 122.08   |
| 1   | F     | 183 | ASP  | N-CA-C   | 6.86  | 119.34      | 111.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 55  | MET  | N-CA-C      | 6.86  | 120.11      | 109.07   |
| 1   | E     | 183 | ASP  | CA-CB-CG    | 6.86  | 119.46      | 112.60   |
| 1   | M     | 271 | GLN  | CA-C-N      | 6.86  | 130.32      | 120.79   |
| 1   | M     | 271 | GLN  | C-N-CA      | 6.86  | 130.32      | 120.79   |
| 1   | E     | 170 | SER  | O-C-N       | -6.85 | 113.48      | 122.39   |
| 1   | G     | 322 | ARG  | N-CA-C      | 6.85  | 120.53      | 111.28   |
| 1   | M     | 39  | VAL  | O-C-N       | -6.85 | 115.19      | 121.91   |
| 1   | S     | 204 | LEU  | N-CA-C      | 6.85  | 120.52      | 111.75   |
| 1   | S     | 433 | ALA  | CA-C-N      | 6.85  | 128.41      | 119.84   |
| 1   | S     | 433 | ALA  | C-N-CA      | 6.85  | 128.41      | 119.84   |
| 1   | B     | 233 | VAL  | N-CA-C      | 6.85  | 118.43      | 110.62   |
| 1   | E     | 146 | ILE  | CA-C-O      | 6.84  | 128.06      | 120.46   |
| 1   | N     | 171 | SER  | O-C-N       | -6.84 | 113.45      | 122.42   |
| 1   | S     | 243 | ASN  | CA-CB-CG    | -6.84 | 105.75      | 112.60   |
| 1   | P     | 428 | LYS  | N-CA-C      | 6.84  | 118.74      | 111.28   |
| 1   | N     | 287 | VAL  | O-C-N       | -6.84 | 115.20      | 121.91   |
| 1   | B     | 493 | GLN  | CA-C-N      | 6.84  | 127.22      | 119.83   |
| 1   | B     | 493 | GLN  | C-N-CA      | 6.84  | 127.22      | 119.83   |
| 1   | O     | 281 | ASN  | CA-C-N      | 6.84  | 130.00      | 120.29   |
| 1   | O     | 281 | ASN  | C-N-CA      | 6.84  | 130.00      | 120.29   |
| 1   | D     | 479 | ASN  | CA-C-N      | 6.84  | 132.06      | 121.19   |
| 1   | D     | 479 | ASN  | C-N-CA      | 6.84  | 132.06      | 121.19   |
| 1   | R     | 349 | GLN  | OE1-CD-NE2  | 6.84  | 129.44      | 122.60   |
| 1   | H     | 458 | LEU  | CA-C-N      | 6.83  | 129.17      | 120.56   |
| 1   | H     | 458 | LEU  | C-N-CA      | 6.83  | 129.17      | 120.56   |
| 1   | I     | 260 | LEU  | N-CA-C      | 6.83  | 118.42      | 110.97   |
| 1   | R     | 437 | GLY  | CA-C-O      | -6.83 | 112.51      | 121.12   |
| 1   | A     | 423 | ILE  | CA-C-N      | 6.83  | 129.73      | 120.44   |
| 1   | A     | 423 | ILE  | C-N-CA      | 6.83  | 129.73      | 120.44   |
| 1   | G     | 42  | VAL  | N-CA-C      | 6.83  | 117.58      | 110.62   |
| 1   | P     | 137 | LYS  | N-CA-C      | 6.83  | 120.49      | 111.75   |
| 1   | D     | 216 | SER  | N-CA-C      | 6.83  | 120.36      | 109.24   |
| 1   | G     | 273 | GLN  | OE1-CD-NE2  | -6.83 | 115.77      | 122.60   |
| 1   | N     | 127 | HIS  | CE1-NE2-CD2 | -6.82 | 102.18      | 109.00   |
| 1   | Q     | 42  | VAL  | O-C-N       | -6.82 | 115.25      | 121.87   |
| 1   | K     | 278 | GLU  | CA-C-N      | 6.82  | 130.68      | 120.31   |
| 1   | K     | 278 | GLU  | C-N-CA      | 6.82  | 130.68      | 120.31   |
| 1   | F     | 40  | LYS  | N-CA-C      | 6.82  | 119.58      | 111.33   |
| 1   | Q     | 263 | GLU  | N-CA-C      | 6.82  | 119.10      | 110.24   |
| 1   | S     | 118 | ALA  | CA-C-N      | 6.82  | 129.41      | 120.28   |
| 1   | S     | 118 | ALA  | C-N-CA      | 6.82  | 129.41      | 120.28   |
| 1   | I     | 115 | VAL  | CA-C-N      | 6.81  | 129.64      | 120.65   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | I     | 115 | VAL  | C-N-CA    | 6.81  | 129.64      | 120.65   |
| 1   | I     | 170 | SER  | O-C-N     | -6.81 | 113.47      | 122.33   |
| 1   | R     | 34  | ALA  | CA-C-N    | 6.81  | 130.26      | 120.79   |
| 1   | R     | 34  | ALA  | C-N-CA    | 6.81  | 130.26      | 120.79   |
| 1   | I     | 242 | GLU  | CB-CG-CD  | 6.81  | 124.18      | 112.60   |
| 1   | M     | 178 | ARG  | NE-CZ-NH2 | 6.81  | 125.33      | 119.20   |
| 1   | M     | 347 | SER  | O-C-N     | -6.81 | 116.11      | 123.26   |
| 1   | N     | 496 | ASP  | CA-C-N    | 6.81  | 129.70      | 120.44   |
| 1   | N     | 496 | ASP  | C-N-CA    | 6.81  | 129.70      | 120.44   |
| 1   | R     | 477 | HIS  | O-C-N     | -6.81 | 114.00      | 122.24   |
| 1   | P     | 442 | LEU  | CA-C-N    | 6.81  | 129.29      | 120.44   |
| 1   | P     | 442 | LEU  | C-N-CA    | 6.81  | 129.29      | 120.44   |
| 1   | B     | 65  | ASP  | N-CA-C    | 6.80  | 120.10      | 110.23   |
| 1   | K     | 480 | GLU  | N-CA-C    | 6.80  | 120.84      | 112.54   |
| 1   | O     | 413 | ARG  | CA-C-O    | 6.80  | 127.92      | 120.71   |
| 1   | K     | 213 | ALA  | CA-C-N    | 6.80  | 131.31      | 121.44   |
| 1   | K     | 213 | ALA  | C-N-CA    | 6.80  | 131.31      | 121.44   |
| 1   | Q     | 481 | ASN  | CA-CB-CG  | -6.80 | 105.80      | 112.60   |
| 1   | K     | 350 | ASP  | CA-C-O    | 6.80  | 127.27      | 119.18   |
| 1   | P     | 274 | LYS  | CA-C-O    | 6.80  | 127.64      | 119.61   |
| 1   | D     | 313 | ALA  | CB-CA-C   | -6.80 | 100.16      | 110.90   |
| 1   | I     | 88  | LEU  | CA-C-O    | 6.80  | 127.62      | 120.42   |
| 1   | C     | 42  | VAL  | CB-CA-C   | -6.79 | 102.97      | 112.14   |
| 1   | K     | 493 | GLN  | O-C-N     | -6.79 | 113.51      | 121.32   |
| 1   | C     | 183 | ASP  | O-C-N     | -6.79 | 115.08      | 122.07   |
| 1   | I     | 69  | THR  | CA-C-O    | 6.79  | 128.57      | 121.31   |
| 1   | A     | 131 | ILE  | O-C-N     | -6.79 | 115.02      | 121.87   |
| 1   | F     | 185 | VAL  | N-CA-C    | 6.78  | 118.35      | 110.62   |
| 1   | G     | 400 | ASP  | CA-C-N    | 6.78  | 129.37      | 120.28   |
| 1   | G     | 400 | ASP  | C-N-CA    | 6.78  | 129.37      | 120.28   |
| 1   | L     | 83  | HIS  | CA-C-N    | 6.78  | 126.03      | 118.97   |
| 1   | L     | 83  | HIS  | C-N-CA    | 6.78  | 126.03      | 118.97   |
| 1   | N     | 267 | ASN  | CA-C-O    | 6.78  | 126.51      | 119.05   |
| 1   | I     | 510 | MET  | N-CA-C    | -6.78 | 105.01      | 113.55   |
| 1   | B     | 69  | THR  | CA-C-N    | 6.78  | 131.55      | 120.23   |
| 1   | B     | 69  | THR  | C-N-CA    | 6.78  | 131.55      | 120.23   |
| 1   | I     | 430 | ARG  | N-CA-C    | 6.78  | 118.67      | 111.28   |
| 1   | G     | 515 | ALA  | N-CA-C    | 6.78  | 118.36      | 110.97   |
| 1   | I     | 511 | ASN  | N-CA-C    | 6.77  | 119.68      | 111.82   |
| 1   | M     | 371 | GLU  | N-CA-CB   | 6.77  | 120.04      | 110.36   |
| 1   | C     | 262 | ALA  | O-C-N     | -6.77 | 116.18      | 123.42   |
| 1   | C     | 312 | LEU  | N-CA-C    | 6.76  | 119.67      | 111.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 396 | ARG  | N-CA-CB    | 6.76  | 119.79      | 109.98   |
| 1   | B     | 504 | GLU  | CA-C-O     | -6.76 | 113.02      | 119.91   |
| 1   | N     | 127 | HIS  | CG-CD2-NE2 | 6.76  | 113.96      | 107.20   |
| 1   | C     | 97  | ASP  | CA-CB-CG   | -6.75 | 105.84      | 112.60   |
| 1   | L     | 293 | THR  | N-CA-CB    | 6.75  | 120.46      | 110.53   |
| 1   | S     | 91  | GLN  | OE1-CD-NE2 | -6.75 | 115.85      | 122.60   |
| 1   | R     | 33  | ARG  | CA-C-N     | 6.75  | 129.65      | 120.54   |
| 1   | R     | 33  | ARG  | C-N-CA     | 6.75  | 129.65      | 120.54   |
| 1   | K     | 470 | LEU  | N-CA-C     | 6.75  | 118.63      | 111.28   |
| 1   | Q     | 93  | ALA  | CA-C-N     | 6.75  | 130.16      | 120.79   |
| 1   | Q     | 93  | ALA  | C-N-CA     | 6.75  | 130.16      | 120.79   |
| 1   | F     | 404 | THR  | N-CA-C     | 6.74  | 119.20      | 111.11   |
| 1   | Q     | 152 | THR  | N-CA-C     | 6.74  | 118.86      | 109.15   |
| 1   | F     | 41  | ALA  | N-CA-C     | 6.74  | 118.28      | 111.07   |
| 1   | F     | 405 | VAL  | O-C-N      | -6.74 | 115.33      | 121.87   |
| 1   | M     | 85  | ALA  | N-CA-C     | 6.74  | 119.20      | 111.11   |
| 1   | N     | 523 | VAL  | O-C-N      | -6.74 | 115.33      | 121.87   |
| 1   | C     | 457 | ILE  | CA-C-N     | 6.74  | 129.20      | 120.44   |
| 1   | C     | 457 | ILE  | C-N-CA     | 6.74  | 129.20      | 120.44   |
| 1   | L     | 437 | GLY  | CA-C-O     | -6.74 | 113.72      | 121.47   |
| 1   | D     | 421 | VAL  | CA-C-O     | 6.74  | 127.74      | 120.47   |
| 1   | E     | 430 | ARG  | NE-CZ-NH2  | -6.74 | 113.14      | 119.20   |
| 1   | D     | 453 | SER  | O-C-N      | -6.73 | 114.98      | 122.12   |
| 1   | S     | 93  | ALA  | N-CA-C     | 6.73  | 118.50      | 111.03   |
| 1   | K     | 43  | GLU  | N-CA-C     | 6.73  | 118.27      | 111.07   |
| 1   | O     | 474 | ARG  | NE-CZ-NH1  | -6.73 | 114.77      | 121.50   |
| 1   | D     | 88  | LEU  | CA-C-O     | -6.73 | 113.29      | 120.42   |
| 1   | P     | 410 | LYS  | O-C-N      | -6.73 | 114.35      | 122.22   |
| 1   | G     | 233 | VAL  | CA-C-O     | -6.72 | 113.96      | 120.95   |
| 1   | C     | 428 | LYS  | N-CA-C     | 6.72  | 119.44      | 111.71   |
| 1   | S     | 453 | SER  | CA-C-N     | 6.72  | 129.18      | 120.44   |
| 1   | S     | 453 | SER  | C-N-CA     | 6.72  | 129.18      | 120.44   |
| 1   | A     | 364 | GLU  | O-C-N      | -6.72 | 114.08      | 122.35   |
| 1   | O     | 417 | GLY  | O-C-N      | -6.72 | 117.47      | 122.71   |
| 1   | F     | 286 | LYS  | CA-C-N     | 6.72  | 129.03      | 120.56   |
| 1   | F     | 286 | LYS  | C-N-CA     | 6.72  | 129.03      | 120.56   |
| 1   | I     | 349 | GLN  | N-CA-C     | 6.72  | 119.43      | 111.71   |
| 1   | R     | 252 | SER  | N-CA-C     | 6.72  | 119.48      | 110.35   |
| 1   | H     | 271 | GLN  | CA-C-N     | 6.71  | 130.12      | 120.79   |
| 1   | H     | 271 | GLN  | C-N-CA     | 6.71  | 130.12      | 120.79   |
| 1   | S     | 35  | ASN  | CA-CB-CG   | -6.71 | 105.89      | 112.60   |
| 1   | I     | 200 | TRP  | N-CA-C     | 6.71  | 120.21      | 110.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | N     | 264 | ILE  | N-CA-C     | 6.71  | 118.24      | 109.58   |
| 1   | D     | 377 | LYS  | O-C-N      | -6.71 | 115.16      | 122.07   |
| 1   | E     | 387 | LEU  | CA-C-O     | 6.71  | 127.82      | 120.71   |
| 1   | P     | 360 | ARG  | NE-CZ-NH1  | -6.71 | 114.79      | 121.50   |
| 1   | D     | 183 | ASP  | CA-CB-CG   | -6.70 | 105.90      | 112.60   |
| 1   | Q     | 116 | LYS  | O-C-N      | -6.70 | 114.91      | 122.08   |
| 1   | Q     | 503 | ILE  | CA-C-O     | -6.70 | 113.84      | 121.75   |
| 1   | R     | 218 | ASN  | CA-C-O     | 6.70  | 127.62      | 119.38   |
| 1   | R     | 257 | LYS  | N-CA-C     | 6.70  | 120.03      | 110.24   |
| 1   | O     | 272 | MET  | CG-SD-CE   | -6.70 | 86.17       | 100.90   |
| 1   | C     | 339 | VAL  | O-C-N      | -6.70 | 115.38      | 122.81   |
| 1   | E     | 162 | ARG  | CA-C-O     | 6.69  | 127.66      | 120.10   |
| 1   | N     | 79  | MET  | CG-SD-CE   | -6.69 | 86.18       | 100.90   |
| 1   | Q     | 271 | GLN  | OE1-CD-NE2 | -6.69 | 115.91      | 122.60   |
| 1   | C     | 50  | TYR  | CA-C-N     | 6.69  | 132.37      | 121.87   |
| 1   | C     | 50  | TYR  | C-N-CA     | 6.69  | 132.37      | 121.87   |
| 1   | H     | 245 | LYS  | CA-C-N     | 6.69  | 129.46      | 120.50   |
| 1   | H     | 245 | LYS  | C-N-CA     | 6.69  | 129.46      | 120.50   |
| 1   | C     | 482 | ASN  | CA-CB-CG   | -6.69 | 105.91      | 112.60   |
| 1   | D     | 218 | ASN  | OD1-CG-ND2 | -6.69 | 115.91      | 122.60   |
| 1   | S     | 28  | GLY  | CA-C-N     | 6.69  | 129.54      | 120.38   |
| 1   | S     | 28  | GLY  | C-N-CA     | 6.69  | 129.54      | 120.38   |
| 1   | Q     | 121 | LEU  | CA-C-N     | 6.68  | 129.24      | 120.28   |
| 1   | Q     | 121 | LEU  | C-N-CA     | 6.68  | 129.24      | 120.28   |
| 1   | R     | 398 | LEU  | CA-C-N     | 6.68  | 129.13      | 120.44   |
| 1   | R     | 398 | LEU  | C-N-CA     | 6.68  | 129.13      | 120.44   |
| 1   | B     | 312 | LEU  | CA-C-O     | 6.68  | 127.66      | 119.97   |
| 1   | C     | 278 | GLU  | CA-C-N     | 6.68  | 129.23      | 120.28   |
| 1   | C     | 278 | GLU  | C-N-CA     | 6.68  | 129.23      | 120.28   |
| 1   | G     | 436 | VAL  | N-CA-C     | 6.68  | 117.44      | 110.62   |
| 1   | L     | 302 | LYS  | O-C-N      | -6.68 | 113.70      | 122.59   |
| 1   | L     | 514 | LYS  | CA-C-N     | 6.68  | 129.47      | 120.65   |
| 1   | L     | 514 | LYS  | C-N-CA     | 6.68  | 129.47      | 120.65   |
| 1   | M     | 399 | ARG  | NE-CZ-NH1  | -6.68 | 114.82      | 121.50   |
| 1   | L     | 74  | THR  | CA-C-O     | 6.68  | 127.84      | 120.63   |
| 1   | S     | 333 | ARG  | NE-CZ-NH2  | 6.68  | 125.21      | 119.20   |
| 1   | C     | 516 | ALA  | N-CA-C     | 6.67  | 119.12      | 111.11   |
| 1   | Q     | 414 | ALA  | O-C-N      | -6.67 | 115.60      | 123.41   |
| 1   | H     | 487 | ILE  | O-C-N      | -6.67 | 115.85      | 122.99   |
| 1   | G     | 181 | ILE  | CA-C-N     | 6.67  | 129.54      | 120.54   |
| 1   | G     | 181 | ILE  | C-N-CA     | 6.67  | 129.54      | 120.54   |
| 1   | N     | 191 | GLN  | CB-CG-CD   | 6.67  | 123.94      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | P     | 157 | ASP  | CA-CB-CG   | -6.67 | 105.93      | 112.60   |
| 1   | Q     | 480 | GLU  | CB-CG-CD   | 6.67  | 123.94      | 112.60   |
| 1   | G     | 90  | VAL  | N-CA-C     | 6.67  | 119.38      | 111.05   |
| 1   | D     | 222 | LEU  | O-C-N      | -6.66 | 115.43      | 123.29   |
| 1   | G     | 264 | ILE  | N-CA-C     | 6.66  | 118.37      | 109.37   |
| 1   | M     | 51  | GLY  | CA-C-N     | 6.66  | 126.80      | 119.87   |
| 1   | M     | 51  | GLY  | C-N-CA     | 6.66  | 126.80      | 119.87   |
| 1   | G     | 329 | GLU  | CA-C-N     | 6.66  | 130.10      | 120.38   |
| 1   | G     | 329 | GLU  | C-N-CA     | 6.66  | 130.10      | 120.38   |
| 1   | A     | 102 | ASP  | N-CA-C     | 6.66  | 120.14      | 110.28   |
| 1   | P     | 180 | TYR  | CA-C-N     | 6.66  | 129.87      | 120.42   |
| 1   | P     | 180 | TYR  | C-N-CA     | 6.66  | 129.87      | 120.42   |
| 1   | S     | 175 | ALA  | CA-C-N     | 6.66  | 127.69      | 120.44   |
| 1   | S     | 175 | ALA  | C-N-CA     | 6.66  | 127.69      | 120.44   |
| 1   | L     | 515 | ALA  | CA-C-N     | 6.65  | 129.52      | 120.54   |
| 1   | L     | 515 | ALA  | C-N-CA     | 6.65  | 129.52      | 120.54   |
| 1   | A     | 286 | LYS  | N-CA-C     | 6.65  | 118.53      | 111.28   |
| 1   | D     | 240 | ARG  | NE-CZ-NH2  | -6.65 | 113.22      | 119.20   |
| 1   | R     | 220 | THR  | CA-CB-OG1  | 6.65  | 119.58      | 109.60   |
| 1   | A     | 33  | ARG  | CA-C-N     | 6.65  | 129.51      | 120.54   |
| 1   | A     | 33  | ARG  | C-N-CA     | 6.65  | 129.51      | 120.54   |
| 1   | L     | 237 | MET  | CA-C-N     | 6.65  | 126.68      | 119.90   |
| 1   | L     | 237 | MET  | C-N-CA     | 6.65  | 126.68      | 119.90   |
| 1   | S     | 174 | VAL  | CB-CA-C    | -6.64 | 102.43      | 111.33   |
| 1   | R     | 281 | ASN  | OD1-CG-ND2 | -6.64 | 115.96      | 122.60   |
| 1   | C     | 494 | PRO  | O-C-N      | -6.64 | 115.37      | 123.01   |
| 1   | I     | 195 | LEU  | CA-C-N     | 6.64  | 132.13      | 122.77   |
| 1   | I     | 195 | LEU  | C-N-CA     | 6.64  | 132.13      | 122.77   |
| 1   | S     | 29  | LYS  | CA-C-N     | 6.64  | 134.22      | 121.54   |
| 1   | S     | 29  | LYS  | C-N-CA     | 6.64  | 134.22      | 121.54   |
| 1   | S     | 357 | ILE  | O-C-N      | -6.64 | 116.37      | 123.14   |
| 1   | A     | 36  | ILE  | CA-C-N     | 6.64  | 130.02      | 120.79   |
| 1   | A     | 36  | ILE  | C-N-CA     | 6.64  | 130.02      | 120.79   |
| 1   | H     | 207 | ILE  | O-C-N      | -6.64 | 116.28      | 123.18   |
| 1   | A     | 53  | ARG  | NH1-CZ-NH2 | -6.64 | 110.67      | 119.30   |
| 1   | A     | 495 | VAL  | O-C-N      | -6.64 | 114.62      | 122.58   |
| 1   | F     | 72  | GLY  | CA-C-N     | 6.64  | 131.74      | 121.19   |
| 1   | F     | 72  | GLY  | C-N-CA     | 6.64  | 131.74      | 121.19   |
| 1   | K     | 487 | ILE  | N-CA-C     | 6.63  | 117.83      | 107.28   |
| 1   | A     | 119 | GLU  | N-CA-CB    | -6.63 | 100.37      | 110.12   |
| 1   | C     | 191 | GLN  | OE1-CD-NE2 | -6.63 | 115.97      | 122.60   |
| 1   | E     | 210 | VAL  | CA-CB-CG1  | 6.63  | 121.67      | 110.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | R     | 453 | SER  | CA-C-N      | 6.63  | 129.06      | 120.44   |
| 1   | R     | 453 | SER  | C-N-CA      | 6.63  | 129.06      | 120.44   |
| 1   | M     | 243 | ASN  | CA-C-N      | 6.63  | 130.16      | 120.82   |
| 1   | M     | 243 | ASN  | C-N-CA      | 6.63  | 130.16      | 120.82   |
| 1   | G     | 127 | HIS  | N-CA-C      | 6.62  | 118.14      | 109.93   |
| 1   | G     | 229 | ASP  | N-CA-CB     | -6.62 | 100.03      | 110.49   |
| 1   | A     | 412 | GLY  | O-C-N       | -6.62 | 114.70      | 122.38   |
| 1   | B     | 169 | LEU  | O-C-N       | -6.62 | 113.46      | 122.33   |
| 1   | G     | 343 | ILE  | O-C-N       | -6.62 | 115.21      | 121.90   |
| 1   | L     | 144 | GLN  | O-C-N       | -6.62 | 113.79      | 122.39   |
| 1   | F     | 348 | GLU  | CA-C-O      | 6.62  | 127.44      | 119.10   |
| 1   | H     | 83  | HIS  | CG-CD2-NE2  | 6.62  | 113.82      | 107.20   |
| 1   | P     | 421 | VAL  | CA-C-N      | 6.61  | 129.38      | 120.65   |
| 1   | P     | 421 | VAL  | C-N-CA      | 6.61  | 129.38      | 120.65   |
| 1   | F     | 365 | ASP  | CA-CB-CG    | 6.61  | 119.21      | 112.60   |
| 1   | H     | 450 | ALA  | O-C-N       | -6.61 | 115.12      | 122.12   |
| 1   | R     | 227 | VAL  | O-C-N       | -6.61 | 116.31      | 123.18   |
| 1   | K     | 293 | THR  | O-C-N       | -6.61 | 113.64      | 122.49   |
| 1   | H     | 498 | TRP  | CG-CD2-CE3  | -6.60 | 127.30      | 133.90   |
| 1   | Q     | 286 | LYS  | N-CA-C      | 6.60  | 118.14      | 111.07   |
| 1   | C     | 151 | GLN  | CA-C-N      | 6.60  | 130.75      | 121.24   |
| 1   | C     | 151 | GLN  | C-N-CA      | 6.60  | 130.75      | 121.24   |
| 1   | F     | 173 | ALA  | N-CA-C      | 6.60  | 118.13      | 111.07   |
| 1   | F     | 496 | ASP  | CA-C-O      | 6.60  | 128.06      | 120.60   |
| 1   | R     | 91  | GLN  | CA-C-O      | -6.60 | 113.89      | 120.82   |
| 1   | F     | 433 | ALA  | CA-C-O      | -6.60 | 111.12      | 120.16   |
| 1   | I     | 328 | LEU  | CA-C-N      | 6.60  | 129.02      | 120.44   |
| 1   | I     | 328 | LEU  | C-N-CA      | 6.60  | 129.02      | 120.44   |
| 1   | O     | 33  | ARG  | CA-C-N      | 6.60  | 129.96      | 120.79   |
| 1   | O     | 33  | ARG  | C-N-CA      | 6.60  | 129.96      | 120.79   |
| 1   | N     | 80  | ASP  | CA-C-O      | -6.60 | 114.06      | 120.92   |
| 1   | A     | 459 | ILE  | O-C-N       | -6.59 | 115.45      | 121.91   |
| 1   | S     | 512 | ALA  | O-C-N       | -6.59 | 115.28      | 122.07   |
| 1   | L     | 40  | LYS  | CA-C-N      | 6.59  | 129.44      | 120.54   |
| 1   | L     | 40  | LYS  | C-N-CA      | 6.59  | 129.44      | 120.54   |
| 1   | R     | 496 | ASP  | CA-CB-CG    | 6.59  | 119.19      | 112.60   |
| 1   | A     | 40  | LYS  | O-C-N       | -6.59 | 115.13      | 122.12   |
| 1   | A     | 477 | HIS  | ND1-CE1-NE2 | 6.59  | 114.99      | 108.40   |
| 1   | H     | 228 | VAL  | N-CA-CB     | -6.59 | 103.50      | 111.21   |
| 1   | H     | 381 | ILE  | O-C-N       | -6.59 | 116.06      | 123.18   |
| 1   | L     | 94  | LYS  | CA-C-N      | 6.59  | 134.32      | 121.41   |
| 1   | L     | 94  | LYS  | C-N-CA      | 6.59  | 134.32      | 121.41   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 220 | THR  | O-C-N      | -6.59 | 115.33      | 123.04   |
| 1   | R     | 502 | VAL  | CA-CB-CG1  | 6.59  | 121.60      | 110.40   |
| 1   | L     | 454 | LEU  | CA-C-O     | 6.59  | 127.73      | 120.82   |
| 1   | N     | 369 | PHE  | CA-CB-CG   | -6.59 | 107.21      | 113.80   |
| 1   | B     | 115 | VAL  | CA-C-N     | 6.58  | 129.34      | 120.65   |
| 1   | B     | 115 | VAL  | C-N-CA     | 6.58  | 129.34      | 120.65   |
| 1   | D     | 307 | VAL  | CA-CB-CG2  | -6.58 | 99.21       | 110.40   |
| 1   | N     | 193 | ALA  | O-C-N      | 6.58  | 131.35      | 122.59   |
| 1   | H     | 155 | ILE  | N-CA-C     | 6.58  | 118.12      | 110.62   |
| 1   | S     | 377 | LYS  | N-CA-C     | 6.58  | 118.45      | 111.28   |
| 1   | M     | 41  | ALA  | CA-C-N     | 6.58  | 128.85      | 120.56   |
| 1   | M     | 41  | ALA  | C-N-CA     | 6.58  | 128.85      | 120.56   |
| 1   | E     | 464 | PHE  | O-C-N      | -6.58 | 113.72      | 122.14   |
| 1   | E     | 65  | ASP  | CA-CB-CG   | -6.58 | 106.03      | 112.60   |
| 1   | H     | 42  | VAL  | CA-C-O     | 6.57  | 127.79      | 120.95   |
| 1   | N     | 140 | GLU  | O-C-N      | -6.57 | 114.25      | 122.20   |
| 1   | R     | 261 | ASP  | CA-CB-CG   | -6.57 | 106.03      | 112.60   |
| 1   | G     | 268 | ASP  | CA-C-O     | -6.57 | 114.27      | 119.66   |
| 1   | D     | 94  | LYS  | N-CA-C     | 6.57  | 118.13      | 110.97   |
| 1   | M     | 478 | GLU  | CA-C-O     | 6.57  | 127.51      | 120.55   |
| 1   | N     | 171 | SER  | CA-C-O     | 6.57  | 126.64      | 119.15   |
| 1   | C     | 450 | ALA  | N-CA-C     | 6.57  | 118.44      | 111.28   |
| 1   | D     | 159 | ASP  | O-C-N      | -6.57 | 113.40      | 122.46   |
| 1   | K     | 88  | LEU  | CA-C-N     | 6.57  | 128.98      | 120.44   |
| 1   | K     | 88  | LEU  | C-N-CA     | 6.57  | 128.98      | 120.44   |
| 1   | P     | 308 | ALA  | CA-C-N     | 6.57  | 129.37      | 120.44   |
| 1   | P     | 308 | ALA  | C-N-CA     | 6.57  | 129.37      | 120.44   |
| 1   | M     | 349 | GLN  | OE1-CD-NE2 | 6.56  | 129.16      | 122.60   |
| 1   | Q     | 126 | VAL  | O-C-N      | -6.56 | 115.46      | 122.61   |
| 1   | D     | 91  | GLN  | O-C-N      | 6.56  | 129.08      | 122.12   |
| 1   | E     | 137 | LYS  | O-C-N      | -6.56 | 115.17      | 122.12   |
| 1   | R     | 519 | ALA  | N-CA-C     | 6.56  | 118.98      | 111.11   |
| 1   | B     | 508 | VAL  | O-C-N      | -6.56 | 115.48      | 121.91   |
| 1   | F     | 391 | VAL  | CA-CB-CG1  | 6.56  | 121.55      | 110.40   |
| 1   | I     | 189 | VAL  | CA-C-O     | -6.56 | 112.83      | 120.83   |
| 1   | C     | 315 | LYS  | CA-C-N     | 6.56  | 131.05      | 122.26   |
| 1   | C     | 315 | LYS  | C-N-CA     | 6.56  | 131.05      | 122.26   |
| 1   | M     | 202 | VAL  | CA-C-O     | -6.56 | 113.88      | 120.31   |
| 1   | L     | 445 | GLU  | N-CA-CB    | 6.56  | 119.89      | 110.06   |
| 1   | E     | 298 | ILE  | O-C-N      | -6.55 | 114.38      | 122.57   |
| 1   | F     | 458 | LEU  | N-CA-C     | 6.55  | 118.08      | 111.07   |
| 1   | Q     | 349 | GLN  | OE1-CD-NE2 | -6.55 | 116.05      | 122.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 157 | ASP  | CA-CB-CG    | -6.55 | 106.05      | 112.60   |
| 1   | E     | 147 | GLN  | CA-C-O      | -6.55 | 114.12      | 121.00   |
| 1   | P     | 184 | ILE  | CA-C-N      | 6.55  | 129.76      | 120.53   |
| 1   | P     | 184 | ILE  | C-N-CA      | 6.55  | 129.76      | 120.53   |
| 1   | I     | 349 | GLN  | N-CA-CB     | -6.54 | 100.14      | 110.22   |
| 1   | D     | 322 | ARG  | O-C-N       | -6.54 | 114.44      | 122.55   |
| 1   | O     | 514 | LYS  | O-C-N       | -6.54 | 115.19      | 122.12   |
| 1   | Q     | 94  | LYS  | CA-CB-CG    | 6.54  | 127.19      | 114.10   |
| 1   | D     | 298 | ILE  | CA-C-O      | 6.54  | 126.73      | 120.25   |
| 1   | N     | 127 | HIS  | N-CA-C      | 6.54  | 118.93      | 109.84   |
| 1   | S     | 321 | ARG  | CD-NE-CZ    | 6.54  | 133.56      | 124.40   |
| 1   | A     | 102 | ASP  | N-CA-CB     | -6.54 | 100.36      | 109.97   |
| 1   | L     | 284 | LYS  | N-CA-C      | 6.54  | 119.23      | 111.71   |
| 1   | O     | 93  | ALA  | CA-C-N      | 6.54  | 129.28      | 120.65   |
| 1   | O     | 93  | ALA  | C-N-CA      | 6.54  | 129.28      | 120.65   |
| 1   | O     | 243 | ASN  | CA-CB-CG    | -6.54 | 106.06      | 112.60   |
| 1   | O     | 350 | ASP  | O-C-N       | -6.54 | 113.50      | 122.46   |
| 1   | R     | 35  | ASN  | CA-CB-CG    | -6.54 | 106.06      | 112.60   |
| 1   | C     | 459 | ILE  | CA-C-N      | 6.54  | 131.58      | 121.19   |
| 1   | C     | 459 | ILE  | C-N-CA      | 6.54  | 131.58      | 121.19   |
| 1   | K     | 280 | GLU  | CB-CG-CD    | -6.53 | 101.49      | 112.60   |
| 1   | R     | 402 | LEU  | N-CA-C      | -6.53 | 104.08      | 111.07   |
| 1   | Q     | 287 | VAL  | N-CA-C      | 6.53  | 116.69      | 110.42   |
| 1   | D     | 268 | ASP  | CA-CB-CG    | 6.53  | 119.13      | 112.60   |
| 1   | L     | 69  | THR  | CA-C-N      | 6.52  | 134.00      | 121.54   |
| 1   | L     | 69  | THR  | C-N-CA      | 6.52  | 134.00      | 121.54   |
| 1   | L     | 304 | ILE  | CA-C-O      | 6.52  | 127.54      | 120.43   |
| 1   | C     | 504 | GLU  | O-C-N       | 6.52  | 126.41      | 121.85   |
| 1   | F     | 420 | ALA  | N-CA-C      | 6.52  | 118.97      | 111.02   |
| 1   | F     | 497 | MET  | CG-SD-CE    | -6.52 | 86.56       | 100.90   |
| 1   | M     | 243 | ASN  | N-CA-C      | 6.52  | 119.17      | 111.02   |
| 1   | I     | 74  | THR  | CA-C-N      | 6.52  | 131.46      | 120.64   |
| 1   | I     | 74  | THR  | C-N-CA      | 6.52  | 131.46      | 120.64   |
| 1   | K     | 432 | TYR  | CA-C-O      | 6.52  | 127.41      | 120.70   |
| 1   | R     | 298 | ILE  | CB-CA-C     | -6.52 | 101.25      | 110.12   |
| 1   | C     | 236 | GLY  | CA-C-N      | 6.52  | 129.45      | 120.39   |
| 1   | C     | 236 | GLY  | C-N-CA      | 6.52  | 129.45      | 120.39   |
| 1   | R     | 234 | HIS  | ND1-CE1-NE2 | 6.51  | 114.91      | 108.40   |
| 1   | S     | 340 | VAL  | N-CA-C      | 6.51  | 117.44      | 108.84   |
| 1   | A     | 268 | ASP  | CA-CB-CG    | -6.51 | 106.09      | 112.60   |
| 1   | H     | 264 | ILE  | O-C-N       | -6.51 | 115.73      | 122.63   |
| 1   | H     | 341 | SER  | CB-CA-C     | -6.51 | 98.78       | 110.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | L     | 454 | LEU  | O-C-N       | -6.51 | 115.36      | 122.07   |
| 1   | I     | 76  | LEU  | N-CA-C      | -6.51 | 105.47      | 113.41   |
| 1   | N     | 312 | LEU  | CA-C-N      | 6.51  | 129.00      | 120.28   |
| 1   | N     | 312 | LEU  | C-N-CA      | 6.51  | 129.00      | 120.28   |
| 1   | I     | 83  | HIS  | CE1-NE2-CD2 | -6.51 | 102.49      | 109.00   |
| 1   | C     | 281 | ASN  | OD1-CG-ND2  | -6.50 | 116.09      | 122.60   |
| 1   | G     | 67  | THR  | CA-C-O      | 6.50  | 128.14      | 120.20   |
| 1   | L     | 93  | ALA  | N-CA-C      | 6.50  | 118.25      | 111.03   |
| 1   | A     | 461 | ASN  | CA-CB-CG    | -6.50 | 106.10      | 112.60   |
| 1   | I     | 456 | SER  | CA-C-N      | 6.50  | 128.99      | 120.60   |
| 1   | I     | 456 | SER  | C-N-CA      | 6.50  | 128.99      | 120.60   |
| 1   | I     | 409 | ILE  | CA-C-N      | 6.50  | 129.64      | 120.28   |
| 1   | I     | 409 | ILE  | C-N-CA      | 6.50  | 129.64      | 120.28   |
| 1   | Q     | 97  | ASP  | CA-CB-CG    | -6.50 | 106.10      | 112.60   |
| 1   | F     | 270 | THR  | CA-C-N      | 6.50  | 129.52      | 120.29   |
| 1   | F     | 270 | THR  | C-N-CA      | 6.50  | 129.52      | 120.29   |
| 1   | F     | 487 | ILE  | CB-CA-C     | -6.50 | 102.54      | 110.99   |
| 1   | K     | 465 | ASP  | CA-CB-CG    | -6.50 | 106.10      | 112.60   |
| 1   | S     | 271 | GLN  | N-CA-C      | 6.50  | 118.44      | 111.36   |
| 1   | E     | 389 | ARG  | NE-CZ-NH1   | 6.49  | 127.99      | 121.50   |
| 1   | M     | 460 | GLU  | CA-C-O      | 6.49  | 128.62      | 121.02   |
| 1   | M     | 234 | HIS  | CE1-NE2-CD2 | -6.49 | 102.51      | 109.00   |
| 1   | B     | 234 | HIS  | CA-CB-CG    | 6.49  | 120.29      | 113.80   |
| 1   | L     | 325 | LYS  | CA-C-N      | 6.49  | 129.85      | 120.38   |
| 1   | L     | 325 | LYS  | C-N-CA      | 6.49  | 129.85      | 120.38   |
| 1   | D     | 449 | ASN  | OD1-CG-ND2  | 6.49  | 129.09      | 122.60   |
| 1   | I     | 505 | PRO  | CA-C-N      | 6.49  | 129.62      | 120.28   |
| 1   | I     | 505 | PRO  | C-N-CA      | 6.49  | 129.62      | 120.28   |
| 1   | G     | 405 | VAL  | CA-C-N      | 6.48  | 129.50      | 120.29   |
| 1   | G     | 405 | VAL  | C-N-CA      | 6.48  | 129.50      | 120.29   |
| 1   | B     | 391 | VAL  | CA-C-N      | 6.48  | 128.86      | 120.44   |
| 1   | B     | 391 | VAL  | C-N-CA      | 6.48  | 128.86      | 120.44   |
| 1   | C     | 109 | ILE  | N-CA-CB     | 6.48  | 117.42      | 110.62   |
| 1   | D     | 453 | SER  | CA-C-N      | 6.48  | 129.29      | 120.54   |
| 1   | D     | 453 | SER  | C-N-CA      | 6.48  | 129.29      | 120.54   |
| 1   | I     | 179 | GLU  | N-CA-C      | 6.48  | 118.34      | 111.28   |
| 1   | L     | 262 | ALA  | CA-C-O      | -6.48 | 112.31      | 120.28   |
| 1   | L     | 354 | ALA  | CA-C-N      | 6.47  | 128.96      | 120.28   |
| 1   | L     | 354 | ALA  | C-N-CA      | 6.47  | 128.96      | 120.28   |
| 1   | A     | 265 | ARG  | NE-CZ-NH2   | 6.47  | 125.02      | 119.20   |
| 1   | F     | 257 | LYS  | N-CA-C      | 6.47  | 119.01      | 110.08   |
| 1   | L     | 512 | ALA  | CA-C-N      | 6.47  | 128.95      | 120.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 512 | ALA  | C-N-CA     | 6.47  | 128.95      | 120.60   |
| 1   | Q     | 257 | LYS  | CA-C-O     | -6.47 | 113.74      | 120.02   |
| 1   | B     | 500 | LYS  | N-CA-C     | -6.47 | 102.83      | 113.50   |
| 1   | S     | 104 | THR  | N-CA-C     | 6.47  | 118.41      | 111.36   |
| 1   | S     | 168 | SER  | O-C-N      | -6.47 | 113.72      | 122.19   |
| 1   | B     | 238 | PRO  | N-CA-C     | 6.46  | 121.80      | 111.26   |
| 1   | C     | 511 | ASN  | CA-C-N     | 6.46  | 129.18      | 120.65   |
| 1   | C     | 511 | ASN  | C-N-CA     | 6.46  | 129.18      | 120.65   |
| 1   | M     | 186 | VAL  | N-CA-C     | 6.46  | 116.57      | 110.30   |
| 1   | P     | 138 | ALA  | CA-C-N     | 6.46  | 128.84      | 120.44   |
| 1   | P     | 138 | ALA  | C-N-CA     | 6.46  | 128.84      | 120.44   |
| 1   | F     | 304 | ILE  | N-CA-CB    | 6.46  | 121.56      | 111.99   |
| 1   | P     | 53  | ARG  | CA-C-N     | 6.46  | 126.24      | 120.10   |
| 1   | P     | 53  | ARG  | C-N-CA     | 6.46  | 126.24      | 120.10   |
| 1   | B     | 360 | ARG  | O-C-N      | -6.46 | 115.75      | 123.31   |
| 1   | F     | 292 | ALA  | CA-C-O     | 6.46  | 127.31      | 119.49   |
| 1   | S     | 441 | GLN  | CA-C-N     | 6.46  | 128.94      | 120.28   |
| 1   | S     | 441 | GLN  | C-N-CA     | 6.46  | 128.94      | 120.28   |
| 1   | I     | 206 | ASN  | CA-CB-CG   | -6.46 | 106.14      | 112.60   |
| 1   | K     | 309 | GLN  | O-C-N      | -6.46 | 114.36      | 122.17   |
| 1   | N     | 152 | THR  | N-CA-C     | 6.46  | 118.44      | 109.15   |
| 1   | F     | 430 | ARG  | NE-CZ-NH2  | -6.45 | 113.39      | 119.20   |
| 1   | M     | 232 | VAL  | O-C-N      | -6.45 | 115.67      | 122.57   |
| 1   | P     | 309 | GLN  | CA-C-O     | 6.45  | 127.35      | 120.70   |
| 1   | P     | 449 | ASN  | OD1-CG-ND2 | -6.45 | 116.15      | 122.60   |
| 1   | R     | 69  | THR  | CA-CB-OG1  | 6.45  | 119.28      | 109.60   |
| 1   | A     | 190 | THR  | CA-C-N     | 6.45  | 129.45      | 120.29   |
| 1   | A     | 190 | THR  | C-N-CA     | 6.45  | 129.45      | 120.29   |
| 1   | C     | 474 | ARG  | NE-CZ-NH2  | 6.45  | 125.00      | 119.20   |
| 1   | B     | 162 | ARG  | N-CA-C     | 6.45  | 119.12      | 111.71   |
| 1   | G     | 414 | ALA  | CA-C-N     | 6.45  | 129.77      | 122.48   |
| 1   | G     | 414 | ALA  | C-N-CA     | 6.45  | 129.77      | 122.48   |
| 1   | L     | 328 | LEU  | O-C-N      | -6.45 | 115.28      | 122.12   |
| 1   | M     | 187 | LYS  | CA-C-N     | 6.45  | 128.92      | 120.28   |
| 1   | M     | 187 | LYS  | C-N-CA     | 6.45  | 128.92      | 120.28   |
| 1   | N     | 74  | THR  | CA-C-N     | 6.45  | 131.34      | 120.64   |
| 1   | N     | 74  | THR  | C-N-CA     | 6.45  | 131.34      | 120.64   |
| 1   | Q     | 424 | GLU  | O-C-N      | -6.45 | 115.06      | 122.03   |
| 1   | G     | 69  | THR  | CA-C-O     | 6.45  | 128.21      | 121.31   |
| 1   | F     | 395 | GLU  | N-CA-C     | 6.45  | 119.30      | 111.82   |
| 1   | F     | 432 | TYR  | N-CA-C     | 6.45  | 118.10      | 111.14   |
| 1   | P     | 256 | GLU  | N-CA-C     | 6.45  | 121.14      | 113.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | S     | 250 | ASP  | CA-C-N     | 6.45  | 133.85      | 121.54   |
| 1   | S     | 250 | ASP  | C-N-CA     | 6.45  | 133.85      | 121.54   |
| 1   | A     | 304 | ILE  | CA-C-N     | 6.44  | 129.86      | 120.71   |
| 1   | A     | 304 | ILE  | C-N-CA     | 6.44  | 129.86      | 120.71   |
| 1   | C     | 274 | LYS  | N-CA-C     | 6.44  | 120.60      | 112.87   |
| 1   | I     | 482 | ASN  | CA-CB-CG   | -6.44 | 106.16      | 112.60   |
| 1   | Q     | 43  | GLU  | CB-CA-C    | 6.44  | 121.00      | 110.88   |
| 1   | S     | 356 | LEU  | O-C-N      | -6.44 | 115.52      | 123.44   |
| 1   | D     | 229 | ASP  | CA-C-N     | 6.44  | 133.25      | 121.85   |
| 1   | D     | 229 | ASP  | C-N-CA     | 6.44  | 133.25      | 121.85   |
| 1   | S     | 90  | VAL  | O-C-N      | -6.44 | 115.36      | 121.87   |
| 1   | S     | 107 | ALA  | N-CA-C     | 6.44  | 122.00      | 111.37   |
| 1   | C     | 479 | ASN  | OD1-CG-ND2 | -6.44 | 116.16      | 122.60   |
| 1   | H     | 68  | ILE  | N-CA-C     | -6.44 | 99.16       | 108.36   |
| 1   | K     | 159 | ASP  | CA-CB-CG   | -6.44 | 106.16      | 112.60   |
| 1   | L     | 446 | ALA  | N-CA-C     | 6.44  | 117.99      | 110.97   |
| 1   | M     | 529 | VAL  | CB-CA-C    | -6.44 | 101.63      | 110.77   |
| 1   | B     | 62  | SER  | O-C-N      | -6.43 | 115.44      | 122.07   |
| 1   | E     | 162 | ARG  | NE-CZ-NH2  | -6.43 | 113.41      | 119.20   |
| 1   | L     | 257 | LYS  | N-CA-C     | 6.43  | 118.00      | 109.83   |
| 1   | M     | 310 | SER  | O-C-N      | -6.43 | 114.69      | 122.22   |
| 1   | G     | 437 | GLY  | N-CA-C     | -6.43 | 101.75      | 110.43   |
| 1   | L     | 150 | ALA  | O-C-N      | -6.43 | 114.90      | 122.81   |
| 1   | A     | 131 | ILE  | CA-C-O     | 6.43  | 127.45      | 120.57   |
| 1   | A     | 166 | MET  | CG-SD-CE   | -6.43 | 86.75       | 100.90   |
| 1   | K     | 274 | LYS  | O-C-N      | -6.43 | 113.88      | 122.43   |
| 1   | M     | 365 | ASP  | CA-C-N     | 6.43  | 132.64      | 122.74   |
| 1   | M     | 365 | ASP  | C-N-CA     | 6.43  | 132.64      | 122.74   |
| 1   | P     | 274 | LYS  | N-CA-C     | 6.43  | 120.70      | 112.34   |
| 1   | Q     | 268 | ASP  | O-C-N      | -6.43 | 113.93      | 121.32   |
| 1   | E     | 313 | ALA  | N-CA-C     | 6.43  | 118.37      | 111.36   |
| 1   | F     | 30  | GLU  | O-C-N      | -6.43 | 114.04      | 122.59   |
| 1   | H     | 433 | ALA  | CA-C-O     | -6.43 | 111.35      | 120.16   |
| 1   | P     | 183 | ASP  | N-CA-C     | 6.43  | 117.95      | 111.07   |
| 1   | A     | 197 | GLY  | CA-C-N     | 6.43  | 131.25      | 122.19   |
| 1   | A     | 197 | GLY  | C-N-CA     | 6.43  | 131.25      | 122.19   |
| 1   | I     | 344 | ASP  | CA-CB-CG   | -6.43 | 106.17      | 112.60   |
| 1   | A     | 444 | VAL  | N-CA-C     | 6.42  | 116.59      | 110.42   |
| 1   | I     | 392 | ASP  | O-C-N      | -6.42 | 115.45      | 122.07   |
| 1   | L     | 179 | GLU  | CA-C-N     | 6.42  | 128.79      | 120.44   |
| 1   | L     | 179 | GLU  | C-N-CA     | 6.42  | 128.79      | 120.44   |
| 1   | A     | 242 | GLU  | N-CA-C     | 6.42  | 120.75      | 109.96   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 270 | THR  | N-CA-C    | -6.42 | 104.28      | 111.28   |
| 1   | E     | 430 | ARG  | O-C-N     | -6.42 | 115.46      | 122.07   |
| 1   | F     | 530 | VAL  | CA-C-O    | 6.42  | 127.86      | 120.67   |
| 1   | G     | 351 | LEU  | CA-C-N    | 6.42  | 129.03      | 122.80   |
| 1   | G     | 351 | LEU  | C-N-CA    | 6.42  | 129.03      | 122.80   |
| 1   | L     | 389 | ARG  | NE-CZ-NH2 | -6.42 | 113.42      | 119.20   |
| 1   | P     | 270 | THR  | CA-C-N    | 6.42  | 129.41      | 120.29   |
| 1   | P     | 270 | THR  | C-N-CA    | 6.42  | 129.41      | 120.29   |
| 1   | L     | 496 | ASP  | CA-C-N    | 6.42  | 129.41      | 120.29   |
| 1   | L     | 496 | ASP  | C-N-CA    | 6.42  | 129.41      | 120.29   |
| 1   | G     | 33  | ARG  | CA-C-O    | -6.42 | 114.08      | 120.82   |
| 1   | P     | 521 | THR  | CA-C-N    | 6.42  | 129.41      | 120.29   |
| 1   | P     | 521 | THR  | C-N-CA    | 6.42  | 129.41      | 120.29   |
| 1   | B     | 426 | ALA  | CA-C-O    | -6.42 | 114.15      | 120.89   |
| 1   | D     | 201 | TYR  | CA-C-N    | 6.42  | 131.01      | 122.93   |
| 1   | D     | 201 | TYR  | C-N-CA    | 6.42  | 131.01      | 122.93   |
| 1   | D     | 459 | ILE  | CB-CA-C   | -6.42 | 103.76      | 111.97   |
| 1   | N     | 227 | VAL  | CA-C-O    | 6.42  | 126.75      | 120.27   |
| 1   | I     | 342 | ASN  | O-C-N     | -6.42 | 115.42      | 123.05   |
| 1   | L     | 232 | VAL  | N-CA-C    | 6.41  | 118.33      | 109.80   |
| 1   | O     | 250 | ASP  | N-CA-CB   | -6.41 | 100.44      | 110.44   |
| 1   | K     | 404 | THR  | O-C-N     | -6.41 | 115.47      | 122.07   |
| 1   | Q     | 398 | LEU  | CA-C-N    | 6.41  | 128.78      | 120.44   |
| 1   | Q     | 398 | LEU  | C-N-CA    | 6.41  | 128.78      | 120.44   |
| 1   | C     | 514 | LYS  | CA-C-N    | 6.41  | 129.11      | 120.65   |
| 1   | C     | 514 | LYS  | C-N-CA    | 6.41  | 129.11      | 120.65   |
| 1   | Q     | 348 | GLU  | N-CA-C    | 6.41  | 118.27      | 111.28   |
| 1   | S     | 388 | GLU  | N-CA-C    | 6.41  | 120.20      | 112.38   |
| 1   | O     | 507 | LEU  | O-C-N     | -6.41 | 112.86      | 122.28   |
| 1   | G     | 443 | ALA  | CA-C-O    | 6.41  | 127.30      | 120.70   |
| 1   | N     | 500 | LYS  | CA-C-O    | 6.41  | 125.50      | 118.65   |
| 1   | K     | 68  | ILE  | O-C-N     | -6.40 | 116.46      | 123.18   |
| 1   | B     | 123 | TYR  | CA-C-O    | 6.40  | 127.34      | 120.55   |
| 1   | G     | 157 | ASP  | CA-CB-CG  | -6.40 | 106.20      | 112.60   |
| 1   | N     | 400 | ASP  | CB-CA-C   | 6.40  | 121.73      | 110.85   |
| 1   | R     | 260 | LEU  | O-C-N     | -6.40 | 115.33      | 122.12   |
| 1   | F     | 38  | ALA  | CA-C-N    | 6.40  | 128.62      | 120.56   |
| 1   | F     | 38  | ALA  | C-N-CA    | 6.40  | 128.62      | 120.56   |
| 1   | S     | 514 | LYS  | CA-C-N    | 6.40  | 129.10      | 120.65   |
| 1   | S     | 514 | LYS  | C-N-CA    | 6.40  | 129.10      | 120.65   |
| 1   | C     | 512 | ALA  | N-CA-CB   | 6.40  | 119.25      | 109.91   |
| 1   | D     | 389 | ARG  | CD-NE-CZ  | 6.39  | 133.35      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 90  | VAL  | CA-C-N     | 6.39  | 128.85      | 120.28   |
| 1   | F     | 90  | VAL  | C-N-CA     | 6.39  | 128.85      | 120.28   |
| 1   | A     | 458 | LEU  | N-CA-CB    | -6.39 | 100.74      | 110.01   |
| 1   | C     | 108 | VAL  | N-CA-C     | 6.39  | 116.54      | 110.53   |
| 1   | I     | 262 | ALA  | CA-C-N     | 6.39  | 130.40      | 120.75   |
| 1   | I     | 262 | ALA  | C-N-CA     | 6.39  | 130.40      | 120.75   |
| 1   | Q     | 387 | LEU  | N-CA-C     | 6.39  | 119.18      | 110.55   |
| 1   | B     | 496 | ASP  | CA-CB-CG   | 6.39  | 118.99      | 112.60   |
| 1   | C     | 113 | GLU  | N-CA-C     | 6.39  | 118.33      | 111.36   |
| 1   | H     | 206 | ASN  | CA-CB-CG   | -6.39 | 106.21      | 112.60   |
| 1   | K     | 115 | VAL  | CA-C-N     | 6.39  | 129.08      | 120.65   |
| 1   | K     | 115 | VAL  | C-N-CA     | 6.39  | 129.08      | 120.65   |
| 1   | M     | 58  | MET  | CA-C-O     | 6.39  | 127.48      | 120.71   |
| 1   | Q     | 258 | PRO  | N-CA-C     | -6.39 | 103.89      | 114.75   |
| 1   | H     | 259 | GLU  | CA-C-N     | 6.39  | 129.36      | 120.29   |
| 1   | H     | 259 | GLU  | C-N-CA     | 6.39  | 129.36      | 120.29   |
| 1   | N     | 265 | ARG  | NE-CZ-NH1  | -6.39 | 115.11      | 121.50   |
| 1   | H     | 497 | MET  | N-CA-C     | 6.39  | 118.32      | 111.36   |
| 1   | I     | 276 | LEU  | CA-C-O     | 6.39  | 127.23      | 119.31   |
| 1   | B     | 35  | ASN  | CA-C-O     | 6.38  | 128.09      | 121.07   |
| 1   | E     | 354 | ALA  | CA-C-N     | 6.38  | 129.36      | 120.29   |
| 1   | E     | 354 | ALA  | C-N-CA     | 6.38  | 129.36      | 120.29   |
| 1   | F     | 444 | VAL  | N-CA-C     | -6.38 | 104.53      | 110.53   |
| 1   | L     | 414 | ALA  | CA-C-O     | 6.38  | 128.83      | 120.21   |
| 1   | B     | 422 | GLU  | CA-C-O     | -6.38 | 111.39      | 120.51   |
| 1   | E     | 417 | GLY  | O-C-N      | -6.38 | 117.73      | 122.71   |
| 1   | P     | 50  | TYR  | O-C-N      | -6.38 | 114.52      | 123.01   |
| 1   | Q     | 278 | GLU  | CA-C-O     | 6.38  | 127.31      | 120.10   |
| 1   | S     | 161 | LEU  | CA-C-N     | 6.38  | 129.47      | 120.28   |
| 1   | S     | 161 | LEU  | C-N-CA     | 6.38  | 129.47      | 120.28   |
| 1   | E     | 35  | ASN  | OD1-CG-ND2 | -6.38 | 116.22      | 122.60   |
| 1   | C     | 131 | ILE  | CB-CA-C    | -6.38 | 102.27      | 112.16   |
| 1   | L     | 88  | LEU  | N-CA-CB    | -6.38 | 100.72      | 110.16   |
| 1   | L     | 152 | THR  | CB-CA-C    | -6.38 | 100.97      | 110.67   |
| 1   | E     | 267 | ASN  | CA-CB-CG   | -6.37 | 106.23      | 112.60   |
| 1   | E     | 295 | ALA  | N-CA-C     | 6.37  | 119.45      | 109.96   |
| 1   | F     | 155 | ILE  | CA-CB-CG2  | 6.37  | 121.33      | 110.50   |
| 1   | R     | 140 | GLU  | CA-C-N     | 6.37  | 128.59      | 120.56   |
| 1   | R     | 140 | GLU  | C-N-CA     | 6.37  | 128.59      | 120.56   |
| 1   | K     | 455 | VAL  | CA-C-O     | 6.37  | 127.35      | 120.47   |
| 1   | D     | 79  | MET  | CG-SD-CE   | -6.37 | 86.89       | 100.90   |
| 1   | S     | 70  | ASN  | CA-C-O     | 6.37  | 125.77      | 119.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 320 | VAL  | CA-C-O      | 6.36  | 127.11      | 120.36   |
| 1   | H     | 35  | ASN  | CA-C-N      | 6.36  | 129.11      | 120.77   |
| 1   | H     | 35  | ASN  | C-N-CA      | 6.36  | 129.11      | 120.77   |
| 1   | O     | 399 | ARG  | NE-CZ-NH1   | -6.36 | 115.14      | 121.50   |
| 1   | F     | 476 | THR  | CA-C-N      | 6.36  | 132.52      | 122.60   |
| 1   | F     | 476 | THR  | C-N-CA      | 6.36  | 132.52      | 122.60   |
| 1   | H     | 496 | ASP  | O-C-N       | -6.36 | 114.55      | 122.82   |
| 1   | R     | 455 | VAL  | CA-C-O      | 6.36  | 127.34      | 120.47   |
| 1   | C     | 519 | ALA  | O-C-N       | -6.36 | 115.52      | 122.07   |
| 1   | F     | 239 | LYS  | N-CA-C      | -6.36 | 104.45      | 111.82   |
| 1   | L     | 130 | ILE  | N-CA-CB     | -6.36 | 102.43      | 110.57   |
| 1   | S     | 113 | GLU  | CA-C-N      | 6.36  | 128.80      | 120.28   |
| 1   | S     | 113 | GLU  | C-N-CA      | 6.36  | 128.80      | 120.28   |
| 1   | S     | 436 | VAL  | O-C-N       | -6.36 | 115.70      | 121.87   |
| 1   | H     | 272 | MET  | CG-SD-CE    | -6.35 | 86.92       | 100.90   |
| 1   | S     | 246 | ILE  | O-C-N       | -6.35 | 115.90      | 122.63   |
| 1   | F     | 268 | ASP  | O-C-N       | -6.35 | 112.67      | 121.12   |
| 1   | A     | 114 | LEU  | CB-CA-C     | 6.35  | 121.64      | 110.85   |
| 1   | A     | 483 | LYS  | O-C-N       | -6.35 | 115.39      | 122.12   |
| 1   | C     | 365 | ASP  | CA-CB-CG    | -6.35 | 106.25      | 112.60   |
| 1   | G     | 119 | GLU  | O-C-N       | -6.35 | 115.39      | 122.12   |
| 1   | O     | 185 | VAL  | N-CA-C      | 6.35  | 117.03      | 110.36   |
| 1   | C     | 128 | PRO  | N-CA-C      | 6.35  | 122.09      | 113.84   |
| 1   | S     | 135 | TYR  | CA-C-N      | 6.35  | 129.61      | 120.79   |
| 1   | S     | 135 | TYR  | C-N-CA      | 6.35  | 129.61      | 120.79   |
| 1   | C     | 127 | HIS  | CE1-NE2-CD2 | -6.34 | 102.66      | 109.00   |
| 1   | M     | 174 | VAL  | CB-CA-C     | 6.34  | 119.90      | 111.21   |
| 1   | Q     | 122 | LEU  | CA-C-N      | 6.34  | 128.78      | 120.28   |
| 1   | Q     | 122 | LEU  | C-N-CA      | 6.34  | 128.78      | 120.28   |
| 1   | S     | 504 | GLU  | CA-C-N      | 6.34  | 127.77      | 119.84   |
| 1   | S     | 504 | GLU  | C-N-CA      | 6.34  | 127.77      | 119.84   |
| 1   | B     | 137 | LYS  | N-CA-CB     | -6.34 | 100.80      | 110.12   |
| 1   | C     | 265 | ARG  | O-C-N       | -6.34 | 114.16      | 122.59   |
| 1   | E     | 430 | ARG  | CA-C-N      | 6.34  | 129.95      | 120.31   |
| 1   | E     | 430 | ARG  | C-N-CA      | 6.34  | 129.95      | 120.31   |
| 1   | N     | 471 | MET  | CG-SD-CE    | -6.34 | 86.95       | 100.90   |
| 1   | O     | 422 | GLU  | CA-C-O      | -6.34 | 114.34      | 121.00   |
| 1   | Q     | 32  | VAL  | CA-C-N      | 6.34  | 128.69      | 120.44   |
| 1   | Q     | 32  | VAL  | C-N-CA      | 6.34  | 128.69      | 120.44   |
| 1   | S     | 150 | ALA  | N-CA-CB     | -6.34 | 100.72      | 110.04   |
| 1   | B     | 203 | ASP  | CA-C-N      | 6.34  | 129.64      | 120.38   |
| 1   | B     | 203 | ASP  | C-N-CA      | 6.34  | 129.64      | 120.38   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 40  | LYS  | CA-C-N     | 6.34  | 128.68      | 120.44   |
| 1   | E     | 40  | LYS  | C-N-CA     | 6.34  | 128.68      | 120.44   |
| 1   | K     | 377 | LYS  | CB-CA-C    | -6.34 | 100.07      | 110.85   |
| 1   | I     | 32  | VAL  | N-CA-C     | 6.34  | 119.92      | 111.17   |
| 1   | P     | 398 | LEU  | O-C-N      | -6.34 | 114.92      | 122.15   |
| 1   | E     | 62  | SER  | CA-C-O     | 6.34  | 127.47      | 120.63   |
| 1   | L     | 128 | PRO  | CA-C-O     | -6.34 | 109.92      | 119.55   |
| 1   | Q     | 257 | LYS  | CA-CB-CG   | -6.34 | 101.43      | 114.10   |
| 1   | B     | 286 | LYS  | CA-C-O     | 6.33  | 127.67      | 120.90   |
| 1   | C     | 305 | ASP  | CA-CB-CG   | 6.33  | 118.93      | 112.60   |
| 1   | K     | 483 | LYS  | N-CA-C     | 6.33  | 118.18      | 111.28   |
| 1   | A     | 457 | ILE  | N-CA-C     | 6.33  | 117.84      | 110.62   |
| 1   | R     | 406 | ALA  | CA-C-N     | 6.33  | 129.28      | 120.29   |
| 1   | R     | 406 | ALA  | C-N-CA     | 6.33  | 129.28      | 120.29   |
| 1   | A     | 299 | ILE  | N-CA-C     | -6.33 | 99.37       | 108.48   |
| 1   | C     | 153 | VAL  | CA-C-O     | 6.33  | 126.97      | 120.39   |
| 1   | K     | 444 | VAL  | CA-C-N     | 6.33  | 129.05      | 120.38   |
| 1   | K     | 444 | VAL  | C-N-CA     | 6.33  | 129.05      | 120.38   |
| 1   | L     | 76  | LEU  | CA-C-N     | 6.33  | 129.05      | 120.44   |
| 1   | L     | 76  | LEU  | C-N-CA     | 6.33  | 129.05      | 120.44   |
| 1   | N     | 84  | PRO  | N-CA-C     | 6.33  | 124.03      | 113.78   |
| 1   | O     | 305 | ASP  | CA-CB-CG   | -6.33 | 106.27      | 112.60   |
| 1   | S     | 34  | ALA  | CA-C-O     | -6.33 | 114.13      | 120.90   |
| 1   | S     | 352 | GLY  | CA-C-O     | -6.32 | 115.37      | 120.81   |
| 1   | A     | 421 | VAL  | CA-C-N     | 6.32  | 129.23      | 120.63   |
| 1   | A     | 421 | VAL  | C-N-CA     | 6.32  | 129.23      | 120.63   |
| 1   | C     | 310 | SER  | CA-C-N     | 6.32  | 129.04      | 120.44   |
| 1   | C     | 310 | SER  | C-N-CA     | 6.32  | 129.04      | 120.44   |
| 1   | E     | 360 | ARG  | NH1-CZ-NH2 | -6.32 | 111.08      | 119.30   |
| 1   | P     | 53  | ARG  | NE-CZ-NH1  | 6.32  | 127.82      | 121.50   |
| 1   | E     | 85  | ALA  | CA-C-N     | 6.32  | 129.58      | 120.79   |
| 1   | E     | 85  | ALA  | C-N-CA     | 6.32  | 129.58      | 120.79   |
| 1   | L     | 170 | SER  | N-CA-C     | 6.32  | 120.09      | 112.38   |
| 1   | I     | 209 | ILE  | O-C-N      | -6.32 | 116.90      | 123.03   |
| 1   | Q     | 94  | LYS  | CB-CA-C    | -6.32 | 100.87      | 110.92   |
| 1   | Q     | 401 | ALA  | CA-C-N     | 6.32  | 129.22      | 120.63   |
| 1   | Q     | 401 | ALA  | C-N-CA     | 6.32  | 129.22      | 120.63   |
| 1   | S     | 326 | SER  | CA-C-O     | 6.32  | 127.45      | 120.63   |
| 1   | K     | 433 | ALA  | CA-C-O     | -6.32 | 111.51      | 120.16   |
| 1   | M     | 350 | ASP  | CA-C-O     | 6.32  | 127.14      | 119.31   |
| 1   | O     | 233 | VAL  | N-CA-C     | 6.32  | 118.98      | 111.09   |
| 1   | Q     | 94  | LYS  | N-CA-CB    | 6.32  | 119.42      | 109.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 249 | ILE  | CA-C-O     | 6.31  | 128.48      | 120.97   |
| 1   | K     | 163 | LYS  | N-CA-C     | -6.31 | 103.09      | 111.24   |
| 1   | A     | 402 | LEU  | N-CA-C     | -6.31 | 104.32      | 111.14   |
| 1   | L     | 265 | ARG  | CA-C-N     | 6.31  | 129.99      | 120.77   |
| 1   | L     | 265 | ARG  | C-N-CA     | 6.31  | 129.99      | 120.77   |
| 1   | S     | 420 | ALA  | N-CA-C     | 6.31  | 118.72      | 111.02   |
| 1   | C     | 388 | GLU  | N-CA-C     | 6.31  | 120.54      | 112.34   |
| 1   | L     | 33  | ARG  | NE-CZ-NH2  | -6.31 | 113.52      | 119.20   |
| 1   | L     | 352 | GLY  | N-CA-C     | 6.31  | 122.25      | 112.60   |
| 1   | K     | 322 | ARG  | NE-CZ-NH2  | 6.31  | 124.88      | 119.20   |
| 1   | S     | 208 | GLN  | OE1-CD-NE2 | 6.31  | 128.91      | 122.60   |
| 1   | K     | 320 | VAL  | O-C-N      | -6.31 | 116.45      | 123.26   |
| 1   | O     | 115 | VAL  | CA-C-N     | 6.31  | 129.56      | 120.79   |
| 1   | O     | 115 | VAL  | C-N-CA     | 6.31  | 129.56      | 120.79   |
| 1   | S     | 309 | GLN  | OE1-CD-NE2 | -6.31 | 116.29      | 122.60   |
| 1   | C     | 284 | LYS  | CA-C-O     | 6.30  | 127.22      | 120.10   |
| 1   | G     | 227 | VAL  | O-C-N      | -6.30 | 116.92      | 123.03   |
| 1   | I     | 70  | ASN  | CA-C-O     | 6.30  | 125.57      | 119.08   |
| 1   | N     | 430 | ARG  | O-C-N      | 6.30  | 128.56      | 122.07   |
| 1   | O     | 263 | GLU  | N-CA-C     | 6.30  | 118.92      | 110.35   |
| 1   | C     | 522 | LEU  | O-C-N      | -6.30 | 114.97      | 122.15   |
| 1   | H     | 305 | ASP  | O-C-N      | -6.30 | 115.06      | 122.81   |
| 1   | N     | 114 | LEU  | CA-C-N     | 6.30  | 128.50      | 120.56   |
| 1   | N     | 114 | LEU  | C-N-CA     | 6.30  | 128.50      | 120.56   |
| 1   | D     | 287 | VAL  | O-C-N      | -6.30 | 115.74      | 121.91   |
| 1   | E     | 30  | GLU  | N-CA-C     | 6.30  | 124.21      | 110.80   |
| 1   | R     | 208 | GLN  | O-C-N      | -6.29 | 115.86      | 123.10   |
| 1   | B     | 242 | GLU  | N-CA-C     | 6.29  | 120.53      | 109.96   |
| 1   | B     | 257 | LYS  | CB-CA-C    | 6.29  | 119.46      | 109.52   |
| 1   | C     | 221 | GLN  | CA-C-N     | 6.29  | 131.40      | 122.72   |
| 1   | C     | 221 | GLN  | C-N-CA     | 6.29  | 131.40      | 122.72   |
| 1   | K     | 528 | ASP  | CA-CB-CG   | 6.29  | 118.89      | 112.60   |
| 1   | Q     | 152 | THR  | CA-C-N     | 6.29  | 131.22      | 123.10   |
| 1   | Q     | 152 | THR  | C-N-CA     | 6.29  | 131.22      | 123.10   |
| 1   | O     | 406 | ALA  | N-CA-C     | 6.29  | 118.14      | 111.28   |
| 1   | B     | 127 | HIS  | O-C-N      | -6.29 | 114.82      | 121.30   |
| 1   | C     | 87  | LYS  | CA-C-N     | 6.29  | 129.22      | 120.29   |
| 1   | C     | 87  | LYS  | C-N-CA     | 6.29  | 129.22      | 120.29   |
| 1   | C     | 279 | GLU  | CA-C-O     | 6.29  | 127.22      | 120.55   |
| 1   | N     | 85  | ALA  | CA-C-N     | 6.29  | 129.03      | 120.54   |
| 1   | N     | 85  | ALA  | C-N-CA     | 6.29  | 129.03      | 120.54   |
| 1   | L     | 431 | LYS  | CA-C-N     | 6.29  | 128.99      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 431 | LYS  | C-N-CA     | 6.29  | 128.99      | 120.44   |
| 1   | R     | 120 | ASP  | CA-C-N     | 6.29  | 129.22      | 120.29   |
| 1   | R     | 120 | ASP  | C-N-CA     | 6.29  | 129.22      | 120.29   |
| 1   | F     | 525 | ARG  | NE-CZ-NH2  | 6.28  | 124.85      | 119.20   |
| 1   | O     | 488 | ASP  | CA-CB-CG   | -6.28 | 106.32      | 112.60   |
| 1   | Q     | 151 | GLN  | OE1-CD-NE2 | -6.28 | 116.32      | 122.60   |
| 1   | Q     | 265 | ARG  | CA-C-N     | 6.28  | 129.64      | 120.91   |
| 1   | Q     | 265 | ARG  | C-N-CA     | 6.28  | 129.64      | 120.91   |
| 1   | K     | 109 | ILE  | CA-C-N     | 6.28  | 128.69      | 120.28   |
| 1   | K     | 109 | ILE  | C-N-CA     | 6.28  | 128.69      | 120.28   |
| 1   | L     | 133 | SER  | N-CA-C     | 6.28  | 118.12      | 111.28   |
| 1   | M     | 119 | GLU  | O-C-N      | -6.28 | 115.47      | 122.12   |
| 1   | K     | 270 | THR  | O-C-N      | -6.28 | 115.00      | 122.15   |
| 1   | L     | 210 | VAL  | N-CA-C     | -6.28 | 99.44       | 108.48   |
| 1   | L     | 244 | ALA  | N-CA-C     | 6.28  | 119.37      | 109.96   |
| 1   | F     | 391 | VAL  | CA-C-N     | 6.27  | 128.60      | 120.44   |
| 1   | F     | 391 | VAL  | C-N-CA     | 6.27  | 128.60      | 120.44   |
| 1   | O     | 322 | ARG  | N-CA-C     | 6.27  | 119.90      | 111.24   |
| 1   | P     | 301 | GLN  | CA-C-N     | 6.27  | 132.40      | 122.36   |
| 1   | P     | 301 | GLN  | C-N-CA     | 6.27  | 132.40      | 122.36   |
| 1   | M     | 470 | LEU  | CA-C-N     | 6.27  | 128.97      | 120.44   |
| 1   | M     | 470 | LEU  | C-N-CA     | 6.27  | 128.97      | 120.44   |
| 1   | Q     | 33  | ARG  | NE-CZ-NH2  | -6.27 | 113.56      | 119.20   |
| 1   | I     | 229 | ASP  | CA-C-N     | 6.27  | 131.03      | 122.19   |
| 1   | I     | 229 | ASP  | C-N-CA     | 6.27  | 131.03      | 122.19   |
| 1   | I     | 127 | HIS  | CA-CB-CG   | -6.27 | 107.53      | 113.80   |
| 1   | M     | 205 | ASP  | O-C-N      | -6.26 | 114.19      | 122.33   |
| 1   | B     | 202 | VAL  | CA-C-N     | 6.26  | 133.50      | 121.54   |
| 1   | B     | 202 | VAL  | C-N-CA     | 6.26  | 133.50      | 121.54   |
| 1   | P     | 59  | LEU  | CB-CA-C    | 6.26  | 120.16      | 110.14   |
| 1   | P     | 277 | ASP  | CA-CB-CG   | -6.26 | 106.34      | 112.60   |
| 1   | I     | 144 | GLN  | OE1-CD-NE2 | 6.26  | 128.86      | 122.60   |
| 1   | M     | 125 | ASP  | O-C-N      | -6.26 | 114.02      | 122.41   |
| 1   | F     | 186 | VAL  | CA-C-N     | 6.26  | 128.66      | 120.28   |
| 1   | F     | 186 | VAL  | C-N-CA     | 6.26  | 128.66      | 120.28   |
| 1   | N     | 246 | ILE  | CA-C-O     | -6.26 | 114.48      | 121.36   |
| 1   | O     | 288 | ASP  | N-CA-CB    | -6.26 | 100.58      | 110.28   |
| 1   | H     | 477 | HIS  | CA-C-O     | 6.26  | 127.04      | 119.78   |
| 1   | M     | 318 | LEU  | O-C-N      | -6.26 | 115.25      | 123.13   |
| 1   | C     | 281 | ASN  | CA-CB-CG   | 6.25  | 118.86      | 112.60   |
| 1   | M     | 142 | ALA  | N-CA-C     | 6.25  | 118.90      | 111.33   |
| 1   | H     | 42  | VAL  | O-C-N      | -6.25 | 115.80      | 121.87   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 420 | ALA  | N-CA-C     | 6.25  | 118.65      | 111.02   |
| 1   | S     | 370 | VAL  | CA-C-O     | 6.25  | 128.60      | 120.78   |
| 1   | A     | 452 | GLU  | CA-C-O     | 6.25  | 127.05      | 120.42   |
| 1   | G     | 127 | HIS  | CA-CB-CG   | -6.25 | 107.55      | 113.80   |
| 1   | L     | 124 | LYS  | CA-C-O     | 6.25  | 126.84      | 119.28   |
| 1   | I     | 146 | ILE  | CA-C-N     | 6.25  | 128.90      | 120.65   |
| 1   | I     | 146 | ILE  | C-N-CA     | 6.25  | 128.90      | 120.65   |
| 1   | A     | 478 | GLU  | O-C-N      | 6.25  | 128.84      | 122.09   |
| 1   | C     | 93  | ALA  | CA-C-N     | 6.25  | 128.90      | 120.65   |
| 1   | C     | 93  | ALA  | C-N-CA     | 6.25  | 128.90      | 120.65   |
| 1   | G     | 231 | GLU  | O-C-N      | -6.25 | 115.73      | 122.85   |
| 1   | I     | 479 | ASN  | OD1-CG-ND2 | -6.25 | 116.35      | 122.60   |
| 1   | C     | 466 | PRO  | O-C-N      | -6.25 | 115.43      | 122.18   |
| 1   | E     | 365 | ASP  | N-CA-C     | 6.25  | 118.78      | 110.53   |
| 1   | G     | 78  | LYS  | O-C-N      | -6.25 | 113.84      | 122.46   |
| 1   | K     | 269 | PRO  | N-CA-CB    | 6.25  | 109.51      | 103.51   |
| 1   | F     | 512 | ALA  | CA-C-O     | -6.24 | 114.27      | 120.82   |
| 1   | G     | 35  | ASN  | CA-CB-CG   | -6.24 | 106.36      | 112.60   |
| 1   | L     | 479 | ASN  | OD1-CG-ND2 | -6.24 | 116.36      | 122.60   |
| 1   | K     | 309 | GLN  | CA-C-N     | 6.24  | 129.27      | 120.28   |
| 1   | K     | 309 | GLN  | C-N-CA     | 6.24  | 129.27      | 120.28   |
| 1   | B     | 344 | ASP  | CA-CB-CG   | -6.24 | 106.36      | 112.60   |
| 1   | C     | 238 | PRO  | N-CA-C     | 6.24  | 125.32      | 112.47   |
| 1   | L     | 240 | ARG  | NE-CZ-NH2  | -6.24 | 113.59      | 119.20   |
| 1   | N     | 448 | ALA  | CA-C-N     | 6.24  | 128.96      | 120.54   |
| 1   | N     | 448 | ALA  | C-N-CA     | 6.24  | 128.96      | 120.54   |
| 1   | Q     | 196 | ARG  | NE-CZ-NH2  | 6.24  | 124.81      | 119.20   |
| 1   | E     | 42  | VAL  | O-C-N      | -6.24 | 115.82      | 121.87   |
| 1   | C     | 126 | VAL  | O-C-N      | -6.24 | 116.63      | 123.18   |
| 1   | C     | 402 | LEU  | N-CA-CB    | 6.24  | 119.01      | 109.91   |
| 1   | M     | 389 | ARG  | O-C-N      | -6.24 | 112.78      | 122.13   |
| 1   | R     | 250 | ASP  | CA-C-N     | 6.24  | 130.73      | 120.94   |
| 1   | R     | 250 | ASP  | C-N-CA     | 6.24  | 130.73      | 120.94   |
| 1   | B     | 146 | ILE  | N-CA-C     | -6.23 | 104.97      | 111.58   |
| 1   | D     | 231 | GLU  | CA-C-O     | 6.23  | 129.08      | 121.72   |
| 1   | K     | 104 | THR  | N-CA-C     | 6.23  | 119.05      | 111.82   |
| 1   | P     | 139 | GLU  | CA-C-O     | -6.23 | 114.28      | 120.82   |
| 1   | C     | 184 | ILE  | N-CA-CB    | 6.23  | 117.43      | 110.51   |
| 1   | H     | 418 | GLY  | O-C-N      | 6.23  | 129.94      | 122.34   |
| 1   | O     | 50  | TYR  | O-C-N      | -6.23 | 115.51      | 122.86   |
| 1   | P     | 257 | LYS  | O-C-N      | -6.23 | 114.16      | 121.32   |
| 1   | G     | 289 | LYS  | CA-C-O     | 6.23  | 127.04      | 119.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | H     | 459 | ILE  | N-CA-CB     | 6.23  | 117.84      | 110.55   |
| 1   | O     | 507 | LEU  | CA-C-O      | 6.23  | 127.60      | 120.00   |
| 1   | Q     | 67  | THR  | CB-CA-C     | -6.23 | 100.55      | 110.14   |
| 1   | A     | 134 | GLY  | CA-C-N      | 6.23  | 128.62      | 120.28   |
| 1   | A     | 134 | GLY  | C-N-CA      | 6.23  | 128.62      | 120.28   |
| 1   | I     | 53  | ARG  | N-CA-C      | -6.23 | 104.85      | 112.88   |
| 1   | I     | 297 | VAL  | CA-CB-CG1   | 6.23  | 120.99      | 110.40   |
| 1   | S     | 74  | THR  | CA-C-O      | 6.23  | 127.35      | 120.63   |
| 1   | A     | 498 | TRP  | CB-CG-CD2   | -6.22 | 118.08      | 126.80   |
| 1   | C     | 188 | ALA  | N-CA-C      | 6.22  | 118.06      | 111.28   |
| 1   | K     | 132 | ILE  | CA-C-N      | 6.22  | 128.53      | 120.44   |
| 1   | K     | 132 | ILE  | C-N-CA      | 6.22  | 128.53      | 120.44   |
| 1   | L     | 51  | GLY  | O-C-N       | -6.22 | 115.55      | 121.77   |
| 1   | R     | 82  | GLN  | OE1-CD-NE2  | -6.22 | 116.38      | 122.60   |
| 1   | E     | 179 | GLU  | CA-C-N      | 6.22  | 128.53      | 120.44   |
| 1   | E     | 179 | GLU  | C-N-CA      | 6.22  | 128.53      | 120.44   |
| 1   | E     | 445 | GLU  | O-C-N       | -6.22 | 115.53      | 122.12   |
| 1   | E     | 502 | VAL  | CB-CA-C     | -6.22 | 105.59      | 112.68   |
| 1   | H     | 385 | GLY  | O-C-N       | -6.22 | 115.52      | 122.68   |
| 1   | K     | 430 | ARG  | NE-CZ-NH1   | 6.22  | 127.72      | 121.50   |
| 1   | N     | 339 | VAL  | CA-C-O      | -6.22 | 114.57      | 121.23   |
| 1   | S     | 320 | VAL  | CA-CB-CG1   | 6.22  | 120.98      | 110.40   |
| 1   | B     | 481 | ASN  | CA-CB-CG    | -6.22 | 106.38      | 112.60   |
| 1   | Q     | 452 | GLU  | CB-CG-CD    | 6.22  | 123.17      | 112.60   |
| 1   | G     | 219 | ASP  | CA-C-N      | 6.21  | 129.53      | 120.71   |
| 1   | G     | 219 | ASP  | C-N-CA      | 6.21  | 129.53      | 120.71   |
| 1   | G     | 467 | ILE  | N-CA-C      | 6.21  | 116.39      | 110.42   |
| 1   | E     | 107 | ALA  | CA-C-N      | 6.21  | 129.62      | 120.74   |
| 1   | E     | 107 | ALA  | C-N-CA      | 6.21  | 129.62      | 120.74   |
| 1   | Q     | 384 | ARG  | O-C-N       | 6.21  | 131.04      | 122.78   |
| 1   | A     | 268 | ASP  | CA-C-O      | -6.21 | 114.23      | 119.76   |
| 1   | K     | 430 | ARG  | NE-CZ-NH2   | -6.21 | 113.61      | 119.20   |
| 1   | R     | 248 | LEU  | CA-C-N      | 6.21  | 131.06      | 122.93   |
| 1   | R     | 248 | LEU  | C-N-CA      | 6.21  | 131.06      | 122.93   |
| 1   | S     | 389 | ARG  | N-CA-C      | -6.21 | 105.73      | 113.55   |
| 1   | A     | 53  | ARG  | NE-CZ-NH2   | 6.21  | 124.79      | 119.20   |
| 1   | R     | 109 | ILE  | N-CA-C      | 6.21  | 116.32      | 110.30   |
| 1   | S     | 90  | VAL  | CA-C-O      | 6.21  | 127.21      | 120.57   |
| 1   | I     | 477 | HIS  | ND1-CE1-NE2 | 6.21  | 114.61      | 108.40   |
| 1   | D     | 69  | THR  | CA-C-N      | 6.20  | 130.59      | 120.23   |
| 1   | D     | 69  | THR  | C-N-CA      | 6.20  | 130.59      | 120.23   |
| 1   | A     | 182 | ALA  | N-CA-C      | 6.20  | 118.55      | 111.11   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 511 | ASN  | N-CA-C    | 6.20  | 119.01      | 111.82   |
| 1   | Q     | 323 | ALA  | CA-C-O    | 6.20  | 127.19      | 120.43   |
| 1   | R     | 531 | SER  | N-CA-C    | -6.20 | 99.61       | 109.59   |
| 1   | A     | 399 | ARG  | NE-CZ-NH2 | 6.20  | 124.78      | 119.20   |
| 1   | B     | 453 | SER  | O-C-N     | -6.20 | 115.55      | 122.12   |
| 1   | N     | 478 | GLU  | CA-C-N    | 6.20  | 129.56      | 120.82   |
| 1   | N     | 478 | GLU  | C-N-CA    | 6.20  | 129.56      | 120.82   |
| 1   | D     | 231 | GLU  | O-C-N     | -6.20 | 116.00      | 122.94   |
| 1   | E     | 423 | ILE  | CA-C-N    | 6.20  | 128.87      | 120.44   |
| 1   | E     | 423 | ILE  | C-N-CA    | 6.20  | 128.87      | 120.44   |
| 1   | E     | 507 | LEU  | CA-C-N    | 6.20  | 128.37      | 120.56   |
| 1   | E     | 507 | LEU  | C-N-CA    | 6.20  | 128.37      | 120.56   |
| 1   | F     | 346 | ILE  | CA-C-O    | 6.20  | 128.32      | 121.13   |
| 1   | S     | 423 | ILE  | CA-CB-CG2 | -6.20 | 99.97       | 110.50   |
| 1   | B     | 396 | ARG  | CA-C-O    | -6.19 | 114.52      | 120.90   |
| 1   | F     | 56  | ASP  | CA-CB-CG  | -6.19 | 106.41      | 112.60   |
| 1   | M     | 150 | ALA  | N-CA-C    | 6.19  | 118.77      | 110.35   |
| 1   | Q     | 288 | ASP  | N-CA-CB   | -6.19 | 100.69      | 110.28   |
| 1   | B     | 477 | HIS  | O-C-N     | -6.19 | 114.54      | 122.21   |
| 1   | B     | 321 | ARG  | NE-CZ-NH2 | -6.19 | 113.63      | 119.20   |
| 1   | K     | 234 | HIS  | CA-C-O    | -6.19 | 113.92      | 119.86   |
| 1   | O     | 355 | SER  | CB-CA-C   | -6.19 | 100.52      | 110.79   |
| 1   | R     | 503 | ILE  | CB-CA-C   | 6.19  | 119.81      | 110.90   |
| 1   | P     | 94  | LYS  | N-CA-C    | 6.19  | 117.71      | 110.97   |
| 1   | C     | 524 | LEU  | CA-C-N    | 6.18  | 129.71      | 120.31   |
| 1   | C     | 524 | LEU  | C-N-CA    | 6.18  | 129.71      | 120.31   |
| 1   | E     | 423 | ILE  | O-C-N     | -6.18 | 115.65      | 121.90   |
| 1   | R     | 139 | GLU  | O-C-N     | -6.18 | 115.70      | 122.07   |
| 1   | F     | 243 | ASN  | CA-CB-CG  | -6.18 | 106.42      | 112.60   |
| 1   | Q     | 268 | ASP  | CA-C-N    | 6.18  | 125.81      | 119.56   |
| 1   | Q     | 268 | ASP  | C-N-CA    | 6.18  | 125.81      | 119.56   |
| 1   | Q     | 485 | TYR  | CA-CB-CG  | -6.18 | 102.78      | 113.90   |
| 1   | R     | 104 | THR  | N-CA-C    | 6.18  | 118.10      | 111.36   |
| 1   | E     | 285 | GLU  | CA-C-N    | 6.18  | 128.88      | 120.54   |
| 1   | E     | 285 | GLU  | C-N-CA    | 6.18  | 128.88      | 120.54   |
| 1   | D     | 188 | ALA  | N-CA-C    | 6.18  | 118.80      | 111.33   |
| 1   | I     | 347 | SER  | N-CA-C    | 6.17  | 118.46      | 109.07   |
| 1   | I     | 517 | THR  | CB-CA-C   | -6.17 | 100.35      | 110.85   |
| 1   | O     | 239 | LYS  | N-CA-C    | 6.17  | 118.81      | 111.71   |
| 1   | B     | 99  | GLU  | CA-C-O    | 6.17  | 126.97      | 119.38   |
| 1   | E     | 59  | LEU  | O-C-N     | -6.17 | 116.05      | 123.27   |
| 1   | F     | 267 | ASN  | CA-C-N    | 6.17  | 131.80      | 122.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 267 | ASN  | C-N-CA     | 6.17  | 131.80      | 122.42   |
| 1   | S     | 244 | ALA  | CB-CA-C    | 6.17  | 120.67      | 109.62   |
| 1   | S     | 406 | ALA  | CA-C-N     | 6.17  | 129.69      | 120.31   |
| 1   | S     | 406 | ALA  | C-N-CA     | 6.17  | 129.69      | 120.31   |
| 1   | C     | 144 | GLN  | O-C-N      | -6.17 | 115.00      | 122.22   |
| 1   | C     | 354 | ALA  | O-C-N      | -6.17 | 115.65      | 123.24   |
| 1   | D     | 238 | PRO  | N-CA-C     | 6.17  | 120.90      | 111.15   |
| 1   | E     | 115 | VAL  | CA-C-N     | 6.17  | 129.37      | 120.79   |
| 1   | E     | 115 | VAL  | C-N-CA     | 6.17  | 129.37      | 120.79   |
| 1   | C     | 202 | VAL  | CB-CA-C    | -6.17 | 103.38      | 110.41   |
| 1   | C     | 281 | ASN  | CB-CG-ND2  | 6.17  | 125.65      | 116.40   |
| 1   | G     | 456 | SER  | CB-CA-C    | -6.17 | 101.20      | 110.88   |
| 1   | H     | 179 | GLU  | CA-C-N     | 6.17  | 128.79      | 120.65   |
| 1   | H     | 179 | GLU  | C-N-CA     | 6.17  | 128.79      | 120.65   |
| 1   | K     | 167 | THR  | CA-C-O     | 6.17  | 126.87      | 119.10   |
| 1   | N     | 407 | ASP  | CA-CB-CG   | -6.17 | 106.43      | 112.60   |
| 1   | E     | 498 | TRP  | CA-C-O     | 6.17  | 127.50      | 120.90   |
| 1   | F     | 157 | ASP  | CA-CB-CG   | 6.17  | 118.77      | 112.60   |
| 1   | O     | 510 | MET  | N-CA-C     | -6.17 | 105.78      | 113.55   |
| 1   | E     | 263 | GLU  | CB-CG-CD   | -6.16 | 102.12      | 112.60   |
| 1   | S     | 249 | ILE  | N-CA-C     | 6.16  | 116.69      | 107.51   |
| 1   | L     | 144 | GLN  | OE1-CD-NE2 | -6.16 | 116.44      | 122.60   |
| 1   | L     | 203 | ASP  | CA-C-O     | 6.16  | 129.32      | 120.51   |
| 1   | M     | 384 | ARG  | N-CA-C     | -6.16 | 99.78       | 108.96   |
| 1   | O     | 277 | ASP  | CA-CB-CG   | -6.16 | 106.44      | 112.60   |
| 1   | R     | 451 | LEU  | N-CA-C     | 6.16  | 118.80      | 111.71   |
| 1   | K     | 191 | GLN  | CA-CB-CG   | 6.16  | 126.42      | 114.10   |
| 1   | R     | 394 | THR  | CA-C-O     | 6.16  | 127.05      | 119.97   |
| 1   | S     | 167 | THR  | CA-C-O     | 6.16  | 129.31      | 120.51   |
| 1   | R     | 154 | SER  | CA-C-N     | 6.15  | 130.86      | 120.64   |
| 1   | R     | 154 | SER  | C-N-CA     | 6.15  | 130.86      | 120.64   |
| 1   | I     | 398 | LEU  | CA-C-N     | 6.15  | 128.44      | 120.44   |
| 1   | I     | 398 | LEU  | C-N-CA     | 6.15  | 128.44      | 120.44   |
| 1   | P     | 33  | ARG  | N-CA-C     | 6.15  | 117.78      | 111.14   |
| 1   | Q     | 416 | ALA  | O-C-N      | -6.15 | 115.36      | 122.93   |
| 1   | F     | 65  | ASP  | CA-CB-CG   | -6.15 | 106.45      | 112.60   |
| 1   | I     | 474 | ARG  | NE-CZ-NH2  | 6.15  | 124.73      | 119.20   |
| 1   | P     | 53  | ARG  | NH1-CZ-NH2 | -6.15 | 111.31      | 119.30   |
| 1   | P     | 340 | VAL  | N-CA-C     | 6.15  | 116.78      | 108.17   |
| 1   | Q     | 404 | THR  | N-CA-C     | 6.15  | 118.49      | 111.11   |
| 1   | A     | 120 | ASP  | CA-CB-CG   | 6.15  | 118.75      | 112.60   |
| 1   | H     | 458 | LEU  | CA-C-O     | 6.14  | 127.27      | 120.82   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | K     | 270 | THR  | CA-C-N    | 6.14  | 129.01      | 120.29   |
| 1   | K     | 270 | THR  | C-N-CA    | 6.14  | 129.01      | 120.29   |
| 1   | N     | 32  | VAL  | CA-CB-CG1 | 6.14  | 120.84      | 110.40   |
| 1   | P     | 229 | ASP  | N-CA-C    | 6.14  | 120.28      | 113.21   |
| 1   | E     | 93  | ALA  | CA-C-N    | 6.14  | 128.76      | 120.65   |
| 1   | E     | 93  | ALA  | C-N-CA    | 6.14  | 128.76      | 120.65   |
| 1   | B     | 142 | ALA  | CA-C-N    | 6.14  | 128.98      | 120.63   |
| 1   | B     | 142 | ALA  | C-N-CA    | 6.14  | 128.98      | 120.63   |
| 1   | C     | 334 | ALA  | N-CA-C    | -6.14 | 105.95      | 113.50   |
| 1   | F     | 399 | ARG  | NE-CZ-NH2 | 6.14  | 124.73      | 119.20   |
| 1   | L     | 233 | VAL  | N-CA-CB   | -6.14 | 103.93      | 110.62   |
| 1   | A     | 316 | GLY  | CA-C-O    | 6.14  | 125.86      | 118.86   |
| 1   | G     | 132 | ILE  | N-CA-C    | 6.14  | 116.30      | 110.53   |
| 1   | H     | 437 | GLY  | CA-C-N    | 6.14  | 133.44      | 121.41   |
| 1   | H     | 437 | GLY  | C-N-CA    | 6.14  | 133.44      | 121.41   |
| 1   | B     | 60  | VAL  | O-C-N     | -6.13 | 114.84      | 122.88   |
| 1   | O     | 158 | THR  | O-C-N     | -6.13 | 114.00      | 122.46   |
| 1   | C     | 525 | ARG  | CA-C-N    | 6.13  | 130.39      | 121.80   |
| 1   | C     | 525 | ARG  | C-N-CA    | 6.13  | 130.39      | 121.80   |
| 1   | I     | 50  | TYR  | CB-CG-CD1 | 6.13  | 130.00      | 120.80   |
| 1   | R     | 465 | ASP  | CA-CB-CG  | -6.13 | 106.47      | 112.60   |
| 1   | E     | 487 | ILE  | N-CA-C    | 6.13  | 117.03      | 107.28   |
| 1   | P     | 438 | GLY  | CA-C-N    | 6.13  | 129.00      | 120.29   |
| 1   | P     | 438 | GLY  | C-N-CA    | 6.13  | 129.00      | 120.29   |
| 1   | N     | 100 | THR  | N-CA-C    | 6.13  | 118.69      | 110.35   |
| 1   | G     | 326 | SER  | O-C-N     | -6.13 | 115.22      | 122.20   |
| 1   | G     | 368 | VAL  | CA-CB-CG2 | -6.13 | 99.99       | 110.40   |
| 1   | R     | 162 | ARG  | CA-C-O    | 6.13  | 127.02      | 120.10   |
| 1   | P     | 484 | TRP  | N-CA-C    | 6.12  | 119.79      | 112.93   |
| 1   | L     | 475 | SER  | N-CA-C    | 6.12  | 120.96      | 112.45   |
| 1   | M     | 451 | LEU  | O-C-N     | -6.12 | 115.17      | 122.15   |
| 1   | G     | 169 | LEU  | N-CA-C    | 6.12  | 119.94      | 112.23   |
| 1   | M     | 202 | VAL  | O-C-N     | 6.12  | 128.97      | 123.03   |
| 1   | F     | 153 | VAL  | CA-C-O    | 6.12  | 127.82      | 120.66   |
| 1   | O     | 444 | VAL  | O-C-N     | -6.12 | 115.91      | 121.91   |
| 1   | A     | 34  | ALA  | CA-C-N    | 6.12  | 129.29      | 120.79   |
| 1   | A     | 34  | ALA  | C-N-CA    | 6.12  | 129.29      | 120.79   |
| 1   | B     | 442 | LEU  | CA-C-N    | 6.12  | 128.39      | 120.44   |
| 1   | B     | 442 | LEU  | C-N-CA    | 6.12  | 128.39      | 120.44   |
| 1   | Q     | 242 | GLU  | CA-C-N    | 6.12  | 131.09      | 122.46   |
| 1   | Q     | 242 | GLU  | C-N-CA    | 6.12  | 131.09      | 122.46   |
| 1   | S     | 531 | SER  | O-C-N     | 6.12  | 129.94      | 123.03   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | M     | 440 | GLU  | N-CA-CB  | -6.12 | 100.48      | 110.14   |
| 1   | G     | 288 | ASP  | O-C-N    | -6.11 | 115.07      | 122.22   |
| 1   | Q     | 297 | VAL  | N-CA-C   | -6.11 | 98.91       | 108.81   |
| 1   | B     | 30  | GLU  | CB-CG-CD | 6.11  | 122.99      | 112.60   |
| 1   | Q     | 195 | LEU  | O-C-N    | -6.11 | 116.36      | 123.27   |
| 1   | K     | 322 | ARG  | CG-CD-NE | -6.11 | 98.56       | 112.00   |
| 1   | P     | 183 | ASP  | CA-C-N   | 6.11  | 128.48      | 120.60   |
| 1   | P     | 183 | ASP  | C-N-CA   | 6.11  | 128.48      | 120.60   |
| 1   | B     | 83  | HIS  | CA-C-N   | 6.11  | 125.59      | 119.24   |
| 1   | B     | 83  | HIS  | C-N-CA   | 6.11  | 125.59      | 119.24   |
| 1   | H     | 394 | THR  | CA-C-O   | 6.11  | 126.99      | 119.97   |
| 1   | E     | 134 | GLY  | CA-C-N   | 6.11  | 128.46      | 120.28   |
| 1   | E     | 134 | GLY  | C-N-CA   | 6.11  | 128.46      | 120.28   |
| 1   | L     | 494 | PRO  | CA-C-O   | -6.11 | 114.70      | 121.23   |
| 1   | N     | 104 | THR  | N-CA-C   | 6.11  | 118.01      | 111.36   |
| 1   | I     | 354 | ALA  | CA-C-N   | 6.10  | 128.46      | 120.28   |
| 1   | I     | 354 | ALA  | C-N-CA   | 6.10  | 128.46      | 120.28   |
| 1   | B     | 365 | ASP  | CA-C-O   | 6.10  | 129.64      | 121.89   |
| 1   | E     | 310 | SER  | CA-C-N   | 6.10  | 130.90      | 120.71   |
| 1   | E     | 310 | SER  | C-N-CA   | 6.10  | 130.90      | 120.71   |
| 1   | Q     | 282 | LEU  | CA-C-O   | 6.10  | 126.89      | 120.42   |
| 1   | M     | 219 | ASP  | CA-CB-CG | 6.10  | 118.70      | 112.60   |
| 1   | S     | 110 | PHE  | CA-CB-CG | -6.10 | 107.70      | 113.80   |
| 1   | P     | 479 | ASN  | CA-C-N   | 6.10  | 129.58      | 120.31   |
| 1   | P     | 479 | ASN  | C-N-CA   | 6.10  | 129.58      | 120.31   |
| 1   | R     | 435 | GLN  | N-CA-CB  | -6.10 | 100.93      | 110.44   |
| 1   | S     | 522 | LEU  | O-C-N    | -6.10 | 115.20      | 122.15   |
| 1   | I     | 178 | ARG  | N-CA-CB  | -6.09 | 100.83      | 110.28   |
| 1   | R     | 285 | GLU  | O-C-N    | -6.09 | 115.51      | 122.09   |
| 1   | S     | 417 | GLY  | O-C-N    | -6.09 | 117.57      | 122.81   |
| 1   | I     | 306 | GLU  | N-CA-C   | 6.09  | 118.89      | 111.82   |
| 1   | N     | 337 | GLY  | O-C-N    | -6.09 | 117.96      | 122.71   |
| 1   | G     | 375 | ASN  | CA-C-O   | -6.09 | 111.81      | 120.16   |
| 1   | I     | 359 | GLU  | CA-C-O   | -6.09 | 113.78      | 120.36   |
| 1   | D     | 387 | LEU  | CA-C-N   | 6.09  | 130.34      | 120.60   |
| 1   | D     | 387 | LEU  | C-N-CA   | 6.09  | 130.34      | 120.60   |
| 1   | D     | 440 | GLU  | N-CA-C   | 6.09  | 119.54      | 111.75   |
| 1   | P     | 516 | ALA  | N-CA-C   | 6.09  | 118.42      | 111.11   |
| 1   | S     | 110 | PHE  | CA-C-O   | -6.09 | 114.09      | 120.55   |
| 1   | D     | 445 | GLU  | CA-C-N   | 6.09  | 128.69      | 120.65   |
| 1   | D     | 445 | GLU  | C-N-CA   | 6.09  | 128.69      | 120.65   |
| 1   | K     | 444 | VAL  | N-CA-C   | -6.09 | 104.81      | 110.53   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 75  | ILE  | CA-C-O    | 6.09  | 127.40      | 119.85   |
| 1   | L     | 504 | GLU  | CA-C-N    | 6.08  | 127.45      | 119.84   |
| 1   | L     | 504 | GLU  | C-N-CA    | 6.08  | 127.45      | 119.84   |
| 1   | M     | 428 | LYS  | O-C-N     | -6.08 | 115.67      | 122.12   |
| 1   | N     | 28  | GLY  | CA-C-N    | 6.08  | 128.72      | 120.38   |
| 1   | N     | 28  | GLY  | C-N-CA    | 6.08  | 128.72      | 120.38   |
| 1   | N     | 219 | ASP  | CA-CB-CG  | 6.08  | 118.68      | 112.60   |
| 1   | N     | 254 | GLU  | N-CA-CB   | -6.08 | 100.68      | 111.08   |
| 1   | O     | 128 | PRO  | O-C-N     | -6.08 | 114.38      | 122.22   |
| 1   | E     | 59  | LEU  | CA-C-O    | 6.08  | 126.69      | 120.24   |
| 1   | F     | 445 | GLU  | CA-C-O    | 6.08  | 127.20      | 120.63   |
| 1   | A     | 91  | GLN  | O-C-N     | -6.08 | 115.68      | 122.12   |
| 1   | G     | 391 | VAL  | CA-C-N    | 6.08  | 128.34      | 120.44   |
| 1   | G     | 391 | VAL  | C-N-CA    | 6.08  | 128.34      | 120.44   |
| 1   | G     | 261 | ASP  | CA-C-O    | 6.08  | 125.82      | 119.14   |
| 1   | P     | 291 | LEU  | O-C-N     | -6.08 | 114.07      | 122.46   |
| 1   | L     | 517 | THR  | N-CA-C    | 6.08  | 117.90      | 111.28   |
| 1   | M     | 451 | LEU  | CA-C-N    | 6.08  | 129.54      | 120.31   |
| 1   | M     | 451 | LEU  | C-N-CA    | 6.08  | 129.54      | 120.31   |
| 1   | R     | 218 | ASN  | O-C-N     | -6.08 | 114.29      | 122.43   |
| 1   | C     | 470 | LEU  | CA-C-O    | -6.07 | 114.44      | 120.82   |
| 1   | K     | 156 | ASN  | CA-C-N    | 6.07  | 133.14      | 121.54   |
| 1   | K     | 156 | ASN  | C-N-CA    | 6.07  | 133.14      | 121.54   |
| 1   | P     | 115 | VAL  | CA-C-N    | 6.07  | 129.23      | 120.79   |
| 1   | P     | 115 | VAL  | C-N-CA    | 6.07  | 129.23      | 120.79   |
| 1   | S     | 392 | ASP  | CA-C-O    | 6.07  | 127.20      | 120.82   |
| 1   | A     | 157 | ASP  | CA-CB-CG  | 6.07  | 118.67      | 112.60   |
| 1   | C     | 53  | ARG  | NE-CZ-NH1 | 6.07  | 127.57      | 121.50   |
| 1   | H     | 417 | GLY  | CA-C-O    | -6.07 | 115.92      | 122.47   |
| 1   | G     | 106 | THR  | N-CA-C    | -6.07 | 104.29      | 111.03   |
| 1   | A     | 402 | LEU  | N-CA-CB   | 6.07  | 118.87      | 110.07   |
| 1   | G     | 511 | ASN  | CA-C-N    | 6.07  | 128.33      | 120.44   |
| 1   | G     | 511 | ASN  | C-N-CA    | 6.07  | 128.33      | 120.44   |
| 1   | K     | 202 | VAL  | CA-C-O    | 6.07  | 126.25      | 120.31   |
| 1   | P     | 467 | ILE  | CA-C-N    | 6.07  | 129.22      | 120.79   |
| 1   | P     | 467 | ILE  | C-N-CA    | 6.07  | 129.22      | 120.79   |
| 1   | D     | 342 | ASN  | O-C-N     | -6.07 | 115.52      | 123.28   |
| 1   | E     | 68  | ILE  | CA-C-O    | 6.07  | 127.06      | 120.57   |
| 1   | G     | 423 | ILE  | O-C-N     | -6.07 | 115.77      | 121.90   |
| 1   | H     | 289 | LYS  | O-C-N     | -6.07 | 114.30      | 122.43   |
| 1   | F     | 482 | ASN  | CA-C-N    | 6.06  | 128.41      | 120.28   |
| 1   | F     | 482 | ASN  | C-N-CA    | 6.06  | 128.41      | 120.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 265 | ARG  | CA-C-O     | 6.06  | 126.62      | 119.28   |
| 1   | I     | 529 | VAL  | N-CA-C     | 6.06  | 116.60      | 108.11   |
| 1   | L     | 178 | ARG  | CA-C-O     | 6.06  | 126.94      | 119.97   |
| 1   | D     | 482 | ASN  | CA-CB-CG   | 6.06  | 118.66      | 112.60   |
| 1   | P     | 155 | ILE  | N-CA-C     | 6.06  | 117.53      | 110.62   |
| 1   | B     | 53  | ARG  | NE-CZ-NH1  | 6.06  | 127.56      | 121.50   |
| 1   | F     | 301 | GLN  | CB-CG-CD   | 6.06  | 122.90      | 112.60   |
| 1   | H     | 375 | ASN  | CB-CA-C    | 6.06  | 117.41      | 108.87   |
| 1   | I     | 479 | ASN  | CA-CB-CG   | -6.06 | 106.54      | 112.60   |
| 1   | K     | 477 | HIS  | CG-CD2-NE2 | 6.06  | 113.26      | 107.20   |
| 1   | S     | 389 | ARG  | NE-CZ-NH1  | 6.06  | 127.56      | 121.50   |
| 1   | M     | 102 | ASP  | CA-C-O     | -6.06 | 114.79      | 121.33   |
| 1   | L     | 405 | VAL  | N-CA-C     | 6.05  | 116.80      | 110.62   |
| 1   | H     | 205 | ASP  | CA-C-O     | 6.05  | 126.75      | 119.61   |
| 1   | R     | 236 | GLY  | CA-C-N     | 6.05  | 131.60      | 121.92   |
| 1   | R     | 236 | GLY  | C-N-CA     | 6.05  | 131.60      | 121.92   |
| 1   | A     | 453 | SER  | CA-C-N     | 6.05  | 128.31      | 120.44   |
| 1   | A     | 453 | SER  | C-N-CA     | 6.05  | 128.31      | 120.44   |
| 1   | D     | 80  | ASP  | O-C-N      | -6.05 | 116.32      | 123.22   |
| 1   | D     | 487 | ILE  | N-CA-C     | 6.05  | 116.90      | 107.28   |
| 1   | K     | 418 | GLY  | O-C-N      | -6.05 | 116.48      | 122.41   |
| 1   | M     | 126 | VAL  | O-C-N      | -6.05 | 115.58      | 122.72   |
| 1   | E     | 106 | THR  | CA-C-O     | 6.05  | 127.13      | 120.90   |
| 1   | M     | 169 | LEU  | N-CA-C     | 6.05  | 117.95      | 111.36   |
| 1   | N     | 459 | ILE  | CA-C-O     | 6.05  | 127.58      | 121.17   |
| 1   | P     | 384 | ARG  | NE-CZ-NH2  | -6.05 | 113.75      | 119.20   |
| 1   | P     | 390 | LEU  | CA-C-N     | 6.05  | 128.75      | 120.46   |
| 1   | P     | 390 | LEU  | C-N-CA     | 6.05  | 128.75      | 120.46   |
| 1   | R     | 60  | VAL  | CA-C-N     | 6.05  | 132.43      | 121.06   |
| 1   | R     | 60  | VAL  | C-N-CA     | 6.05  | 132.43      | 121.06   |
| 1   | S     | 178 | ARG  | CA-C-N     | 6.05  | 128.67      | 120.38   |
| 1   | S     | 178 | ARG  | C-N-CA     | 6.05  | 128.67      | 120.38   |
| 1   | P     | 221 | GLN  | N-CA-C     | 6.05  | 118.26      | 109.07   |
| 1   | R     | 396 | ARG  | CD-NE-CZ   | -6.05 | 115.93      | 124.40   |
| 1   | E     | 257 | LYS  | O-C-N      | -6.05 | 115.56      | 121.18   |
| 1   | G     | 140 | GLU  | CA-C-N     | 6.05  | 128.18      | 120.56   |
| 1   | G     | 140 | GLU  | C-N-CA     | 6.05  | 128.18      | 120.56   |
| 1   | H     | 407 | ASP  | CA-CB-CG   | -6.05 | 106.55      | 112.60   |
| 1   | K     | 342 | ASN  | CA-CB-CG   | -6.05 | 106.55      | 112.60   |
| 1   | S     | 489 | LEU  | CA-C-O     | 6.05  | 126.91      | 119.05   |
| 1   | E     | 89  | LEU  | O-C-N      | -6.04 | 115.50      | 122.03   |
| 1   | G     | 243 | ASN  | CA-CB-CG   | -6.04 | 106.56      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 415 | ILE  | O-C-N     | -6.04 | 116.62      | 122.97   |
| 1   | A     | 343 | ILE  | CA-CB-CG1 | 6.04  | 120.67      | 110.40   |
| 1   | I     | 114 | LEU  | N-CA-C    | 6.04  | 117.86      | 111.28   |
| 1   | I     | 439 | LYS  | CA-C-O    | 6.04  | 126.92      | 120.70   |
| 1   | N     | 290 | ILE  | CB-CA-C   | -6.04 | 104.14      | 112.24   |
| 1   | N     | 512 | ALA  | CB-CA-C   | -6.04 | 101.66      | 110.96   |
| 1   | P     | 262 | ALA  | CA-C-N    | 6.04  | 129.29      | 120.71   |
| 1   | P     | 262 | ALA  | C-N-CA    | 6.04  | 129.29      | 120.71   |
| 1   | P     | 437 | GLY  | CA-C-O    | -6.04 | 115.58      | 121.86   |
| 1   | M     | 238 | PRO  | CA-C-N    | 6.04  | 128.37      | 120.28   |
| 1   | M     | 238 | PRO  | C-N-CA    | 6.04  | 128.37      | 120.28   |
| 1   | N     | 40  | LYS  | CA-C-N    | 6.04  | 128.29      | 120.44   |
| 1   | N     | 40  | LYS  | C-N-CA    | 6.04  | 128.29      | 120.44   |
| 1   | N     | 288 | ASP  | CA-CB-CG  | -6.04 | 106.56      | 112.60   |
| 1   | E     | 321 | ARG  | N-CA-C    | 6.04  | 119.55      | 109.95   |
| 1   | I     | 77  | ASP  | N-CA-C    | 6.04  | 117.66      | 111.14   |
| 1   | P     | 504 | GLU  | CA-C-O    | -6.04 | 114.78      | 120.34   |
| 1   | C     | 440 | GLU  | CA-C-O    | -6.04 | 113.44      | 120.20   |
| 1   | E     | 387 | LEU  | O-C-N     | -6.04 | 115.54      | 123.21   |
| 1   | A     | 76  | LEU  | CA-C-O    | -6.04 | 112.59      | 119.41   |
| 1   | B     | 170 | SER  | N-CA-C    | 6.04  | 119.74      | 112.38   |
| 1   | M     | 36  | ILE  | N-CA-C    | 6.04  | 116.70      | 110.36   |
| 1   | N     | 157 | ASP  | CA-CB-CG  | -6.04 | 106.56      | 112.60   |
| 1   | D     | 317 | VAL  | O-C-N     | -6.03 | 116.33      | 122.54   |
| 1   | H     | 32  | VAL  | N-CA-C    | 6.03  | 117.50      | 110.62   |
| 1   | F     | 231 | GLU  | N-CA-C    | 6.03  | 119.34      | 110.59   |
| 1   | O     | 288 | ASP  | CA-C-O    | -6.03 | 113.03      | 119.97   |
| 1   | E     | 444 | VAL  | O-C-N     | -6.03 | 116.00      | 121.91   |
| 1   | P     | 120 | ASP  | CA-C-N    | 6.03  | 128.85      | 120.29   |
| 1   | P     | 120 | ASP  | C-N-CA    | 6.03  | 128.85      | 120.29   |
| 1   | P     | 523 | VAL  | CA-C-O    | 6.03  | 127.22      | 120.95   |
| 1   | D     | 43  | GLU  | CA-C-O    | -6.03 | 114.49      | 120.82   |
| 1   | R     | 446 | ALA  | CA-C-O    | -6.03 | 114.67      | 121.00   |
| 1   | L     | 90  | VAL  | CA-C-O    | -6.03 | 114.68      | 120.95   |
| 1   | L     | 281 | ASN  | CA-CB-CG  | -6.03 | 106.57      | 112.60   |
| 1   | G     | 114 | LEU  | CA-C-N    | 6.03  | 128.15      | 120.56   |
| 1   | G     | 114 | LEU  | C-N-CA    | 6.03  | 128.15      | 120.56   |
| 1   | P     | 114 | LEU  | CA-C-N    | 6.03  | 128.15      | 120.56   |
| 1   | P     | 114 | LEU  | C-N-CA    | 6.03  | 128.15      | 120.56   |
| 1   | E     | 457 | ILE  | O-C-N     | -6.02 | 115.92      | 121.94   |
| 1   | F     | 423 | ILE  | N-CA-C    | 6.02  | 117.48      | 110.62   |
| 1   | M     | 458 | LEU  | CB-CA-C   | 6.02  | 120.34      | 110.88   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 200 | TRP  | CB-CG-CD1  | 6.02  | 135.93      | 126.90   |
| 1   | F     | 76  | LEU  | N-CA-C     | -6.02 | 106.07      | 113.41   |
| 1   | Q     | 170 | SER  | N-CA-C     | 6.02  | 119.72      | 112.38   |
| 1   | Q     | 204 | LEU  | CA-C-O     | 6.02  | 126.90      | 120.10   |
| 1   | Q     | 445 | GLU  | CA-C-N     | 6.02  | 128.63      | 120.44   |
| 1   | Q     | 445 | GLU  | C-N-CA     | 6.02  | 128.63      | 120.44   |
| 1   | S     | 196 | ARG  | N-CA-C     | -6.02 | 97.48       | 108.02   |
| 1   | B     | 82  | GLN  | OE1-CD-NE2 | 6.02  | 128.62      | 122.60   |
| 1   | E     | 410 | LYS  | N-CA-C     | 6.02  | 118.63      | 111.71   |
| 1   | P     | 184 | ILE  | CB-CA-C    | -6.02 | 104.18      | 111.88   |
| 1   | A     | 87  | LYS  | N-CA-C     | 6.01  | 118.63      | 111.71   |
| 1   | A     | 276 | LEU  | CA-C-N     | 6.01  | 128.62      | 120.44   |
| 1   | A     | 276 | LEU  | C-N-CA     | 6.01  | 128.62      | 120.44   |
| 1   | B     | 33  | ARG  | N-CA-C     | 6.01  | 117.51      | 111.07   |
| 1   | C     | 45  | ALA  | N-CA-C     | -6.01 | 105.77      | 113.23   |
| 1   | H     | 71  | ASP  | N-CA-C     | 6.01  | 117.81      | 109.15   |
| 1   | I     | 281 | ASN  | CA-C-N     | 6.01  | 128.83      | 120.29   |
| 1   | I     | 281 | ASN  | C-N-CA     | 6.01  | 128.83      | 120.29   |
| 1   | R     | 291 | LEU  | CA-C-N     | 6.01  | 130.22      | 120.60   |
| 1   | R     | 291 | LEU  | C-N-CA     | 6.01  | 130.22      | 120.60   |
| 1   | F     | 327 | ASP  | N-CA-C     | -6.01 | 106.10      | 113.50   |
| 1   | H     | 135 | TYR  | N-CA-C     | 6.01  | 117.83      | 111.28   |
| 1   | S     | 223 | VAL  | O-C-N      | -6.01 | 116.87      | 123.18   |
| 1   | A     | 342 | ASN  | CA-C-O     | 6.01  | 126.82      | 120.33   |
| 1   | C     | 343 | ILE  | N-CA-C     | 6.01  | 118.56      | 111.05   |
| 1   | D     | 121 | LEU  | N-CA-C     | 6.01  | 117.91      | 111.36   |
| 1   | H     | 499 | GLN  | OE1-CD-NE2 | 6.01  | 128.61      | 122.60   |
| 1   | K     | 35  | ASN  | CA-CB-CG   | -6.01 | 106.59      | 112.60   |
| 1   | Q     | 355 | SER  | CB-CA-C    | -6.01 | 100.63      | 110.85   |
| 1   | E     | 196 | ARG  | CD-NE-CZ   | -6.01 | 115.99      | 124.40   |
| 1   | I     | 246 | ILE  | N-CA-C     | 6.01  | 118.10      | 109.51   |
| 1   | M     | 144 | GLN  | CA-C-N     | 6.01  | 130.22      | 120.60   |
| 1   | M     | 144 | GLN  | C-N-CA     | 6.01  | 130.22      | 120.60   |
| 1   | L     | 382 | LEU  | O-C-N      | -6.01 | 115.19      | 123.12   |
| 1   | O     | 405 | VAL  | CA-CB-CG1  | 6.01  | 120.61      | 110.40   |
| 1   | R     | 401 | ALA  | N-CA-C     | 6.01  | 117.83      | 111.28   |
| 1   | R     | 523 | VAL  | CA-C-N     | 6.01  | 129.44      | 120.31   |
| 1   | R     | 523 | VAL  | C-N-CA     | 6.01  | 129.44      | 120.31   |
| 1   | C     | 364 | GLU  | N-CA-CB    | -6.00 | 101.86      | 110.80   |
| 1   | C     | 495 | VAL  | CA-C-N     | 6.00  | 130.94      | 121.99   |
| 1   | C     | 495 | VAL  | C-N-CA     | 6.00  | 130.94      | 121.99   |
| 1   | K     | 428 | LYS  | CA-C-O     | 6.00  | 126.88      | 120.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M     | 504 | GLU  | CA-C-O      | -6.00 | 114.10      | 120.28   |
| 1   | C     | 513 | ILE  | CB-CA-C     | -6.00 | 104.20      | 111.88   |
| 1   | F     | 219 | ASP  | CA-CB-CG    | -6.00 | 106.60      | 112.60   |
| 1   | M     | 205 | ASP  | CA-C-O      | 6.00  | 126.69      | 119.61   |
| 1   | N     | 131 | ILE  | CA-CB-CG2   | -6.00 | 100.30      | 110.50   |
| 1   | D     | 68  | ILE  | CB-CG1-CD1  | 6.00  | 126.40      | 113.80   |
| 1   | E     | 304 | ILE  | CA-C-O      | -6.00 | 114.09      | 120.39   |
| 1   | I     | 238 | PRO  | N-CA-C      | 6.00  | 120.65      | 111.11   |
| 1   | M     | 509 | LYS  | N-CA-C      | 6.00  | 120.29      | 113.15   |
| 1   | S     | 127 | HIS  | O-C-N       | -6.00 | 115.12      | 121.30   |
| 1   | Q     | 244 | ALA  | N-CA-C      | 6.00  | 119.16      | 110.28   |
| 1   | D     | 515 | ALA  | N-CA-C      | 6.00  | 117.51      | 110.97   |
| 1   | O     | 178 | ARG  | NE-CZ-NH1   | -6.00 | 115.50      | 121.50   |
| 1   | E     | 79  | MET  | O-C-N       | -6.00 | 115.65      | 123.02   |
| 1   | R     | 60  | VAL  | N-CA-C      | 6.00  | 116.24      | 107.37   |
| 1   | E     | 384 | ARG  | NE-CZ-NH1   | 5.99  | 127.49      | 121.50   |
| 1   | L     | 250 | ASP  | N-CA-CB     | -5.99 | 101.34      | 110.33   |
| 1   | N     | 389 | ARG  | NE-CZ-NH2   | -5.99 | 113.81      | 119.20   |
| 1   | C     | 379 | ILE  | N-CA-CB     | -5.99 | 104.14      | 112.52   |
| 1   | D     | 127 | HIS  | CE1-NE2-CD2 | -5.99 | 103.01      | 109.00   |
| 1   | D     | 521 | THR  | CA-CB-CG2   | -5.99 | 100.31      | 110.50   |
| 1   | H     | 38  | ALA  | CA-C-N      | 5.99  | 128.19      | 120.70   |
| 1   | H     | 38  | ALA  | C-N-CA      | 5.99  | 128.19      | 120.70   |
| 1   | I     | 428 | LYS  | N-CA-C      | 5.99  | 117.81      | 111.28   |
| 1   | D     | 369 | PHE  | CA-CB-CG    | -5.99 | 107.81      | 113.80   |
| 1   | Q     | 299 | ILE  | CA-C-O      | 5.99  | 127.38      | 120.67   |
| 1   | O     | 194 | GLU  | O-C-N       | -5.99 | 117.01      | 123.42   |
| 1   | C     | 200 | TRP  | CB-CG-CD1   | 5.99  | 135.88      | 126.90   |
| 1   | D     | 114 | LEU  | CA-C-N      | 5.99  | 128.10      | 120.56   |
| 1   | D     | 114 | LEU  | C-N-CA      | 5.99  | 128.10      | 120.56   |
| 1   | Q     | 498 | TRP  | CB-CG-CD2   | -5.99 | 118.42      | 126.80   |
| 1   | A     | 240 | ARG  | NE-CZ-NH1   | 5.98  | 127.48      | 121.50   |
| 1   | G     | 356 | LEU  | O-C-N       | -5.98 | 116.60      | 123.42   |
| 1   | E     | 495 | VAL  | O-C-N       | -5.98 | 115.40      | 122.58   |
| 1   | M     | 119 | GLU  | CA-C-N      | 5.98  | 128.89      | 120.28   |
| 1   | M     | 119 | GLU  | C-N-CA      | 5.98  | 128.89      | 120.28   |
| 1   | N     | 154 | SER  | CA-C-N      | 5.98  | 128.92      | 120.42   |
| 1   | N     | 154 | SER  | C-N-CA      | 5.98  | 128.92      | 120.42   |
| 1   | E     | 483 | LYS  | N-CA-C      | 5.98  | 118.59      | 111.71   |
| 1   | F     | 61  | ASP  | CA-C-N      | 5.98  | 129.79      | 120.82   |
| 1   | F     | 61  | ASP  | C-N-CA      | 5.98  | 129.79      | 120.82   |
| 1   | H     | 496 | ASP  | CA-C-O      | 5.98  | 127.36      | 120.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M     | 323 | ALA  | CA-C-O      | 5.98  | 127.87      | 121.05   |
| 1   | P     | 255 | VAL  | O-C-N       | -5.98 | 116.17      | 122.57   |
| 1   | C     | 239 | LYS  | N-CA-C      | 5.98  | 117.88      | 111.36   |
| 1   | C     | 500 | LYS  | N-CA-C      | -5.98 | 103.64      | 113.50   |
| 1   | O     | 83  | HIS  | ND1-CE1-NE2 | 5.98  | 114.38      | 108.40   |
| 1   | R     | 166 | MET  | CG-SD-CE    | -5.98 | 87.75       | 100.90   |
| 1   | K     | 165 | ALA  | N-CA-C      | 5.98  | 117.59      | 111.14   |
| 1   | M     | 512 | ALA  | N-CA-C      | 5.98  | 117.47      | 111.07   |
| 1   | P     | 143 | LEU  | N-CA-CB     | 5.98  | 118.65      | 109.98   |
| 1   | S     | 424 | GLU  | CA-CB-CG    | 5.98  | 126.06      | 114.10   |
| 1   | D     | 88  | LEU  | N-CA-C      | -5.98 | 104.85      | 111.36   |
| 1   | N     | 181 | ILE  | CA-C-N      | 5.98  | 128.61      | 120.54   |
| 1   | N     | 181 | ILE  | C-N-CA      | 5.98  | 128.61      | 120.54   |
| 1   | P     | 328 | LEU  | N-CA-C      | -5.98 | 104.77      | 111.28   |
| 1   | F     | 164 | ILE  | CA-C-N      | 5.97  | 128.56      | 120.44   |
| 1   | F     | 164 | ILE  | C-N-CA      | 5.97  | 128.56      | 120.44   |
| 1   | S     | 91  | GLN  | CG-CD-OE1   | 5.97  | 132.75      | 120.80   |
| 1   | A     | 124 | LYS  | CA-C-N      | 5.97  | 131.14      | 122.36   |
| 1   | A     | 124 | LYS  | C-N-CA      | 5.97  | 131.14      | 122.36   |
| 1   | O     | 92  | ILE  | N-CA-C      | -5.97 | 104.69      | 110.72   |
| 1   | P     | 504 | GLU  | N-CA-C      | 5.97  | 115.18      | 108.25   |
| 1   | Q     | 420 | ALA  | N-CA-C      | 5.97  | 118.30      | 111.02   |
| 1   | R     | 87  | LYS  | N-CA-CB     | -5.97 | 101.03      | 110.22   |
| 1   | R     | 423 | ILE  | N-CA-C      | 5.97  | 117.43      | 110.62   |
| 1   | R     | 467 | ILE  | N-CA-C      | 5.97  | 116.15      | 110.42   |
| 1   | D     | 349 | GLN  | CB-CG-CD    | -5.97 | 102.45      | 112.60   |
| 1   | A     | 141 | VAL  | N-CA-C      | 5.97  | 116.62      | 110.36   |
| 1   | D     | 191 | GLN  | CA-C-N      | 5.97  | 130.03      | 121.02   |
| 1   | D     | 191 | GLN  | C-N-CA      | 5.97  | 130.03      | 121.02   |
| 1   | L     | 152 | THR  | N-CA-C      | 5.97  | 117.74      | 109.15   |
| 1   | G     | 99  | GLU  | N-CA-C      | 5.96  | 117.86      | 111.36   |
| 1   | H     | 409 | ILE  | O-C-N       | -5.96 | 115.69      | 121.83   |
| 1   | M     | 93  | ALA  | CA-C-N      | 5.96  | 128.52      | 120.65   |
| 1   | M     | 93  | ALA  | C-N-CA      | 5.96  | 128.52      | 120.65   |
| 1   | N     | 176 | GLY  | CA-C-N      | 5.96  | 132.93      | 121.54   |
| 1   | N     | 176 | GLY  | C-N-CA      | 5.96  | 132.93      | 121.54   |
| 1   | P     | 443 | ALA  | CA-C-O      | 5.96  | 127.08      | 120.82   |
| 1   | R     | 268 | ASP  | CA-CB-CG    | 5.96  | 118.56      | 112.60   |
| 1   | N     | 301 | GLN  | CA-C-O      | 5.96  | 125.95      | 119.15   |
| 1   | R     | 83  | HIS  | N-CA-C      | 5.96  | 118.27      | 109.50   |
| 1   | E     | 218 | ASN  | CA-CB-CG    | -5.96 | 106.64      | 112.60   |
| 1   | L     | 503 | ILE  | CA-C-O      | -5.96 | 114.72      | 121.75   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | P     | 415 | ILE  | O-C-N     | -5.96 | 116.71      | 122.97   |
| 1   | N     | 323 | ALA  | O-C-N     | -5.96 | 116.38      | 123.06   |
| 1   | N     | 445 | GLU  | CA-C-O    | -5.96 | 114.19      | 120.63   |
| 1   | R     | 153 | VAL  | N-CA-CB   | 5.96  | 119.39      | 111.64   |
| 1   | L     | 248 | LEU  | CA-C-O    | -5.96 | 114.69      | 121.66   |
| 1   | S     | 184 | ILE  | CA-C-N    | 5.96  | 128.93      | 120.53   |
| 1   | S     | 184 | ILE  | C-N-CA    | 5.96  | 128.93      | 120.53   |
| 1   | E     | 165 | ALA  | N-CA-CB   | 5.96  | 118.71      | 110.07   |
| 1   | C     | 133 | SER  | CA-C-N    | 5.96  | 126.72      | 119.99   |
| 1   | C     | 133 | SER  | C-N-CA    | 5.96  | 126.72      | 119.99   |
| 1   | D     | 101 | ALA  | N-CA-CB   | -5.95 | 102.10      | 111.39   |
| 1   | O     | 237 | MET  | N-CA-C    | 5.95  | 117.39      | 109.83   |
| 1   | E     | 183 | ASP  | CA-C-N    | 5.95  | 128.57      | 120.77   |
| 1   | E     | 183 | ASP  | C-N-CA    | 5.95  | 128.57      | 120.77   |
| 1   | H     | 205 | ASP  | N-CA-C    | 5.95  | 120.08      | 112.34   |
| 1   | Q     | 461 | ASN  | CB-CA-C   | -5.95 | 97.17       | 110.21   |
| 1   | G     | 93  | ALA  | CA-C-N    | 5.95  | 128.50      | 120.65   |
| 1   | G     | 93  | ALA  | C-N-CA    | 5.95  | 128.50      | 120.65   |
| 1   | I     | 128 | PRO  | N-CA-C    | 5.95  | 121.58      | 113.84   |
| 1   | N     | 203 | ASP  | CA-CB-CG  | -5.95 | 106.65      | 112.60   |
| 1   | P     | 397 | ALA  | N-CA-C    | 5.95  | 118.25      | 111.11   |
| 1   | S     | 517 | THR  | CA-C-N    | 5.95  | 128.50      | 120.65   |
| 1   | S     | 517 | THR  | C-N-CA    | 5.95  | 128.50      | 120.65   |
| 1   | B     | 86  | ALA  | CA-C-N    | 5.95  | 128.25      | 120.28   |
| 1   | B     | 86  | ALA  | C-N-CA    | 5.95  | 128.25      | 120.28   |
| 1   | K     | 180 | TYR  | CA-CB-CG  | -5.95 | 103.19      | 113.90   |
| 1   | A     | 32  | VAL  | CA-CB-CG2 | 5.95  | 120.51      | 110.40   |
| 1   | B     | 81  | LEU  | CA-C-N    | 5.95  | 132.89      | 121.54   |
| 1   | B     | 81  | LEU  | C-N-CA    | 5.95  | 132.89      | 121.54   |
| 1   | O     | 75  | ILE  | O-C-N     | -5.94 | 114.26      | 122.05   |
| 1   | A     | 450 | ALA  | CA-C-N    | 5.94  | 129.34      | 120.31   |
| 1   | A     | 450 | ALA  | C-N-CA    | 5.94  | 129.34      | 120.31   |
| 1   | I     | 467 | ILE  | CA-C-N    | 5.94  | 129.05      | 120.79   |
| 1   | I     | 467 | ILE  | C-N-CA    | 5.94  | 129.05      | 120.79   |
| 1   | P     | 190 | THR  | N-CA-C    | 5.94  | 119.35      | 111.75   |
| 1   | R     | 123 | TYR  | CB-CA-C   | 5.94  | 120.65      | 110.79   |
| 1   | H     | 329 | GLU  | N-CA-C    | 5.94  | 117.42      | 111.07   |
| 1   | H     | 496 | ASP  | CA-C-N    | 5.94  | 128.72      | 120.29   |
| 1   | H     | 496 | ASP  | C-N-CA    | 5.94  | 128.72      | 120.29   |
| 1   | N     | 249 | ILE  | N-CA-C    | 5.94  | 115.91      | 106.88   |
| 1   | D     | 244 | ALA  | CA-C-N    | 5.94  | 131.06      | 122.16   |
| 1   | D     | 244 | ALA  | C-N-CA    | 5.94  | 131.06      | 122.16   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 83  | HIS  | CA-C-N     | 5.94  | 125.41      | 119.24   |
| 1   | F     | 83  | HIS  | C-N-CA     | 5.94  | 125.41      | 119.24   |
| 1   | P     | 322 | ARG  | NE-CZ-NH2  | 5.94  | 124.54      | 119.20   |
| 1   | B     | 260 | LEU  | CA-C-O     | -5.93 | 114.20      | 120.55   |
| 1   | C     | 514 | LYS  | CA-C-O     | -5.93 | 114.59      | 120.82   |
| 1   | M     | 67  | THR  | CA-C-N     | -5.93 | 115.83      | 123.19   |
| 1   | M     | 67  | THR  | C-N-CA     | -5.93 | 115.83      | 123.19   |
| 1   | B     | 398 | LEU  | CA-C-N     | 5.93  | 128.15      | 120.44   |
| 1   | B     | 398 | LEU  | C-N-CA     | 5.93  | 128.15      | 120.44   |
| 1   | M     | 345 | GLU  | CA-C-O     | 5.93  | 125.73      | 119.03   |
| 1   | N     | 500 | LYS  | O-C-N      | -5.93 | 114.84      | 121.84   |
| 1   | O     | 173 | ALA  | N-CA-C     | -5.93 | 104.89      | 111.36   |
| 1   | A     | 167 | THR  | O-C-N      | -5.93 | 114.70      | 122.59   |
| 1   | A     | 405 | VAL  | CA-CB-CG1  | 5.93  | 120.48      | 110.40   |
| 1   | H     | 447 | TYR  | CA-C-O     | 5.93  | 127.03      | 120.63   |
| 1   | C     | 138 | ALA  | CA-C-N     | 5.93  | 128.15      | 120.44   |
| 1   | C     | 138 | ALA  | C-N-CA     | 5.93  | 128.15      | 120.44   |
| 1   | H     | 365 | ASP  | O-C-N      | -5.93 | 116.27      | 123.27   |
| 1   | M     | 187 | LYS  | O-C-N      | -5.93 | 115.96      | 122.07   |
| 1   | O     | 83  | HIS  | CG-CD2-NE2 | 5.93  | 113.13      | 107.20   |
| 1   | O     | 223 | VAL  | O-C-N      | -5.93 | 117.09      | 123.14   |
| 1   | O     | 419 | GLY  | N-CA-C     | 5.93  | 123.54      | 115.30   |
| 1   | Q     | 123 | TYR  | CA-CB-CG   | -5.93 | 103.23      | 113.90   |
| 1   | L     | 500 | LYS  | CA-C-O     | 5.93  | 125.30      | 119.08   |
| 1   | B     | 36  | ILE  | CA-C-N     | 5.93  | 130.61      | 121.19   |
| 1   | B     | 36  | ILE  | C-N-CA     | 5.93  | 130.61      | 121.19   |
| 1   | Q     | 233 | VAL  | CA-C-N     | -5.93 | 115.23      | 122.64   |
| 1   | Q     | 233 | VAL  | C-N-CA     | -5.93 | 115.23      | 122.64   |
| 1   | Q     | 296 | ASN  | OD1-CG-ND2 | 5.93  | 128.53      | 122.60   |
| 1   | M     | 163 | LYS  | N-CA-CB    | 5.92  | 118.78      | 110.07   |
| 1   | K     | 92  | ILE  | CA-C-N     | 5.92  | 128.47      | 120.65   |
| 1   | K     | 92  | ILE  | C-N-CA     | 5.92  | 128.47      | 120.65   |
| 1   | K     | 495 | VAL  | CB-CA-C    | -5.92 | 101.22      | 110.52   |
| 1   | R     | 365 | ASP  | CA-C-O     | 5.92  | 127.85      | 121.16   |
| 1   | O     | 72  | GLY  | CA-C-N     | 5.92  | 130.60      | 121.19   |
| 1   | O     | 72  | GLY  | C-N-CA     | 5.92  | 130.60      | 121.19   |
| 1   | R     | 50  | TYR  | CB-CG-CD1  | -5.92 | 111.92      | 120.80   |
| 1   | A     | 280 | GLU  | CA-C-O     | 5.92  | 126.81      | 120.24   |
| 1   | H     | 76  | LEU  | O-C-N      | -5.92 | 114.43      | 122.36   |
| 1   | L     | 138 | ALA  | CA-C-N     | 5.92  | 128.13      | 120.44   |
| 1   | L     | 138 | ALA  | C-N-CA     | 5.92  | 128.13      | 120.44   |
| 1   | N     | 47  | LYS  | N-CA-C     | 5.92  | 123.41      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 456 | SER  | CA-C-N     | 5.92  | 128.23      | 120.60   |
| 1   | O     | 456 | SER  | C-N-CA     | 5.92  | 128.23      | 120.60   |
| 1   | G     | 286 | LYS  | CA-C-N     | 5.92  | 128.01      | 120.56   |
| 1   | G     | 286 | LYS  | C-N-CA     | 5.92  | 128.01      | 120.56   |
| 1   | R     | 114 | LEU  | CA-C-N     | 5.92  | 128.01      | 120.56   |
| 1   | R     | 114 | LEU  | C-N-CA     | 5.92  | 128.01      | 120.56   |
| 1   | R     | 402 | LEU  | N-CA-CB    | 5.92  | 118.59      | 110.01   |
| 1   | S     | 83  | HIS  | O-C-N      | 5.92  | 127.20      | 121.28   |
| 1   | G     | 40  | LYS  | CA-C-N     | 5.92  | 128.13      | 120.44   |
| 1   | G     | 40  | LYS  | C-N-CA     | 5.92  | 128.13      | 120.44   |
| 1   | I     | 83  | HIS  | CB-CG-CD2  | -5.91 | 123.51      | 131.20   |
| 1   | D     | 481 | ASN  | OD1-CG-ND2 | -5.91 | 116.69      | 122.60   |
| 1   | F     | 356 | LEU  | CA-C-O     | -5.91 | 112.23      | 120.21   |
| 1   | L     | 174 | VAL  | CB-CA-C    | -5.91 | 101.60      | 111.29   |
| 1   | O     | 459 | ILE  | N-CA-C     | 5.91  | 116.09      | 110.42   |
| 1   | A     | 398 | LEU  | CA-C-N     | 5.91  | 128.12      | 120.44   |
| 1   | A     | 398 | LEU  | C-N-CA     | 5.91  | 128.12      | 120.44   |
| 1   | D     | 439 | LYS  | CA-C-O     | 5.91  | 126.68      | 120.42   |
| 1   | P     | 202 | VAL  | O-C-N      | -5.91 | 116.82      | 123.20   |
| 1   | Q     | 102 | ASP  | CA-CB-CG   | -5.91 | 106.69      | 112.60   |
| 1   | G     | 191 | GLN  | N-CA-C     | 5.90  | 117.80      | 111.36   |
| 1   | N     | 49  | THR  | CA-C-O     | 5.90  | 126.14      | 119.18   |
| 1   | P     | 397 | ALA  | O-C-N      | -5.90 | 115.95      | 122.09   |
| 1   | F     | 77  | ASP  | O-C-N      | -5.90 | 115.72      | 122.09   |
| 1   | M     | 213 | ALA  | CA-C-O     | -5.90 | 114.76      | 121.72   |
| 1   | N     | 394 | THR  | CA-C-N     | 5.90  | 128.67      | 120.29   |
| 1   | N     | 394 | THR  | C-N-CA     | 5.90  | 128.67      | 120.29   |
| 1   | N     | 292 | ALA  | N-CA-C     | 5.90  | 119.58      | 112.38   |
| 1   | Q     | 327 | ASP  | CA-CB-CG   | -5.90 | 106.70      | 112.60   |
| 1   | L     | 169 | LEU  | O-C-N      | -5.90 | 114.43      | 122.33   |
| 1   | G     | 487 | ILE  | O-C-N      | -5.89 | 116.68      | 122.99   |
| 1   | N     | 93  | ALA  | CA-C-N     | 5.89  | 128.43      | 120.65   |
| 1   | N     | 93  | ALA  | C-N-CA     | 5.89  | 128.43      | 120.65   |
| 1   | R     | 174 | VAL  | N-CA-C     | 5.89  | 117.27      | 108.54   |
| 1   | R     | 370 | VAL  | CA-C-O     | 5.89  | 128.15      | 120.78   |
| 1   | N     | 336 | GLY  | N-CA-C     | -5.89 | 107.19      | 115.32   |
| 1   | P     | 191 | GLN  | OE1-CD-NE2 | -5.89 | 116.71      | 122.60   |
| 1   | C     | 80  | ASP  | CA-CB-CG   | -5.89 | 106.71      | 112.60   |
| 1   | C     | 117 | LYS  | O-C-N      | -5.89 | 115.33      | 122.22   |
| 1   | S     | 496 | ASP  | CA-C-O     | 5.89  | 127.26      | 120.60   |
| 1   | N     | 275 | PHE  | CB-CG-CD2  | 5.89  | 130.71      | 120.70   |
| 1   | N     | 466 | PRO  | CA-C-N     | 5.89  | 128.10      | 120.56   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | N     | 466 | PRO  | C-N-CA     | 5.89  | 128.10      | 120.56   |
| 1   | D     | 252 | SER  | N-CA-C     | 5.89  | 118.99      | 110.28   |
| 1   | M     | 309 | GLN  | CA-C-N     | 5.89  | 128.76      | 120.28   |
| 1   | M     | 309 | GLN  | C-N-CA     | 5.89  | 128.76      | 120.28   |
| 1   | N     | 431 | LYS  | CA-C-O     | 5.89  | 126.74      | 119.97   |
| 1   | Q     | 396 | ARG  | O-C-N      | 5.89  | 128.45      | 122.09   |
| 1   | F     | 75  | ILE  | O-C-N      | -5.89 | 114.34      | 122.05   |
| 1   | H     | 517 | THR  | CA-C-O     | 5.89  | 126.79      | 120.55   |
| 1   | I     | 83  | HIS  | CA-CB-CG   | 5.89  | 119.69      | 113.80   |
| 1   | H     | 377 | LYS  | N-CA-C     | 5.88  | 117.69      | 111.28   |
| 1   | B     | 408 | VAL  | CA-C-O     | -5.88 | 114.83      | 120.95   |
| 1   | S     | 42  | VAL  | CA-C-N     | 5.88  | 128.09      | 120.44   |
| 1   | S     | 42  | VAL  | C-N-CA     | 5.88  | 128.09      | 120.44   |
| 1   | C     | 463 | GLY  | CA-C-O     | -5.88 | 113.24      | 118.77   |
| 1   | O     | 444 | VAL  | CA-C-N     | 5.88  | 128.44      | 120.38   |
| 1   | O     | 444 | VAL  | C-N-CA     | 5.88  | 128.44      | 120.38   |
| 1   | P     | 136 | LYS  | N-CA-C     | 5.88  | 118.19      | 111.02   |
| 1   | D     | 207 | ILE  | O-C-N      | -5.88 | 117.06      | 123.18   |
| 1   | K     | 32  | VAL  | CB-CA-C    | -5.88 | 104.34      | 112.04   |
| 1   | R     | 265 | ARG  | NE-CZ-NH1  | -5.88 | 115.62      | 121.50   |
| 1   | I     | 166 | MET  | CA-C-O     | 5.88  | 126.65      | 120.42   |
| 1   | L     | 156 | ASN  | OD1-CG-ND2 | -5.88 | 116.72      | 122.60   |
| 1   | E     | 98  | GLU  | CA-C-N     | 5.88  | 128.96      | 120.38   |
| 1   | E     | 98  | GLU  | C-N-CA     | 5.88  | 128.96      | 120.38   |
| 1   | I     | 472 | LYS  | CA-C-O     | 5.88  | 126.74      | 120.10   |
| 1   | Q     | 32  | VAL  | O-C-N      | -5.88 | 115.97      | 121.90   |
| 1   | D     | 119 | GLU  | CA-C-O     | 5.88  | 126.78      | 120.55   |
| 1   | M     | 73  | ALA  | CA-C-O     | -5.88 | 114.15      | 121.02   |
| 1   | A     | 114 | LEU  | CA-C-N     | 5.87  | 127.96      | 120.56   |
| 1   | A     | 114 | LEU  | C-N-CA     | 5.87  | 127.96      | 120.56   |
| 1   | B     | 209 | ILE  | O-C-N      | -5.87 | 117.33      | 123.03   |
| 1   | H     | 201 | TYR  | O-C-N      | -5.87 | 116.02      | 123.24   |
| 1   | P     | 307 | VAL  | CB-CA-C    | -5.87 | 104.37      | 112.24   |
| 1   | B     | 131 | ILE  | O-C-N      | -5.87 | 115.94      | 121.87   |
| 1   | H     | 411 | ASP  | O-C-N      | -5.87 | 114.78      | 122.59   |
| 1   | C     | 469 | LEU  | N-CA-CB    | 5.87  | 118.84      | 110.16   |
| 1   | O     | 344 | ASP  | O-C-N      | -5.87 | 112.97      | 122.42   |
| 1   | R     | 372 | GLY  | CA-C-O     | 5.87  | 127.01      | 119.68   |
| 1   | C     | 287 | VAL  | N-CA-C     | 5.87  | 116.60      | 110.62   |
| 1   | M     | 459 | ILE  | CA-C-N     | 5.87  | 130.51      | 121.19   |
| 1   | M     | 459 | ILE  | C-N-CA     | 5.87  | 130.51      | 121.19   |
| 1   | O     | 183 | ASP  | N-CA-C     | 5.87  | 118.15      | 111.11   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | O     | 398 | LEU  | O-C-N       | 5.87  | 128.84      | 122.15   |
| 1   | M     | 164 | ILE  | CA-C-N      | 5.86  | 128.41      | 120.44   |
| 1   | M     | 164 | ILE  | C-N-CA      | 5.86  | 128.41      | 120.44   |
| 1   | N     | 286 | LYS  | CA-C-O      | -5.86 | 114.30      | 120.63   |
| 1   | O     | 234 | HIS  | CE1-NE2-CD2 | -5.86 | 103.14      | 109.00   |
| 1   | C     | 231 | GLU  | CB-CG-CD    | 5.86  | 122.56      | 112.60   |
| 1   | F     | 494 | PRO  | N-CD-CG     | 5.86  | 111.99      | 103.20   |
| 1   | G     | 388 | GLU  | N-CA-C      | 5.86  | 119.96      | 112.34   |
| 1   | L     | 94  | LYS  | O-C-N       | -5.86 | 115.94      | 122.03   |
| 1   | N     | 30  | GLU  | N-CA-C      | 5.86  | 123.28      | 110.80   |
| 1   | N     | 388 | GLU  | O-C-N       | -5.86 | 115.52      | 122.20   |
| 1   | R     | 344 | ASP  | N-CA-CB     | -5.86 | 101.44      | 110.46   |
| 1   | M     | 373 | ALA  | N-CA-CB     | 5.86  | 118.65      | 110.04   |
| 1   | Q     | 389 | ARG  | CA-C-N      | 5.86  | 128.13      | 120.28   |
| 1   | Q     | 389 | ARG  | C-N-CA      | 5.86  | 128.13      | 120.28   |
| 1   | S     | 112 | GLY  | N-CA-C      | 5.86  | 121.22      | 113.37   |
| 1   | B     | 430 | ARG  | N-CA-C      | 5.86  | 117.66      | 111.28   |
| 1   | F     | 243 | ASN  | OD1-CG-ND2  | -5.86 | 116.74      | 122.60   |
| 1   | M     | 399 | ARG  | CA-C-N      | 5.86  | 128.13      | 120.28   |
| 1   | M     | 399 | ARG  | C-N-CA      | 5.86  | 128.13      | 120.28   |
| 1   | M     | 264 | ILE  | O-C-N       | -5.86 | 116.51      | 122.54   |
| 1   | P     | 322 | ARG  | O-C-N       | -5.86 | 115.66      | 122.86   |
| 1   | P     | 480 | GLU  | N-CA-C      | 5.85  | 118.61      | 111.82   |
| 1   | B     | 331 | LEU  | N-CA-C      | -5.85 | 105.23      | 112.90   |
| 1   | E     | 74  | THR  | N-CA-C      | 5.85  | 118.41      | 111.33   |
| 1   | K     | 321 | ARG  | NE-CZ-NH1   | 5.85  | 127.35      | 121.50   |
| 1   | L     | 434 | PRO  | CA-C-N      | 5.85  | 131.96      | 121.66   |
| 1   | L     | 434 | PRO  | C-N-CA      | 5.85  | 131.96      | 121.66   |
| 1   | N     | 75  | ILE  | CA-C-O      | 5.85  | 127.11      | 119.85   |
| 1   | N     | 183 | ASP  | N-CA-C      | 5.85  | 118.13      | 111.11   |
| 1   | O     | 255 | VAL  | CA-C-O      | 5.85  | 127.71      | 121.04   |
| 1   | S     | 365 | ASP  | N-CA-C      | 5.85  | 119.17      | 109.46   |
| 1   | C     | 391 | VAL  | N-CA-C      | 5.85  | 116.59      | 110.62   |
| 1   | F     | 510 | MET  | CA-C-O      | 5.85  | 126.40      | 119.67   |
| 1   | M     | 127 | HIS  | CE1-NE2-CD2 | -5.85 | 103.15      | 109.00   |
| 1   | S     | 301 | GLN  | N-CA-C      | -5.85 | 106.48      | 113.97   |
| 1   | A     | 389 | ARG  | CG-CD-NE    | -5.85 | 99.14       | 112.00   |
| 1   | B     | 452 | GLU  | CB-CG-CD    | 5.85  | 122.54      | 112.60   |
| 1   | D     | 216 | SER  | CB-CA-C     | -5.85 | 100.10      | 109.75   |
| 1   | M     | 419 | GLY  | N-CA-C      | -5.85 | 107.32      | 114.92   |
| 1   | Q     | 205 | ASP  | CA-CB-CG    | -5.85 | 106.75      | 112.60   |
| 1   | O     | 271 | GLN  | CA-C-O      | 5.84  | 126.62      | 120.42   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 478 | GLU  | CA-C-O    | 5.84  | 126.72      | 120.70   |
| 1   | L     | 272 | MET  | CA-C-O    | -5.84 | 114.64      | 121.07   |
| 1   | P     | 316 | GLY  | O-C-N     | 5.84  | 129.33      | 122.38   |
| 1   | R     | 327 | ASP  | CA-CB-CG  | -5.84 | 106.76      | 112.60   |
| 1   | S     | 249 | ILE  | CA-CB-CG1 | 5.84  | 120.33      | 110.40   |
| 1   | D     | 97  | ASP  | CA-C-N    | 5.84  | 129.57      | 120.75   |
| 1   | D     | 97  | ASP  | C-N-CA    | 5.84  | 129.57      | 120.75   |
| 1   | K     | 451 | LEU  | N-CA-C    | -5.84 | 104.99      | 111.36   |
| 1   | L     | 57  | LYS  | CA-C-O    | 5.84  | 126.90      | 120.71   |
| 1   | H     | 451 | LEU  | N-CA-C    | 5.84  | 117.72      | 111.36   |
| 1   | D     | 400 | ASP  | CA-C-N    | 5.84  | 128.38      | 120.38   |
| 1   | D     | 400 | ASP  | C-N-CA    | 5.84  | 128.38      | 120.38   |
| 1   | G     | 62  | SER  | N-CA-C    | 5.84  | 119.22      | 111.75   |
| 1   | I     | 444 | VAL  | CA-C-N    | 5.84  | 128.10      | 120.28   |
| 1   | I     | 444 | VAL  | C-N-CA    | 5.84  | 128.10      | 120.28   |
| 1   | P     | 455 | VAL  | CA-C-N    | 5.84  | 128.38      | 120.44   |
| 1   | P     | 455 | VAL  | C-N-CA    | 5.84  | 128.38      | 120.44   |
| 1   | B     | 70  | ASN  | CA-CB-CG  | -5.83 | 106.77      | 112.60   |
| 1   | P     | 103 | GLY  | CA-C-N    | 5.83  | 128.58      | 120.29   |
| 1   | P     | 103 | GLY  | C-N-CA    | 5.83  | 128.58      | 120.29   |
| 1   | Q     | 437 | GLY  | O-C-N     | -5.83 | 118.32      | 123.92   |
| 1   | E     | 323 | ALA  | O-C-N     | -5.83 | 116.40      | 123.16   |
| 1   | H     | 291 | LEU  | CA-C-N    | 5.83  | 129.93      | 120.60   |
| 1   | H     | 291 | LEU  | C-N-CA    | 5.83  | 129.93      | 120.60   |
| 1   | H     | 312 | LEU  | CA-C-O    | 5.83  | 126.68      | 119.97   |
| 1   | L     | 297 | VAL  | O-C-N     | -5.83 | 116.35      | 123.00   |
| 1   | Q     | 478 | GLU  | O-C-N     | -5.83 | 115.94      | 122.12   |
| 1   | S     | 394 | THR  | O-C-N     | -5.83 | 115.10      | 122.27   |
| 1   | A     | 436 | VAL  | CB-CA-C   | -5.83 | 104.17      | 112.22   |
| 1   | E     | 465 | ASP  | CA-C-O    | -5.83 | 115.50      | 119.29   |
| 1   | H     | 180 | TYR  | CA-C-N    | 5.83  | 128.70      | 120.42   |
| 1   | H     | 180 | TYR  | C-N-CA    | 5.83  | 128.70      | 120.42   |
| 1   | N     | 225 | GLY  | O-C-N     | -5.83 | 117.62      | 124.15   |
| 1   | P     | 474 | ARG  | NE-CZ-NH2 | 5.83  | 124.45      | 119.20   |
| 1   | R     | 325 | LYS  | CA-C-N    | 5.83  | 128.89      | 120.38   |
| 1   | R     | 325 | LYS  | C-N-CA    | 5.83  | 128.89      | 120.38   |
| 1   | A     | 60  | VAL  | CA-C-O    | 5.83  | 127.48      | 120.66   |
| 1   | D     | 277 | ASP  | CA-C-O    | 5.83  | 126.70      | 120.70   |
| 1   | F     | 204 | LEU  | CA-C-O    | -5.83 | 113.67      | 120.20   |
| 1   | O     | 31  | ALA  | CA-C-N    | 5.83  | 130.18      | 120.62   |
| 1   | O     | 31  | ALA  | C-N-CA    | 5.83  | 130.18      | 120.62   |
| 1   | R     | 66  | ILE  | N-CA-C    | 5.83  | 116.98      | 108.53   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 525 | ARG  | N-CA-C     | 5.83  | 118.58      | 111.82   |
| 1   | Q     | 470 | LEU  | O-C-N      | -5.83 | 115.94      | 122.12   |
| 1   | S     | 323 | ALA  | O-C-N      | -5.83 | 116.13      | 123.01   |
| 1   | C     | 183 | ASP  | CA-C-O     | 5.83  | 126.94      | 120.82   |
| 1   | O     | 471 | MET  | CG-SD-CE   | -5.83 | 88.08       | 100.90   |
| 1   | A     | 393 | GLU  | CA-C-N     | 5.82  | 130.58      | 120.68   |
| 1   | A     | 393 | GLU  | C-N-CA     | 5.82  | 130.58      | 120.68   |
| 1   | B     | 507 | LEU  | N-CA-C     | -5.82 | 105.27      | 112.90   |
| 1   | I     | 328 | LEU  | CB-CA-C    | -5.82 | 101.12      | 110.79   |
| 1   | N     | 190 | THR  | CA-CB-OG1  | 5.82  | 118.33      | 109.60   |
| 1   | S     | 83  | HIS  | CA-C-O     | -5.82 | 113.98      | 119.80   |
| 1   | A     | 482 | ASN  | CA-CB-CG   | -5.82 | 106.78      | 112.60   |
| 1   | F     | 268 | ASP  | CA-CB-CG   | 5.82  | 118.42      | 112.60   |
| 1   | I     | 480 | GLU  | N-CA-CB    | -5.82 | 102.53      | 110.56   |
| 1   | I     | 510 | MET  | CA-C-O     | 5.82  | 126.36      | 119.67   |
| 1   | K     | 185 | VAL  | O-C-N      | -5.82 | 116.19      | 121.89   |
| 1   | S     | 394 | THR  | OG1-CB-CG2 | -5.82 | 97.66       | 109.30   |
| 1   | G     | 174 | VAL  | O-C-N      | -5.82 | 116.27      | 122.61   |
| 1   | L     | 401 | ALA  | CB-CA-C    | -5.82 | 101.50      | 110.81   |
| 1   | E     | 395 | GLU  | CA-C-N     | 5.82  | 128.54      | 120.63   |
| 1   | E     | 395 | GLU  | C-N-CA     | 5.82  | 128.54      | 120.63   |
| 1   | F     | 469 | LEU  | N-CA-C     | 5.82  | 117.62      | 111.28   |
| 1   | N     | 184 | ILE  | CA-C-N     | 5.82  | 128.73      | 120.53   |
| 1   | N     | 184 | ILE  | C-N-CA     | 5.82  | 128.73      | 120.53   |
| 1   | E     | 531 | SER  | N-CA-C     | 5.81  | 119.15      | 110.14   |
| 1   | K     | 38  | ALA  | CA-C-O     | 5.81  | 127.12      | 120.90   |
| 1   | P     | 35  | ASN  | CA-C-N     | 5.81  | 128.39      | 120.77   |
| 1   | P     | 35  | ASN  | C-N-CA     | 5.81  | 128.39      | 120.77   |
| 1   | R     | 234 | HIS  | CB-CG-CD2  | -5.81 | 123.64      | 131.20   |
| 1   | L     | 39  | VAL  | N-CA-CB    | 5.81  | 116.96      | 110.62   |
| 1   | O     | 179 | GLU  | O-C-N      | -5.81 | 115.96      | 122.12   |
| 1   | E     | 174 | VAL  | CA-C-O     | -5.81 | 113.37      | 120.69   |
| 1   | K     | 373 | ALA  | CA-C-N     | 5.81  | 128.38      | 120.54   |
| 1   | K     | 373 | ALA  | C-N-CA     | 5.81  | 128.38      | 120.54   |
| 1   | O     | 203 | ASP  | O-C-N      | -5.81 | 114.86      | 122.59   |
| 1   | Q     | 415 | ILE  | CA-CB-CG1  | 5.81  | 120.28      | 110.40   |
| 1   | A     | 309 | GLN  | N-CA-C     | -5.81 | 104.31      | 111.40   |
| 1   | A     | 433 | ALA  | CA-C-N     | 5.81  | 127.10      | 119.84   |
| 1   | A     | 433 | ALA  | C-N-CA     | 5.81  | 127.10      | 119.84   |
| 1   | D     | 526 | ILE  | N-CA-C     | 5.81  | 115.90      | 108.12   |
| 1   | F     | 396 | ARG  | CA-C-N     | 5.81  | 128.34      | 120.38   |
| 1   | F     | 396 | ARG  | C-N-CA     | 5.81  | 128.34      | 120.38   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | Q     | 49  | THR  | CA-C-O    | 5.81  | 126.03      | 119.18   |
| 1   | R     | 256 | GLU  | O-C-N     | -5.81 | 115.33      | 123.11   |
| 1   | G     | 402 | LEU  | CB-CA-C   | -5.81 | 101.95      | 110.95   |
| 1   | H     | 203 | ASP  | CA-C-N    | 5.81  | 128.86      | 120.38   |
| 1   | H     | 203 | ASP  | C-N-CA    | 5.81  | 128.86      | 120.38   |
| 1   | M     | 38  | ALA  | N-CA-C    | 5.81  | 118.08      | 111.11   |
| 1   | I     | 50  | TYR  | N-CA-C    | 5.80  | 118.65      | 110.23   |
| 1   | Q     | 84  | PRO  | CA-C-N    | 5.80  | 128.38      | 120.54   |
| 1   | Q     | 84  | PRO  | C-N-CA    | 5.80  | 128.38      | 120.54   |
| 1   | O     | 424 | GLU  | CA-C-N    | 5.80  | 130.14      | 120.62   |
| 1   | O     | 424 | GLU  | C-N-CA    | 5.80  | 130.14      | 120.62   |
| 1   | F     | 142 | ALA  | CA-C-N    | 5.80  | 128.52      | 120.63   |
| 1   | F     | 142 | ALA  | C-N-CA    | 5.80  | 128.52      | 120.63   |
| 1   | H     | 474 | ARG  | N-CA-C    | 5.80  | 119.83      | 112.87   |
| 1   | R     | 168 | SER  | N-CA-C    | -5.80 | 104.97      | 112.68   |
| 1   | R     | 465 | ASP  | CA-C-N    | 5.80  | 125.93      | 119.32   |
| 1   | R     | 465 | ASP  | C-N-CA    | 5.80  | 125.93      | 119.32   |
| 1   | H     | 412 | GLY  | O-C-N     | -5.80 | 115.66      | 122.38   |
| 1   | G     | 82  | GLN  | O-C-N     | -5.80 | 115.09      | 122.34   |
| 1   | K     | 67  | THR  | CB-CA-C   | -5.80 | 101.22      | 110.14   |
| 1   | M     | 250 | ASP  | O-C-N     | -5.80 | 115.83      | 122.09   |
| 1   | E     | 392 | ASP  | N-CA-CB   | -5.79 | 101.61      | 110.01   |
| 1   | G     | 408 | VAL  | CA-CB-CG1 | 5.79  | 120.25      | 110.40   |
| 1   | C     | 444 | VAL  | N-CA-CB   | 5.79  | 117.33      | 110.55   |
| 1   | O     | 162 | ARG  | NE-CZ-NH1 | 5.79  | 127.29      | 121.50   |
| 1   | Q     | 204 | LEU  | O-C-N     | -5.79 | 115.44      | 122.22   |
| 1   | I     | 367 | MET  | O-C-N     | -5.79 | 116.55      | 123.27   |
| 1   | D     | 502 | VAL  | N-CA-C    | 5.79  | 115.64      | 106.32   |
| 1   | C     | 471 | MET  | CG-SD-CE  | -5.79 | 88.17       | 100.90   |
| 1   | R     | 449 | ASN  | CB-CA-C   | -5.79 | 101.55      | 110.81   |
| 1   | H     | 322 | ARG  | NE-CZ-NH2 | -5.79 | 113.99      | 119.20   |
| 1   | R     | 314 | LYS  | N-CA-C    | 5.79  | 119.60      | 112.54   |
| 1   | H     | 390 | LEU  | N-CA-C    | 5.78  | 117.58      | 111.28   |
| 1   | D     | 62  | SER  | CA-C-N    | 5.78  | 131.90      | 122.65   |
| 1   | D     | 62  | SER  | C-N-CA    | 5.78  | 131.90      | 122.65   |
| 1   | H     | 474 | ARG  | NE-CZ-NH1 | -5.78 | 115.72      | 121.50   |
| 1   | N     | 297 | VAL  | CA-C-O    | 5.78  | 127.12      | 120.76   |
| 1   | L     | 182 | ALA  | CA-C-O    | -5.78 | 114.71      | 121.07   |
| 1   | A     | 277 | ASP  | CA-CB-CG  | 5.78  | 118.38      | 112.60   |
| 1   | D     | 265 | ARG  | CA-C-N    | 5.78  | 128.31      | 120.63   |
| 1   | D     | 265 | ARG  | C-N-CA    | 5.78  | 128.31      | 120.63   |
| 1   | F     | 328 | LEU  | CA-C-O    | 5.78  | 126.89      | 120.82   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 364 | GLU  | CA-C-N    | 5.78  | 131.14      | 123.05   |
| 1   | H     | 364 | GLU  | C-N-CA    | 5.78  | 131.14      | 123.05   |
| 1   | I     | 504 | GLU  | CA-C-O    | -5.78 | 115.18      | 120.50   |
| 1   | Q     | 468 | ASP  | CA-CB-CG  | -5.78 | 106.82      | 112.60   |
| 1   | D     | 30  | GLU  | O-C-N     | -5.78 | 114.91      | 122.59   |
| 1   | K     | 490 | TYR  | CA-CB-CG  | -5.78 | 103.50      | 113.90   |
| 1   | O     | 78  | LYS  | CG-CD-CE  | 5.78  | 124.58      | 111.30   |
| 1   | Q     | 448 | ALA  | N-CA-C    | 5.78  | 117.38      | 111.14   |
| 1   | B     | 57  | LYS  | CB-CA-C   | -5.77 | 99.78       | 109.48   |
| 1   | D     | 207 | ILE  | CA-C-O    | 5.77  | 126.10      | 120.27   |
| 1   | M     | 334 | ALA  | N-CA-C    | -5.77 | 104.59      | 111.69   |
| 1   | O     | 512 | ALA  | N-CA-CB   | 5.77  | 118.38      | 110.01   |
| 1   | F     | 372 | GLY  | O-C-N     | -5.77 | 116.17      | 122.41   |
| 1   | L     | 321 | ARG  | CA-C-O    | -5.77 | 114.47      | 120.70   |
| 1   | M     | 237 | MET  | CA-C-N    | 5.77  | 126.11      | 119.93   |
| 1   | M     | 237 | MET  | C-N-CA    | 5.77  | 126.11      | 119.93   |
| 1   | M     | 420 | ALA  | CA-C-O    | 5.77  | 127.42      | 121.07   |
| 1   | Q     | 368 | VAL  | N-CA-CB   | 5.77  | 117.01      | 110.72   |
| 1   | R     | 152 | THR  | CB-CA-C   | -5.77 | 101.89      | 110.67   |
| 1   | H     | 445 | GLU  | CA-C-N    | 5.77  | 127.94      | 120.44   |
| 1   | H     | 445 | GLU  | C-N-CA    | 5.77  | 127.94      | 120.44   |
| 1   | F     | 473 | LEU  | O-C-N     | -5.77 | 114.51      | 122.30   |
| 1   | I     | 327 | ASP  | CA-C-O    | 5.77  | 125.48      | 119.14   |
| 1   | I     | 517 | THR  | CA-C-N    | 5.77  | 128.81      | 120.79   |
| 1   | I     | 517 | THR  | C-N-CA    | 5.77  | 128.81      | 120.79   |
| 1   | G     | 360 | ARG  | NE-CZ-NH2 | 5.77  | 124.39      | 119.20   |
| 1   | S     | 294 | GLY  | O-C-N     | 5.77  | 128.90      | 122.50   |
| 1   | A     | 287 | VAL  | CB-CA-C   | -5.76 | 104.59      | 111.97   |
| 1   | D     | 165 | ALA  | CA-C-N    | 5.76  | 128.01      | 120.28   |
| 1   | D     | 165 | ALA  | C-N-CA    | 5.76  | 128.01      | 120.28   |
| 1   | G     | 115 | VAL  | CA-C-N    | 5.76  | 128.80      | 120.79   |
| 1   | G     | 115 | VAL  | C-N-CA    | 5.76  | 128.80      | 120.79   |
| 1   | R     | 61  | ASP  | CA-CB-CG  | -5.76 | 106.84      | 112.60   |
| 1   | B     | 407 | ASP  | CA-CB-CG  | -5.76 | 106.84      | 112.60   |
| 1   | C     | 296 | ASN  | CA-CB-CG  | -5.76 | 106.84      | 112.60   |
| 1   | S     | 287 | VAL  | CA-C-N    | 5.76  | 129.07      | 120.31   |
| 1   | S     | 287 | VAL  | C-N-CA    | 5.76  | 129.07      | 120.31   |
| 1   | D     | 404 | THR  | N-CA-C    | 5.76  | 118.03      | 111.11   |
| 1   | K     | 46  | LEU  | CA-C-N    | 5.76  | 132.54      | 121.54   |
| 1   | K     | 46  | LEU  | C-N-CA    | 5.76  | 132.54      | 121.54   |
| 1   | Q     | 465 | ASP  | CA-C-O    | -5.76 | 113.86      | 119.51   |
| 1   | R     | 427 | LYS  | O-C-N     | -5.76 | 114.93      | 122.59   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | S     | 272 | MET  | CG-SD-CE    | -5.76 | 88.22       | 100.90   |
| 1   | S     | 297 | VAL  | N-CA-C      | -5.76 | 99.48       | 108.81   |
| 1   | R     | 83  | HIS  | CE1-NE2-CD2 | -5.76 | 103.24      | 109.00   |
| 1   | E     | 115 | VAL  | O-C-N       | -5.76 | 116.27      | 121.91   |
| 1   | E     | 266 | ILE  | CB-CG1-CD1  | -5.76 | 101.71      | 113.80   |
| 1   | E     | 461 | ASN  | CA-CB-CG    | -5.76 | 106.84      | 112.60   |
| 1   | R     | 127 | HIS  | CG-CD2-NE2  | 5.76  | 112.96      | 107.20   |
| 1   | H     | 125 | ASP  | N-CA-CB     | 5.75  | 120.22      | 110.49   |
| 1   | P     | 260 | LEU  | CA-C-N      | 5.75  | 128.46      | 120.63   |
| 1   | P     | 260 | LEU  | C-N-CA      | 5.75  | 128.46      | 120.63   |
| 1   | S     | 272 | MET  | CA-C-O      | -5.75 | 114.96      | 121.00   |
| 1   | Q     | 95  | GLY  | N-CA-C      | 5.75  | 118.09      | 111.36   |
| 1   | M     | 322 | ARG  | N-CA-C      | 5.75  | 119.32      | 111.39   |
| 1   | R     | 309 | GLN  | OE1-CD-NE2  | 5.75  | 128.35      | 122.60   |
| 1   | P     | 339 | VAL  | CB-CA-C     | 5.75  | 117.80      | 111.08   |
| 1   | R     | 461 | ASN  | O-C-N       | -5.75 | 114.92      | 122.39   |
| 1   | B     | 404 | THR  | N-CA-C      | 5.75  | 117.54      | 111.28   |
| 1   | B     | 471 | MET  | O-C-N       | -5.75 | 115.89      | 122.09   |
| 1   | G     | 62  | SER  | CB-CA-C     | -5.74 | 99.32       | 110.46   |
| 1   | H     | 39  | VAL  | CA-C-O      | -5.74 | 115.14      | 121.29   |
| 1   | I     | 315 | LYS  | CA-C-O      | 5.74  | 126.43      | 119.31   |
| 1   | P     | 90  | VAL  | N-CA-C      | 5.74  | 118.23      | 111.05   |
| 1   | F     | 488 | ASP  | CA-C-O      | -5.74 | 114.10      | 120.70   |
| 1   | O     | 434 | PRO  | CA-C-N      | 5.74  | 131.77      | 121.66   |
| 1   | O     | 434 | PRO  | C-N-CA      | 5.74  | 131.77      | 121.66   |
| 1   | P     | 493 | GLN  | CA-C-N      | 5.74  | 126.03      | 119.83   |
| 1   | P     | 493 | GLN  | C-N-CA      | 5.74  | 126.03      | 119.83   |
| 1   | B     | 235 | PRO  | N-CA-CB     | 5.74  | 109.22      | 103.48   |
| 1   | P     | 420 | ALA  | N-CA-C      | 5.74  | 117.23      | 110.97   |
| 1   | Q     | 325 | LYS  | N-CA-C      | 5.74  | 119.10      | 111.75   |
| 1   | A     | 190 | THR  | CB-CA-C     | -5.74 | 99.33       | 110.46   |
| 1   | R     | 40  | LYS  | CA-C-N      | 5.74  | 127.90      | 120.44   |
| 1   | R     | 40  | LYS  | C-N-CA      | 5.74  | 127.90      | 120.44   |
| 1   | O     | 179 | GLU  | CA-C-O      | 5.74  | 126.63      | 120.55   |
| 1   | O     | 520 | ALA  | CA-C-O      | 5.74  | 127.38      | 121.07   |
| 1   | L     | 243 | ASN  | OD1-CG-ND2  | -5.74 | 116.86      | 122.60   |
| 1   | N     | 365 | ASP  | N-CA-CB     | 5.74  | 118.43      | 110.17   |
| 1   | P     | 73  | ALA  | CA-C-N      | 5.74  | 128.24      | 120.38   |
| 1   | P     | 73  | ALA  | C-N-CA      | 5.74  | 128.24      | 120.38   |
| 1   | H     | 72  | GLY  | N-CA-C      | 5.73  | 119.58      | 112.64   |
| 1   | K     | 303 | GLY  | O-C-N       | -5.73 | 115.25      | 122.70   |
| 1   | L     | 306 | GLU  | CA-C-N      | 5.73  | 130.15      | 120.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | L     | 306 | GLU  | C-N-CA      | 5.73  | 130.15      | 120.29   |
| 1   | P     | 367 | MET  | O-C-N       | -5.73 | 116.85      | 123.33   |
| 1   | R     | 389 | ARG  | CA-C-O      | 5.73  | 125.72      | 119.24   |
| 1   | A     | 458 | LEU  | CA-C-O      | -5.73 | 114.81      | 120.82   |
| 1   | M     | 474 | ARG  | NE-CZ-NH1   | -5.73 | 115.77      | 121.50   |
| 1   | O     | 514 | LYS  | CA-C-O      | 5.73  | 126.62      | 120.55   |
| 1   | P     | 344 | ASP  | N-CA-CB     | -5.73 | 101.64      | 110.46   |
| 1   | P     | 500 | LYS  | N-CA-C      | -5.73 | 103.77      | 112.99   |
| 1   | R     | 363 | GLY  | O-C-N       | -5.73 | 115.25      | 122.70   |
| 1   | A     | 83  | HIS  | CE1-NE2-CD2 | -5.73 | 103.27      | 109.00   |
| 1   | C     | 243 | ASN  | CA-CB-CG    | -5.73 | 106.87      | 112.60   |
| 1   | B     | 400 | ASP  | N-CA-C      | 5.72  | 117.52      | 111.28   |
| 1   | D     | 103 | GLY  | CA-C-O      | 5.72  | 125.64      | 119.06   |
| 1   | F     | 114 | LEU  | N-CA-CB     | -5.72 | 101.70      | 110.12   |
| 1   | N     | 480 | GLU  | CA-C-N      | 5.72  | 128.22      | 120.38   |
| 1   | N     | 480 | GLU  | C-N-CA      | 5.72  | 128.22      | 120.38   |
| 1   | E     | 463 | GLY  | CA-C-O      | 5.72  | 125.38      | 118.86   |
| 1   | I     | 74  | THR  | N-CA-C      | 5.72  | 118.25      | 111.33   |
| 1   | N     | 119 | GLU  | CA-C-N      | 5.72  | 128.52      | 120.28   |
| 1   | N     | 119 | GLU  | C-N-CA      | 5.72  | 128.52      | 120.28   |
| 1   | P     | 295 | ALA  | N-CA-CB     | -5.72 | 101.19      | 109.83   |
| 1   | G     | 262 | ALA  | O-C-N       | -5.72 | 117.50      | 123.56   |
| 1   | A     | 322 | ARG  | N-CA-C      | 5.72  | 119.53      | 111.52   |
| 1   | H     | 127 | HIS  | ND1-CE1-NE2 | 5.72  | 114.12      | 108.40   |
| 1   | L     | 53  | ARG  | NE-CZ-NH2   | 5.72  | 124.35      | 119.20   |
| 1   | M     | 295 | ALA  | CB-CA-C     | -5.72 | 99.04       | 110.42   |
| 1   | Q     | 116 | LYS  | CA-C-O      | 5.72  | 127.36      | 121.07   |
| 1   | F     | 423 | ILE  | N-CA-CB     | 5.72  | 117.62      | 110.47   |
| 1   | R     | 388 | GLU  | N-CA-C      | 5.72  | 119.07      | 111.75   |
| 1   | B     | 200 | TRP  | N-CA-CB     | 5.72  | 118.37      | 109.97   |
| 1   | F     | 100 | THR  | CA-CB-CG2   | 5.72  | 120.22      | 110.50   |
| 1   | Q     | 255 | VAL  | O-C-N       | -5.71 | 116.45      | 122.68   |
| 1   | E     | 35  | ASN  | CA-C-N      | 5.71  | 128.25      | 120.77   |
| 1   | E     | 35  | ASN  | C-N-CA      | 5.71  | 128.25      | 120.77   |
| 1   | E     | 139 | GLU  | CB-CG-CD    | -5.71 | 102.89      | 112.60   |
| 1   | F     | 255 | VAL  | CA-C-O      | 5.71  | 127.47      | 121.59   |
| 1   | I     | 220 | THR  | CA-CB-OG1   | 5.71  | 118.17      | 109.60   |
| 1   | O     | 517 | THR  | CA-C-N      | 5.71  | 128.19      | 120.65   |
| 1   | O     | 517 | THR  | C-N-CA      | 5.71  | 128.19      | 120.65   |
| 1   | S     | 34  | ALA  | O-C-N       | 5.71  | 128.03      | 122.09   |
| 1   | E     | 323 | ALA  | CA-C-O      | 5.71  | 127.48      | 120.92   |
| 1   | K     | 127 | HIS  | CA-CB-CG    | 5.71  | 119.51      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 410 | LYS  | N-CA-CB    | -5.71 | 101.43      | 110.22   |
| 1   | D     | 119 | GLU  | N-CA-C     | 5.71  | 117.50      | 111.28   |
| 1   | M     | 365 | ASP  | O-C-N      | -5.71 | 115.52      | 122.82   |
| 1   | M     | 487 | ILE  | CB-CA-C    | -5.71 | 103.57      | 110.99   |
| 1   | Q     | 405 | VAL  | O-C-N      | -5.71 | 116.33      | 121.87   |
| 1   | R     | 243 | ASN  | CB-CA-C    | -5.71 | 103.30      | 112.09   |
| 1   | F     | 470 | LEU  | N-CA-C     | 5.71  | 117.17      | 111.07   |
| 1   | F     | 380 | SER  | CA-C-N     | -5.70 | 115.19      | 123.06   |
| 1   | F     | 380 | SER  | C-N-CA     | -5.70 | 115.19      | 123.06   |
| 1   | L     | 409 | ILE  | CA-C-N     | 5.70  | 128.49      | 120.28   |
| 1   | L     | 409 | ILE  | C-N-CA     | 5.70  | 128.49      | 120.28   |
| 1   | N     | 457 | ILE  | CA-C-N     | 5.70  | 127.85      | 120.44   |
| 1   | N     | 457 | ILE  | C-N-CA     | 5.70  | 127.85      | 120.44   |
| 1   | C     | 465 | ASP  | CA-C-N     | 5.70  | 125.17      | 119.24   |
| 1   | C     | 465 | ASP  | C-N-CA     | 5.70  | 125.17      | 119.24   |
| 1   | G     | 531 | SER  | CA-C-N     | 5.70  | 131.96      | 121.70   |
| 1   | G     | 531 | SER  | C-N-CA     | 5.70  | 131.96      | 121.70   |
| 1   | H     | 340 | VAL  | N-CA-C     | 5.70  | 116.59      | 107.98   |
| 1   | M     | 323 | ALA  | O-C-N      | -5.70 | 116.29      | 123.01   |
| 1   | F     | 138 | ALA  | CA-C-N     | 5.70  | 127.84      | 120.44   |
| 1   | F     | 138 | ALA  | C-N-CA     | 5.70  | 127.84      | 120.44   |
| 1   | F     | 396 | ARG  | NE-CZ-NH2  | 5.70  | 124.33      | 119.20   |
| 1   | I     | 371 | GLU  | N-CA-CB    | 5.70  | 118.37      | 110.17   |
| 1   | L     | 183 | ASP  | O-C-N      | 5.70  | 127.94      | 122.07   |
| 1   | C     | 185 | VAL  | CA-CB-CG1  | 5.70  | 120.08      | 110.40   |
| 1   | H     | 104 | THR  | N-CA-C     | 5.70  | 117.57      | 111.36   |
| 1   | H     | 485 | TYR  | CG-CD1-CE1 | -5.70 | 112.66      | 121.20   |
| 1   | L     | 304 | ILE  | O-C-N      | -5.70 | 116.92      | 123.07   |
| 1   | P     | 80  | ASP  | CA-CB-CG   | -5.70 | 106.90      | 112.60   |
| 1   | A     | 202 | VAL  | N-CA-CB    | -5.69 | 105.58      | 112.35   |
| 1   | E     | 441 | GLN  | CG-CD-NE2  | 5.69  | 124.94      | 116.40   |
| 1   | K     | 134 | GLY  | O-C-N      | -5.69 | 115.30      | 122.70   |
| 1   | L     | 342 | ASN  | O-C-N      | -5.69 | 115.61      | 123.12   |
| 1   | A     | 220 | THR  | O-C-N      | -5.69 | 116.56      | 123.16   |
| 1   | D     | 101 | ALA  | O-C-N      | -5.69 | 114.58      | 122.20   |
| 1   | H     | 342 | ASN  | OD1-CG-ND2 | -5.69 | 116.91      | 122.60   |
| 1   | R     | 458 | LEU  | CA-C-N     | 5.69  | 127.73      | 120.56   |
| 1   | R     | 458 | LEU  | C-N-CA     | 5.69  | 127.73      | 120.56   |
| 1   | M     | 243 | ASN  | CA-C-O     | -5.69 | 115.06      | 122.45   |
| 1   | O     | 345 | GLU  | O-C-N      | -5.69 | 116.03      | 122.23   |
| 1   | R     | 148 | GLU  | CA-C-N     | 5.69  | 132.41      | 121.54   |
| 1   | R     | 148 | GLU  | C-N-CA     | 5.69  | 132.41      | 121.54   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | R     | 528 | ASP  | CA-CB-CG  | -5.69 | 106.91      | 112.60   |
| 1   | C     | 88  | LEU  | N-CA-C    | -5.69 | 105.16      | 111.36   |
| 1   | D     | 58  | MET  | CA-C-O    | 5.69  | 126.74      | 120.71   |
| 1   | F     | 255 | VAL  | CA-C-N    | 5.69  | 130.23      | 122.84   |
| 1   | F     | 255 | VAL  | C-N-CA    | 5.69  | 130.23      | 122.84   |
| 1   | K     | 342 | ASN  | N-CA-CB   | -5.69 | 102.03      | 110.90   |
| 1   | L     | 114 | LEU  | CA-C-N    | 5.69  | 127.73      | 120.56   |
| 1   | L     | 114 | LEU  | C-N-CA    | 5.69  | 127.73      | 120.56   |
| 1   | R     | 118 | ALA  | CA-C-N    | 5.69  | 127.90      | 120.28   |
| 1   | R     | 118 | ALA  | C-N-CA    | 5.69  | 127.90      | 120.28   |
| 1   | R     | 232 | VAL  | CB-CA-C   | -5.69 | 103.86      | 110.91   |
| 1   | E     | 281 | ASN  | CA-CB-CG  | -5.68 | 106.92      | 112.60   |
| 1   | F     | 453 | SER  | O-C-N     | -5.68 | 116.09      | 122.12   |
| 1   | N     | 32  | VAL  | N-CA-C    | 5.68  | 119.02      | 111.17   |
| 1   | Q     | 449 | ASN  | CA-CB-CG  | -5.68 | 106.92      | 112.60   |
| 1   | A     | 241 | LEU  | O-C-N     | -5.68 | 116.58      | 123.29   |
| 1   | I     | 512 | ALA  | CA-C-O    | -5.68 | 114.85      | 120.82   |
| 1   | M     | 272 | MET  | O-C-N     | 5.68  | 128.16      | 122.08   |
| 1   | O     | 69  | THR  | O-C-N     | -5.68 | 116.91      | 122.99   |
| 1   | M     | 448 | ALA  | CA-C-O    | 5.68  | 126.55      | 120.70   |
| 1   | D     | 209 | ILE  | O-C-N     | -5.68 | 116.91      | 122.99   |
| 1   | E     | 359 | GLU  | O-C-N     | -5.68 | 116.68      | 123.27   |
| 1   | N     | 297 | VAL  | O-C-N     | -5.68 | 116.75      | 123.05   |
| 1   | E     | 77  | ASP  | O-C-N     | -5.68 | 116.22      | 122.07   |
| 1   | L     | 515 | ALA  | N-CA-C    | -5.68 | 104.78      | 110.97   |
| 1   | S     | 490 | TYR  | CB-CG-CD2 | -5.68 | 112.28      | 120.80   |
| 1   | A     | 357 | ILE  | CA-C-O    | 5.68  | 127.19      | 120.72   |
| 1   | B     | 98  | GLU  | N-CA-C    | 5.68  | 122.89      | 110.80   |
| 1   | C     | 40  | LYS  | CA-C-N    | 5.68  | 128.20      | 120.54   |
| 1   | C     | 40  | LYS  | C-N-CA    | 5.68  | 128.20      | 120.54   |
| 1   | F     | 372 | GLY  | CA-C-O    | 5.68  | 126.65      | 119.72   |
| 1   | L     | 146 | ILE  | N-CA-C    | -5.68 | 105.56      | 111.58   |
| 1   | N     | 98  | GLU  | N-CA-C    | 5.68  | 117.65      | 110.33   |
| 1   | D     | 503 | ILE  | O-C-N     | -5.67 | 116.74      | 123.04   |
| 1   | E     | 335 | THR  | CA-C-O    | 5.67  | 125.99      | 119.35   |
| 1   | O     | 98  | GLU  | N-CA-CB   | 5.67  | 118.92      | 110.29   |
| 1   | O     | 459 | ILE  | CA-C-N    | 5.67  | 130.21      | 121.19   |
| 1   | O     | 459 | ILE  | C-N-CA    | 5.67  | 130.21      | 121.19   |
| 1   | Q     | 77  | ASP  | CA-CB-CG  | -5.67 | 106.93      | 112.60   |
| 1   | A     | 109 | ILE  | O-C-N     | -5.67 | 115.83      | 121.96   |
| 1   | C     | 68  | ILE  | N-CA-C    | -5.67 | 100.23      | 108.17   |
| 1   | C     | 200 | TRP  | N-CA-C    | 5.67  | 118.55      | 110.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 257 | LYS  | CG-CD-CE    | 5.67  | 124.35      | 111.30   |
| 1   | F     | 187 | LYS  | CA-C-N      | 5.67  | 127.88      | 120.28   |
| 1   | F     | 187 | LYS  | C-N-CA      | 5.67  | 127.88      | 120.28   |
| 1   | F     | 442 | LEU  | CB-CA-C     | -5.67 | 101.38      | 110.79   |
| 1   | G     | 316 | GLY  | N-CA-C      | -5.67 | 107.16      | 115.72   |
| 1   | H     | 330 | LYS  | N-CA-C      | 5.67  | 118.23      | 111.71   |
| 1   | F     | 525 | ARG  | O-C-N       | -5.67 | 115.30      | 122.27   |
| 1   | H     | 162 | ARG  | CB-CG-CD    | 5.67  | 124.34      | 111.30   |
| 1   | H     | 246 | ILE  | N-CA-C      | 5.67  | 117.79      | 109.63   |
| 1   | K     | 374 | LYS  | N-CA-C      | 5.67  | 117.91      | 111.11   |
| 1   | N     | 249 | ILE  | CA-C-N      | 5.67  | 128.44      | 120.28   |
| 1   | N     | 249 | ILE  | C-N-CA      | 5.67  | 128.44      | 120.28   |
| 1   | G     | 342 | ASN  | CA-C-N      | 5.67  | 129.91      | 120.62   |
| 1   | G     | 342 | ASN  | C-N-CA      | 5.67  | 129.91      | 120.62   |
| 1   | I     | 295 | ALA  | CA-C-O      | -5.67 | 114.01      | 120.58   |
| 1   | C     | 509 | LYS  | CB-CG-CD    | 5.66  | 124.32      | 111.30   |
| 1   | K     | 481 | ASN  | CA-CB-CG    | -5.66 | 106.94      | 112.60   |
| 1   | O     | 192 | VAL  | CA-C-O      | 5.66  | 125.87      | 119.92   |
| 1   | C     | 525 | ARG  | N-CA-C      | 5.66  | 118.39      | 111.82   |
| 1   | K     | 282 | LEU  | CA-C-O      | 5.66  | 126.42      | 120.42   |
| 1   | N     | 500 | LYS  | N-CA-C      | -5.66 | 104.16      | 113.50   |
| 1   | P     | 164 | ILE  | CA-C-N      | 5.66  | 128.14      | 120.44   |
| 1   | P     | 164 | ILE  | C-N-CA      | 5.66  | 128.14      | 120.44   |
| 1   | A     | 370 | VAL  | O-C-N       | -5.66 | 115.50      | 122.57   |
| 1   | E     | 75  | ILE  | CA-C-O      | 5.66  | 126.88      | 120.03   |
| 1   | K     | 183 | ASP  | CA-C-N      | 5.66  | 128.18      | 120.77   |
| 1   | K     | 183 | ASP  | C-N-CA      | 5.66  | 128.18      | 120.77   |
| 1   | K     | 424 | GLU  | CB-CG-CD    | 5.66  | 122.22      | 112.60   |
| 1   | G     | 477 | HIS  | CA-CB-CG    | 5.66  | 119.46      | 113.80   |
| 1   | K     | 402 | LEU  | CB-CA-C     | -5.66 | 102.25      | 110.96   |
| 1   | R     | 151 | GLN  | CB-CG-CD    | 5.66  | 122.22      | 112.60   |
| 1   | C     | 234 | HIS  | ND1-CE1-NE2 | 5.66  | 114.06      | 108.40   |
| 1   | S     | 35  | ASN  | OD1-CG-ND2  | -5.66 | 116.94      | 122.60   |
| 1   | A     | 90  | VAL  | O-C-N       | -5.65 | 116.16      | 121.87   |
| 1   | A     | 116 | LYS  | N-CA-CB     | -5.65 | 100.94      | 110.49   |
| 1   | H     | 448 | ALA  | CA-C-N      | 5.65  | 127.86      | 120.28   |
| 1   | H     | 448 | ALA  | C-N-CA      | 5.65  | 127.86      | 120.28   |
| 1   | L     | 405 | VAL  | CA-CB-CG1   | 5.65  | 120.01      | 110.40   |
| 1   | A     | 91  | GLN  | CA-C-N      | 5.65  | 128.45      | 120.42   |
| 1   | A     | 91  | GLN  | C-N-CA      | 5.65  | 128.45      | 120.42   |
| 1   | D     | 87  | LYS  | CA-C-N      | 5.65  | 128.32      | 120.29   |
| 1   | D     | 87  | LYS  | C-N-CA      | 5.65  | 128.32      | 120.29   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 453 | SER  | CA-C-N     | 5.65  | 128.17      | 120.54   |
| 1   | H     | 453 | SER  | C-N-CA     | 5.65  | 128.17      | 120.54   |
| 1   | L     | 245 | LYS  | CA-C-N     | 5.65  | 128.29      | 120.49   |
| 1   | L     | 245 | LYS  | C-N-CA     | 5.65  | 128.29      | 120.49   |
| 1   | P     | 497 | MET  | CA-C-N     | 5.65  | 128.17      | 120.54   |
| 1   | P     | 497 | MET  | C-N-CA     | 5.65  | 128.17      | 120.54   |
| 1   | R     | 72  | GLY  | CA-C-N     | 5.65  | 128.65      | 120.79   |
| 1   | R     | 72  | GLY  | C-N-CA     | 5.65  | 128.65      | 120.79   |
| 1   | R     | 500 | LYS  | N-CA-C     | -5.65 | 103.89      | 112.99   |
| 1   | G     | 234 | HIS  | CA-C-N     | 5.65  | 126.90      | 119.84   |
| 1   | G     | 234 | HIS  | C-N-CA     | 5.65  | 126.90      | 119.84   |
| 1   | D     | 120 | ASP  | CA-C-N     | 5.65  | 128.31      | 120.29   |
| 1   | D     | 120 | ASP  | C-N-CA     | 5.65  | 128.31      | 120.29   |
| 1   | D     | 182 | ALA  | CA-C-N     | 5.65  | 127.78      | 120.44   |
| 1   | D     | 182 | ALA  | C-N-CA     | 5.65  | 127.78      | 120.44   |
| 1   | F     | 319 | ALA  | CA-C-N     | 5.65  | 130.79      | 122.94   |
| 1   | F     | 319 | ALA  | C-N-CA     | 5.65  | 130.79      | 122.94   |
| 1   | F     | 459 | ILE  | N-CA-C     | 5.65  | 115.78      | 110.30   |
| 1   | I     | 39  | VAL  | N-CA-CB    | 5.65  | 116.77      | 110.62   |
| 1   | K     | 258 | PRO  | O-C-N      | 5.65  | 128.55      | 122.17   |
| 1   | A     | 61  | ASP  | CA-C-N     | 5.64  | 127.84      | 120.28   |
| 1   | A     | 61  | ASP  | C-N-CA     | 5.64  | 127.84      | 120.28   |
| 1   | C     | 221 | GLN  | OE1-CD-NE2 | -5.64 | 116.95      | 122.60   |
| 1   | D     | 357 | ILE  | N-CA-C     | -5.64 | 100.34      | 108.53   |
| 1   | H     | 446 | ALA  | CA-C-N     | 5.64  | 128.11      | 120.38   |
| 1   | H     | 446 | ALA  | C-N-CA     | 5.64  | 128.11      | 120.38   |
| 1   | I     | 120 | ASP  | O-C-N      | -5.64 | 115.61      | 122.22   |
| 1   | I     | 462 | ALA  | O-C-N      | -5.64 | 114.73      | 122.46   |
| 1   | L     | 148 | GLU  | O-C-N      | -5.64 | 115.08      | 122.59   |
| 1   | L     | 210 | VAL  | O-C-N      | -5.64 | 117.08      | 123.18   |
| 1   | L     | 458 | LEU  | N-CA-C     | 5.64  | 117.11      | 111.07   |
| 1   | P     | 60  | VAL  | CA-C-N     | 5.64  | 129.27      | 120.75   |
| 1   | P     | 60  | VAL  | C-N-CA     | 5.64  | 129.27      | 120.75   |
| 1   | R     | 147 | GLN  | O-C-N      | -5.64 | 116.16      | 122.03   |
| 1   | S     | 212 | LYS  | O-C-N      | -5.64 | 116.34      | 123.17   |
| 1   | D     | 247 | ALA  | N-CA-C     | 5.64  | 119.49      | 107.70   |
| 1   | H     | 142 | ALA  | N-CA-C     | 5.64  | 118.16      | 111.33   |
| 1   | L     | 82  | GLN  | CB-CA-C    | -5.64 | 100.33      | 109.13   |
| 1   | L     | 439 | LYS  | O-C-N      | -5.64 | 115.72      | 122.15   |
| 1   | M     | 72  | GLY  | CA-C-N     | 5.64  | 130.16      | 121.19   |
| 1   | M     | 72  | GLY  | C-N-CA     | 5.64  | 130.16      | 121.19   |
| 1   | Q     | 92  | ILE  | N-CA-C     | -5.64 | 104.85      | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | R     | 39  | VAL  | CB-CA-C    | -5.64 | 104.75      | 111.97   |
| 1   | B     | 356 | LEU  | CB-CA-C    | -5.64 | 100.36      | 109.89   |
| 1   | D     | 191 | GLN  | N-CA-C     | 5.64  | 117.51      | 111.36   |
| 1   | D     | 384 | ARG  | N-CA-CB    | 5.64  | 120.63      | 111.21   |
| 1   | K     | 253 | LEU  | N-CA-CB    | 5.64  | 120.85      | 111.49   |
| 1   | M     | 399 | ARG  | O-C-N      | -5.64 | 116.26      | 122.07   |
| 1   | O     | 426 | ALA  | CA-C-O     | -5.64 | 114.97      | 120.89   |
| 1   | A     | 379 | ILE  | CA-C-O     | 5.64  | 127.42      | 121.67   |
| 1   | L     | 531 | SER  | CA-C-N     | 5.64  | 131.85      | 121.70   |
| 1   | L     | 531 | SER  | C-N-CA     | 5.64  | 131.85      | 121.70   |
| 1   | M     | 205 | ASP  | N-CA-C     | 5.64  | 119.67      | 112.34   |
| 1   | M     | 413 | ARG  | NH1-CZ-NH2 | -5.64 | 111.97      | 119.30   |
| 1   | N     | 484 | TRP  | CA-CB-CG   | 5.64  | 124.31      | 113.60   |
| 1   | Q     | 109 | ILE  | CB-CA-C    | 5.64  | 119.10      | 111.88   |
| 1   | Q     | 141 | VAL  | O-C-N      | -5.64 | 116.30      | 121.94   |
| 1   | L     | 326 | SER  | N-CA-C     | 5.64  | 118.97      | 111.75   |
| 1   | M     | 413 | ARG  | O-C-N      | -5.64 | 115.90      | 123.23   |
| 1   | M     | 517 | THR  | OG1-CB-CG2 | -5.64 | 98.03       | 109.30   |
| 1   | B     | 368 | VAL  | N-CA-CB    | 5.63  | 118.34      | 110.56   |
| 1   | C     | 471 | MET  | N-CA-CB    | 5.63  | 118.18      | 110.01   |
| 1   | C     | 480 | GLU  | O-C-N      | -5.63 | 114.69      | 122.46   |
| 1   | H     | 237 | MET  | CA-C-N     | 5.63  | 126.88      | 119.84   |
| 1   | H     | 237 | MET  | C-N-CA     | 5.63  | 126.88      | 119.84   |
| 1   | G     | 401 | ALA  | N-CA-C     | 5.63  | 117.42      | 111.28   |
| 1   | P     | 65  | ASP  | O-C-N      | -5.63 | 115.94      | 122.87   |
| 1   | P     | 69  | THR  | N-CA-C     | 5.63  | 115.98      | 108.38   |
| 1   | I     | 79  | MET  | N-CA-C     | 5.63  | 118.61      | 110.28   |
| 1   | P     | 187 | LYS  | N-CA-C     | 5.63  | 117.42      | 111.28   |
| 1   | Q     | 336 | GLY  | CA-C-N     | 5.63  | 128.75      | 122.55   |
| 1   | Q     | 336 | GLY  | C-N-CA     | 5.63  | 128.75      | 122.55   |
| 1   | S     | 311 | TYR  | CB-CG-CD2  | 5.63  | 129.25      | 120.80   |
| 1   | C     | 32  | VAL  | N-CA-C     | 5.63  | 118.94      | 111.17   |
| 1   | F     | 429 | LEU  | CA-C-O     | 5.63  | 126.49      | 120.24   |
| 1   | H     | 458 | LEU  | O-C-N      | -5.63 | 116.27      | 122.07   |
| 1   | M     | 475 | SER  | N-CA-C     | -5.63 | 104.62      | 112.45   |
| 1   | D     | 283 | ILE  | CA-CB-CG1  | 5.63  | 119.97      | 110.40   |
| 1   | G     | 143 | LEU  | O-C-N      | -5.63 | 115.95      | 122.03   |
| 1   | G     | 459 | ILE  | CA-C-N     | 5.63  | 130.14      | 121.19   |
| 1   | G     | 459 | ILE  | C-N-CA     | 5.63  | 130.14      | 121.19   |
| 1   | N     | 101 | ALA  | CA-C-O     | 5.63  | 125.39      | 119.03   |
| 1   | D     | 239 | LYS  | O-C-N      | 5.62  | 128.16      | 122.09   |
| 1   | H     | 201 | TYR  | CA-CB-CG   | -5.62 | 103.78      | 113.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | S     | 211 | LYS  | N-CA-C    | 5.62  | 118.62      | 109.06   |
| 1   | C     | 28  | GLY  | CA-C-N    | 5.62  | 128.08      | 120.38   |
| 1   | C     | 28  | GLY  | C-N-CA    | 5.62  | 128.08      | 120.38   |
| 1   | H     | 471 | MET  | CA-C-O    | -5.62 | 114.92      | 120.82   |
| 1   | P     | 144 | GLN  | CA-C-N    | 5.62  | 130.11      | 120.72   |
| 1   | P     | 144 | GLN  | C-N-CA    | 5.62  | 130.11      | 120.72   |
| 1   | R     | 526 | ILE  | N-CA-C    | 5.62  | 116.47      | 107.98   |
| 1   | S     | 469 | LEU  | CA-C-N    | 5.62  | 127.75      | 120.44   |
| 1   | S     | 469 | LEU  | C-N-CA    | 5.62  | 127.75      | 120.44   |
| 1   | S     | 526 | ILE  | N-CA-C    | 5.62  | 115.66      | 108.12   |
| 1   | H     | 51  | GLY  | N-CA-C    | 5.62  | 123.81      | 112.34   |
| 1   | I     | 162 | ARG  | CD-NE-CZ  | 5.62  | 132.27      | 124.40   |
| 1   | N     | 269 | PRO  | N-CD-CG   | 5.62  | 111.63      | 103.20   |
| 1   | O     | 203 | ASP  | CA-C-N    | 5.62  | 128.38      | 120.28   |
| 1   | O     | 203 | ASP  | C-N-CA    | 5.62  | 128.38      | 120.28   |
| 1   | A     | 476 | THR  | CA-C-N    | 5.62  | 130.30      | 121.08   |
| 1   | A     | 476 | THR  | C-N-CA    | 5.62  | 130.30      | 121.08   |
| 1   | E     | 413 | ARG  | NE-CZ-NH2 | 5.62  | 124.26      | 119.20   |
| 1   | P     | 38  | ALA  | N-CA-C    | 5.62  | 117.85      | 111.11   |
| 1   | C     | 453 | SER  | CA-C-N    | 5.62  | 127.74      | 120.44   |
| 1   | C     | 453 | SER  | C-N-CA    | 5.62  | 127.74      | 120.44   |
| 1   | G     | 46  | LEU  | CA-C-N    | 5.62  | 132.27      | 121.54   |
| 1   | G     | 46  | LEU  | C-N-CA    | 5.62  | 132.27      | 121.54   |
| 1   | G     | 63  | LEU  | N-CA-C    | 5.62  | 117.48      | 111.36   |
| 1   | G     | 422 | GLU  | O-C-N     | -5.62 | 115.12      | 122.59   |
| 1   | I     | 448 | ALA  | CA-C-N    | 5.62  | 127.81      | 120.28   |
| 1   | I     | 448 | ALA  | C-N-CA    | 5.62  | 127.81      | 120.28   |
| 1   | M     | 507 | LEU  | N-CA-C    | -5.62 | 105.54      | 112.90   |
| 1   | P     | 196 | ARG  | CG-CD-NE  | -5.62 | 99.64       | 112.00   |
| 1   | R     | 106 | THR  | CA-C-N    | 5.62  | 129.25      | 120.82   |
| 1   | R     | 106 | THR  | C-N-CA    | 5.62  | 129.25      | 120.82   |
| 1   | K     | 120 | ASP  | N-CA-CB   | -5.62 | 100.77      | 110.32   |
| 1   | K     | 247 | ALA  | CA-C-N    | 5.62  | 131.24      | 122.26   |
| 1   | K     | 247 | ALA  | C-N-CA    | 5.62  | 131.24      | 122.26   |
| 1   | K     | 374 | LYS  | O-C-N     | -5.62 | 116.25      | 122.09   |
| 1   | N     | 475 | SER  | N-CA-CB   | 5.62  | 118.89      | 110.19   |
| 1   | Q     | 287 | VAL  | CA-C-O    | 5.62  | 127.12      | 121.17   |
| 1   | C     | 179 | GLU  | CB-CG-CD  | -5.61 | 103.06      | 112.60   |
| 1   | O     | 401 | ALA  | CA-C-N    | 5.61  | 128.06      | 120.65   |
| 1   | O     | 401 | ALA  | C-N-CA    | 5.61  | 128.06      | 120.65   |
| 1   | A     | 188 | ALA  | N-CA-C    | 5.61  | 117.40      | 111.28   |
| 1   | A     | 262 | ALA  | CA-C-O    | 5.61  | 127.27      | 121.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 263 | GLU  | CA-C-N     | 5.61  | 128.02      | 120.50   |
| 1   | H     | 263 | GLU  | C-N-CA     | 5.61  | 128.02      | 120.50   |
| 1   | N     | 299 | ILE  | N-CA-C     | -5.61 | 100.40      | 108.48   |
| 1   | A     | 190 | THR  | N-CA-CB    | 5.61  | 119.00      | 110.14   |
| 1   | G     | 531 | SER  | CA-C-O     | 5.61  | 127.03      | 120.80   |
| 1   | D     | 68  | ILE  | N-CA-C     | -5.61 | 100.32      | 108.17   |
| 1   | E     | 479 | ASN  | CA-C-N     | 5.61  | 129.57      | 120.60   |
| 1   | E     | 479 | ASN  | C-N-CA     | 5.61  | 129.57      | 120.60   |
| 1   | I     | 343 | ILE  | CA-C-O     | 5.61  | 126.57      | 120.57   |
| 1   | M     | 255 | VAL  | CA-C-N     | -5.61 | 113.79      | 122.09   |
| 1   | M     | 255 | VAL  | C-N-CA     | -5.61 | 113.79      | 122.09   |
| 1   | Q     | 402 | LEU  | CB-CA-C    | -5.61 | 102.26      | 110.95   |
| 1   | R     | 435 | GLN  | OE1-CD-NE2 | -5.61 | 116.99      | 122.60   |
| 1   | L     | 335 | THR  | CA-C-O     | 5.61  | 125.99      | 119.32   |
| 1   | Q     | 240 | ARG  | O-C-N      | -5.61 | 116.71      | 123.27   |
| 1   | F     | 33  | ARG  | NE-CZ-NH2  | -5.60 | 114.16      | 119.20   |
| 1   | B     | 405 | VAL  | N-CA-C     | 5.60  | 116.34      | 110.62   |
| 1   | D     | 40  | LYS  | CA-C-N     | 5.60  | 127.72      | 120.44   |
| 1   | D     | 40  | LYS  | C-N-CA     | 5.60  | 127.72      | 120.44   |
| 1   | E     | 341 | SER  | CB-CA-C    | -5.60 | 99.91       | 110.67   |
| 1   | F     | 338 | ARG  | CD-NE-CZ   | 5.60  | 132.24      | 124.40   |
| 1   | N     | 270 | THR  | CA-CB-CG2  | 5.60  | 120.03      | 110.50   |
| 1   | Q     | 405 | VAL  | CA-C-O     | 5.60  | 126.78      | 120.95   |
| 1   | I     | 474 | ARG  | CA-C-O     | 5.60  | 126.16      | 119.10   |
| 1   | Q     | 423 | ILE  | CA-CB-CG1  | 5.60  | 119.92      | 110.40   |
| 1   | E     | 137 | LYS  | CA-C-O     | 5.60  | 126.48      | 120.55   |
| 1   | G     | 387 | LEU  | O-C-N      | -5.60 | 115.15      | 122.59   |
| 1   | G     | 453 | SER  | CB-CA-C    | -5.60 | 101.17      | 110.68   |
| 1   | M     | 147 | GLN  | OE1-CD-NE2 | 5.60  | 128.20      | 122.60   |
| 1   | N     | 120 | ASP  | O-C-N      | -5.60 | 115.67      | 122.22   |
| 1   | G     | 65  | ASP  | N-CA-C     | 5.59  | 118.18      | 110.35   |
| 1   | O     | 237 | MET  | N-CA-CB    | -5.59 | 101.18      | 110.02   |
| 1   | R     | 447 | TYR  | CA-C-N     | 5.59  | 128.05      | 120.44   |
| 1   | R     | 447 | TYR  | C-N-CA     | 5.59  | 128.05      | 120.44   |
| 1   | S     | 299 | ILE  | O-C-N      | -5.59 | 117.14      | 123.18   |
| 1   | O     | 381 | ILE  | N-CA-C     | -5.59 | 100.43      | 108.48   |
| 1   | H     | 388 | GLU  | N-CA-C     | 5.59  | 118.91      | 111.75   |
| 1   | M     | 227 | VAL  | CB-CA-C    | -5.59 | 102.87      | 110.42   |
| 1   | O     | 264 | ILE  | N-CA-C     | 5.59  | 118.62      | 109.78   |
| 1   | S     | 97  | ASP  | CA-CB-CG   | -5.59 | 107.01      | 112.60   |
| 1   | B     | 361 | LYS  | CA-C-O     | 5.59  | 126.35      | 120.54   |
| 1   | F     | 459 | ILE  | CA-C-N     | 5.59  | 130.08      | 121.19   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 459 | ILE  | C-N-CA    | 5.59  | 130.08      | 121.19   |
| 1   | R     | 242 | GLU  | CA-C-N    | 5.59  | 130.90      | 122.68   |
| 1   | R     | 242 | GLU  | C-N-CA    | 5.59  | 130.90      | 122.68   |
| 1   | S     | 276 | LEU  | CB-CA-C   | -5.59 | 98.63       | 110.31   |
| 1   | C     | 432 | TYR  | N-CA-CB   | -5.59 | 101.97      | 110.07   |
| 1   | G     | 170 | SER  | O-C-N     | -5.59 | 115.12      | 122.39   |
| 1   | K     | 237 | MET  | CA-C-O    | -5.59 | 114.72      | 120.87   |
| 1   | A     | 450 | ALA  | O-C-N     | -5.59 | 116.20      | 122.12   |
| 1   | L     | 31  | ALA  | CA-C-N    | 5.59  | 129.78      | 120.62   |
| 1   | L     | 31  | ALA  | C-N-CA    | 5.59  | 129.78      | 120.62   |
| 1   | O     | 120 | ASP  | N-CA-CB   | -5.59 | 100.82      | 110.32   |
| 1   | R     | 259 | GLU  | CA-C-N    | 5.59  | 127.77      | 120.28   |
| 1   | R     | 259 | GLU  | C-N-CA    | 5.59  | 127.77      | 120.28   |
| 1   | R     | 290 | ILE  | N-CA-C    | -5.59 | 105.66      | 111.58   |
| 1   | Q     | 506 | ALA  | N-CA-C    | 5.58  | 119.57      | 112.87   |
| 1   | I     | 59  | LEU  | N-CA-C    | -5.58 | 99.18       | 108.34   |
| 1   | O     | 443 | ALA  | CA-C-N    | 5.58  | 127.59      | 120.56   |
| 1   | O     | 443 | ALA  | C-N-CA    | 5.58  | 127.59      | 120.56   |
| 1   | Q     | 135 | TYR  | CB-CG-CD2 | 5.58  | 129.18      | 120.80   |
| 1   | E     | 124 | LYS  | N-CA-C    | 5.58  | 119.79      | 113.15   |
| 1   | G     | 83  | HIS  | CA-C-N    | 5.58  | 125.05      | 119.24   |
| 1   | G     | 83  | HIS  | C-N-CA    | 5.58  | 125.05      | 119.24   |
| 1   | L     | 458 | LEU  | O-C-N     | 5.58  | 127.82      | 122.07   |
| 1   | L     | 484 | TRP  | CA-CB-CG  | 5.58  | 124.21      | 113.60   |
| 1   | O     | 299 | ILE  | CA-CB-CG1 | 5.58  | 119.89      | 110.40   |
| 1   | F     | 141 | VAL  | CA-C-N    | 5.58  | 128.02      | 120.38   |
| 1   | F     | 141 | VAL  | C-N-CA    | 5.58  | 128.02      | 120.38   |
| 1   | P     | 237 | MET  | CG-SD-CE  | -5.58 | 88.63       | 100.90   |
| 1   | Q     | 336 | GLY  | CA-C-O    | 5.58  | 125.93      | 119.13   |
| 1   | A     | 396 | ARG  | CA-C-N    | 5.58  | 128.02      | 120.38   |
| 1   | A     | 396 | ARG  | C-N-CA    | 5.58  | 128.02      | 120.38   |
| 1   | R     | 484 | TRP  | O-C-N     | 5.58  | 129.21      | 122.35   |
| 1   | S     | 56  | ASP  | CA-C-N    | 5.58  | 131.01      | 122.93   |
| 1   | S     | 56  | ASP  | C-N-CA    | 5.58  | 131.01      | 122.93   |
| 1   | B     | 427 | LYS  | CA-C-N    | 5.57  | 127.75      | 120.28   |
| 1   | B     | 427 | LYS  | C-N-CA    | 5.57  | 127.75      | 120.28   |
| 1   | D     | 327 | ASP  | N-CA-C    | -5.57 | 106.64      | 113.50   |
| 1   | I     | 514 | LYS  | CA-C-O    | -5.57 | 114.97      | 120.82   |
| 1   | K     | 55  | MET  | CA-C-O    | 5.57  | 126.99      | 120.80   |
| 1   | P     | 395 | GLU  | CA-C-N    | 5.57  | 128.01      | 120.65   |
| 1   | P     | 395 | GLU  | C-N-CA    | 5.57  | 128.01      | 120.65   |
| 1   | R     | 147 | GLN  | CG-CD-NE2 | 5.57  | 124.76      | 116.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 372 | GLY  | CA-C-N     | 5.57  | 129.16      | 120.75   |
| 1   | M     | 372 | GLY  | C-N-CA     | 5.57  | 129.16      | 120.75   |
| 1   | B     | 311 | TYR  | CA-CB-CG   | -5.57 | 103.87      | 113.90   |
| 1   | D     | 123 | TYR  | CA-C-O     | 5.57  | 126.45      | 120.55   |
| 1   | F     | 379 | ILE  | CA-C-O     | 5.57  | 127.35      | 121.67   |
| 1   | H     | 325 | LYS  | N-CA-C     | 5.57  | 118.88      | 111.75   |
| 1   | K     | 417 | GLY  | CA-C-O     | 5.57  | 127.69      | 121.67   |
| 1   | Q     | 500 | LYS  | CA-C-O     | 5.57  | 124.93      | 119.08   |
| 1   | S     | 184 | ILE  | N-CA-C     | 5.57  | 115.70      | 110.30   |
| 1   | A     | 316 | GLY  | O-C-N      | -5.57 | 116.31      | 122.55   |
| 1   | K     | 98  | GLU  | N-CA-C     | 5.57  | 118.76      | 110.52   |
| 1   | P     | 325 | LYS  | O-C-N      | 5.57  | 128.55      | 122.20   |
| 1   | B     | 333 | ARG  | NE-CZ-NH1  | 5.57  | 127.07      | 121.50   |
| 1   | D     | 223 | VAL  | O-C-N      | -5.57 | 117.33      | 123.18   |
| 1   | N     | 203 | ASP  | CA-C-N     | 5.57  | 128.29      | 120.28   |
| 1   | N     | 203 | ASP  | C-N-CA     | 5.57  | 128.29      | 120.28   |
| 1   | L     | 196 | ARG  | CA-C-O     | 5.56  | 127.12      | 120.28   |
| 1   | L     | 389 | ARG  | N-CA-C     | -5.56 | 106.62      | 113.41   |
| 1   | R     | 504 | GLU  | N-CA-C     | 5.56  | 118.22      | 108.82   |
| 1   | D     | 61  | ASP  | O-C-N      | -5.56 | 116.24      | 122.75   |
| 1   | D     | 144 | GLN  | OE1-CD-NE2 | -5.56 | 117.04      | 122.60   |
| 1   | F     | 529 | VAL  | CA-C-N     | 5.56  | 130.67      | 122.94   |
| 1   | F     | 529 | VAL  | C-N-CA     | 5.56  | 130.67      | 122.94   |
| 1   | G     | 487 | ILE  | CB-CA-C    | 5.56  | 118.22      | 110.99   |
| 1   | M     | 478 | GLU  | O-C-N      | -5.56 | 116.22      | 122.12   |
| 1   | S     | 271 | GLN  | CA-C-N     | 5.56  | 127.99      | 120.65   |
| 1   | S     | 271 | GLN  | C-N-CA     | 5.56  | 127.99      | 120.65   |
| 1   | F     | 259 | GLU  | CA-C-N     | 5.56  | 128.05      | 120.54   |
| 1   | F     | 259 | GLU  | C-N-CA     | 5.56  | 128.05      | 120.54   |
| 1   | C     | 161 | LEU  | CA-C-N     | 5.56  | 128.29      | 120.28   |
| 1   | C     | 161 | LEU  | C-N-CA     | 5.56  | 128.29      | 120.28   |
| 1   | C     | 54  | GLY  | N-CA-C     | 5.56  | 121.01      | 112.51   |
| 1   | E     | 66  | ILE  | N-CA-C     | 5.56  | 116.59      | 108.53   |
| 1   | I     | 90  | VAL  | N-CA-CB    | 5.56  | 120.15      | 110.65   |
| 1   | I     | 234 | HIS  | CG-CD2-NE2 | 5.56  | 112.76      | 107.20   |
| 1   | N     | 61  | ASP  | CA-C-N     | 5.56  | 127.99      | 120.38   |
| 1   | N     | 61  | ASP  | C-N-CA     | 5.56  | 127.99      | 120.38   |
| 1   | B     | 429 | LEU  | N-CA-CB    | -5.55 | 101.94      | 110.16   |
| 1   | D     | 389 | ARG  | N-CA-C     | -5.55 | 107.05      | 113.88   |
| 1   | E     | 67  | THR  | CA-CB-CG2  | 5.55  | 119.94      | 110.50   |
| 1   | N     | 490 | TYR  | N-CA-CB    | -5.55 | 102.00      | 110.33   |
| 1   | Q     | 469 | LEU  | CA-C-O     | -5.55 | 114.53      | 120.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 93  | ALA  | O-C-N      | -5.55 | 116.03      | 122.03   |
| 1   | E     | 139 | GLU  | CA-C-N     | 5.55  | 128.51      | 120.79   |
| 1   | E     | 139 | GLU  | C-N-CA     | 5.55  | 128.51      | 120.79   |
| 1   | H     | 270 | THR  | CA-C-N     | 5.55  | 128.17      | 120.29   |
| 1   | H     | 270 | THR  | C-N-CA     | 5.55  | 128.17      | 120.29   |
| 1   | L     | 422 | GLU  | CA-C-O     | -5.55 | 115.17      | 121.00   |
| 1   | Q     | 186 | VAL  | O-C-N      | 5.55  | 127.35      | 121.91   |
| 1   | R     | 171 | SER  | CA-C-O     | 5.55  | 126.14      | 119.59   |
| 1   | S     | 66  | ILE  | N-CA-C     | 5.55  | 116.58      | 108.53   |
| 1   | C     | 203 | ASP  | CA-C-N     | 5.55  | 128.27      | 120.28   |
| 1   | C     | 203 | ASP  | C-N-CA     | 5.55  | 128.27      | 120.28   |
| 1   | F     | 234 | HIS  | O-C-N      | -5.55 | 117.60      | 121.65   |
| 1   | I     | 71  | ASP  | CA-CB-CG   | -5.55 | 107.05      | 112.60   |
| 1   | G     | 272 | MET  | O-C-N      | 5.55  | 128.02      | 122.08   |
| 1   | O     | 504 | GLU  | N-CA-C     | 5.55  | 118.20      | 108.82   |
| 1   | A     | 481 | ASN  | CB-CA-C    | -5.55 | 101.58      | 110.79   |
| 1   | C     | 155 | ILE  | CA-CB-CG1  | 5.55  | 119.83      | 110.40   |
| 1   | N     | 35  | ASN  | O-C-N      | -5.55 | 116.32      | 122.09   |
| 1   | P     | 397 | ALA  | CA-C-N     | 5.55  | 128.16      | 120.29   |
| 1   | P     | 397 | ALA  | C-N-CA     | 5.55  | 128.16      | 120.29   |
| 1   | D     | 39  | VAL  | CA-C-N     | 5.54  | 127.97      | 120.38   |
| 1   | D     | 39  | VAL  | C-N-CA     | 5.54  | 127.97      | 120.38   |
| 1   | I     | 244 | ALA  | CA-C-N     | -5.54 | 115.05      | 122.42   |
| 1   | I     | 244 | ALA  | C-N-CA     | -5.54 | 115.05      | 122.42   |
| 1   | I     | 494 | PRO  | N-CA-C     | 5.54  | 119.57      | 111.03   |
| 1   | N     | 393 | GLU  | CA-C-N     | 5.54  | 128.74      | 120.31   |
| 1   | N     | 393 | GLU  | C-N-CA     | 5.54  | 128.74      | 120.31   |
| 1   | C     | 362 | VAL  | CB-CA-C    | -5.54 | 104.61      | 111.32   |
| 1   | G     | 281 | ASN  | CA-CB-CG   | -5.54 | 107.06      | 112.60   |
| 1   | Q     | 122 | LEU  | CD1-CG-CD2 | -5.54 | 98.61       | 110.80   |
| 1   | Q     | 190 | THR  | CA-C-N     | 5.54  | 128.16      | 120.29   |
| 1   | Q     | 190 | THR  | C-N-CA     | 5.54  | 128.16      | 120.29   |
| 1   | R     | 253 | LEU  | N-CA-C     | -5.54 | 104.76      | 112.30   |
| 1   | D     | 204 | LEU  | O-C-N      | -5.54 | 115.74      | 122.22   |
| 1   | K     | 400 | ASP  | CA-C-N     | 5.54  | 127.70      | 120.28   |
| 1   | K     | 400 | ASP  | C-N-CA     | 5.54  | 127.70      | 120.28   |
| 1   | L     | 239 | LYS  | CA-C-N     | 5.54  | 130.61      | 121.86   |
| 1   | L     | 239 | LYS  | C-N-CA     | 5.54  | 130.61      | 121.86   |
| 1   | P     | 193 | ALA  | N-CA-C     | 5.54  | 118.38      | 110.24   |
| 1   | B     | 104 | THR  | N-CA-C     | 5.54  | 117.40      | 111.36   |
| 1   | B     | 377 | LYS  | O-C-N      | 5.54  | 129.08      | 122.27   |
| 1   | L     | 98  | GLU  | CA-C-N     | 5.54  | 127.70      | 120.28   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | L     | 98  | GLU  | C-N-CA    | 5.54  | 127.70      | 120.28   |
| 1   | K     | 518 | GLU  | O-C-N     | 5.54  | 127.79      | 122.03   |
| 1   | K     | 171 | SER  | O-C-N     | -5.54 | 114.55      | 122.41   |
| 1   | O     | 407 | ASP  | CA-CB-CG  | -5.54 | 107.06      | 112.60   |
| 1   | K     | 437 | GLY  | CA-C-N    | 5.53  | 132.25      | 121.41   |
| 1   | K     | 437 | GLY  | C-N-CA    | 5.53  | 132.25      | 121.41   |
| 1   | M     | 303 | GLY  | CA-C-O    | 5.53  | 129.78      | 122.75   |
| 1   | M     | 517 | THR  | N-CA-C    | 5.53  | 118.07      | 111.71   |
| 1   | B     | 481 | ASN  | N-CA-C    | 5.53  | 117.31      | 111.28   |
| 1   | L     | 294 | GLY  | O-C-N     | -5.53 | 116.36      | 122.55   |
| 1   | P     | 244 | ALA  | N-CA-CB   | -5.53 | 100.53      | 109.60   |
| 1   | O     | 40  | LYS  | N-CA-C    | 5.53  | 118.02      | 111.33   |
| 1   | R     | 158 | THR  | CB-CA-C   | 5.53  | 121.55      | 109.99   |
| 1   | R     | 189 | VAL  | O-C-N     | -5.53 | 114.71      | 121.90   |
| 1   | N     | 37  | ALA  | CA-C-N    | 5.53  | 128.00      | 120.54   |
| 1   | N     | 37  | ALA  | C-N-CA    | 5.53  | 128.00      | 120.54   |
| 1   | K     | 275 | PHE  | CA-C-O    | -5.53 | 114.64      | 120.55   |
| 1   | L     | 244 | ALA  | CA-C-O    | 5.53  | 127.17      | 120.81   |
| 1   | R     | 276 | LEU  | CA-C-N    | 5.53  | 128.14      | 120.63   |
| 1   | R     | 276 | LEU  | C-N-CA    | 5.53  | 128.14      | 120.63   |
| 1   | E     | 200 | TRP  | CA-C-O    | 5.52  | 127.82      | 121.47   |
| 1   | N     | 445 | GLU  | O-C-N     | 5.52  | 127.97      | 122.12   |
| 1   | A     | 481 | ASN  | CA-C-O    | 5.52  | 126.40      | 120.55   |
| 1   | K     | 529 | VAL  | O-C-N     | -5.52 | 117.30      | 123.26   |
| 1   | P     | 416 | ALA  | N-CA-CB   | -5.52 | 101.39      | 109.95   |
| 1   | Q     | 525 | ARG  | NE-CZ-NH2 | -5.52 | 114.23      | 119.20   |
| 1   | O     | 195 | LEU  | O-C-N     | -5.52 | 116.00      | 122.96   |
| 1   | R     | 315 | LYS  | CB-CG-CD  | 5.52  | 124.00      | 111.30   |
| 1   | A     | 58  | MET  | CA-C-N    | 5.52  | 130.70      | 122.86   |
| 1   | A     | 58  | MET  | C-N-CA    | 5.52  | 130.70      | 122.86   |
| 1   | B     | 471 | MET  | CA-C-O    | 5.52  | 126.39      | 120.70   |
| 1   | C     | 228 | VAL  | CA-C-O    | 5.52  | 127.48      | 120.75   |
| 1   | F     | 283 | ILE  | O-C-N     | -5.52 | 116.14      | 121.83   |
| 1   | M     | 353 | TYR  | CA-C-O    | 5.52  | 126.20      | 120.30   |
| 1   | R     | 172 | LYS  | CA-C-N    | 5.52  | 127.67      | 120.28   |
| 1   | R     | 172 | LYS  | C-N-CA    | 5.52  | 127.67      | 120.28   |
| 1   | F     | 492 | GLY  | O-C-N     | -5.52 | 115.89      | 122.34   |
| 1   | N     | 353 | TYR  | CA-CB-CG  | -5.52 | 103.97      | 113.90   |
| 1   | R     | 50  | TYR  | O-C-N     | -5.52 | 116.14      | 122.93   |
| 1   | B     | 263 | GLU  | CA-C-N    | 5.52  | 131.90      | 121.97   |
| 1   | B     | 263 | GLU  | C-N-CA    | 5.52  | 131.90      | 121.97   |
| 1   | C     | 192 | VAL  | O-C-N     | -5.52 | 115.67      | 122.18   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 90  | VAL  | CB-CA-C    | -5.52 | 103.61      | 112.16   |
| 1   | M     | 113 | GLU  | CA-C-N     | 5.52  | 128.12      | 120.29   |
| 1   | M     | 113 | GLU  | C-N-CA     | 5.52  | 128.12      | 120.29   |
| 1   | Q     | 459 | ILE  | CB-CA-C    | -5.52 | 104.91      | 111.97   |
| 1   | A     | 263 | GLU  | N-CA-C     | 5.51  | 118.31      | 110.10   |
| 1   | B     | 259 | GLU  | N-CA-C     | 5.51  | 119.99      | 112.88   |
| 1   | B     | 424 | GLU  | CA-C-O     | -5.51 | 115.02      | 120.70   |
| 1   | M     | 74  | THR  | CA-CB-CG2  | 5.51  | 119.87      | 110.50   |
| 1   | O     | 32  | VAL  | N-CA-C     | 5.51  | 118.78      | 111.17   |
| 1   | S     | 226 | ILE  | O-C-N      | -5.51 | 116.60      | 122.61   |
| 1   | G     | 178 | ARG  | NE-CZ-NH1  | -5.51 | 115.99      | 121.50   |
| 1   | B     | 387 | LEU  | CD1-CG-CD2 | -5.51 | 98.68       | 110.80   |
| 1   | H     | 202 | VAL  | O-C-N      | -5.51 | 117.45      | 123.18   |
| 1   | I     | 400 | ASP  | CA-C-N     | 5.51  | 127.60      | 120.44   |
| 1   | I     | 400 | ASP  | C-N-CA     | 5.51  | 127.60      | 120.44   |
| 1   | M     | 360 | ARG  | NE-CZ-NH2  | 5.51  | 124.16      | 119.20   |
| 1   | N     | 189 | VAL  | N-CA-C     | -5.51 | 105.47      | 110.82   |
| 1   | P     | 243 | ASN  | CA-CB-CG   | -5.51 | 107.09      | 112.60   |
| 1   | P     | 394 | THR  | CA-C-N     | 5.51  | 128.12      | 120.29   |
| 1   | P     | 394 | THR  | C-N-CA     | 5.51  | 128.12      | 120.29   |
| 1   | Q     | 376 | PRO  | N-CD-CG    | 5.51  | 111.47      | 103.20   |
| 1   | D     | 261 | ASP  | CB-CA-C    | -5.51 | 99.70       | 110.11   |
| 1   | E     | 137 | LYS  | CA-C-N     | 5.51  | 128.12      | 120.29   |
| 1   | E     | 137 | LYS  | C-N-CA     | 5.51  | 128.12      | 120.29   |
| 1   | I     | 313 | ALA  | O-C-N      | -5.51 | 115.87      | 122.15   |
| 1   | M     | 35  | ASN  | CA-CB-CG   | -5.51 | 107.09      | 112.60   |
| 1   | R     | 431 | LYS  | CA-C-N     | 5.51  | 127.93      | 120.44   |
| 1   | R     | 431 | LYS  | C-N-CA     | 5.51  | 127.93      | 120.44   |
| 1   | B     | 91  | GLN  | CA-C-N     | 5.50  | 128.24      | 120.42   |
| 1   | B     | 91  | GLN  | C-N-CA     | 5.50  | 128.24      | 120.42   |
| 1   | K     | 423 | ILE  | CA-C-N     | 5.50  | 127.93      | 120.44   |
| 1   | K     | 423 | ILE  | C-N-CA     | 5.50  | 127.93      | 120.44   |
| 1   | R     | 292 | ALA  | CA-C-O     | 5.50  | 126.15      | 119.49   |
| 1   | D     | 234 | HIS  | CG-CD2-NE2 | 5.50  | 112.70      | 107.20   |
| 1   | D     | 301 | GLN  | CA-C-O     | 5.50  | 125.67      | 119.18   |
| 1   | H     | 324 | LYS  | CA-C-N     | 5.50  | 128.42      | 120.38   |
| 1   | H     | 324 | LYS  | C-N-CA     | 5.50  | 128.42      | 120.38   |
| 1   | L     | 378 | SER  | N-CA-C     | 5.50  | 117.70      | 108.23   |
| 1   | S     | 456 | SER  | O-C-N      | -5.50 | 116.40      | 122.07   |
| 1   | A     | 73  | ALA  | N-CA-C     | 5.50  | 117.73      | 111.02   |
| 1   | D     | 208 | GLN  | CB-CA-C    | 5.50  | 118.80      | 109.50   |
| 1   | L     | 465 | ASP  | N-CA-C     | 5.50  | 117.59      | 109.50   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | M     | 61  | ASP  | CA-CB-CG  | -5.50 | 107.10      | 112.60   |
| 1   | Q     | 512 | ALA  | CA-C-N    | 5.50  | 128.00      | 120.46   |
| 1   | Q     | 512 | ALA  | C-N-CA    | 5.50  | 128.00      | 120.46   |
| 1   | L     | 221 | GLN  | N-CA-C    | 5.50  | 117.20      | 108.79   |
| 1   | P     | 357 | ILE  | CA-CB-CG1 | 5.50  | 119.75      | 110.40   |
| 1   | S     | 368 | VAL  | N-CA-CB   | -5.50 | 102.06      | 110.86   |
| 1   | A     | 194 | GLU  | CB-CG-CD  | 5.50  | 121.95      | 112.60   |
| 1   | E     | 400 | ASP  | CA-CB-CG  | -5.50 | 107.10      | 112.60   |
| 1   | E     | 504 | GLU  | CA-C-N    | 5.50  | 126.71      | 119.84   |
| 1   | E     | 504 | GLU  | C-N-CA    | 5.50  | 126.71      | 119.84   |
| 1   | H     | 231 | GLU  | N-CA-C    | 5.50  | 118.56      | 110.59   |
| 1   | K     | 246 | ILE  | N-CA-C    | 5.50  | 117.37      | 109.51   |
| 1   | M     | 389 | ARG  | NE-CZ-NH1 | 5.50  | 127.00      | 121.50   |
| 1   | O     | 85  | ALA  | N-CA-C    | 5.50  | 117.71      | 111.11   |
| 1   | O     | 508 | VAL  | CA-C-O    | 5.50  | 127.00      | 121.17   |
| 1   | A     | 118 | ALA  | CA-C-N    | 5.50  | 127.64      | 120.28   |
| 1   | A     | 118 | ALA  | C-N-CA    | 5.50  | 127.64      | 120.28   |
| 1   | G     | 120 | ASP  | CA-CB-CG  | 5.50  | 118.10      | 112.60   |
| 1   | I     | 396 | ARG  | NE-CZ-NH1 | 5.50  | 127.00      | 121.50   |
| 1   | L     | 96  | GLN  | CA-C-O    | 5.50  | 127.04      | 120.28   |
| 1   | L     | 180 | TYR  | N-CA-CB   | 5.50  | 117.98      | 110.01   |
| 1   | N     | 113 | GLU  | CA-C-O    | 5.50  | 126.25      | 120.42   |
| 1   | N     | 240 | ARG  | N-CA-CB   | 5.50  | 120.31      | 110.80   |
| 1   | Q     | 80  | ASP  | CA-CB-CG  | -5.50 | 107.10      | 112.60   |
| 1   | S     | 321 | ARG  | CA-C-N    | 5.50  | 130.16      | 122.36   |
| 1   | S     | 321 | ARG  | C-N-CA    | 5.50  | 130.16      | 122.36   |
| 1   | C     | 264 | ILE  | N-CA-C    | 5.50  | 117.11      | 109.80   |
| 1   | D     | 531 | SER  | O-C-N     | -5.50 | 116.96      | 123.22   |
| 1   | M     | 428 | LYS  | CG-CD-CE  | 5.50  | 123.94      | 111.30   |
| 1   | M     | 481 | ASN  | N-CA-C    | -5.50 | 105.45      | 111.82   |
| 1   | O     | 34  | ALA  | CA-C-N    | 5.50  | 127.96      | 120.54   |
| 1   | O     | 34  | ALA  | C-N-CA    | 5.50  | 127.96      | 120.54   |
| 1   | B     | 35  | ASN  | O-C-N     | -5.49 | 116.20      | 122.08   |
| 1   | M     | 398 | LEU  | CA-C-N    | 5.49  | 127.58      | 120.44   |
| 1   | M     | 398 | LEU  | C-N-CA    | 5.49  | 127.58      | 120.44   |
| 1   | N     | 398 | LEU  | CA-C-N    | 5.49  | 127.58      | 120.44   |
| 1   | N     | 398 | LEU  | C-N-CA    | 5.49  | 127.58      | 120.44   |
| 1   | N     | 409 | ILE  | N-CA-C    | 5.49  | 115.69      | 110.53   |
| 1   | N     | 479 | ASN  | CA-C-N    | 5.49  | 127.64      | 120.28   |
| 1   | N     | 479 | ASN  | C-N-CA    | 5.49  | 127.64      | 120.28   |
| 1   | Q     | 299 | ILE  | O-C-N     | -5.49 | 117.22      | 123.10   |
| 1   | R     | 420 | ALA  | N-CA-C    | 5.49  | 116.96      | 110.97   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 80  | ASP  | CA-C-N    | 5.49  | 128.09      | 120.29   |
| 1   | B     | 80  | ASP  | C-N-CA    | 5.49  | 128.09      | 120.29   |
| 1   | D     | 63  | LEU  | CA-C-N    | 5.49  | 132.58      | 121.93   |
| 1   | D     | 63  | LEU  | C-N-CA    | 5.49  | 132.58      | 121.93   |
| 1   | D     | 67  | THR  | CA-C-O    | -5.49 | 114.42      | 120.24   |
| 1   | G     | 408 | VAL  | CB-CA-C   | -5.49 | 104.73      | 112.14   |
| 1   | L     | 389 | ARG  | CG-CD-NE  | -5.49 | 99.92       | 112.00   |
| 1   | N     | 163 | LYS  | N-CA-C    | -5.49 | 104.16      | 111.24   |
| 1   | O     | 462 | ALA  | N-CA-C    | 5.49  | 119.70      | 112.89   |
| 1   | B     | 430 | ARG  | CB-CA-C   | -5.49 | 101.68      | 110.79   |
| 1   | G     | 401 | ALA  | CA-C-O    | 5.49  | 126.37      | 120.55   |
| 1   | I     | 240 | ARG  | NE-CZ-NH2 | -5.49 | 114.26      | 119.20   |
| 1   | L     | 329 | GLU  | N-CA-C    | 5.49  | 116.94      | 111.07   |
| 1   | L     | 501 | GLY  | CA-C-O    | -5.49 | 113.02      | 119.72   |
| 1   | N     | 64  | GLY  | CA-C-N    | 5.49  | 128.64      | 120.90   |
| 1   | N     | 64  | GLY  | C-N-CA    | 5.49  | 128.64      | 120.90   |
| 1   | C     | 55  | MET  | CG-SD-CE  | -5.49 | 88.83       | 100.90   |
| 1   | I     | 347 | SER  | CA-C-N    | 5.49  | 127.63      | 120.28   |
| 1   | I     | 347 | SER  | C-N-CA    | 5.49  | 127.63      | 120.28   |
| 1   | K     | 364 | GLU  | O-C-N     | -5.49 | 115.75      | 122.34   |
| 1   | F     | 79  | MET  | O-C-N     | -5.49 | 116.76      | 122.96   |
| 1   | K     | 68  | ILE  | CA-C-O    | 5.49  | 126.29      | 120.48   |
| 1   | K     | 505 | PRO  | N-CA-C    | 5.49  | 123.77      | 112.47   |
| 1   | L     | 304 | ILE  | CA-C-N    | 5.49  | 129.03      | 120.75   |
| 1   | L     | 304 | ILE  | C-N-CA    | 5.49  | 129.03      | 120.75   |
| 1   | N     | 126 | VAL  | N-CA-CB   | 5.49  | 119.53      | 111.52   |
| 1   | O     | 238 | PRO  | N-CA-C    | 5.49  | 119.48      | 111.03   |
| 1   | R     | 146 | ILE  | N-CA-C    | -5.49 | 105.77      | 111.58   |
| 1   | B     | 97  | ASP  | CA-CB-CG  | -5.48 | 107.12      | 112.60   |
| 1   | E     | 328 | LEU  | CA-C-N    | 5.48  | 127.57      | 120.44   |
| 1   | E     | 328 | LEU  | C-N-CA    | 5.48  | 127.57      | 120.44   |
| 1   | L     | 178 | ARG  | NE-CZ-NH2 | 5.48  | 124.13      | 119.20   |
| 1   | P     | 31  | ALA  | N-CA-C    | -5.48 | 104.83      | 112.45   |
| 1   | A     | 47  | LYS  | N-CA-C    | 5.48  | 122.47      | 110.80   |
| 1   | L     | 121 | LEU  | CA-C-O    | 5.48  | 126.23      | 120.42   |
| 1   | P     | 154 | SER  | CA-C-N    | 5.48  | 128.26      | 120.53   |
| 1   | P     | 154 | SER  | C-N-CA    | 5.48  | 128.26      | 120.53   |
| 1   | Q     | 222 | LEU  | O-C-N     | -5.48 | 116.78      | 123.19   |
| 1   | R     | 189 | VAL  | CA-C-N    | 5.48  | 128.38      | 120.38   |
| 1   | R     | 189 | VAL  | C-N-CA    | 5.48  | 128.38      | 120.38   |
| 1   | Q     | 142 | ALA  | N-CA-C    | 5.48  | 117.96      | 111.33   |
| 1   | C     | 371 | GLU  | CA-C-O    | 5.48  | 127.77      | 121.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 449 | ASN  | N-CA-C     | 5.48  | 117.25      | 111.28   |
| 1   | L     | 471 | MET  | CG-SD-CE   | -5.48 | 88.85       | 100.90   |
| 1   | Q     | 127 | HIS  | CA-C-O     | -5.48 | 115.59      | 120.19   |
| 1   | G     | 139 | GLU  | CA-C-N     | 5.48  | 129.90      | 121.19   |
| 1   | G     | 139 | GLU  | C-N-CA     | 5.48  | 129.90      | 121.19   |
| 1   | H     | 517 | THR  | CA-C-N     | 5.48  | 127.88      | 120.65   |
| 1   | H     | 517 | THR  | C-N-CA     | 5.48  | 127.88      | 120.65   |
| 1   | Q     | 481 | ASN  | N-CA-C     | -5.48 | 105.86      | 112.54   |
| 1   | C     | 389 | ARG  | CA-C-N     | 5.47  | 127.62      | 120.28   |
| 1   | C     | 389 | ARG  | C-N-CA     | 5.47  | 127.62      | 120.28   |
| 1   | F     | 63  | LEU  | CA-C-O     | 5.47  | 126.41      | 119.95   |
| 1   | M     | 220 | THR  | CA-C-O     | -5.47 | 115.17      | 121.19   |
| 1   | A     | 329 | GLU  | N-CA-C     | 5.47  | 116.93      | 111.07   |
| 1   | G     | 191 | GLN  | CA-C-O     | 5.47  | 126.22      | 120.42   |
| 1   | H     | 304 | ILE  | O-C-N      | -5.47 | 117.29      | 123.20   |
| 1   | S     | 484 | TRP  | O-C-N      | -5.47 | 115.19      | 122.20   |
| 1   | E     | 165 | ALA  | CA-C-N     | 5.47  | 127.61      | 120.28   |
| 1   | E     | 165 | ALA  | C-N-CA     | 5.47  | 127.61      | 120.28   |
| 1   | E     | 68  | ILE  | O-C-N      | -5.47 | 116.96      | 123.03   |
| 1   | E     | 111 | SER  | N-CA-CB    | 5.47  | 117.94      | 110.01   |
| 1   | G     | 285 | GLU  | N-CA-CB    | 5.47  | 117.91      | 109.98   |
| 1   | L     | 512 | ALA  | CA-C-O     | 5.47  | 126.74      | 121.00   |
| 1   | K     | 375 | ASN  | CB-CG-ND2  | 5.47  | 124.60      | 116.40   |
| 1   | L     | 151 | GLN  | OE1-CD-NE2 | 5.47  | 128.07      | 122.60   |
| 1   | A     | 471 | MET  | CA-C-O     | -5.47 | 115.08      | 120.82   |
| 1   | F     | 104 | THR  | O-C-N      | -5.46 | 115.92      | 122.15   |
| 1   | L     | 487 | ILE  | CA-CB-CG1  | 5.46  | 119.69      | 110.40   |
| 1   | N     | 429 | LEU  | N-CA-C     | -5.46 | 105.40      | 111.36   |
| 1   | N     | 430 | ARG  | CA-C-O     | -5.46 | 115.08      | 120.82   |
| 1   | E     | 398 | LEU  | CA-C-N     | 5.46  | 127.54      | 120.44   |
| 1   | E     | 398 | LEU  | C-N-CA     | 5.46  | 127.54      | 120.44   |
| 1   | G     | 481 | ASN  | O-C-N      | -5.46 | 116.33      | 122.12   |
| 1   | L     | 515 | ALA  | O-C-N      | -5.46 | 116.35      | 122.03   |
| 1   | S     | 201 | TYR  | CB-CG-CD1  | -5.46 | 112.61      | 120.80   |
| 1   | A     | 83  | HIS  | CG-CD2-NE2 | 5.46  | 112.66      | 107.20   |
| 1   | C     | 325 | LYS  | CA-C-N     | 5.46  | 128.35      | 120.38   |
| 1   | C     | 325 | LYS  | C-N-CA     | 5.46  | 128.35      | 120.38   |
| 1   | C     | 502 | VAL  | N-CA-CB    | 5.46  | 117.74      | 112.28   |
| 1   | G     | 354 | ALA  | CA-C-N     | 5.46  | 127.60      | 120.28   |
| 1   | G     | 354 | ALA  | C-N-CA     | 5.46  | 127.60      | 120.28   |
| 1   | I     | 273 | GLN  | CA-C-N     | 5.46  | 129.42      | 120.63   |
| 1   | I     | 273 | GLN  | C-N-CA     | 5.46  | 129.42      | 120.63   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 453 | SER  | N-CA-C     | 5.46  | 117.23      | 111.28   |
| 1   | N     | 271 | GLN  | OE1-CD-NE2 | -5.46 | 117.14      | 122.60   |
| 1   | K     | 209 | ILE  | CB-CA-C    | -5.46 | 104.23      | 110.73   |
| 1   | I     | 506 | ALA  | N-CA-C     | 5.46  | 117.99      | 111.71   |
| 1   | K     | 219 | ASP  | CA-CB-CG   | 5.46  | 118.06      | 112.60   |
| 1   | N     | 401 | ALA  | CA-C-N     | 5.46  | 127.86      | 120.65   |
| 1   | N     | 401 | ALA  | C-N-CA     | 5.46  | 127.86      | 120.65   |
| 1   | B     | 264 | ILE  | CA-CB-CG1  | 5.46  | 119.68      | 110.40   |
| 1   | E     | 246 | ILE  | O-C-N      | -5.46 | 116.85      | 122.63   |
| 1   | H     | 275 | PHE  | N-CA-CB    | -5.46 | 102.05      | 110.07   |
| 1   | R     | 170 | SER  | N-CA-C     | 5.46  | 119.43      | 112.34   |
| 1   | C     | 507 | LEU  | CA-C-N     | 5.46  | 127.43      | 120.56   |
| 1   | C     | 507 | LEU  | C-N-CA     | 5.46  | 127.43      | 120.56   |
| 1   | E     | 510 | MET  | N-CA-C     | -5.46 | 105.67      | 112.93   |
| 1   | F     | 144 | GLN  | N-CA-C     | 5.46  | 118.73      | 111.75   |
| 1   | A     | 35  | ASN  | CA-C-N     | 5.45  | 127.91      | 120.77   |
| 1   | A     | 35  | ASN  | C-N-CA     | 5.45  | 127.91      | 120.77   |
| 1   | H     | 83  | HIS  | CA-C-N     | 5.45  | 124.91      | 119.24   |
| 1   | H     | 83  | HIS  | C-N-CA     | 5.45  | 124.91      | 119.24   |
| 1   | I     | 382 | LEU  | CA-C-O     | 5.45  | 126.13      | 120.40   |
| 1   | B     | 70  | ASN  | OD1-CG-ND2 | -5.45 | 117.15      | 122.60   |
| 1   | K     | 165 | ALA  | CA-C-N     | 5.45  | 127.58      | 120.28   |
| 1   | K     | 165 | ALA  | C-N-CA     | 5.45  | 127.58      | 120.28   |
| 1   | R     | 137 | LYS  | N-CA-C     | 5.45  | 117.93      | 111.33   |
| 1   | D     | 82  | GLN  | N-CA-CB    | 5.45  | 119.70      | 110.49   |
| 1   | G     | 187 | LYS  | CA-C-N     | 5.45  | 127.58      | 120.28   |
| 1   | G     | 187 | LYS  | C-N-CA     | 5.45  | 127.58      | 120.28   |
| 1   | G     | 320 | VAL  | N-CA-C     | -5.45 | 100.63      | 108.48   |
| 1   | I     | 259 | GLU  | CB-CG-CD   | -5.45 | 103.33      | 112.60   |
| 1   | I     | 511 | ASN  | CA-C-N     | 5.45  | 127.53      | 120.44   |
| 1   | I     | 511 | ASN  | C-N-CA     | 5.45  | 127.53      | 120.44   |
| 1   | P     | 214 | GLY  | CA-C-O     | -5.45 | 117.88      | 122.29   |
| 1   | Q     | 458 | LEU  | CA-C-O     | 5.45  | 126.54      | 120.82   |
| 1   | A     | 362 | VAL  | O-C-N      | -5.45 | 115.76      | 122.57   |
| 1   | I     | 253 | LEU  | CA-C-N     | 5.45  | 131.12      | 122.62   |
| 1   | I     | 253 | LEU  | C-N-CA     | 5.45  | 131.12      | 122.62   |
| 1   | M     | 179 | GLU  | O-C-N      | 5.45  | 127.89      | 122.12   |
| 1   | N     | 127 | HIS  | ND1-CG-CD2 | -5.45 | 100.65      | 106.10   |
| 1   | S     | 512 | ALA  | CA-C-O     | 5.45  | 126.54      | 120.82   |
| 1   | D     | 504 | GLU  | CA-C-O     | -5.45 | 114.35      | 119.91   |
| 1   | C     | 340 | VAL  | CA-C-N     | 5.45  | 128.02      | 120.29   |
| 1   | C     | 340 | VAL  | C-N-CA     | 5.45  | 128.02      | 120.29   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | I     | 528 | ASP  | CA-C-N     | 5.45  | 130.27      | 123.14   |
| 1   | I     | 528 | ASP  | C-N-CA     | 5.45  | 130.27      | 123.14   |
| 1   | N     | 29  | LYS  | CA-C-N     | 5.45  | 131.94      | 121.54   |
| 1   | N     | 29  | LYS  | C-N-CA     | 5.45  | 131.94      | 121.54   |
| 1   | R     | 383 | ILE  | CB-CA-C    | -5.45 | 103.75      | 111.21   |
| 1   | S     | 327 | ASP  | N-CA-CB    | -5.45 | 102.53      | 110.53   |
| 1   | K     | 425 | ILE  | CA-C-N     | 5.44  | 129.06      | 120.89   |
| 1   | K     | 425 | ILE  | C-N-CA     | 5.44  | 129.06      | 120.89   |
| 1   | M     | 530 | VAL  | O-C-N      | -5.44 | 117.32      | 122.98   |
| 1   | N     | 474 | ARG  | NH1-CZ-NH2 | -5.44 | 112.22      | 119.30   |
| 1   | O     | 122 | LEU  | CA-C-N     | 5.44  | 127.57      | 120.28   |
| 1   | O     | 122 | LEU  | C-N-CA     | 5.44  | 127.57      | 120.28   |
| 1   | Q     | 156 | ASN  | O-C-N      | -5.44 | 115.78      | 122.25   |
| 1   | B     | 305 | ASP  | CA-CB-CG   | -5.44 | 107.16      | 112.60   |
| 1   | C     | 117 | LYS  | N-CA-C     | 5.44  | 117.97      | 111.71   |
| 1   | K     | 171 | SER  | CA-C-O     | 5.44  | 125.65      | 119.18   |
| 1   | L     | 463 | GLY  | N-CA-C     | -5.44 | 107.51      | 115.72   |
| 1   | O     | 199 | LYS  | CG-CD-CE   | 5.44  | 123.81      | 111.30   |
| 1   | R     | 441 | GLN  | N-CA-C     | 5.44  | 117.64      | 111.11   |
| 1   | S     | 110 | PHE  | CA-C-N     | 5.44  | 127.83      | 120.65   |
| 1   | S     | 110 | PHE  | C-N-CA     | 5.44  | 127.83      | 120.65   |
| 1   | S     | 400 | ASP  | O-C-N      | -5.44 | 116.36      | 122.12   |
| 1   | C     | 525 | ARG  | CD-NE-CZ   | 5.44  | 132.01      | 124.40   |
| 1   | L     | 29  | LYS  | CA-C-N     | 5.44  | 131.92      | 121.54   |
| 1   | L     | 29  | LYS  | C-N-CA     | 5.44  | 131.92      | 121.54   |
| 1   | N     | 491 | ALA  | CA-C-N     | 5.44  | 132.07      | 121.41   |
| 1   | N     | 491 | ALA  | C-N-CA     | 5.44  | 132.07      | 121.41   |
| 1   | O     | 392 | ASP  | N-CA-C     | 5.44  | 116.89      | 111.07   |
| 1   | P     | 86  | ALA  | O-C-N      | -5.44 | 116.44      | 122.09   |
| 1   | K     | 362 | VAL  | CA-C-O     | 5.44  | 125.64      | 120.31   |
| 1   | P     | 129 | THR  | CA-C-N     | 5.43  | 127.52      | 120.56   |
| 1   | P     | 129 | THR  | C-N-CA     | 5.43  | 127.52      | 120.56   |
| 1   | P     | 404 | THR  | O-C-N      | -5.43 | 116.44      | 122.09   |
| 1   | B     | 131 | ILE  | N-CA-C     | 5.43  | 117.84      | 111.05   |
| 1   | M     | 400 | ASP  | CA-C-N     | 5.43  | 127.88      | 120.54   |
| 1   | M     | 400 | ASP  | C-N-CA     | 5.43  | 127.88      | 120.54   |
| 1   | M     | 447 | TYR  | N-CA-C     | 5.43  | 117.90      | 111.33   |
| 1   | N     | 104 | THR  | CA-C-N     | 5.43  | 128.00      | 120.29   |
| 1   | N     | 104 | THR  | C-N-CA     | 5.43  | 128.00      | 120.29   |
| 1   | P     | 414 | ALA  | CA-C-N     | 5.43  | 130.32      | 122.77   |
| 1   | P     | 414 | ALA  | C-N-CA     | 5.43  | 130.32      | 122.77   |
| 1   | R     | 86  | ALA  | CA-C-O     | -5.43 | 115.09      | 121.07   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | S     | 37  | ALA  | CA-C-N    | 5.43  | 127.87      | 120.54   |
| 1   | S     | 37  | ALA  | C-N-CA    | 5.43  | 127.87      | 120.54   |
| 1   | S     | 362 | VAL  | O-C-N     | -5.43 | 117.44      | 123.20   |
| 1   | A     | 371 | GLU  | O-C-N     | -5.43 | 116.45      | 122.86   |
| 1   | B     | 455 | VAL  | CA-C-O    | 5.43  | 126.33      | 120.47   |
| 1   | B     | 489 | LEU  | N-CA-C    | 5.43  | 119.61      | 113.15   |
| 1   | H     | 339 | VAL  | N-CA-C    | 5.43  | 116.58      | 108.54   |
| 1   | I     | 70  | ASN  | CA-C-N    | 5.43  | 130.13      | 121.66   |
| 1   | I     | 70  | ASN  | C-N-CA    | 5.43  | 130.13      | 121.66   |
| 1   | L     | 434 | PRO  | N-CA-C    | 5.43  | 123.66      | 112.47   |
| 1   | E     | 36  | ILE  | O-C-N     | -5.43 | 116.10      | 121.96   |
| 1   | O     | 258 | PRO  | N-CA-CB   | -5.43 | 96.96       | 102.88   |
| 1   | H     | 270 | THR  | N-CA-C    | 5.43  | 117.20      | 111.28   |
| 1   | A     | 373 | ALA  | CA-C-O    | -5.43 | 115.08      | 121.16   |
| 1   | B     | 328 | LEU  | CA-C-N    | 5.43  | 127.49      | 120.44   |
| 1   | B     | 328 | LEU  | C-N-CA    | 5.43  | 127.49      | 120.44   |
| 1   | B     | 462 | ALA  | O-C-N     | -5.43 | 114.97      | 122.46   |
| 1   | N     | 161 | LEU  | O-C-N     | -5.43 | 115.87      | 122.22   |
| 1   | O     | 496 | ASP  | CA-CB-CG  | 5.43  | 118.03      | 112.60   |
| 1   | Q     | 396 | ARG  | N-CA-C    | -5.43 | 105.28      | 111.14   |
| 1   | D     | 240 | ARG  | CD-NE-CZ  | -5.42 | 116.81      | 124.40   |
| 1   | G     | 113 | GLU  | O-C-N     | -5.42 | 115.97      | 122.15   |
| 1   | P     | 252 | SER  | CA-CB-OG  | 5.42  | 121.95      | 111.10   |
| 1   | R     | 83  | HIS  | CA-C-N    | 5.42  | 125.50      | 119.32   |
| 1   | R     | 83  | HIS  | C-N-CA    | 5.42  | 125.50      | 119.32   |
| 1   | N     | 124 | LYS  | CA-C-N    | 5.42  | 131.12      | 122.93   |
| 1   | N     | 124 | LYS  | C-N-CA    | 5.42  | 131.12      | 122.93   |
| 1   | H     | 353 | TYR  | CB-CG-CD2 | -5.42 | 112.67      | 120.80   |
| 1   | K     | 141 | VAL  | CA-C-N    | 5.42  | 127.81      | 120.38   |
| 1   | K     | 141 | VAL  | C-N-CA    | 5.42  | 127.81      | 120.38   |
| 1   | M     | 264 | ILE  | CA-C-N    | 5.42  | 131.19      | 122.14   |
| 1   | M     | 264 | ILE  | C-N-CA    | 5.42  | 131.19      | 122.14   |
| 1   | N     | 419 | GLY  | CA-C-O    | -5.42 | 113.19      | 119.10   |
| 1   | S     | 496 | ASP  | O-C-N     | -5.42 | 115.77      | 122.82   |
| 1   | C     | 515 | ALA  | CA-C-O    | 5.42  | 126.69      | 121.00   |
| 1   | F     | 496 | ASP  | CA-C-N    | 5.42  | 127.99      | 120.29   |
| 1   | F     | 496 | ASP  | C-N-CA    | 5.42  | 127.99      | 120.29   |
| 1   | G     | 198 | ASP  | CA-C-O    | 5.42  | 127.53      | 120.81   |
| 1   | H     | 503 | ILE  | N-CA-C    | -5.42 | 100.53      | 108.99   |
| 1   | M     | 191 | GLN  | N-CA-CB   | -5.42 | 102.14      | 110.16   |
| 1   | C     | 136 | LYS  | CA-C-N    | 5.42  | 127.80      | 120.38   |
| 1   | C     | 136 | LYS  | C-N-CA    | 5.42  | 127.80      | 120.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M     | 129 | THR  | CA-C-O      | 5.42  | 126.22      | 120.10   |
| 1   | C     | 463 | GLY  | O-C-N       | 5.42  | 128.14      | 122.51   |
| 1   | R     | 234 | HIS  | CE1-NE2-CD2 | -5.42 | 103.58      | 109.00   |
| 1   | S     | 183 | ASP  | O-C-N       | -5.42 | 116.49      | 122.07   |
| 1   | I     | 274 | LYS  | N-CA-C      | 5.42  | 119.38      | 112.34   |
| 1   | M     | 385 | GLY  | CA-C-N      | 5.42  | 131.01      | 121.32   |
| 1   | M     | 385 | GLY  | C-N-CA      | 5.42  | 131.01      | 121.32   |
| 1   | S     | 468 | ASP  | N-CA-C      | 5.42  | 117.63      | 111.02   |
| 1   | K     | 447 | TYR  | CA-C-O      | 5.41  | 128.25      | 120.51   |
| 1   | O     | 45  | ALA  | N-CA-C      | -5.41 | 106.52      | 113.23   |
| 1   | Q     | 219 | ASP  | CA-C-O      | 5.41  | 125.98      | 119.43   |
| 1   | B     | 105 | LYS  | CA-C-N      | 5.41  | 127.79      | 120.65   |
| 1   | B     | 105 | LYS  | C-N-CA      | 5.41  | 127.79      | 120.65   |
| 1   | D     | 298 | ILE  | O-C-N       | -5.41 | 117.46      | 123.03   |
| 1   | M     | 502 | VAL  | CA-CB-CG2   | -5.41 | 101.20      | 110.40   |
| 1   | P     | 498 | TRP  | N-CA-CB     | 5.41  | 118.00      | 109.94   |
| 1   | R     | 296 | ASN  | N-CA-C      | -5.41 | 107.33      | 114.31   |
| 1   | A     | 77  | ASP  | CA-CB-CG    | -5.41 | 107.19      | 112.60   |
| 1   | N     | 91  | GLN  | N-CA-C      | 5.41  | 117.18      | 111.28   |
| 1   | P     | 173 | ALA  | N-CA-CB     | -5.41 | 101.66      | 110.42   |
| 1   | R     | 429 | LEU  | CA-C-N      | 5.41  | 127.53      | 120.28   |
| 1   | R     | 429 | LEU  | C-N-CA      | 5.41  | 127.53      | 120.28   |
| 1   | S     | 523 | VAL  | CA-CB-CG1   | 5.41  | 119.59      | 110.40   |
| 1   | A     | 244 | ALA  | O-C-N       | -5.41 | 115.13      | 122.48   |
| 1   | B     | 322 | ARG  | N-CA-C      | 5.41  | 118.85      | 111.39   |
| 1   | D     | 62  | SER  | N-CA-CB     | 5.41  | 118.55      | 110.22   |
| 1   | G     | 396 | ARG  | CA-C-N      | 5.41  | 127.79      | 120.38   |
| 1   | G     | 396 | ARG  | C-N-CA      | 5.41  | 127.79      | 120.38   |
| 1   | M     | 109 | ILE  | N-CA-C      | 5.41  | 115.85      | 110.23   |
| 1   | C     | 315 | LYS  | N-CA-CB     | 5.41  | 119.21      | 110.40   |
| 1   | N     | 413 | ARG  | NE-CZ-NH1   | -5.41 | 116.09      | 121.50   |
| 1   | P     | 429 | LEU  | O-C-N       | -5.41 | 115.99      | 122.15   |
| 1   | S     | 224 | TYR  | CA-C-O      | 5.41  | 128.24      | 120.51   |
| 1   | B     | 320 | VAL  | CB-CA-C     | -5.40 | 102.44      | 110.33   |
| 1   | D     | 145 | THR  | CA-C-O      | 5.40  | 126.03      | 119.38   |
| 1   | G     | 347 | SER  | CA-C-N      | 5.40  | 129.75      | 120.72   |
| 1   | G     | 347 | SER  | C-N-CA      | 5.40  | 129.75      | 120.72   |
| 1   | L     | 497 | MET  | N-CA-C      | 5.40  | 117.25      | 111.36   |
| 1   | A     | 84  | PRO  | N-CA-CB     | 5.40  | 109.01      | 103.23   |
| 1   | E     | 286 | LYS  | CA-C-O      | -5.40 | 115.12      | 120.90   |
| 1   | G     | 216 | SER  | O-C-N       | -5.40 | 116.87      | 123.19   |
| 1   | L     | 237 | MET  | CG-SD-CE    | -5.40 | 89.01       | 100.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 135 | TYR  | CB-CG-CD2  | 5.40  | 128.90      | 120.80   |
| 1   | O     | 488 | ASP  | CB-CG-OD2  | -5.40 | 105.97      | 118.40   |
| 1   | B     | 318 | LEU  | CB-CA-C    | 5.40  | 119.59      | 110.79   |
| 1   | E     | 487 | ILE  | CB-CA-C    | -5.40 | 103.97      | 110.99   |
| 1   | L     | 469 | LEU  | CA-C-N     | 5.40  | 127.46      | 120.44   |
| 1   | L     | 469 | LEU  | C-N-CA     | 5.40  | 127.46      | 120.44   |
| 1   | Q     | 296 | ASN  | CA-CB-CG   | 5.40  | 118.00      | 112.60   |
| 1   | S     | 458 | LEU  | O-C-N      | -5.40 | 116.51      | 122.07   |
| 1   | E     | 225 | GLY  | CA-C-O     | -5.40 | 116.19      | 121.05   |
| 1   | I     | 40  | LYS  | CG-CD-CE   | 5.40  | 123.72      | 111.30   |
| 1   | I     | 150 | ALA  | CB-CA-C    | -5.40 | 101.48      | 109.90   |
| 1   | K     | 256 | GLU  | CB-CG-CD   | 5.40  | 121.78      | 112.60   |
| 1   | L     | 234 | HIS  | CA-CB-CG   | 5.40  | 119.20      | 113.80   |
| 1   | M     | 124 | LYS  | CA-C-O     | 5.40  | 126.19      | 119.12   |
| 1   | N     | 290 | ILE  | O-C-N      | -5.40 | 114.72      | 121.84   |
| 1   | H     | 530 | VAL  | O-C-N      | -5.40 | 117.35      | 123.18   |
| 1   | P     | 149 | LEU  | O-C-N      | -5.40 | 115.41      | 122.59   |
| 1   | D     | 461 | ASN  | N-CA-C     | 5.39  | 119.34      | 112.87   |
| 1   | F     | 424 | GLU  | CB-CA-C    | -5.39 | 102.41      | 110.88   |
| 1   | L     | 472 | LYS  | N-CA-C     | 5.39  | 117.91      | 111.71   |
| 1   | R     | 152 | THR  | CA-C-O     | 5.39  | 127.04      | 120.62   |
| 1   | C     | 333 | ARG  | CB-CG-CD   | 5.39  | 123.70      | 111.30   |
| 1   | N     | 29  | LYS  | N-CA-C     | 5.39  | 117.86      | 111.33   |
| 1   | K     | 508 | VAL  | N-CA-C     | 5.39  | 115.59      | 110.42   |
| 1   | Q     | 194 | GLU  | N-CA-C     | -5.39 | 101.16      | 109.52   |
| 1   | C     | 53  | ARG  | NE-CZ-NH2  | -5.39 | 114.35      | 119.20   |
| 1   | M     | 435 | GLN  | CB-CG-CD   | -5.39 | 103.44      | 112.60   |
| 1   | N     | 74  | THR  | N-CA-C     | 5.39  | 117.85      | 111.33   |
| 1   | A     | 250 | ASP  | N-CA-CB    | -5.39 | 102.20      | 110.44   |
| 1   | L     | 414 | ALA  | O-C-N      | -5.39 | 116.81      | 123.44   |
| 1   | O     | 135 | TYR  | CB-CG-CD2  | 5.39  | 128.88      | 120.80   |
| 1   | S     | 344 | ASP  | CA-CB-CG   | -5.39 | 107.21      | 112.60   |
| 1   | A     | 108 | VAL  | CA-C-O     | -5.39 | 115.07      | 121.05   |
| 1   | E     | 69  | THR  | O-C-N      | -5.39 | 117.22      | 122.99   |
| 1   | E     | 463 | GLY  | O-C-N      | -5.39 | 116.52      | 122.55   |
| 1   | N     | 360 | ARG  | NH1-CZ-NH2 | -5.39 | 112.30      | 119.30   |
| 1   | N     | 462 | ALA  | CA-C-O     | 5.39  | 126.15      | 119.79   |
| 1   | R     | 69  | THR  | O-C-N      | 5.39  | 128.75      | 122.99   |
| 1   | B     | 65  | ASP  | CA-CB-CG   | -5.38 | 107.22      | 112.60   |
| 1   | N     | 170 | SER  | N-CA-C     | 5.38  | 118.95      | 112.38   |
| 1   | P     | 70  | ASN  | O-C-N      | 5.38  | 128.24      | 122.05   |
| 1   | Q     | 483 | LYS  | CG-CD-CE   | 5.38  | 123.68      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | S     | 112 | GLY  | CA-C-N     | 5.38  | 127.94      | 120.29   |
| 1   | S     | 112 | GLY  | C-N-CA     | 5.38  | 127.94      | 120.29   |
| 1   | D     | 525 | ARG  | N-CA-C     | 5.38  | 117.90      | 111.71   |
| 1   | A     | 83  | HIS  | CB-CG-CD2  | 5.38  | 138.20      | 131.20   |
| 1   | K     | 104 | THR  | CA-CB-CG2  | 5.38  | 119.65      | 110.50   |
| 1   | K     | 254 | GLU  | CA-C-O     | 5.38  | 126.90      | 120.28   |
| 1   | L     | 344 | ASP  | CA-C-N     | 5.38  | 130.38      | 121.99   |
| 1   | L     | 344 | ASP  | C-N-CA     | 5.38  | 130.38      | 121.99   |
| 1   | L     | 458 | LEU  | CA-C-O     | -5.38 | 115.17      | 120.82   |
| 1   | N     | 389 | ARG  | NE-CZ-NH1  | 5.38  | 126.88      | 121.50   |
| 1   | G     | 456 | SER  | CA-C-N     | 5.38  | 127.83      | 120.46   |
| 1   | G     | 456 | SER  | C-N-CA     | 5.38  | 127.83      | 120.46   |
| 1   | D     | 420 | ALA  | O-C-N      | -5.38 | 116.44      | 122.03   |
| 1   | G     | 375 | ASN  | CA-CB-CG   | -5.38 | 107.22      | 112.60   |
| 1   | N     | 92  | ILE  | CB-CA-C    | -5.38 | 105.03      | 112.24   |
| 1   | O     | 345 | GLU  | N-CA-CB    | -5.38 | 103.20      | 110.95   |
| 1   | S     | 187 | LYS  | CA-C-N     | 5.38  | 127.49      | 120.28   |
| 1   | S     | 187 | LYS  | C-N-CA     | 5.38  | 127.49      | 120.28   |
| 1   | F     | 407 | ASP  | CA-CB-CG   | -5.38 | 107.22      | 112.60   |
| 1   | G     | 344 | ASP  | O-C-N      | -5.38 | 113.77      | 122.42   |
| 1   | R     | 285 | GLU  | CA-C-N     | 5.38  | 127.75      | 120.38   |
| 1   | R     | 285 | GLU  | C-N-CA     | 5.38  | 127.75      | 120.38   |
| 1   | R     | 229 | ASP  | CA-CB-CG   | 5.38  | 117.97      | 112.60   |
| 1   | C     | 158 | THR  | CA-CB-OG1  | 5.37  | 117.66      | 109.60   |
| 1   | F     | 51  | GLY  | O-C-N      | -5.37 | 116.40      | 121.77   |
| 1   | H     | 385 | GLY  | CA-C-O     | 5.37  | 127.51      | 122.57   |
| 1   | L     | 61  | ASP  | N-CA-C     | 5.37  | 117.26      | 110.33   |
| 1   | C     | 447 | TYR  | CA-C-N     | 5.37  | 127.75      | 120.44   |
| 1   | C     | 447 | TYR  | C-N-CA     | 5.37  | 127.75      | 120.44   |
| 1   | H     | 251 | ALA  | CA-C-N     | 5.37  | 128.34      | 120.71   |
| 1   | H     | 251 | ALA  | C-N-CA     | 5.37  | 128.34      | 120.71   |
| 1   | F     | 55  | MET  | CA-C-N     | 5.37  | 128.50      | 120.87   |
| 1   | F     | 55  | MET  | C-N-CA     | 5.37  | 128.50      | 120.87   |
| 1   | B     | 426 | ALA  | N-CA-C     | -5.37 | 102.72      | 111.04   |
| 1   | K     | 325 | LYS  | O-C-N      | -5.37 | 115.94      | 122.22   |
| 1   | R     | 413 | ARG  | NH1-CZ-NH2 | -5.37 | 112.32      | 119.30   |
| 1   | K     | 281 | ASN  | CA-CB-CG   | -5.37 | 107.23      | 112.60   |
| 1   | E     | 154 | SER  | N-CA-C     | 5.37  | 116.14      | 108.74   |
| 1   | M     | 111 | SER  | N-CA-C     | -5.37 | 105.12      | 110.97   |
| 1   | P     | 526 | ILE  | CB-CA-C    | -5.37 | 105.44      | 111.23   |
| 1   | Q     | 69  | THR  | O-C-N      | -5.37 | 116.64      | 122.92   |
| 1   | A     | 179 | GLU  | CA-C-N     | 5.36  | 127.41      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 179 | GLU  | C-N-CA     | 5.36  | 127.41      | 120.44   |
| 1   | F     | 320 | VAL  | O-C-N      | -5.36 | 117.36      | 123.10   |
| 1   | Q     | 449 | ASN  | CA-C-N     | 5.36  | 127.47      | 120.28   |
| 1   | Q     | 449 | ASN  | C-N-CA     | 5.36  | 127.47      | 120.28   |
| 1   | C     | 184 | ILE  | CA-C-N     | 5.36  | 128.09      | 120.53   |
| 1   | C     | 184 | ILE  | C-N-CA     | 5.36  | 128.09      | 120.53   |
| 1   | I     | 374 | LYS  | N-CA-C     | 5.36  | 116.81      | 111.07   |
| 1   | A     | 69  | THR  | CA-C-O     | 5.36  | 127.04      | 121.36   |
| 1   | C     | 455 | VAL  | CA-C-N     | 5.36  | 127.41      | 120.44   |
| 1   | C     | 455 | VAL  | C-N-CA     | 5.36  | 127.41      | 120.44   |
| 1   | D     | 111 | SER  | N-CA-C     | 5.36  | 116.81      | 111.07   |
| 1   | L     | 172 | LYS  | O-C-N      | -5.36 | 116.97      | 123.03   |
| 1   | L     | 510 | MET  | N-CA-C     | -5.36 | 106.80      | 113.55   |
| 1   | O     | 530 | VAL  | O-C-N      | -5.36 | 117.40      | 122.98   |
| 1   | R     | 251 | ALA  | N-CA-CB    | -5.36 | 102.45      | 110.17   |
| 1   | R     | 411 | ASP  | O-C-N      | -5.36 | 115.46      | 122.59   |
| 1   | I     | 393 | GLU  | N-CA-CB    | -5.36 | 101.66      | 110.40   |
| 1   | L     | 328 | LEU  | CA-C-O     | 5.36  | 126.23      | 120.55   |
| 1   | B     | 259 | GLU  | N-CA-CB    | -5.36 | 102.42      | 110.73   |
| 1   | E     | 525 | ARG  | NE-CZ-NH1  | 5.36  | 126.86      | 121.50   |
| 1   | K     | 399 | ARG  | NE-CZ-NH2  | 5.36  | 124.02      | 119.20   |
| 1   | K     | 439 | LYS  | CA-C-N     | 5.36  | 128.20      | 120.38   |
| 1   | K     | 439 | LYS  | C-N-CA     | 5.36  | 128.20      | 120.38   |
| 1   | N     | 450 | ALA  | O-C-N      | -5.36 | 116.44      | 122.12   |
| 1   | F     | 176 | GLY  | N-CA-C     | 5.36  | 118.53      | 111.03   |
| 1   | M     | 87  | LYS  | CA-C-N     | 5.36  | 127.89      | 120.29   |
| 1   | M     | 87  | LYS  | C-N-CA     | 5.36  | 127.89      | 120.29   |
| 1   | O     | 111 | SER  | CB-CA-C    | -5.36 | 102.71      | 110.96   |
| 1   | N     | 321 | ARG  | NE-CZ-NH2  | -5.35 | 114.38      | 119.20   |
| 1   | O     | 106 | THR  | CA-C-O     | -5.35 | 115.39      | 120.90   |
| 1   | A     | 404 | THR  | N-CA-C     | 5.35  | 116.80      | 111.07   |
| 1   | C     | 449 | ASN  | CA-CB-CG   | -5.35 | 107.25      | 112.60   |
| 1   | E     | 53  | ARG  | CB-CA-C    | -5.35 | 101.15      | 110.09   |
| 1   | K     | 221 | GLN  | N-CA-C     | 5.35  | 117.21      | 109.07   |
| 1   | P     | 125 | ASP  | N-CA-C     | 5.35  | 119.11      | 112.58   |
| 1   | Q     | 192 | VAL  | CA-C-O     | 5.35  | 125.54      | 119.92   |
| 1   | Q     | 319 | ALA  | CA-C-N     | 5.35  | 130.45      | 123.06   |
| 1   | Q     | 319 | ALA  | C-N-CA     | 5.35  | 130.45      | 123.06   |
| 1   | D     | 321 | ARG  | NH1-CZ-NH2 | -5.35 | 112.34      | 119.30   |
| 1   | D     | 348 | GLU  | N-CA-CB    | -5.35 | 101.98      | 110.22   |
| 1   | Q     | 321 | ARG  | NE-CZ-NH1  | -5.35 | 116.15      | 121.50   |
| 1   | C     | 493 | GLN  | CA-C-O     | -5.35 | 112.83      | 120.16   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 119 | GLU  | CB-CG-CD  | -5.35 | 103.51      | 112.60   |
| 1   | E     | 126 | VAL  | N-CA-CB   | 5.35  | 117.10      | 111.00   |
| 1   | E     | 283 | ILE  | O-C-N     | -5.35 | 116.32      | 121.83   |
| 1   | I     | 229 | ASP  | N-CA-C    | 5.35  | 119.52      | 113.15   |
| 1   | N     | 459 | ILE  | O-C-N     | -5.35 | 116.67      | 121.91   |
| 1   | P     | 511 | ASN  | CA-C-N    | 5.35  | 127.39      | 120.44   |
| 1   | P     | 511 | ASN  | C-N-CA    | 5.35  | 127.39      | 120.44   |
| 1   | B     | 342 | ASN  | O-C-N     | -5.35 | 116.19      | 123.14   |
| 1   | G     | 442 | LEU  | CA-C-O    | 5.35  | 126.41      | 120.63   |
| 1   | H     | 221 | GLN  | O-C-N     | -5.35 | 117.70      | 123.42   |
| 1   | C     | 149 | LEU  | CA-C-N    | 5.34  | 128.69      | 121.05   |
| 1   | C     | 149 | LEU  | C-N-CA    | 5.34  | 128.69      | 121.05   |
| 1   | D     | 270 | THR  | CA-C-O    | 5.34  | 126.22      | 120.55   |
| 1   | L     | 115 | VAL  | CA-C-N    | 5.34  | 127.70      | 120.65   |
| 1   | L     | 115 | VAL  | C-N-CA    | 5.34  | 127.70      | 120.65   |
| 1   | M     | 325 | LYS  | CA-C-N    | 5.34  | 128.18      | 120.38   |
| 1   | M     | 325 | LYS  | C-N-CA    | 5.34  | 128.18      | 120.38   |
| 1   | S     | 73  | ALA  | N-CA-C    | 5.34  | 117.54      | 111.02   |
| 1   | C     | 433 | ALA  | CA-C-N    | 5.34  | 126.52      | 119.84   |
| 1   | C     | 433 | ALA  | C-N-CA    | 5.34  | 126.52      | 119.84   |
| 1   | E     | 170 | SER  | CA-C-N    | 5.34  | 129.76      | 120.68   |
| 1   | E     | 170 | SER  | C-N-CA    | 5.34  | 129.76      | 120.68   |
| 1   | L     | 322 | ARG  | NE-CZ-NH2 | -5.34 | 114.39      | 119.20   |
| 1   | B     | 57  | LYS  | N-CA-CB   | 5.34  | 119.33      | 110.52   |
| 1   | B     | 248 | LEU  | N-CA-CB   | -5.34 | 102.88      | 110.46   |
| 1   | C     | 425 | ILE  | O-C-N     | -5.34 | 116.51      | 121.90   |
| 1   | D     | 321 | ARG  | NE-CZ-NH2 | 5.34  | 124.01      | 119.20   |
| 1   | D     | 466 | PRO  | N-CA-CB   | 5.34  | 108.97      | 103.15   |
| 1   | F     | 198 | ASP  | CB-CA-C   | 5.34  | 119.47      | 111.89   |
| 1   | I     | 148 | GLU  | CB-CG-CD  | 5.34  | 121.68      | 112.60   |
| 1   | N     | 378 | SER  | CA-C-N    | 5.34  | 130.61      | 122.92   |
| 1   | N     | 378 | SER  | C-N-CA    | 5.34  | 130.61      | 122.92   |
| 1   | P     | 351 | LEU  | CA-C-O    | 5.34  | 127.74      | 121.87   |
| 1   | Q     | 145 | THR  | CA-CB-CG2 | 5.34  | 119.58      | 110.50   |
| 1   | S     | 409 | ILE  | CA-C-O    | 5.34  | 126.51      | 120.85   |
| 1   | B     | 380 | SER  | CA-C-N    | -5.34 | 115.69      | 123.06   |
| 1   | B     | 380 | SER  | C-N-CA    | -5.34 | 115.69      | 123.06   |
| 1   | B     | 433 | ALA  | CA-C-N    | 5.34  | 126.51      | 119.84   |
| 1   | B     | 433 | ALA  | C-N-CA    | 5.34  | 126.51      | 119.84   |
| 1   | I     | 502 | VAL  | N-CA-CB   | -5.34 | 106.34      | 111.89   |
| 1   | B     | 396 | ARG  | CD-NE-CZ  | 5.34  | 131.87      | 124.40   |
| 1   | C     | 283 | ILE  | CA-C-N    | 5.34  | 127.97      | 120.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 283 | ILE  | C-N-CA     | 5.34  | 127.97      | 120.28   |
| 1   | H     | 172 | LYS  | O-C-N      | -5.34 | 116.77      | 122.85   |
| 1   | I     | 402 | LEU  | O-C-N      | 5.34  | 127.85      | 122.09   |
| 1   | K     | 435 | GLN  | CA-C-O     | 5.34  | 125.52      | 119.27   |
| 1   | N     | 35  | ASN  | CA-C-N     | 5.34  | 127.48      | 120.60   |
| 1   | N     | 35  | ASN  | C-N-CA     | 5.34  | 127.48      | 120.60   |
| 1   | B     | 271 | GLN  | CA-C-N     | 5.33  | 128.21      | 120.79   |
| 1   | B     | 271 | GLN  | C-N-CA     | 5.33  | 128.21      | 120.79   |
| 1   | B     | 441 | GLN  | CA-C-N     | 5.33  | 127.69      | 120.38   |
| 1   | B     | 441 | GLN  | C-N-CA     | 5.33  | 127.69      | 120.38   |
| 1   | F     | 421 | VAL  | CA-C-N     | 5.33  | 131.73      | 121.54   |
| 1   | F     | 421 | VAL  | C-N-CA     | 5.33  | 131.73      | 121.54   |
| 1   | P     | 126 | VAL  | CB-CA-C    | -5.33 | 104.22      | 111.15   |
| 1   | B     | 216 | SER  | O-C-N      | -5.33 | 116.97      | 123.16   |
| 1   | N     | 257 | LYS  | CA-C-O     | -5.33 | 114.21      | 119.49   |
| 1   | O     | 62  | SER  | N-CA-C     | -5.33 | 106.28      | 112.89   |
| 1   | O     | 320 | VAL  | O-C-N      | -5.33 | 117.42      | 123.18   |
| 1   | O     | 329 | GLU  | CA-C-N     | 5.33  | 127.96      | 120.28   |
| 1   | O     | 329 | GLU  | C-N-CA     | 5.33  | 127.96      | 120.28   |
| 1   | O     | 420 | ALA  | N-CA-C     | 5.33  | 117.52      | 111.02   |
| 1   | P     | 63  | LEU  | N-CA-CB    | -5.33 | 102.76      | 110.70   |
| 1   | P     | 206 | ASN  | N-CA-CB    | -5.33 | 102.84      | 110.57   |
| 1   | B     | 275 | PHE  | N-CA-C     | -5.33 | 103.41      | 111.56   |
| 1   | K     | 514 | LYS  | CA-C-N     | 5.33  | 127.69      | 120.65   |
| 1   | K     | 514 | LYS  | C-N-CA     | 5.33  | 127.69      | 120.65   |
| 1   | M     | 448 | ALA  | CA-C-N     | 5.33  | 127.37      | 120.44   |
| 1   | M     | 448 | ALA  | C-N-CA     | 5.33  | 127.37      | 120.44   |
| 1   | C     | 83  | HIS  | CA-C-O     | 5.33  | 123.26      | 119.32   |
| 1   | K     | 273 | GLN  | OE1-CD-NE2 | 5.33  | 127.93      | 122.60   |
| 1   | K     | 407 | ASP  | CA-C-N     | 5.33  | 127.27      | 120.56   |
| 1   | K     | 407 | ASP  | C-N-CA     | 5.33  | 127.27      | 120.56   |
| 1   | L     | 155 | ILE  | N-CA-C     | 5.33  | 118.52      | 111.17   |
| 1   | M     | 255 | VAL  | N-CA-C     | 5.33  | 116.56      | 109.37   |
| 1   | Q     | 460 | GLU  | CB-CA-C    | -5.33 | 102.00      | 110.84   |
| 1   | Q     | 53  | ARG  | CA-C-N     | 5.33  | 126.25      | 120.44   |
| 1   | Q     | 53  | ARG  | C-N-CA     | 5.33  | 126.25      | 120.44   |
| 1   | D     | 257 | LYS  | O-C-N      | -5.33 | 115.47      | 121.43   |
| 1   | E     | 523 | VAL  | N-CA-C     | 5.33  | 116.05      | 110.62   |
| 1   | Q     | 493 | GLN  | OE1-CD-NE2 | -5.33 | 117.27      | 122.60   |
| 1   | D     | 206 | ASN  | OD1-CG-ND2 | -5.32 | 117.28      | 122.60   |
| 1   | K     | 239 | LYS  | CA-CB-CG   | 5.32  | 124.75      | 114.10   |
| 1   | O     | 255 | VAL  | CA-CB-CG1  | 5.32  | 119.45      | 110.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | Q     | 440 | GLU  | CA-CB-CG    | 5.32  | 124.75      | 114.10   |
| 1   | R     | 421 | VAL  | CA-CB-CG2   | -5.32 | 101.35      | 110.40   |
| 1   | C     | 474 | ARG  | NE-CZ-NH1   | -5.32 | 116.18      | 121.50   |
| 1   | O     | 127 | HIS  | CA-C-N      | 5.32  | 125.13      | 119.28   |
| 1   | O     | 127 | HIS  | C-N-CA      | 5.32  | 125.13      | 119.28   |
| 1   | C     | 38  | ALA  | CB-CA-C     | 5.32  | 119.32      | 110.81   |
| 1   | C     | 303 | GLY  | N-CA-C      | 5.32  | 121.24      | 112.30   |
| 1   | H     | 56  | ASP  | N-CA-CB     | 5.32  | 118.85      | 110.23   |
| 1   | L     | 476 | THR  | CA-C-O      | 5.32  | 126.09      | 119.12   |
| 1   | N     | 326 | SER  | N-CA-C      | 5.32  | 118.56      | 111.75   |
| 1   | R     | 55  | MET  | CA-C-N      | 5.32  | 128.64      | 120.82   |
| 1   | R     | 55  | MET  | C-N-CA      | 5.32  | 128.64      | 120.82   |
| 1   | R     | 482 | ASN  | OD1-CG-ND2  | 5.32  | 127.92      | 122.60   |
| 1   | P     | 261 | ASP  | O-C-N       | -5.32 | 116.28      | 122.03   |
| 1   | Q     | 272 | MET  | CG-SD-CE    | -5.32 | 89.20       | 100.90   |
| 1   | C     | 78  | LYS  | CA-C-O      | 5.32  | 126.09      | 119.12   |
| 1   | F     | 120 | ASP  | N-CA-CB     | -5.32 | 102.04      | 110.28   |
| 1   | F     | 508 | VAL  | N-CA-CB     | 5.32  | 116.77      | 110.55   |
| 1   | G     | 32  | VAL  | N-CA-C      | 5.32  | 118.51      | 111.17   |
| 1   | I     | 183 | ASP  | CA-C-N      | 5.32  | 127.26      | 120.56   |
| 1   | I     | 183 | ASP  | C-N-CA      | 5.32  | 127.26      | 120.56   |
| 1   | L     | 382 | LEU  | CA-C-N      | 5.32  | 131.01      | 122.50   |
| 1   | L     | 382 | LEU  | C-N-CA      | 5.32  | 131.01      | 122.50   |
| 1   | B     | 281 | ASN  | CA-C-O      | 5.32  | 125.92      | 119.38   |
| 1   | D     | 243 | ASN  | OD1-CG-ND2  | -5.32 | 117.28      | 122.60   |
| 1   | E     | 396 | ARG  | CA-C-N      | 5.32  | 127.66      | 120.38   |
| 1   | E     | 396 | ARG  | C-N-CA      | 5.32  | 127.66      | 120.38   |
| 1   | H     | 150 | ALA  | O-C-N       | -5.32 | 116.59      | 122.86   |
| 1   | O     | 327 | ASP  | CA-C-O      | 5.32  | 124.99      | 119.14   |
| 1   | C     | 119 | GLU  | O-C-N       | 5.31  | 127.75      | 122.12   |
| 1   | G     | 158 | THR  | N-CA-C      | -5.31 | 106.30      | 112.89   |
| 1   | O     | 33  | ARG  | CG-CD-NE    | -5.31 | 100.31      | 112.00   |
| 1   | C     | 511 | ASN  | OD1-CG-ND2  | -5.31 | 117.29      | 122.60   |
| 1   | D     | 364 | GLU  | O-C-N       | -5.31 | 115.82      | 122.35   |
| 1   | F     | 164 | ILE  | N-CA-C      | 5.31  | 120.39      | 109.34   |
| 1   | F     | 274 | LYS  | N-CA-C      | 5.31  | 122.11      | 110.80   |
| 1   | G     | 434 | PRO  | CA-N-CD     | -5.31 | 104.56      | 112.00   |
| 1   | H     | 107 | ALA  | N-CA-C      | 5.31  | 120.13      | 111.37   |
| 1   | H     | 184 | ILE  | N-CA-CB     | 5.31  | 116.41      | 110.51   |
| 1   | K     | 477 | HIS  | CE1-NE2-CD2 | -5.31 | 103.69      | 109.00   |
| 1   | N     | 508 | VAL  | CA-CB-CG1   | 5.31  | 119.43      | 110.40   |
| 1   | O     | 153 | VAL  | N-CA-C      | 5.31  | 116.96      | 108.89   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 69  | THR  | CA-CB-OG1  | 5.31  | 117.57      | 109.60   |
| 1   | R     | 73  | ALA  | CA-C-N     | 5.31  | 127.66      | 120.38   |
| 1   | R     | 73  | ALA  | C-N-CA     | 5.31  | 127.66      | 120.38   |
| 1   | A     | 298 | ILE  | CA-C-O     | 5.31  | 127.42      | 120.78   |
| 1   | B     | 287 | VAL  | N-CA-C     | 5.31  | 115.52      | 110.42   |
| 1   | D     | 496 | ASP  | CA-CB-CG   | 5.31  | 117.91      | 112.60   |
| 1   | K     | 487 | ILE  | CB-CA-C    | -5.31 | 104.09      | 110.99   |
| 1   | S     | 520 | ALA  | N-CA-C     | 5.31  | 117.50      | 111.02   |
| 1   | B     | 321 | ARG  | NH1-CZ-NH2 | 5.31  | 126.20      | 119.30   |
| 1   | M     | 220 | THR  | N-CA-CB    | 5.31  | 117.84      | 109.83   |
| 1   | P     | 459 | ILE  | CA-C-N     | 5.31  | 129.63      | 121.19   |
| 1   | P     | 459 | ILE  | C-N-CA     | 5.31  | 129.63      | 121.19   |
| 1   | B     | 424 | GLU  | CA-C-N     | 5.31  | 128.85      | 120.47   |
| 1   | B     | 424 | GLU  | C-N-CA     | 5.31  | 128.85      | 120.47   |
| 1   | H     | 239 | LYS  | N-CA-C     | 5.31  | 117.97      | 111.82   |
| 1   | L     | 144 | GLN  | N-CA-C     | 5.31  | 118.85      | 112.38   |
| 1   | M     | 121 | LEU  | CA-C-N     | 5.31  | 127.39      | 120.28   |
| 1   | M     | 121 | LEU  | C-N-CA     | 5.31  | 127.39      | 120.28   |
| 1   | B     | 413 | ARG  | N-CA-C     | 5.30  | 118.05      | 109.40   |
| 1   | B     | 425 | ILE  | CB-CG1-CD1 | -5.30 | 102.66      | 113.80   |
| 1   | D     | 30  | GLU  | N-CA-C     | 5.30  | 122.10      | 110.80   |
| 1   | E     | 515 | ALA  | CA-C-O     | 5.30  | 126.91      | 121.07   |
| 1   | I     | 457 | ILE  | CB-CA-C    | -5.30 | 105.09      | 111.88   |
| 1   | Q     | 347 | SER  | CA-C-O     | 5.30  | 126.98      | 121.36   |
| 1   | C     | 460 | GLU  | CA-C-O     | 5.30  | 127.22      | 121.02   |
| 1   | E     | 196 | ARG  | NE-CZ-NH2  | 5.30  | 123.97      | 119.20   |
| 1   | G     | 405 | VAL  | CB-CA-C    | 5.30  | 119.30      | 112.14   |
| 1   | L     | 195 | LEU  | N-CA-CB    | 5.30  | 117.76      | 109.97   |
| 1   | P     | 488 | ASP  | CA-C-N     | 5.30  | 127.64      | 120.38   |
| 1   | P     | 488 | ASP  | C-N-CA     | 5.30  | 127.64      | 120.38   |
| 1   | S     | 397 | ALA  | O-C-N      | -5.30 | 116.50      | 122.12   |
| 1   | C     | 203 | ASP  | CA-C-O     | 5.30  | 126.56      | 120.84   |
| 1   | H     | 333 | ARG  | CB-CA-C    | -5.30 | 99.99       | 110.27   |
| 1   | I     | 77  | ASP  | O-C-N      | -5.30 | 116.37      | 122.09   |
| 1   | N     | 133 | SER  | CA-C-O     | 5.30  | 126.38      | 120.82   |
| 1   | O     | 424 | GLU  | N-CA-C     | 5.30  | 116.74      | 111.07   |
| 1   | A     | 423 | ILE  | CB-CG1-CD1 | -5.30 | 102.67      | 113.80   |
| 1   | D     | 305 | ASP  | CA-C-N     | 5.30  | 128.36      | 120.31   |
| 1   | D     | 305 | ASP  | C-N-CA     | 5.30  | 128.36      | 120.31   |
| 1   | Q     | 144 | GLN  | OE1-CD-NE2 | -5.30 | 117.30      | 122.60   |
| 1   | S     | 508 | VAL  | CA-C-O     | -5.30 | 115.55      | 121.17   |
| 1   | B     | 320 | VAL  | O-C-N      | -5.30 | 117.48      | 123.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | E     | 309 | GLN  | CB-CG-CD    | -5.30 | 103.59      | 112.60   |
| 1   | F     | 269 | PRO  | N-CD-CG     | 5.30  | 111.14      | 103.20   |
| 1   | G     | 61  | ASP  | N-CA-C      | 5.30  | 117.91      | 110.23   |
| 1   | L     | 491 | ALA  | CA-C-O      | 5.30  | 126.03      | 120.42   |
| 1   | N     | 458 | LEU  | N-CA-CB     | -5.30 | 102.33      | 110.01   |
| 1   | S     | 246 | ILE  | CA-C-O      | 5.30  | 127.19      | 121.36   |
| 1   | D     | 240 | ARG  | O-C-N       | -5.29 | 117.35      | 123.33   |
| 1   | L     | 83  | HIS  | ND1-CE1-NE2 | 5.29  | 113.69      | 108.40   |
| 1   | L     | 209 | ILE  | CA-C-O      | 5.29  | 125.50      | 120.31   |
| 1   | M     | 307 | VAL  | O-C-N       | -5.29 | 114.85      | 121.84   |
| 1   | F     | 186 | VAL  | N-CA-C      | 5.29  | 115.50      | 110.42   |
| 1   | M     | 467 | ILE  | O-C-N       | 5.29  | 127.10      | 121.91   |
| 1   | P     | 338 | ARG  | CD-NE-CZ    | -5.29 | 116.99      | 124.40   |
| 1   | B     | 67  | THR  | CA-CB-OG1   | 5.29  | 117.54      | 109.60   |
| 1   | E     | 187 | LYS  | N-CA-C      | 5.29  | 116.73      | 111.07   |
| 1   | F     | 161 | LEU  | CA-C-N      | 5.29  | 127.90      | 120.28   |
| 1   | F     | 161 | LEU  | C-N-CA      | 5.29  | 127.90      | 120.28   |
| 1   | F     | 301 | GLN  | OE1-CD-NE2  | -5.29 | 117.31      | 122.60   |
| 1   | G     | 391 | VAL  | CA-C-O      | 5.29  | 126.45      | 120.95   |
| 1   | K     | 166 | MET  | CG-SD-CE    | -5.29 | 89.26       | 100.90   |
| 1   | L     | 172 | LYS  | CA-C-N      | 5.29  | 127.37      | 120.28   |
| 1   | L     | 172 | LYS  | C-N-CA      | 5.29  | 127.37      | 120.28   |
| 1   | O     | 36  | ILE  | CA-C-N      | 5.29  | 129.60      | 121.19   |
| 1   | O     | 36  | ILE  | C-N-CA      | 5.29  | 129.60      | 121.19   |
| 1   | P     | 210 | VAL  | N-CA-C      | -5.29 | 100.86      | 108.48   |
| 1   | F     | 374 | LYS  | N-CA-C      | 5.29  | 117.05      | 111.28   |
| 1   | M     | 246 | ILE  | N-CA-CB     | -5.29 | 101.62      | 110.14   |
| 1   | M     | 522 | LEU  | N-CA-C      | 5.29  | 117.12      | 111.36   |
| 1   | G     | 299 | ILE  | CA-CB-CG2   | -5.29 | 101.51      | 110.50   |
| 1   | Q     | 213 | ALA  | CB-CA-C     | 5.29  | 119.08      | 109.62   |
| 1   | M     | 439 | LYS  | N-CA-C      | -5.29 | 105.60      | 111.36   |
| 1   | O     | 371 | GLU  | O-C-N       | -5.29 | 116.76      | 122.79   |
| 1   | G     | 504 | GLU  | CA-C-O      | -5.28 | 114.52      | 119.91   |
| 1   | L     | 471 | MET  | CB-CA-C     | 5.28  | 119.25      | 110.90   |
| 1   | O     | 31  | ALA  | N-CA-C      | 5.28  | 118.19      | 111.69   |
| 1   | F     | 127 | HIS  | CA-C-N      | 5.28  | 125.09      | 119.28   |
| 1   | F     | 127 | HIS  | C-N-CA      | 5.28  | 125.09      | 119.28   |
| 1   | Q     | 369 | PHE  | CA-CB-CG    | -5.28 | 108.52      | 113.80   |
| 1   | S     | 158 | THR  | N-CA-C      | -5.28 | 106.34      | 112.89   |
| 1   | B     | 516 | ALA  | CB-CA-C     | 5.28  | 119.26      | 110.81   |
| 1   | E     | 361 | LYS  | CA-C-O      | 5.28  | 126.01      | 120.36   |
| 1   | L     | 101 | ALA  | CA-C-N      | 5.28  | 129.23      | 120.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | L     | 101 | ALA  | C-N-CA      | 5.28  | 129.23      | 120.94   |
| 1   | R     | 138 | ALA  | CA-C-N      | 5.28  | 127.31      | 120.44   |
| 1   | R     | 138 | ALA  | C-N-CA      | 5.28  | 127.31      | 120.44   |
| 1   | S     | 493 | GLN  | O-C-N       | -5.28 | 115.25      | 121.32   |
| 1   | E     | 351 | LEU  | CA-C-O      | -5.28 | 115.39      | 121.19   |
| 1   | G     | 249 | ILE  | CA-C-O      | 5.28  | 126.86      | 120.74   |
| 1   | O     | 194 | GLU  | CA-C-O      | 5.28  | 126.88      | 121.23   |
| 1   | Q     | 468 | ASP  | CA-C-N      | 5.28  | 127.78      | 120.29   |
| 1   | Q     | 468 | ASP  | C-N-CA      | 5.28  | 127.78      | 120.29   |
| 1   | S     | 180 | TYR  | CA-C-N      | 5.28  | 127.92      | 120.42   |
| 1   | S     | 180 | TYR  | C-N-CA      | 5.28  | 127.92      | 120.42   |
| 1   | A     | 510 | MET  | CG-SD-CE    | -5.28 | 89.29       | 100.90   |
| 1   | E     | 234 | HIS  | ND1-CE1-NE2 | 5.28  | 113.67      | 108.40   |
| 1   | F     | 397 | ALA  | CA-C-N      | 5.28  | 127.78      | 120.29   |
| 1   | F     | 397 | ALA  | C-N-CA      | 5.28  | 127.78      | 120.29   |
| 1   | G     | 270 | THR  | CA-CB-CG2   | 5.28  | 119.47      | 110.50   |
| 1   | L     | 84  | PRO  | CA-C-N      | 5.28  | 127.66      | 120.54   |
| 1   | L     | 84  | PRO  | C-N-CA      | 5.28  | 127.66      | 120.54   |
| 1   | Q     | 187 | LYS  | CA-C-N      | 5.28  | 127.35      | 120.28   |
| 1   | Q     | 187 | LYS  | C-N-CA      | 5.28  | 127.35      | 120.28   |
| 1   | B     | 247 | ALA  | CA-C-N      | 5.27  | 131.60      | 122.32   |
| 1   | B     | 247 | ALA  | C-N-CA      | 5.27  | 131.60      | 122.32   |
| 1   | S     | 514 | LYS  | CA-C-O      | 5.27  | 126.14      | 120.55   |
| 1   | C     | 395 | GLU  | CA-C-N      | 5.27  | 127.30      | 120.44   |
| 1   | C     | 395 | GLU  | C-N-CA      | 5.27  | 127.30      | 120.44   |
| 1   | M     | 391 | VAL  | CA-CB-CG1   | 5.27  | 119.36      | 110.40   |
| 1   | P     | 208 | GLN  | CB-CA-C     | 5.27  | 118.41      | 109.50   |
| 1   | R     | 314 | LYS  | CA-C-O      | 5.27  | 125.86      | 119.38   |
| 1   | R     | 383 | ILE  | CA-C-N      | 5.27  | 130.99      | 122.29   |
| 1   | R     | 383 | ILE  | C-N-CA      | 5.27  | 130.99      | 122.29   |
| 1   | R     | 469 | LEU  | O-C-N       | -5.27 | 116.53      | 122.12   |
| 1   | A     | 487 | ILE  | CA-C-O      | 5.27  | 126.28      | 120.48   |
| 1   | E     | 214 | GLY  | O-C-N       | -5.27 | 118.21      | 122.64   |
| 1   | A     | 384 | ARG  | NE-CZ-NH1   | 5.27  | 126.77      | 121.50   |
| 1   | F     | 94  | LYS  | CA-C-N      | 5.27  | 131.74      | 121.41   |
| 1   | F     | 94  | LYS  | C-N-CA      | 5.27  | 131.74      | 121.41   |
| 1   | H     | 100 | THR  | CB-CA-C     | -5.27 | 101.42      | 110.22   |
| 1   | L     | 140 | GLU  | CA-C-N      | 5.27  | 127.40      | 120.60   |
| 1   | L     | 140 | GLU  | C-N-CA      | 5.27  | 127.40      | 120.60   |
| 1   | L     | 342 | ASN  | N-CA-CB     | -5.27 | 102.33      | 110.65   |
| 1   | L     | 473 | LEU  | CB-CA-C     | -5.27 | 100.92      | 110.56   |
| 1   | R     | 177 | ALA  | O-C-N       | -5.27 | 115.58      | 122.59   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | R     | 514 | LYS  | CA-C-N    | 5.27  | 127.60      | 120.65   |
| 1   | R     | 514 | LYS  | C-N-CA    | 5.27  | 127.60      | 120.65   |
| 1   | A     | 423 | ILE  | O-C-N     | -5.27 | 116.58      | 121.90   |
| 1   | C     | 314 | LYS  | O-C-N     | -5.27 | 115.37      | 122.43   |
| 1   | H     | 394 | THR  | O-C-N     | -5.27 | 115.79      | 122.27   |
| 1   | N     | 121 | LEU  | CA-C-N    | 5.27  | 127.34      | 120.28   |
| 1   | N     | 121 | LEU  | C-N-CA    | 5.27  | 127.34      | 120.28   |
| 1   | P     | 200 | TRP  | CB-CG-CD2 | -5.27 | 119.43      | 126.80   |
| 1   | R     | 137 | LYS  | CA-C-N    | 5.27  | 127.77      | 120.29   |
| 1   | R     | 137 | LYS  | C-N-CA    | 5.27  | 127.77      | 120.29   |
| 1   | R     | 353 | TYR  | CA-C-O    | 5.27  | 126.29      | 120.71   |
| 1   | B     | 239 | LYS  | N-CA-C    | 5.26  | 117.93      | 111.82   |
| 1   | C     | 527 | ASP  | CA-CB-CG  | -5.26 | 107.33      | 112.60   |
| 1   | E     | 84  | PRO  | N-CA-CB   | 5.26  | 108.89      | 103.15   |
| 1   | S     | 375 | ASN  | CA-C-O    | -5.26 | 115.87      | 119.29   |
| 1   | D     | 49  | THR  | CB-CA-C   | -5.26 | 100.83      | 109.99   |
| 1   | H     | 92  | ILE  | CA-C-O    | 5.26  | 126.43      | 120.85   |
| 1   | H     | 358 | GLU  | CA-C-N    | 5.26  | 130.42      | 123.00   |
| 1   | H     | 358 | GLU  | C-N-CA    | 5.26  | 130.42      | 123.00   |
| 1   | C     | 179 | GLU  | CA-C-O    | -5.26 | 114.95      | 120.63   |
| 1   | E     | 375 | ASN  | O-C-N     | -5.26 | 115.27      | 121.32   |
| 1   | F     | 345 | GLU  | CB-CA-C   | -5.26 | 100.70      | 109.75   |
| 1   | K     | 295 | ALA  | N-CA-C    | 5.26  | 117.08      | 110.24   |
| 1   | M     | 397 | ALA  | N-CA-CB   | -5.26 | 102.10      | 109.94   |
| 1   | Q     | 160 | LEU  | CA-C-O    | 5.26  | 126.89      | 120.31   |
| 1   | K     | 397 | ALA  | CA-C-N    | 5.26  | 127.76      | 120.29   |
| 1   | K     | 397 | ALA  | C-N-CA    | 5.26  | 127.76      | 120.29   |
| 1   | L     | 56  | ASP  | CA-CB-CG  | -5.26 | 107.34      | 112.60   |
| 1   | R     | 37  | ALA  | CA-C-N    | 5.26  | 127.64      | 120.54   |
| 1   | R     | 37  | ALA  | C-N-CA    | 5.26  | 127.64      | 120.54   |
| 1   | E     | 165 | ALA  | CB-CA-C   | -5.26 | 102.59      | 110.90   |
| 1   | F     | 102 | ASP  | N-CA-CB   | -5.26 | 102.74      | 110.26   |
| 1   | H     | 420 | ALA  | N-CA-C    | 5.26  | 117.43      | 111.02   |
| 1   | N     | 453 | SER  | CA-C-N    | 5.26  | 127.27      | 120.44   |
| 1   | N     | 453 | SER  | C-N-CA    | 5.26  | 127.27      | 120.44   |
| 1   | Q     | 319 | ALA  | O-C-N     | -5.26 | 116.36      | 123.19   |
| 1   | H     | 202 | VAL  | CA-C-O    | 5.25  | 125.58      | 120.27   |
| 1   | O     | 453 | SER  | N-CA-C    | 5.25  | 117.69      | 111.33   |
| 1   | A     | 506 | ALA  | N-CA-C    | 5.25  | 119.17      | 112.87   |
| 1   | L     | 399 | ARG  | CG-CD-NE  | -5.25 | 100.44      | 112.00   |
| 1   | P     | 50  | TYR  | CA-C-N    | 5.25  | 130.12      | 121.87   |
| 1   | P     | 50  | TYR  | C-N-CA    | 5.25  | 130.12      | 121.87   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 429 | LEU  | O-C-N      | -5.25 | 116.16      | 122.15   |
| 1   | L     | 161 | LEU  | N-CA-C     | 5.25  | 117.75      | 111.71   |
| 1   | O     | 302 | LYS  | CA-C-N     | 5.25  | 127.89      | 121.06   |
| 1   | O     | 302 | LYS  | C-N-CA     | 5.25  | 127.89      | 121.06   |
| 1   | E     | 445 | GLU  | CA-C-N     | 5.25  | 127.58      | 120.65   |
| 1   | E     | 445 | GLU  | C-N-CA     | 5.25  | 127.58      | 120.65   |
| 1   | N     | 32  | VAL  | CB-CA-C    | -5.25 | 104.39      | 112.05   |
| 1   | A     | 142 | ALA  | N-CA-C     | 5.25  | 117.68      | 111.33   |
| 1   | D     | 179 | GLU  | CA-C-N     | 5.25  | 127.26      | 120.44   |
| 1   | D     | 179 | GLU  | C-N-CA     | 5.25  | 127.26      | 120.44   |
| 1   | E     | 291 | LEU  | CA-C-N     | 5.25  | 129.00      | 120.60   |
| 1   | E     | 291 | LEU  | C-N-CA     | 5.25  | 129.00      | 120.60   |
| 1   | F     | 40  | LYS  | N-CA-CB    | 5.25  | 117.93      | 110.06   |
| 1   | G     | 288 | ASP  | CA-C-O     | 5.25  | 126.03      | 120.10   |
| 1   | L     | 388 | GLU  | O-C-N      | -5.25 | 115.57      | 122.39   |
| 1   | N     | 485 | TYR  | CA-C-O     | 5.25  | 127.03      | 121.05   |
| 1   | Q     | 158 | THR  | O-C-N      | -5.25 | 115.81      | 122.27   |
| 1   | B     | 111 | SER  | N-CA-CB    | 5.25  | 117.57      | 109.91   |
| 1   | E     | 92  | ILE  | CA-CB-CG1  | 5.25  | 119.32      | 110.40   |
| 1   | H     | 234 | HIS  | CA-C-N     | 5.25  | 124.91      | 119.56   |
| 1   | H     | 234 | HIS  | C-N-CA     | 5.25  | 124.91      | 119.56   |
| 1   | K     | 499 | GLN  | O-C-N      | -5.25 | 115.61      | 122.59   |
| 1   | M     | 163 | LYS  | CA-C-O     | -5.25 | 115.29      | 120.80   |
| 1   | P     | 34  | ALA  | CA-C-N     | 5.25  | 128.08      | 120.79   |
| 1   | P     | 34  | ALA  | C-N-CA     | 5.25  | 128.08      | 120.79   |
| 1   | P     | 411 | ASP  | CA-CB-CG   | -5.25 | 107.35      | 112.60   |
| 1   | Q     | 200 | TRP  | CA-C-O     | 5.25  | 127.11      | 121.55   |
| 1   | C     | 218 | ASN  | OD1-CG-ND2 | 5.25  | 127.84      | 122.60   |
| 1   | D     | 226 | ILE  | N-CA-C     | -5.25 | 102.31      | 109.55   |
| 1   | G     | 326 | SER  | CA-C-O     | 5.25  | 126.07      | 120.20   |
| 1   | G     | 438 | GLY  | CA-C-O     | 5.25  | 129.70      | 120.57   |
| 1   | H     | 199 | LYS  | O-C-N      | -5.25 | 117.81      | 123.42   |
| 1   | M     | 437 | GLY  | CA-C-N     | 5.25  | 131.69      | 121.41   |
| 1   | M     | 437 | GLY  | C-N-CA     | 5.25  | 131.69      | 121.41   |
| 1   | Q     | 283 | ILE  | CA-C-O     | -5.25 | 115.29      | 120.85   |
| 1   | R     | 33  | ARG  | N-CA-C     | 5.25  | 116.81      | 111.14   |
| 1   | M     | 500 | LYS  | CA-CB-CG   | 5.24  | 124.59      | 114.10   |
| 1   | Q     | 133 | SER  | CA-C-N     | 5.24  | 131.69      | 121.41   |
| 1   | Q     | 133 | SER  | C-N-CA     | 5.24  | 131.69      | 121.41   |
| 1   | R     | 117 | LYS  | N-CA-C     | 5.24  | 118.78      | 112.38   |
| 1   | O     | 351 | LEU  | N-CA-C     | 5.24  | 117.89      | 110.50   |
| 1   | L     | 361 | LYS  | O-C-N      | -5.24 | 117.11      | 123.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | N     | 476 | THR  | CA-CB-OG1   | 5.24  | 117.46      | 109.60   |
| 1   | O     | 134 | GLY  | CA-C-N      | 5.24  | 127.30      | 120.28   |
| 1   | O     | 134 | GLY  | C-N-CA      | 5.24  | 127.30      | 120.28   |
| 1   | R     | 339 | VAL  | N-CA-CB     | 5.24  | 117.56      | 111.90   |
| 1   | R     | 360 | ARG  | NE-CZ-NH1   | 5.24  | 126.74      | 121.50   |
| 1   | D     | 420 | ALA  | N-CA-C      | 5.24  | 116.68      | 110.97   |
| 1   | E     | 136 | LYS  | N-CA-C      | 5.24  | 117.41      | 111.02   |
| 1   | L     | 83  | HIS  | CE1-NE2-CD2 | -5.24 | 103.76      | 109.00   |
| 1   | L     | 129 | THR  | CA-CB-CG2   | 5.24  | 119.41      | 110.50   |
| 1   | M     | 346 | ILE  | N-CA-C      | 5.24  | 117.00      | 109.51   |
| 1   | Q     | 424 | GLU  | CA-C-O      | 5.24  | 126.30      | 120.90   |
| 1   | R     | 400 | ASP  | CA-C-N      | 5.24  | 127.30      | 120.28   |
| 1   | R     | 400 | ASP  | C-N-CA      | 5.24  | 127.30      | 120.28   |
| 1   | D     | 296 | ASN  | CA-C-N      | 5.24  | 130.13      | 122.69   |
| 1   | D     | 296 | ASN  | C-N-CA      | 5.24  | 130.13      | 122.69   |
| 1   | G     | 246 | ILE  | N-CA-C      | 5.24  | 117.17      | 109.63   |
| 1   | C     | 487 | ILE  | CA-CB-CG1   | 5.24  | 119.30      | 110.40   |
| 1   | H     | 275 | PHE  | O-C-N       | 5.24  | 128.18      | 122.11   |
| 1   | L     | 97  | ASP  | CA-C-O      | 5.24  | 125.33      | 119.41   |
| 1   | O     | 395 | GLU  | CA-C-O      | 5.24  | 125.97      | 120.42   |
| 1   | P     | 388 | GLU  | O-C-N       | -5.24 | 115.58      | 122.39   |
| 1   | L     | 404 | THR  | N-CA-C      | 5.23  | 116.67      | 111.07   |
| 1   | L     | 478 | GLU  | O-C-N       | -5.23 | 116.57      | 122.12   |
| 1   | N     | 381 | ILE  | N-CA-C      | -5.23 | 100.94      | 108.48   |
| 1   | M     | 43  | GLU  | CA-C-N      | 5.23  | 131.53      | 121.54   |
| 1   | M     | 43  | GLU  | C-N-CA      | 5.23  | 131.53      | 121.54   |
| 1   | P     | 456 | SER  | CA-C-N      | 5.23  | 127.91      | 120.53   |
| 1   | P     | 456 | SER  | C-N-CA      | 5.23  | 127.91      | 120.53   |
| 1   | R     | 485 | TYR  | CB-CG-CD1   | 5.23  | 128.65      | 120.80   |
| 1   | E     | 333 | ARG  | CD-NE-CZ    | 5.23  | 131.72      | 124.40   |
| 1   | G     | 144 | GLN  | CA-C-N      | 5.23  | 131.54      | 121.18   |
| 1   | G     | 144 | GLN  | C-N-CA      | 5.23  | 131.54      | 121.18   |
| 1   | N     | 423 | ILE  | CA-C-N      | 5.23  | 127.55      | 120.44   |
| 1   | N     | 423 | ILE  | C-N-CA      | 5.23  | 127.55      | 120.44   |
| 1   | O     | 427 | LYS  | O-C-N       | -5.23 | 116.09      | 122.11   |
| 1   | Q     | 271 | GLN  | CA-C-N      | 5.23  | 128.06      | 120.79   |
| 1   | Q     | 271 | GLN  | C-N-CA      | 5.23  | 128.06      | 120.79   |
| 1   | Q     | 360 | ARG  | O-C-N       | -5.23 | 117.19      | 123.31   |
| 1   | S     | 311 | TYR  | CB-CA-C     | 5.23  | 119.58      | 110.79   |
| 1   | A     | 114 | LEU  | N-CA-C      | -5.23 | 105.66      | 111.36   |
| 1   | E     | 433 | ALA  | CB-CA-C     | 5.23  | 120.47      | 110.17   |
| 1   | G     | 285 | GLU  | CB-CA-C     | -5.23 | 102.85      | 110.95   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | K     | 503 | ILE  | O-C-N     | -5.23 | 117.54      | 123.03   |
| 1   | P     | 155 | ILE  | CA-CB-CG2 | 5.23  | 119.39      | 110.50   |
| 1   | S     | 102 | ASP  | N-CA-C    | -5.23 | 100.08      | 108.55   |
| 1   | F     | 167 | THR  | N-CA-CB   | 5.23  | 119.83      | 110.32   |
| 1   | N     | 144 | GLN  | CG-CD-OE1 | 5.23  | 131.25      | 120.80   |
| 1   | C     | 307 | VAL  | CA-CB-CG2 | 5.22  | 119.28      | 110.40   |
| 1   | E     | 203 | ASP  | CA-C-N    | 5.22  | 128.01      | 120.38   |
| 1   | E     | 203 | ASP  | C-N-CA    | 5.22  | 128.01      | 120.38   |
| 1   | F     | 264 | ILE  | CA-CB-CG2 | -5.22 | 101.62      | 110.50   |
| 1   | K     | 39  | VAL  | O-C-N     | -5.22 | 116.56      | 121.94   |
| 1   | L     | 343 | ILE  | N-CA-C    | 5.22  | 118.38      | 111.17   |
| 1   | C     | 527 | ASP  | N-CA-CB   | -5.22 | 102.48      | 110.26   |
| 1   | I     | 165 | ALA  | CA-C-N    | 5.22  | 127.71      | 120.29   |
| 1   | I     | 165 | ALA  | C-N-CA    | 5.22  | 127.71      | 120.29   |
| 1   | K     | 47  | LYS  | CA-C-O    | 5.22  | 127.98      | 120.51   |
| 1   | M     | 178 | ARG  | NE-CZ-NH1 | -5.22 | 116.28      | 121.50   |
| 1   | O     | 187 | LYS  | CA-C-N    | 5.22  | 127.28      | 120.28   |
| 1   | O     | 187 | LYS  | C-N-CA    | 5.22  | 127.28      | 120.28   |
| 1   | O     | 413 | ARG  | O-C-N     | -5.22 | 116.58      | 123.21   |
| 1   | E     | 319 | ALA  | CA-C-N    | 5.22  | 130.26      | 123.06   |
| 1   | E     | 319 | ALA  | C-N-CA    | 5.22  | 130.26      | 123.06   |
| 1   | I     | 399 | ARG  | CG-CD-NE  | -5.22 | 100.51      | 112.00   |
| 1   | K     | 391 | VAL  | CA-C-O    | 5.22  | 126.38      | 120.95   |
| 1   | E     | 198 | ASP  | CA-CB-CG  | 5.22  | 117.82      | 112.60   |
| 1   | H     | 61  | ASP  | CA-CB-CG  | -5.22 | 107.38      | 112.60   |
| 1   | I     | 58  | MET  | O-C-N     | -5.22 | 116.58      | 123.21   |
| 1   | L     | 163 | LYS  | CA-C-N    | 5.22  | 129.18      | 120.62   |
| 1   | L     | 163 | LYS  | C-N-CA    | 5.22  | 129.18      | 120.62   |
| 1   | Q     | 338 | ARG  | N-CA-CB   | 5.22  | 120.77      | 111.69   |
| 1   | C     | 267 | ASN  | CA-CB-CG  | 5.22  | 117.82      | 112.60   |
| 1   | F     | 503 | ILE  | CA-CB-CG1 | 5.22  | 119.27      | 110.40   |
| 1   | S     | 80  | ASP  | CA-CB-CG  | -5.22 | 107.38      | 112.60   |
| 1   | B     | 57  | LYS  | O-C-N     | -5.22 | 117.09      | 123.19   |
| 1   | B     | 485 | TYR  | N-CA-C    | 5.22  | 118.44      | 110.20   |
| 1   | C     | 330 | LYS  | CA-C-O    | 5.22  | 126.04      | 120.20   |
| 1   | G     | 326 | SER  | CB-CA-C   | -5.22 | 100.34      | 110.46   |
| 1   | H     | 42  | VAL  | CB-CA-C   | -5.22 | 105.10      | 112.14   |
| 1   | L     | 166 | MET  | CA-C-O    | 5.22  | 126.08      | 120.55   |
| 1   | O     | 340 | VAL  | CA-C-N    | 5.22  | 129.50      | 120.58   |
| 1   | O     | 340 | VAL  | C-N-CA    | 5.22  | 129.50      | 120.58   |
| 1   | R     | 477 | HIS  | CA-CB-CG  | -5.22 | 108.58      | 113.80   |
| 1   | R     | 522 | LEU  | O-C-N     | -5.22 | 116.20      | 122.15   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 125 | ASP  | CA-C-O    | 5.21  | 127.44      | 120.98   |
| 1   | G     | 291 | LEU  | CA-C-N    | 5.21  | 130.69      | 120.99   |
| 1   | G     | 291 | LEU  | C-N-CA    | 5.21  | 130.69      | 120.99   |
| 1   | M     | 175 | ALA  | CA-C-N    | 5.21  | 125.29      | 120.34   |
| 1   | M     | 175 | ALA  | C-N-CA    | 5.21  | 125.29      | 120.34   |
| 1   | M     | 268 | ASP  | CA-C-N    | 5.21  | 124.83      | 119.56   |
| 1   | M     | 268 | ASP  | C-N-CA    | 5.21  | 124.83      | 119.56   |
| 1   | R     | 253 | LEU  | CA-C-N    | 5.21  | 130.76      | 122.62   |
| 1   | R     | 253 | LEU  | C-N-CA    | 5.21  | 130.76      | 122.62   |
| 1   | A     | 364 | GLU  | CA-C-O    | 5.21  | 125.98      | 119.78   |
| 1   | D     | 98  | GLU  | CA-C-N    | 5.21  | 127.22      | 120.44   |
| 1   | D     | 98  | GLU  | C-N-CA    | 5.21  | 127.22      | 120.44   |
| 1   | N     | 305 | ASP  | CA-CB-CG  | -5.21 | 107.39      | 112.60   |
| 1   | Q     | 83  | HIS  | CA-CB-CG  | -5.21 | 108.59      | 113.80   |
| 1   | S     | 428 | LYS  | CA-CB-CG  | 5.21  | 124.53      | 114.10   |
| 1   | E     | 244 | ALA  | CA-C-N    | 5.21  | 130.25      | 122.23   |
| 1   | E     | 244 | ALA  | C-N-CA    | 5.21  | 130.25      | 122.23   |
| 1   | L     | 139 | GLU  | CA-C-N    | 5.21  | 128.03      | 120.79   |
| 1   | L     | 139 | GLU  | C-N-CA    | 5.21  | 128.03      | 120.79   |
| 1   | Q     | 135 | TYR  | O-C-N     | -5.21 | 116.59      | 122.12   |
| 1   | S     | 426 | ALA  | CA-C-O    | -5.21 | 115.42      | 120.89   |
| 1   | E     | 431 | LYS  | CA-C-N    | 5.21  | 129.32      | 120.88   |
| 1   | E     | 431 | LYS  | C-N-CA    | 5.21  | 129.32      | 120.88   |
| 1   | H     | 508 | VAL  | O-C-N     | -5.21 | 116.81      | 121.91   |
| 1   | I     | 368 | VAL  | CA-CB-CG1 | 5.21  | 119.26      | 110.40   |
| 1   | L     | 326 | SER  | CB-CA-C   | -5.21 | 100.35      | 110.46   |
| 1   | I     | 30  | GLU  | N-CA-CB   | -5.21 | 101.69      | 110.49   |
| 1   | S     | 161 | LEU  | N-CA-CB   | -5.21 | 102.20      | 110.22   |
| 1   | A     | 268 | ASP  | N-CA-C    | 5.21  | 116.21      | 109.65   |
| 1   | D     | 408 | VAL  | CA-C-N    | 5.21  | 127.81      | 120.42   |
| 1   | D     | 408 | VAL  | C-N-CA    | 5.21  | 127.81      | 120.42   |
| 1   | F     | 312 | LEU  | N-CA-C    | -5.21 | 105.78      | 111.82   |
| 1   | F     | 432 | TYR  | O-C-N     | -5.21 | 116.47      | 122.09   |
| 1   | Q     | 485 | TYR  | CA-C-O    | 5.21  | 126.98      | 121.05   |
| 1   | F     | 234 | HIS  | CB-CG-ND1 | 5.21  | 130.51      | 122.70   |
| 1   | G     | 181 | ILE  | N-CA-C    | -5.21 | 105.46      | 110.72   |
| 1   | I     | 356 | LEU  | CA-C-O    | 5.21  | 126.49      | 120.14   |
| 1   | R     | 417 | GLY  | CA-C-O    | -5.21 | 116.05      | 121.67   |
| 1   | L     | 135 | TYR  | CB-CG-CD2 | 5.20  | 128.60      | 120.80   |
| 1   | N     | 38  | ALA  | CA-C-N    | 5.20  | 127.20      | 120.70   |
| 1   | N     | 38  | ALA  | C-N-CA    | 5.20  | 127.20      | 120.70   |
| 1   | N     | 358 | GLU  | O-C-N     | -5.20 | 117.12      | 123.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 520 | ALA  | N-CA-C     | 5.20  | 117.37      | 111.02   |
| 1   | N     | 386 | GLY  | O-C-N      | -5.20 | 115.94      | 122.70   |
| 1   | A     | 366 | LYS  | CG-CD-CE   | 5.20  | 123.26      | 111.30   |
| 1   | B     | 112 | GLY  | N-CA-C     | 5.20  | 120.34      | 113.37   |
| 1   | H     | 279 | GLU  | CB-CG-CD   | 5.20  | 121.44      | 112.60   |
| 1   | M     | 191 | GLN  | N-CA-C     | 5.20  | 117.03      | 111.36   |
| 1   | O     | 298 | ILE  | CA-C-O     | 5.20  | 127.28      | 120.78   |
| 1   | O     | 474 | ARG  | CA-C-O     | 5.20  | 125.65      | 119.10   |
| 1   | P     | 308 | ALA  | N-CA-C     | 5.20  | 118.89      | 112.54   |
| 1   | R     | 263 | GLU  | CA-C-N     | 5.20  | 128.34      | 120.13   |
| 1   | R     | 263 | GLU  | C-N-CA     | 5.20  | 128.34      | 120.13   |
| 1   | C     | 351 | LEU  | O-C-N      | -5.20 | 117.13      | 123.16   |
| 1   | G     | 58  | MET  | O-C-N      | -5.20 | 117.11      | 123.19   |
| 1   | H     | 140 | GLU  | CB-CA-C    | -5.20 | 102.21      | 110.84   |
| 1   | H     | 160 | LEU  | CB-CA-C    | 5.20  | 120.07      | 110.56   |
| 1   | K     | 164 | ILE  | CA-C-N     | 5.20  | 127.51      | 120.44   |
| 1   | K     | 164 | ILE  | C-N-CA     | 5.20  | 127.51      | 120.44   |
| 1   | K     | 270 | THR  | CA-C-O     | 5.20  | 125.93      | 120.42   |
| 1   | K     | 364 | GLU  | N-CA-C     | -5.20 | 106.53      | 112.92   |
| 1   | L     | 149 | LEU  | CA-C-N     | 5.20  | 128.60      | 120.75   |
| 1   | L     | 149 | LEU  | C-N-CA     | 5.20  | 128.60      | 120.75   |
| 1   | L     | 441 | GLN  | CA-C-N     | 5.20  | 127.50      | 120.38   |
| 1   | L     | 441 | GLN  | C-N-CA     | 5.20  | 127.50      | 120.38   |
| 1   | N     | 297 | VAL  | CA-CB-CG2  | 5.20  | 119.24      | 110.40   |
| 1   | A     | 108 | VAL  | CA-C-N     | 5.20  | 127.58      | 120.77   |
| 1   | A     | 108 | VAL  | C-N-CA     | 5.20  | 127.58      | 120.77   |
| 1   | I     | 461 | ASN  | CA-C-O     | -5.20 | 112.55      | 119.10   |
| 1   | S     | 267 | ASN  | CA-C-O     | 5.20  | 124.21      | 118.65   |
| 1   | B     | 158 | THR  | CA-C-O     | -5.20 | 112.87      | 119.31   |
| 1   | C     | 269 | PRO  | CA-C-O     | 5.20  | 126.28      | 119.00   |
| 1   | H     | 311 | TYR  | CB-CG-CD1  | -5.20 | 113.01      | 120.80   |
| 1   | I     | 366 | LYS  | N-CA-CB    | 5.20  | 119.87      | 110.83   |
| 1   | N     | 306 | GLU  | CA-C-O     | 5.20  | 125.94      | 119.97   |
| 1   | N     | 431 | LYS  | CA-C-N     | 5.20  | 127.51      | 120.44   |
| 1   | N     | 431 | LYS  | C-N-CA     | 5.20  | 127.51      | 120.44   |
| 1   | R     | 181 | ILE  | CA-C-N     | 5.20  | 127.55      | 120.54   |
| 1   | R     | 181 | ILE  | C-N-CA     | 5.20  | 127.55      | 120.54   |
| 1   | R     | 340 | VAL  | CA-C-O     | 5.20  | 126.87      | 120.74   |
| 1   | R     | 456 | SER  | CA-C-N     | 5.20  | 127.30      | 120.60   |
| 1   | R     | 456 | SER  | C-N-CA     | 5.20  | 127.30      | 120.60   |
| 1   | E     | 265 | ARG  | NH1-CZ-NH2 | -5.19 | 112.55      | 119.30   |
| 1   | K     | 186 | VAL  | N-CA-C     | 5.19  | 115.41      | 110.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | Q     | 39  | VAL  | N-CA-CB     | -5.19 | 104.96      | 110.62   |
| 1   | A     | 88  | LEU  | CA-C-N      | 5.19  | 127.50      | 120.65   |
| 1   | A     | 88  | LEU  | C-N-CA      | 5.19  | 127.50      | 120.65   |
| 1   | B     | 467 | ILE  | CA-C-O      | -5.19 | 115.67      | 121.17   |
| 1   | E     | 325 | LYS  | N-CA-C      | 5.19  | 118.40      | 111.75   |
| 1   | E     | 527 | ASP  | N-CA-C      | 5.19  | 118.08      | 111.69   |
| 1   | K     | 383 | ILE  | CB-CA-C     | -5.19 | 104.10      | 111.21   |
| 1   | Q     | 30  | GLU  | O-C-N       | -5.19 | 115.69      | 122.59   |
| 1   | Q     | 53  | ARG  | NE-CZ-NH2   | -5.19 | 114.53      | 119.20   |
| 1   | Q     | 461 | ASN  | N-CA-C      | 5.19  | 119.10      | 112.87   |
| 1   | R     | 188 | ALA  | N-CA-C      | 5.19  | 116.94      | 111.28   |
| 1   | B     | 138 | ALA  | CA-C-N      | 5.19  | 127.19      | 120.44   |
| 1   | B     | 138 | ALA  | C-N-CA      | 5.19  | 127.19      | 120.44   |
| 1   | I     | 33  | ARG  | CA-C-N      | 5.19  | 128.00      | 120.79   |
| 1   | I     | 33  | ARG  | C-N-CA      | 5.19  | 128.00      | 120.79   |
| 1   | K     | 317 | VAL  | O-C-N       | -5.19 | 116.21      | 122.59   |
| 1   | O     | 406 | ALA  | O-C-N       | -5.19 | 116.62      | 122.12   |
| 1   | Q     | 404 | THR  | O-C-N       | -5.19 | 116.69      | 122.09   |
| 1   | B     | 419 | GLY  | CA-C-N      | 5.19  | 128.00      | 120.79   |
| 1   | B     | 419 | GLY  | C-N-CA      | 5.19  | 128.00      | 120.79   |
| 1   | F     | 167 | THR  | O-C-N       | -5.19 | 115.53      | 122.43   |
| 1   | G     | 110 | PHE  | CA-CB-CG    | -5.19 | 108.61      | 113.80   |
| 1   | K     | 77  | ASP  | CB-CA-C     | -5.19 | 102.70      | 110.90   |
| 1   | R     | 100 | THR  | CA-CB-OG1   | 5.19  | 117.38      | 109.60   |
| 1   | D     | 425 | ILE  | CA-C-O      | 5.19  | 126.12      | 120.57   |
| 1   | D     | 487 | ILE  | CA-CB-CG1   | 5.19  | 119.22      | 110.40   |
| 1   | A     | 504 | GLU  | N-CA-C      | 5.18  | 117.58      | 108.82   |
| 1   | D     | 273 | GLN  | CB-CG-CD    | 5.18  | 121.41      | 112.60   |
| 1   | I     | 187 | LYS  | CA-C-O      | 5.18  | 126.05      | 120.55   |
| 1   | I     | 200 | TRP  | CE2-CD2-CE3 | -5.18 | 113.61      | 118.80   |
| 1   | Q     | 477 | HIS  | CA-C-N      | 5.18  | 127.23      | 120.28   |
| 1   | Q     | 477 | HIS  | C-N-CA      | 5.18  | 127.23      | 120.28   |
| 1   | B     | 322 | ARG  | CG-CD-NE    | -5.18 | 100.60      | 112.00   |
| 1   | C     | 448 | ALA  | O-C-N       | 5.18  | 127.69      | 122.09   |
| 1   | C     | 528 | ASP  | CB-CA-C     | -5.18 | 98.90       | 109.94   |
| 1   | R     | 421 | VAL  | CA-CB-CG1   | 5.18  | 119.21      | 110.40   |
| 1   | S     | 444 | VAL  | N-CA-C      | 5.18  | 115.39      | 110.42   |
| 1   | E     | 169 | LEU  | CB-CA-C     | -5.18 | 100.72      | 110.67   |
| 1   | A     | 444 | VAL  | CB-CA-C     | -5.18 | 105.34      | 111.97   |
| 1   | C     | 448 | ALA  | N-CA-C      | -5.18 | 105.55      | 111.14   |
| 1   | E     | 107 | ALA  | N-CA-C      | 5.18  | 121.83      | 110.80   |
| 1   | K     | 527 | ASP  | N-CA-CB     | -5.18 | 102.48      | 110.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 490 | TYR  | CA-CB-CG   | -5.18 | 104.58      | 113.90   |
| 1   | B     | 297 | VAL  | O-C-N      | -5.18 | 117.10      | 123.00   |
| 1   | S     | 146 | ILE  | CB-CA-C    | -5.18 | 104.35      | 111.65   |
| 1   | I     | 471 | MET  | N-CA-C     | 5.17  | 116.61      | 111.07   |
| 1   | I     | 490 | TYR  | CA-CB-CG   | -5.17 | 104.59      | 113.90   |
| 1   | L     | 107 | ALA  | N-CA-C     | 5.17  | 119.91      | 111.37   |
| 1   | O     | 306 | GLU  | N-CA-C     | 5.17  | 117.82      | 111.82   |
| 1   | S     | 122 | LEU  | O-C-N      | -5.17 | 116.64      | 122.12   |
| 1   | D     | 233 | VAL  | N-CA-C     | 5.17  | 115.39      | 110.53   |
| 1   | F     | 381 | ILE  | N-CA-C     | -5.17 | 101.03      | 108.48   |
| 1   | H     | 191 | GLN  | CB-CG-CD   | 5.17  | 121.39      | 112.60   |
| 1   | H     | 460 | GLU  | CA-C-O     | 5.17  | 127.07      | 121.02   |
| 1   | H     | 401 | ALA  | CA-C-N     | 5.17  | 127.16      | 120.44   |
| 1   | H     | 401 | ALA  | C-N-CA     | 5.17  | 127.16      | 120.44   |
| 1   | B     | 495 | VAL  | CB-CA-C    | -5.17 | 102.41      | 110.52   |
| 1   | P     | 93  | ALA  | CA-C-N     | 5.17  | 127.47      | 120.65   |
| 1   | P     | 93  | ALA  | C-N-CA     | 5.17  | 127.47      | 120.65   |
| 1   | P     | 283 | ILE  | CB-CA-C    | -5.17 | 105.31      | 112.24   |
| 1   | Q     | 252 | SER  | N-CA-C     | 5.17  | 117.71      | 109.96   |
| 1   | S     | 423 | ILE  | CA-CB-CG1  | 5.17  | 119.19      | 110.40   |
| 1   | C     | 350 | ASP  | O-C-N      | -5.17 | 115.88      | 122.34   |
| 1   | P     | 69  | THR  | CA-C-O     | 5.17  | 126.84      | 121.31   |
| 1   | H     | 256 | GLU  | CA-C-O     | 5.17  | 125.71      | 120.24   |
| 1   | K     | 291 | LEU  | O-C-N      | -5.17 | 115.33      | 122.46   |
| 1   | D     | 391 | VAL  | CA-C-O     | 5.16  | 126.32      | 120.95   |
| 1   | I     | 108 | VAL  | O-C-N      | 5.16  | 127.27      | 121.90   |
| 1   | M     | 406 | ALA  | CA-C-N     | 5.16  | 128.16      | 120.31   |
| 1   | M     | 406 | ALA  | C-N-CA     | 5.16  | 128.16      | 120.31   |
| 1   | N     | 68  | ILE  | O-C-N      | -5.16 | 117.30      | 123.03   |
| 1   | Q     | 346 | ILE  | N-CA-C     | 5.16  | 117.07      | 109.63   |
| 1   | E     | 371 | GLU  | N-CA-C     | 5.16  | 117.52      | 110.55   |
| 1   | F     | 357 | ILE  | O-C-N      | -5.16 | 117.87      | 123.14   |
| 1   | F     | 514 | LYS  | N-CA-CB    | 5.16  | 117.49      | 110.01   |
| 1   | A     | 119 | GLU  | CA-C-N     | 5.16  | 127.71      | 120.28   |
| 1   | A     | 119 | GLU  | C-N-CA     | 5.16  | 127.71      | 120.28   |
| 1   | C     | 310 | SER  | N-CA-C     | 5.16  | 117.64      | 111.71   |
| 1   | F     | 439 | LYS  | CA-C-O     | -5.16 | 114.95      | 120.42   |
| 1   | H     | 340 | VAL  | CB-CA-C    | -5.16 | 105.66      | 111.23   |
| 1   | H     | 483 | LYS  | CG-CD-CE   | 5.16  | 123.17      | 111.30   |
| 1   | I     | 281 | ASN  | OD1-CG-ND2 | 5.16  | 127.76      | 122.60   |
| 1   | P     | 440 | GLU  | N-CA-CB    | -5.16 | 101.99      | 110.14   |
| 1   | S     | 239 | LYS  | O-C-N      | 5.16  | 127.59      | 122.12   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 137 | LYS  | CA-C-N    | 5.16  | 127.61      | 120.29   |
| 1   | C     | 137 | LYS  | C-N-CA    | 5.16  | 127.61      | 120.29   |
| 1   | K     | 286 | LYS  | CA-C-N    | 5.16  | 127.06      | 120.56   |
| 1   | K     | 286 | LYS  | C-N-CA    | 5.16  | 127.06      | 120.56   |
| 1   | C     | 191 | GLN  | N-CA-C    | 5.16  | 116.98      | 111.36   |
| 1   | C     | 235 | PRO  | N-CA-CB   | 5.16  | 108.35      | 103.19   |
| 1   | F     | 29  | LYS  | O-C-N     | 5.16  | 128.08      | 122.20   |
| 1   | K     | 167 | THR  | O-C-N     | -5.16 | 115.57      | 122.43   |
| 1   | S     | 265 | ARG  | N-CA-C    | -5.16 | 106.30      | 112.59   |
| 1   | S     | 345 | GLU  | O-C-N     | -5.16 | 116.61      | 122.23   |
| 1   | B     | 381 | ILE  | O-C-N     | -5.16 | 117.61      | 123.18   |
| 1   | D     | 427 | LYS  | CA-C-O    | 5.16  | 127.88      | 120.51   |
| 1   | G     | 390 | LEU  | CA-C-N    | 5.16  | 127.52      | 120.46   |
| 1   | G     | 390 | LEU  | C-N-CA    | 5.16  | 127.52      | 120.46   |
| 1   | G     | 504 | GLU  | CA-C-N    | 5.16  | 126.28      | 119.84   |
| 1   | G     | 504 | GLU  | C-N-CA    | 5.16  | 126.28      | 119.84   |
| 1   | H     | 311 | TYR  | CA-C-N    | 5.16  | 128.15      | 120.31   |
| 1   | H     | 311 | TYR  | C-N-CA    | 5.16  | 128.15      | 120.31   |
| 1   | I     | 42  | VAL  | N-CA-C    | 5.16  | 115.88      | 110.62   |
| 1   | N     | 136 | LYS  | O-C-N     | -5.16 | 116.56      | 122.08   |
| 1   | N     | 300 | CYS  | CA-C-O    | 5.16  | 127.28      | 121.51   |
| 1   | O     | 318 | LEU  | CA-C-O    | -5.16 | 114.94      | 120.46   |
| 1   | R     | 465 | ASP  | CA-C-O    | -5.16 | 115.49      | 119.46   |
| 1   | S     | 391 | VAL  | CA-CB-CG1 | 5.16  | 119.16      | 110.40   |
| 1   | G     | 400 | ASP  | CA-C-O    | -5.15 | 114.96      | 120.42   |
| 1   | M     | 40  | LYS  | N-CA-C    | 5.15  | 117.57      | 111.33   |
| 1   | D     | 102 | ASP  | CA-CB-CG  | 5.15  | 117.75      | 112.60   |
| 1   | K     | 77  | ASP  | CA-CB-CG  | 5.15  | 117.75      | 112.60   |
| 1   | M     | 143 | LEU  | N-CA-C    | -5.15 | 105.31      | 111.03   |
| 1   | D     | 34  | ALA  | N-CA-C    | 5.15  | 117.30      | 111.02   |
| 1   | D     | 142 | ALA  | N-CA-C    | 5.15  | 117.56      | 111.33   |
| 1   | F     | 123 | TYR  | CB-CG-CD1 | -5.15 | 113.07      | 120.80   |
| 1   | F     | 345 | GLU  | N-CA-C    | -5.15 | 105.75      | 113.89   |
| 1   | G     | 362 | VAL  | O-C-N     | -5.15 | 118.33      | 122.97   |
| 1   | R     | 178 | ARG  | NE-CZ-NH2 | 5.15  | 123.84      | 119.20   |
| 1   | E     | 499 | GLN  | CA-C-N    | 5.15  | 128.10      | 120.17   |
| 1   | E     | 499 | GLN  | C-N-CA    | 5.15  | 128.10      | 120.17   |
| 1   | S     | 340 | VAL  | CA-C-N    | 5.15  | 129.38      | 120.58   |
| 1   | S     | 340 | VAL  | C-N-CA    | 5.15  | 129.38      | 120.58   |
| 1   | S     | 526 | ILE  | CA-CB-CG1 | 5.15  | 119.15      | 110.40   |
| 1   | A     | 193 | ALA  | CA-C-N    | 5.15  | 130.55      | 122.21   |
| 1   | A     | 193 | ALA  | C-N-CA    | 5.15  | 130.55      | 122.21   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 281 | ASN  | N-CA-C     | -5.15 | 106.95      | 113.18   |
| 1   | H     | 120 | ASP  | CA-C-N     | 5.15  | 127.60      | 120.29   |
| 1   | H     | 120 | ASP  | C-N-CA     | 5.15  | 127.60      | 120.29   |
| 1   | H     | 336 | GLY  | O-C-N      | -5.15 | 116.43      | 122.45   |
| 1   | I     | 442 | LEU  | CA-C-N     | 5.15  | 127.13      | 120.44   |
| 1   | I     | 442 | LEU  | C-N-CA     | 5.15  | 127.13      | 120.44   |
| 1   | P     | 126 | VAL  | N-CA-C     | 5.15  | 115.69      | 108.89   |
| 1   | Q     | 141 | VAL  | CA-C-O     | 5.15  | 126.62      | 121.27   |
| 1   | Q     | 421 | VAL  | CA-C-O     | 5.15  | 126.03      | 120.47   |
| 1   | S     | 53  | ARG  | N-CA-C     | -5.15 | 106.85      | 113.23   |
| 1   | S     | 223 | VAL  | N-CA-CB    | 5.15  | 118.25      | 111.25   |
| 1   | D     | 240 | ARG  | NE-CZ-NH1  | 5.15  | 126.65      | 121.50   |
| 1   | E     | 445 | GLU  | CB-CA-C    | -5.15 | 102.25      | 110.79   |
| 1   | F     | 282 | LEU  | CA-C-O     | 5.15  | 125.88      | 120.42   |
| 1   | K     | 170 | SER  | N-CA-C     | 5.15  | 118.66      | 112.38   |
| 1   | O     | 145 | THR  | CA-C-O     | 5.15  | 125.71      | 119.38   |
| 1   | O     | 513 | ILE  | O-C-N      | -5.15 | 116.85      | 121.89   |
| 1   | R     | 447 | TYR  | O-C-N      | -5.15 | 115.75      | 122.59   |
| 1   | E     | 120 | ASP  | CA-C-N     | 5.14  | 127.59      | 120.29   |
| 1   | E     | 120 | ASP  | C-N-CA     | 5.14  | 127.59      | 120.29   |
| 1   | F     | 445 | GLU  | CA-C-N     | 5.14  | 127.44      | 120.65   |
| 1   | F     | 445 | GLU  | C-N-CA     | 5.14  | 127.44      | 120.65   |
| 1   | F     | 460 | GLU  | O-C-N      | -5.14 | 115.97      | 122.20   |
| 1   | P     | 346 | ILE  | O-C-N      | -5.14 | 116.65      | 122.72   |
| 1   | Q     | 448 | ALA  | CA-C-N     | 5.14  | 127.17      | 120.28   |
| 1   | Q     | 448 | ALA  | C-N-CA     | 5.14  | 127.17      | 120.28   |
| 1   | R     | 421 | VAL  | CA-C-N     | 5.14  | 131.37      | 121.54   |
| 1   | R     | 421 | VAL  | C-N-CA     | 5.14  | 131.37      | 121.54   |
| 1   | D     | 342 | ASN  | CA-CB-CG   | 5.14  | 117.74      | 112.60   |
| 1   | K     | 33  | ARG  | NH1-CZ-NH2 | -5.14 | 112.61      | 119.30   |
| 1   | M     | 257 | LYS  | CG-CD-CE   | 5.14  | 123.13      | 111.30   |
| 1   | N     | 127 | HIS  | CA-CB-CG   | -5.14 | 108.66      | 113.80   |
| 1   | C     | 114 | LEU  | CA-C-N     | 5.14  | 127.04      | 120.56   |
| 1   | C     | 114 | LEU  | C-N-CA     | 5.14  | 127.04      | 120.56   |
| 1   | C     | 477 | HIS  | CB-CG-ND1  | 5.14  | 130.41      | 122.70   |
| 1   | P     | 49  | THR  | CA-CB-OG1  | 5.14  | 117.31      | 109.60   |
| 1   | Q     | 234 | HIS  | CA-C-O     | -5.14 | 114.19      | 119.49   |
| 1   | C     | 497 | MET  | CG-SD-CE   | -5.14 | 89.59       | 100.90   |
| 1   | L     | 207 | ILE  | CA-C-O     | 5.14  | 125.46      | 120.27   |
| 1   | M     | 425 | ILE  | CB-CA-C    | -5.14 | 104.19      | 112.16   |
| 1   | R     | 139 | GLU  | CA-C-N     | 5.14  | 129.36      | 121.19   |
| 1   | R     | 139 | GLU  | C-N-CA     | 5.14  | 129.36      | 121.19   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 151 | GLN  | CA-C-O     | 5.14  | 126.16      | 120.71   |
| 1   | E     | 325 | LYS  | CA-C-N     | 5.14  | 127.42      | 120.38   |
| 1   | E     | 325 | LYS  | C-N-CA     | 5.14  | 127.42      | 120.38   |
| 1   | F     | 317 | VAL  | O-C-N      | -5.14 | 116.20      | 122.36   |
| 1   | L     | 354 | ALA  | O-C-N      | -5.14 | 117.73      | 123.48   |
| 1   | A     | 203 | ASP  | O-C-N      | -5.13 | 116.77      | 122.93   |
| 1   | B     | 180 | TYR  | CA-C-N     | 5.13  | 127.13      | 120.56   |
| 1   | B     | 180 | TYR  | C-N-CA     | 5.13  | 127.13      | 120.56   |
| 1   | B     | 290 | ILE  | N-CA-C     | -5.13 | 106.14      | 111.58   |
| 1   | D     | 59  | LEU  | CA-C-N     | 5.13  | 129.66      | 122.93   |
| 1   | D     | 59  | LEU  | C-N-CA     | 5.13  | 129.66      | 122.93   |
| 1   | D     | 187 | LYS  | N-CA-CB    | 5.13  | 117.67      | 110.12   |
| 1   | I     | 267 | ASN  | CA-CB-CG   | -5.13 | 107.47      | 112.60   |
| 1   | L     | 33  | ARG  | CA-C-N     | 5.13  | 127.93      | 120.79   |
| 1   | L     | 33  | ARG  | C-N-CA     | 5.13  | 127.93      | 120.79   |
| 1   | C     | 404 | THR  | O-C-N      | 5.13  | 127.43      | 122.09   |
| 1   | K     | 285 | GLU  | N-CA-CB    | 5.13  | 117.51      | 110.07   |
| 1   | L     | 267 | ASN  | N-CA-C     | 5.13  | 117.66      | 111.40   |
| 1   | N     | 176 | GLY  | O-C-N      | -5.13 | 116.24      | 122.76   |
| 1   | S     | 362 | VAL  | N-CA-CB    | -5.13 | 104.97      | 111.64   |
| 1   | B     | 349 | GLN  | CB-CG-CD   | -5.13 | 103.88      | 112.60   |
| 1   | E     | 346 | ILE  | O-C-N      | -5.13 | 117.33      | 122.62   |
| 1   | H     | 250 | ASP  | N-CA-C     | 5.13  | 116.95      | 111.36   |
| 1   | I     | 133 | SER  | CA-C-N     | 5.13  | 125.79      | 119.99   |
| 1   | I     | 133 | SER  | C-N-CA     | 5.13  | 125.79      | 119.99   |
| 1   | M     | 234 | HIS  | CG-CD2-NE2 | 5.13  | 112.33      | 107.20   |
| 1   | N     | 101 | ALA  | N-CA-C     | -5.13 | 105.78      | 113.89   |
| 1   | P     | 74  | THR  | CB-CA-C    | -5.13 | 101.96      | 110.68   |
| 1   | R     | 471 | MET  | CA-C-N     | 5.13  | 127.87      | 120.38   |
| 1   | R     | 471 | MET  | C-N-CA     | 5.13  | 127.87      | 120.38   |
| 1   | F     | 297 | VAL  | CA-C-N     | 5.13  | 131.20      | 121.97   |
| 1   | F     | 297 | VAL  | C-N-CA     | 5.13  | 131.20      | 121.97   |
| 1   | O     | 133 | SER  | CA-C-N     | 5.13  | 125.79      | 119.99   |
| 1   | O     | 133 | SER  | C-N-CA     | 5.13  | 125.79      | 119.99   |
| 1   | A     | 427 | LYS  | CA-C-N     | 5.13  | 127.15      | 120.28   |
| 1   | A     | 427 | LYS  | C-N-CA     | 5.13  | 127.15      | 120.28   |
| 1   | H     | 255 | VAL  | CA-C-N     | 5.13  | 130.00      | 122.77   |
| 1   | H     | 255 | VAL  | C-N-CA     | 5.13  | 130.00      | 122.77   |
| 1   | K     | 325 | LYS  | N-CA-C     | 5.13  | 117.61      | 111.71   |
| 1   | O     | 343 | ILE  | O-C-N      | -5.13 | 116.72      | 121.90   |
| 1   | A     | 252 | SER  | CB-CA-C    | -5.13 | 102.57      | 110.26   |
| 1   | A     | 510 | MET  | CA-C-N     | 5.13  | 128.10      | 120.31   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 510 | MET  | C-N-CA    | 5.13  | 128.10      | 120.31   |
| 1   | D     | 379 | ILE  | CB-CA-C   | -5.13 | 104.16      | 111.34   |
| 1   | F     | 128 | PRO  | CA-C-N    | 5.13  | 127.66      | 120.28   |
| 1   | F     | 128 | PRO  | C-N-CA    | 5.13  | 127.66      | 120.28   |
| 1   | H     | 138 | ALA  | N-CA-C    | 5.13  | 116.95      | 111.36   |
| 1   | K     | 191 | GLN  | N-CA-C    | 5.13  | 116.95      | 111.36   |
| 1   | N     | 467 | ILE  | N-CA-C    | -5.13 | 105.71      | 110.53   |
| 1   | H     | 300 | CYS  | CA-C-N    | 5.12  | 131.26      | 122.09   |
| 1   | H     | 300 | CYS  | C-N-CA    | 5.12  | 131.26      | 122.09   |
| 1   | N     | 61  | ASP  | N-CA-C    | 5.12  | 116.71      | 110.41   |
| 1   | N     | 176 | GLY  | N-CA-C    | 5.12  | 118.75      | 112.14   |
| 1   | B     | 366 | LYS  | CB-CA-C   | 5.12  | 118.62      | 109.65   |
| 1   | C     | 486 | GLY  | O-C-N     | -5.12 | 116.04      | 122.70   |
| 1   | G     | 92  | ILE  | CB-CA-C   | -5.12 | 105.37      | 112.24   |
| 1   | K     | 351 | LEU  | CB-CA-C   | -5.12 | 101.08      | 109.53   |
| 1   | N     | 496 | ASP  | CA-CB-CG  | -5.12 | 107.48      | 112.60   |
| 1   | D     | 304 | ILE  | CA-C-N    | 5.12  | 128.98      | 120.94   |
| 1   | D     | 304 | ILE  | C-N-CA    | 5.12  | 128.98      | 120.94   |
| 1   | E     | 243 | ASN  | CA-CB-CG  | -5.12 | 107.48      | 112.60   |
| 1   | G     | 33  | ARG  | CA-C-N    | 5.12  | 127.45      | 120.54   |
| 1   | G     | 33  | ARG  | C-N-CA    | 5.12  | 127.45      | 120.54   |
| 1   | L     | 126 | VAL  | CA-CB-CG2 | 5.12  | 119.11      | 110.40   |
| 1   | Q     | 433 | ALA  | CA-C-O    | -5.12 | 113.14      | 120.16   |
| 1   | H     | 432 | TYR  | O-C-N     | 5.12  | 127.62      | 122.09   |
| 1   | M     | 175 | ALA  | N-CA-CB   | 5.12  | 117.81      | 111.00   |
| 1   | P     | 423 | ILE  | N-CA-CB   | 5.12  | 116.87      | 110.47   |
| 1   | P     | 452 | GLU  | CA-C-N    | 5.12  | 127.39      | 120.38   |
| 1   | P     | 452 | GLU  | C-N-CA    | 5.12  | 127.39      | 120.38   |
| 1   | R     | 303 | GLY  | N-CA-C    | 5.12  | 119.11      | 112.25   |
| 1   | D     | 177 | ALA  | N-CA-C    | 5.12  | 118.50      | 111.54   |
| 1   | G     | 59  | LEU  | CA-C-O    | 5.12  | 125.67      | 120.24   |
| 1   | G     | 509 | LYS  | CB-CA-C   | 5.12  | 119.83      | 110.36   |
| 1   | K     | 292 | ALA  | CA-C-N    | 5.12  | 130.78      | 121.92   |
| 1   | K     | 292 | ALA  | C-N-CA    | 5.12  | 130.78      | 121.92   |
| 1   | C     | 54  | GLY  | CA-C-N    | 5.12  | 131.69      | 122.02   |
| 1   | C     | 54  | GLY  | C-N-CA    | 5.12  | 131.69      | 122.02   |
| 1   | Q     | 76  | LEU  | CA-C-N    | 5.12  | 127.09      | 120.44   |
| 1   | Q     | 76  | LEU  | C-N-CA    | 5.12  | 127.09      | 120.44   |
| 1   | C     | 91  | GLN  | CA-C-N    | 5.12  | 128.74      | 120.55   |
| 1   | C     | 91  | GLN  | C-N-CA    | 5.12  | 128.74      | 120.55   |
| 1   | H     | 178 | ARG  | NE-CZ-NH1 | -5.12 | 116.39      | 121.50   |
| 1   | H     | 273 | GLN  | CG-CD-OE1 | 5.12  | 131.03      | 120.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | M     | 517 | THR  | CA-C-N      | 5.12  | 127.40      | 120.65   |
| 1   | M     | 517 | THR  | C-N-CA      | 5.12  | 127.40      | 120.65   |
| 1   | N     | 63  | LEU  | CA-C-N      | 5.12  | 130.54      | 122.51   |
| 1   | N     | 63  | LEU  | C-N-CA      | 5.12  | 130.54      | 122.51   |
| 1   | O     | 144 | GLN  | N-CA-CB     | -5.12 | 101.62      | 110.32   |
| 1   | S     | 157 | ASP  | CA-C-N      | 5.12  | 130.09      | 121.14   |
| 1   | S     | 157 | ASP  | C-N-CA      | 5.12  | 130.09      | 121.14   |
| 1   | S     | 530 | VAL  | CG1-CB-CG2  | -5.12 | 99.55       | 110.80   |
| 1   | D     | 250 | ASP  | CA-CB-CG    | 5.11  | 117.71      | 112.60   |
| 1   | E     | 250 | ASP  | CA-CB-CG    | 5.11  | 117.71      | 112.60   |
| 1   | H     | 459 | ILE  | CA-C-N      | 5.11  | 129.32      | 121.19   |
| 1   | H     | 459 | ILE  | C-N-CA      | 5.11  | 129.32      | 121.19   |
| 1   | M     | 407 | ASP  | CA-C-N      | 5.11  | 127.47      | 120.46   |
| 1   | M     | 407 | ASP  | C-N-CA      | 5.11  | 127.47      | 120.46   |
| 1   | O     | 403 | GLY  | CA-C-N      | 5.11  | 127.09      | 120.44   |
| 1   | O     | 403 | GLY  | C-N-CA      | 5.11  | 127.09      | 120.44   |
| 1   | P     | 177 | ALA  | O-C-N       | -5.11 | 116.06      | 123.07   |
| 1   | D     | 344 | ASP  | CA-C-O      | 5.11  | 127.10      | 119.23   |
| 1   | K     | 471 | MET  | N-CA-C      | 5.11  | 116.66      | 111.14   |
| 1   | O     | 40  | LYS  | CG-CD-CE    | 5.11  | 123.06      | 111.30   |
| 1   | D     | 85  | ALA  | O-C-N       | -5.11 | 116.78      | 122.09   |
| 1   | E     | 482 | ASN  | N-CA-CB     | -5.11 | 101.89      | 110.22   |
| 1   | K     | 190 | THR  | N-CA-C      | 5.11  | 118.29      | 111.75   |
| 1   | L     | 171 | SER  | CB-CA-C     | -5.11 | 101.92      | 110.56   |
| 1   | S     | 47  | LYS  | N-CA-C      | 5.11  | 121.69      | 110.80   |
| 1   | S     | 61  | ASP  | CA-CB-CG    | -5.11 | 107.49      | 112.60   |
| 1   | C     | 395 | GLU  | N-CA-C      | -5.11 | 105.89      | 111.82   |
| 1   | K     | 245 | LYS  | CA-C-N      | 5.11  | 127.54      | 120.49   |
| 1   | K     | 245 | LYS  | C-N-CA      | 5.11  | 127.54      | 120.49   |
| 1   | N     | 290 | ILE  | CA-C-O      | 5.11  | 126.18      | 120.71   |
| 1   | O     | 127 | HIS  | ND1-CE1-NE2 | 5.11  | 113.51      | 108.40   |
| 1   | B     | 480 | GLU  | CA-C-N      | 5.11  | 127.12      | 120.28   |
| 1   | B     | 480 | GLU  | C-N-CA      | 5.11  | 127.12      | 120.28   |
| 1   | F     | 165 | ALA  | CA-C-O      | 5.11  | 125.96      | 120.70   |
| 1   | K     | 302 | LYS  | CA-C-O      | -5.11 | 115.24      | 121.78   |
| 1   | L     | 34  | ALA  | CA-C-N      | 5.11  | 127.43      | 120.54   |
| 1   | L     | 34  | ALA  | C-N-CA      | 5.11  | 127.43      | 120.54   |
| 1   | S     | 323 | ALA  | CA-C-O      | 5.11  | 126.87      | 121.05   |
| 1   | F     | 450 | ALA  | CA-C-O      | 5.11  | 125.96      | 120.55   |
| 1   | Q     | 69  | THR  | N-CA-C      | 5.11  | 115.79      | 108.74   |
| 1   | Q     | 271 | GLN  | N-CA-C      | 5.11  | 116.92      | 111.36   |
| 1   | B     | 445 | GLU  | N-CA-CB     | 5.10  | 117.62      | 110.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 209 | ILE  | CB-CG1-CD1 | 5.10  | 124.52      | 113.80   |
| 1   | A     | 284 | LYS  | CA-C-O     | 5.10  | 125.87      | 120.10   |
| 1   | B     | 102 | ASP  | N-CA-CB    | -5.10 | 103.34      | 110.38   |
| 1   | E     | 32  | VAL  | N-CA-C     | 5.10  | 119.95      | 109.34   |
| 1   | E     | 340 | VAL  | N-CA-C     | 5.10  | 114.96      | 107.15   |
| 1   | G     | 219 | ASP  | N-CA-CB    | -5.10 | 103.07      | 110.47   |
| 1   | K     | 53  | ARG  | CD-NE-CZ   | -5.10 | 117.26      | 124.40   |
| 1   | Q     | 177 | ALA  | O-C-N      | -5.10 | 115.80      | 122.59   |
| 1   | S     | 428 | LYS  | O-C-N      | -5.10 | 116.25      | 122.22   |
| 1   | G     | 170 | SER  | CA-C-O     | 5.10  | 125.66      | 119.49   |
| 1   | R     | 238 | PRO  | N-CA-C     | 5.10  | 118.50      | 110.80   |
| 1   | B     | 152 | THR  | CA-CB-OG1  | 5.10  | 117.25      | 109.60   |
| 1   | C     | 267 | ASN  | N-CA-C     | -5.10 | 106.47      | 113.30   |
| 1   | E     | 409 | ILE  | CA-C-N     | 5.10  | 127.62      | 120.28   |
| 1   | E     | 409 | ILE  | C-N-CA     | 5.10  | 127.62      | 120.28   |
| 1   | G     | 29  | LYS  | N-CA-C     | 5.10  | 121.66      | 110.80   |
| 1   | I     | 168 | SER  | N-CA-C     | -5.10 | 105.90      | 112.68   |
| 1   | R     | 305 | ASP  | O-C-N      | -5.10 | 116.54      | 122.81   |
| 1   | I     | 365 | ASP  | CB-CA-C    | -5.10 | 100.66      | 110.24   |
| 1   | L     | 38  | ALA  | N-CA-C     | 5.10  | 117.23      | 111.11   |
| 1   | L     | 244 | ALA  | O-C-N      | -5.10 | 116.66      | 122.93   |
| 1   | L     | 453 | SER  | CA-C-O     | 5.10  | 126.14      | 120.63   |
| 1   | R     | 477 | HIS  | CB-CG-ND1  | 5.10  | 130.34      | 122.70   |
| 1   | D     | 435 | GLN  | N-CA-CB    | -5.10 | 102.49      | 110.44   |
| 1   | E     | 474 | ARG  | NE-CZ-NH1  | -5.10 | 116.40      | 121.50   |
| 1   | F     | 402 | LEU  | N-CA-C     | 5.10  | 116.53      | 110.97   |
| 1   | M     | 374 | LYS  | CA-C-O     | 5.10  | 125.95      | 120.55   |
| 1   | P     | 493 | GLN  | CA-C-O     | -5.10 | 113.18      | 120.16   |
| 1   | A     | 437 | GLY  | CA-C-O     | -5.09 | 116.44      | 121.48   |
| 1   | D     | 190 | THR  | N-CA-C     | 5.09  | 118.27      | 111.75   |
| 1   | E     | 198 | ASP  | CA-C-N     | 5.09  | 130.56      | 121.75   |
| 1   | E     | 198 | ASP  | C-N-CA     | 5.09  | 130.56      | 121.75   |
| 1   | F     | 240 | ARG  | CA-CB-CG   | 5.09  | 124.29      | 114.10   |
| 1   | P     | 473 | LEU  | O-C-N      | -5.09 | 115.42      | 122.30   |
| 1   | S     | 345 | GLU  | N-CA-C     | -5.09 | 105.84      | 113.89   |
| 1   | H     | 331 | LEU  | CA-C-O     | 5.09  | 125.23      | 119.27   |
| 1   | D     | 109 | ILE  | CA-C-N     | 5.09  | 127.10      | 120.28   |
| 1   | D     | 109 | ILE  | C-N-CA     | 5.09  | 127.10      | 120.28   |
| 1   | H     | 378 | SER  | CB-CA-C    | -5.09 | 102.45      | 111.05   |
| 1   | P     | 384 | ARG  | O-C-N      | -5.09 | 116.96      | 122.92   |
| 1   | H     | 130 | ILE  | O-C-N      | -5.09 | 116.61      | 121.90   |
| 1   | H     | 324 | LYS  | CB-CA-C    | 5.09  | 118.56      | 109.65   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | H     | 499 | GLN  | CB-CG-CD    | -5.09 | 103.95      | 112.60   |
| 1   | K     | 249 | ILE  | CA-C-O      | 5.09  | 126.64      | 120.74   |
| 1   | L     | 391 | VAL  | CA-CB-CG2   | -5.09 | 101.75      | 110.40   |
| 1   | L     | 506 | ALA  | N-CA-C      | 5.09  | 118.98      | 112.87   |
| 1   | A     | 309 | GLN  | CG-CD-NE2   | -5.09 | 108.77      | 116.40   |
| 1   | B     | 282 | LEU  | CA-C-O      | 5.09  | 125.94      | 120.55   |
| 1   | D     | 368 | VAL  | O-C-N       | -5.09 | 116.93      | 122.83   |
| 1   | I     | 343 | ILE  | O-C-N       | -5.09 | 116.73      | 121.87   |
| 1   | I     | 525 | ARG  | NH1-CZ-NH2  | -5.09 | 112.69      | 119.30   |
| 1   | M     | 425 | ILE  | N-CA-C      | 5.09  | 117.41      | 111.05   |
| 1   | P     | 338 | ARG  | NE-CZ-NH1   | 5.09  | 126.59      | 121.50   |
| 1   | E     | 488 | ASP  | O-C-N       | -5.08 | 115.83      | 122.59   |
| 1   | N     | 426 | ALA  | CA-C-O      | -5.08 | 115.55      | 120.89   |
| 1   | S     | 233 | VAL  | CA-CB-CG1   | 5.08  | 119.04      | 110.40   |
| 1   | A     | 137 | LYS  | CA-CB-CG    | -5.08 | 103.94      | 114.10   |
| 1   | I     | 344 | ASP  | CB-CG-OD2   | 5.08  | 130.09      | 118.40   |
| 1   | K     | 275 | PHE  | CA-C-N      | 5.08  | 129.21      | 120.72   |
| 1   | K     | 275 | PHE  | C-N-CA      | 5.08  | 129.21      | 120.72   |
| 1   | K     | 409 | ILE  | CA-C-N      | 5.08  | 127.60      | 120.28   |
| 1   | K     | 409 | ILE  | C-N-CA      | 5.08  | 127.60      | 120.28   |
| 1   | R     | 127 | HIS  | O-C-N       | -5.08 | 116.07      | 121.30   |
| 1   | R     | 127 | HIS  | ND1-CE1-NE2 | 5.08  | 113.48      | 108.40   |
| 1   | R     | 449 | ASN  | N-CA-C      | 5.08  | 117.21      | 111.11   |
| 1   | D     | 57  | LYS  | N-CA-C      | -5.08 | 101.41      | 109.59   |
| 1   | E     | 220 | THR  | O-C-N       | -5.08 | 116.87      | 122.86   |
| 1   | F     | 411 | ASP  | CA-CB-CG    | -5.08 | 107.52      | 112.60   |
| 1   | K     | 91  | GLN  | N-CA-C      | 5.08  | 116.82      | 111.28   |
| 1   | C     | 127 | HIS  | CA-CB-CG    | -5.08 | 108.72      | 113.80   |
| 1   | G     | 172 | LYS  | CA-C-N      | 5.08  | 127.04      | 120.44   |
| 1   | G     | 172 | LYS  | C-N-CA      | 5.08  | 127.04      | 120.44   |
| 1   | L     | 514 | LYS  | N-CA-C      | 5.08  | 116.50      | 111.07   |
| 1   | N     | 225 | GLY  | CA-C-O      | 5.08  | 125.62      | 121.05   |
| 1   | O     | 106 | THR  | CA-CB-OG1   | 5.08  | 117.22      | 109.60   |
| 1   | O     | 389 | ARG  | CG-CD-NE    | -5.08 | 100.83      | 112.00   |
| 1   | R     | 177 | ALA  | N-CA-C      | 5.08  | 121.61      | 110.80   |
| 1   | B     | 192 | VAL  | CB-CA-C     | -5.08 | 104.50      | 111.65   |
| 1   | C     | 484 | TRP  | CA-CB-CG    | 5.08  | 123.24      | 113.60   |
| 1   | E     | 90  | VAL  | CA-CB-CG2   | 5.08  | 119.03      | 110.40   |
| 1   | E     | 234 | HIS  | CA-C-O      | 5.08  | 124.88      | 119.50   |
| 1   | E     | 270 | THR  | CA-CB-OG1   | 5.08  | 117.21      | 109.60   |
| 1   | F     | 135 | TYR  | CA-C-O      | -5.08 | 115.17      | 120.55   |
| 1   | G     | 327 | ASP  | CA-C-O      | 5.08  | 124.40      | 118.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | I     | 251 | ALA  | CA-C-N      | 5.08  | 127.98      | 120.82   |
| 1   | I     | 251 | ALA  | C-N-CA      | 5.08  | 127.98      | 120.82   |
| 1   | I     | 496 | ASP  | CA-CB-CG    | -5.08 | 107.53      | 112.60   |
| 1   | K     | 162 | ARG  | NE-CZ-NH1   | -5.08 | 116.42      | 121.50   |
| 1   | L     | 484 | TRP  | CE2-CD2-CE3 | 5.08  | 123.88      | 118.80   |
| 1   | D     | 69  | THR  | O-C-N       | -5.07 | 117.56      | 122.99   |
| 1   | G     | 149 | LEU  | CB-CA-C     | -5.07 | 100.32      | 110.42   |
| 1   | K     | 127 | HIS  | CA-C-N      | 5.07  | 124.86      | 119.28   |
| 1   | K     | 127 | HIS  | C-N-CA      | 5.07  | 124.86      | 119.28   |
| 1   | K     | 198 | ASP  | O-C-N       | -5.07 | 115.84      | 122.59   |
| 1   | L     | 258 | PRO  | N-CA-C      | -5.07 | 107.42      | 114.27   |
| 1   | Q     | 277 | ASP  | CA-CB-CG    | -5.07 | 107.53      | 112.60   |
| 1   | R     | 168 | SER  | CB-CA-C     | -5.07 | 101.77      | 110.24   |
| 1   | E     | 129 | THR  | O-C-N       | -5.07 | 116.29      | 122.22   |
| 1   | E     | 400 | ASP  | O-C-N       | -5.07 | 116.75      | 122.12   |
| 1   | F     | 399 | ARG  | NE-CZ-NH1   | -5.07 | 116.43      | 121.50   |
| 1   | I     | 146 | ILE  | CB-CA-C     | -5.07 | 105.55      | 111.94   |
| 1   | M     | 156 | ASN  | CA-C-O      | -5.07 | 113.30      | 119.43   |
| 1   | M     | 292 | ALA  | CA-C-O      | 5.07  | 125.62      | 119.49   |
| 1   | O     | 356 | LEU  | CA-C-O      | 5.07  | 126.33      | 120.14   |
| 1   | Q     | 261 | ASP  | CA-CB-CG    | -5.07 | 107.53      | 112.60   |
| 1   | S     | 41  | ALA  | N-CA-CB     | 5.07  | 117.36      | 110.01   |
| 1   | C     | 387 | LEU  | CB-CA-C     | 5.07  | 118.70      | 109.83   |
| 1   | D     | 364 | GLU  | N-CA-C      | -5.07 | 107.13      | 113.72   |
| 1   | H     | 461 | ASN  | O-C-N       | -5.07 | 115.80      | 122.39   |
| 1   | I     | 257 | LYS  | O-C-N       | -5.07 | 117.22      | 121.38   |
| 1   | L     | 39  | VAL  | O-C-N       | -5.07 | 116.72      | 121.94   |
| 1   | N     | 362 | VAL  | CA-CB-CG1   | 5.07  | 119.02      | 110.40   |
| 1   | Q     | 264 | ILE  | N-CA-C      | 5.07  | 119.88      | 109.34   |
| 1   | Q     | 460 | GLU  | O-C-N       | -5.07 | 116.07      | 122.20   |
| 1   | R     | 439 | LYS  | CB-CA-C     | 5.07  | 119.47      | 110.85   |
| 1   | F     | 186 | VAL  | CA-CB-CG1   | 5.07  | 119.02      | 110.40   |
| 1   | F     | 489 | LEU  | O-C-N       | -5.07 | 114.26      | 122.42   |
| 1   | F     | 519 | ALA  | O-C-N       | -5.07 | 116.76      | 122.03   |
| 1   | K     | 43  | GLU  | CB-CA-C     | -5.07 | 102.92      | 110.88   |
| 1   | M     | 447 | TYR  | CB-CG-CD1   | -5.07 | 113.20      | 120.80   |
| 1   | P     | 94  | LYS  | CG-CD-CE    | 5.07  | 122.96      | 111.30   |
| 1   | P     | 168 | SER  | O-C-N       | -5.07 | 115.55      | 122.19   |
| 1   | Q     | 467 | ILE  | CB-CA-C     | -5.07 | 105.38      | 112.02   |
| 1   | B     | 110 | PHE  | N-CA-CB     | -5.07 | 102.67      | 110.12   |
| 1   | E     | 477 | HIS  | CA-CB-CG    | -5.07 | 108.73      | 113.80   |
| 1   | F     | 321 | ARG  | O-C-N       | -5.07 | 116.64      | 123.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 108 | VAL  | CA-C-O     | 5.07  | 126.67      | 121.05   |
| 1   | O     | 388 | GLU  | N-CA-C     | 5.07  | 117.53      | 111.71   |
| 1   | R     | 353 | TYR  | CG-CD2-CE2 | -5.07 | 113.60      | 121.20   |
| 1   | R     | 444 | VAL  | CA-C-N     | 5.07  | 127.32      | 120.38   |
| 1   | R     | 444 | VAL  | C-N-CA     | 5.07  | 127.32      | 120.38   |
| 1   | A     | 113 | GLU  | CA-C-O     | 5.06  | 125.79      | 120.42   |
| 1   | A     | 260 | LEU  | O-C-N      | -5.06 | 116.82      | 122.09   |
| 1   | N     | 355 | SER  | N-CA-C     | 5.06  | 116.49      | 111.07   |
| 1   | N     | 492 | GLY  | O-C-N      | 5.06  | 129.28      | 122.70   |
| 1   | P     | 517 | THR  | N-CA-CB    | 5.06  | 117.56      | 110.12   |
| 1   | B     | 441 | GLN  | O-C-N      | -5.06 | 116.83      | 122.09   |
| 1   | D     | 127 | HIS  | CG-CD2-NE2 | 5.06  | 112.26      | 107.20   |
| 1   | K     | 282 | LEU  | O-C-N      | -5.06 | 116.38      | 122.15   |
| 1   | O     | 303 | GLY  | N-CA-C     | 5.06  | 119.03      | 112.25   |
| 1   | Q     | 187 | LYS  | CA-C-O     | 5.06  | 125.92      | 120.55   |
| 1   | Q     | 265 | ARG  | NE-CZ-NH1  | -5.06 | 116.44      | 121.50   |
| 1   | R     | 409 | ILE  | O-C-N      | -5.06 | 116.61      | 121.83   |
| 1   | S     | 257 | LYS  | N-CA-C     | 5.06  | 115.80      | 109.57   |
| 1   | D     | 195 | LEU  | O-C-N      | 5.06  | 129.32      | 122.59   |
| 1   | O     | 498 | TRP  | CG-CD2-CE3 | -5.06 | 128.84      | 133.90   |
| 1   | C     | 523 | VAL  | CA-C-O     | 5.06  | 126.21      | 120.95   |
| 1   | Q     | 150 | ALA  | N-CA-C     | 5.06  | 117.63      | 110.50   |
| 1   | Q     | 289 | LYS  | O-C-N      | -5.06 | 115.65      | 122.43   |
| 1   | R     | 522 | LEU  | N-CA-C     | -5.06 | 105.84      | 111.36   |
| 1   | A     | 74  | THR  | CB-CA-C    | -5.06 | 102.39      | 110.79   |
| 1   | A     | 92  | ILE  | CA-C-O     | -5.06 | 115.49      | 120.85   |
| 1   | B     | 455 | VAL  | CA-CB-CG1  | -5.06 | 101.80      | 110.40   |
| 1   | E     | 69  | THR  | CA-CB-OG1  | 5.06  | 117.19      | 109.60   |
| 1   | F     | 250 | ASP  | CA-C-O     | 5.06  | 125.78      | 120.42   |
| 1   | H     | 224 | TYR  | CA-C-N     | 5.06  | 127.89      | 120.91   |
| 1   | H     | 224 | TYR  | C-N-CA     | 5.06  | 127.89      | 120.91   |
| 1   | M     | 229 | ASP  | CA-C-O     | 5.06  | 128.26      | 120.37   |
| 1   | M     | 322 | ARG  | N-CA-CB    | -5.06 | 104.21      | 111.70   |
| 1   | A     | 240 | ARG  | NH1-CZ-NH2 | -5.06 | 112.73      | 119.30   |
| 1   | G     | 189 | VAL  | N-CA-CB    | -5.06 | 103.24      | 110.52   |
| 1   | I     | 339 | VAL  | O-C-N      | 5.06  | 127.86      | 122.45   |
| 1   | Q     | 267 | ASN  | OD1-CG-ND2 | -5.06 | 117.54      | 122.60   |
| 1   | L     | 194 | GLU  | O-C-N      | -5.05 | 117.22      | 123.44   |
| 1   | D     | 443 | ALA  | CA-C-N     | 5.05  | 126.92      | 120.56   |
| 1   | D     | 443 | ALA  | C-N-CA     | 5.05  | 126.92      | 120.56   |
| 1   | L     | 238 | PRO  | CA-C-N     | -5.05 | 112.67      | 122.06   |
| 1   | L     | 238 | PRO  | C-N-CA     | -5.05 | 112.67      | 122.06   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | L     | 449 | ASN  | N-CA-CB    | 5.05  | 117.55      | 110.12   |
| 1   | M     | 480 | GLU  | N-CA-CB    | -5.05 | 102.00      | 110.39   |
| 1   | N     | 389 | ARG  | CA-C-O     | 5.05  | 124.95      | 119.24   |
| 1   | R     | 281 | ASN  | CA-CB-CG   | -5.05 | 107.55      | 112.60   |
| 1   | S     | 55  | MET  | CG-SD-CE   | -5.05 | 89.79       | 100.90   |
| 1   | E     | 366 | LYS  | CA-CB-CG   | 5.05  | 124.20      | 114.10   |
| 1   | E     | 503 | ILE  | N-CA-C     | -5.05 | 101.08      | 108.85   |
| 1   | I     | 169 | LEU  | O-C-N      | -5.05 | 115.56      | 122.33   |
| 1   | M     | 311 | TYR  | CA-C-N     | 5.05  | 127.55      | 120.28   |
| 1   | M     | 311 | TYR  | C-N-CA     | 5.05  | 127.55      | 120.28   |
| 1   | N     | 168 | SER  | N-CA-C     | -5.05 | 106.21      | 112.93   |
| 1   | P     | 448 | ALA  | O-C-N      | 5.05  | 127.54      | 122.09   |
| 1   | Q     | 367 | MET  | CA-C-N     | 5.05  | 128.88      | 122.37   |
| 1   | Q     | 367 | MET  | C-N-CA     | 5.05  | 128.88      | 122.37   |
| 1   | L     | 116 | LYS  | N-CA-C     | 5.05  | 116.47      | 110.97   |
| 1   | Q     | 486 | GLY  | O-C-N      | -5.05 | 116.14      | 122.70   |
| 1   | F     | 264 | ILE  | N-CA-C     | 5.05  | 115.91      | 110.21   |
| 1   | K     | 393 | GLU  | N-CA-C     | 5.05  | 118.70      | 112.54   |
| 1   | K     | 517 | THR  | CA-C-N     | 5.05  | 127.31      | 120.65   |
| 1   | K     | 517 | THR  | C-N-CA     | 5.05  | 127.31      | 120.65   |
| 1   | S     | 306 | GLU  | CB-CG-CD   | -5.05 | 104.02      | 112.60   |
| 1   | H     | 157 | ASP  | CA-C-O     | 5.04  | 129.20      | 122.44   |
| 1   | H     | 379 | ILE  | O-C-N      | -5.04 | 117.45      | 123.00   |
| 1   | H     | 526 | ILE  | N-CA-CB    | 5.04  | 116.60      | 110.95   |
| 1   | S     | 471 | MET  | CA-C-O     | 5.04  | 125.90      | 120.70   |
| 1   | B     | 226 | ILE  | N-CA-CB    | -5.04 | 102.23      | 111.91   |
| 1   | C     | 115 | VAL  | CA-C-N     | 5.04  | 127.80      | 120.79   |
| 1   | C     | 115 | VAL  | C-N-CA     | 5.04  | 127.80      | 120.79   |
| 1   | F     | 396 | ARG  | NH1-CZ-NH2 | -5.04 | 112.74      | 119.30   |
| 1   | M     | 141 | VAL  | CA-C-O     | 5.04  | 126.52      | 121.27   |
| 1   | O     | 261 | ASP  | CA-CB-CG   | -5.04 | 107.56      | 112.60   |
| 1   | P     | 391 | VAL  | CA-C-O     | -5.04 | 115.70      | 120.95   |
| 1   | B     | 278 | GLU  | CB-CG-CD   | 5.04  | 121.17      | 112.60   |
| 1   | I     | 110 | PHE  | CB-CG-CD1  | -5.04 | 112.13      | 120.70   |
| 1   | I     | 164 | ILE  | N-CA-C     | 5.04  | 119.83      | 109.34   |
| 1   | M     | 379 | ILE  | N-CA-C     | 5.04  | 116.16      | 108.80   |
| 1   | A     | 262 | ALA  | O-C-N      | -5.04 | 118.47      | 123.46   |
| 1   | C     | 232 | VAL  | CA-CB-CG2  | 5.04  | 118.97      | 110.40   |
| 1   | C     | 523 | VAL  | O-C-N      | -5.04 | 116.98      | 121.87   |
| 1   | F     | 480 | GLU  | N-CA-C     | 5.04  | 118.69      | 112.54   |
| 1   | N     | 82  | GLN  | OE1-CD-NE2 | -5.04 | 117.56      | 122.60   |
| 1   | I     | 227 | VAL  | CB-CA-C    | 5.04  | 117.22      | 110.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | N     | 409 | ILE  | O-C-N      | 5.04  | 127.14      | 121.90   |
| 1   | C     | 384 | ARG  | CG-CD-NE   | -5.04 | 100.92      | 112.00   |
| 1   | G     | 426 | ALA  | CA-C-N     | 5.04  | 129.20      | 121.19   |
| 1   | G     | 426 | ALA  | C-N-CA     | 5.04  | 129.20      | 121.19   |
| 1   | P     | 34  | ALA  | N-CA-C     | -5.04 | 105.07      | 111.11   |
| 1   | E     | 240 | ARG  | NE-CZ-NH2  | -5.04 | 114.67      | 119.20   |
| 1   | I     | 96  | GLN  | CA-C-O     | -5.04 | 115.26      | 120.70   |
| 1   | O     | 384 | ARG  | CG-CD-NE   | -5.04 | 100.92      | 112.00   |
| 1   | Q     | 106 | THR  | N-CA-C     | -5.04 | 105.44      | 111.03   |
| 1   | S     | 405 | VAL  | CA-C-O     | 5.04  | 126.19      | 120.95   |
| 1   | C     | 135 | TYR  | CB-CG-CD2  | 5.03  | 128.35      | 120.80   |
| 1   | E     | 209 | ILE  | CA-C-O     | 5.03  | 125.35      | 120.27   |
| 1   | G     | 342 | ASN  | CA-C-O     | 5.03  | 125.69      | 120.40   |
| 1   | Q     | 132 | ILE  | CA-C-N     | 5.03  | 127.03      | 120.28   |
| 1   | Q     | 132 | ILE  | C-N-CA     | 5.03  | 127.03      | 120.28   |
| 1   | C     | 197 | GLY  | CA-C-O     | 5.03  | 125.89      | 119.80   |
| 1   | P     | 131 | ILE  | N-CA-C     | 5.03  | 117.34      | 111.05   |
| 1   | P     | 522 | LEU  | O-C-N      | -5.03 | 116.41      | 122.15   |
| 1   | G     | 67  | THR  | N-CA-CB    | 5.03  | 118.97      | 110.77   |
| 1   | G     | 455 | VAL  | O-C-N      | -5.03 | 116.12      | 121.80   |
| 1   | H     | 92  | ILE  | O-C-N      | -5.03 | 116.65      | 121.83   |
| 1   | H     | 183 | ASP  | CA-C-N     | 5.03  | 127.09      | 120.60   |
| 1   | H     | 183 | ASP  | C-N-CA     | 5.03  | 127.09      | 120.60   |
| 1   | M     | 288 | ASP  | CA-C-N     | 5.03  | 129.12      | 120.72   |
| 1   | M     | 288 | ASP  | C-N-CA     | 5.03  | 129.12      | 120.72   |
| 1   | P     | 265 | ARG  | CG-CD-NE   | -5.03 | 100.93      | 112.00   |
| 1   | P     | 432 | TYR  | CA-C-O     | 5.03  | 125.88      | 120.70   |
| 1   | Q     | 221 | GLN  | N-CA-C     | 5.03  | 116.72      | 109.07   |
| 1   | R     | 254 | GLU  | CA-C-O     | -5.03 | 115.22      | 121.11   |
| 1   | S     | 277 | ASP  | N-CA-CB    | -5.03 | 102.78      | 110.07   |
| 1   | A     | 234 | HIS  | CB-CG-CD2  | -5.03 | 124.66      | 131.20   |
| 1   | F     | 449 | ASN  | OD1-CG-ND2 | -5.03 | 117.57      | 122.60   |
| 1   | S     | 312 | LEU  | CA-C-N     | 5.03  | 127.28      | 120.44   |
| 1   | S     | 312 | LEU  | C-N-CA     | 5.03  | 127.28      | 120.44   |
| 1   | D     | 153 | VAL  | CA-C-N     | 5.03  | 131.77      | 122.92   |
| 1   | D     | 153 | VAL  | C-N-CA     | 5.03  | 131.77      | 122.92   |
| 1   | D     | 427 | LYS  | CA-C-N     | 5.03  | 127.02      | 120.28   |
| 1   | D     | 427 | LYS  | C-N-CA     | 5.03  | 127.02      | 120.28   |
| 1   | K     | 430 | ARG  | O-C-N      | -5.03 | 116.89      | 122.07   |
| 1   | P     | 460 | GLU  | O-C-N      | -5.03 | 116.12      | 122.20   |
| 1   | S     | 187 | LYS  | N-CA-C     | 5.03  | 116.76      | 111.28   |
| 1   | A     | 442 | LEU  | N-CA-C     | 5.03  | 116.76      | 111.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 384 | ARG  | NE-CZ-NH2  | -5.03 | 114.68      | 119.20   |
| 1   | D     | 193 | ALA  | O-C-N      | -5.03 | 116.72      | 122.95   |
| 1   | H     | 399 | ARG  | O-C-N      | -5.03 | 116.89      | 122.07   |
| 1   | H     | 487 | ILE  | CA-C-O     | 5.03  | 126.01      | 120.48   |
| 1   | K     | 448 | ALA  | N-CA-C     | 5.03  | 116.57      | 111.14   |
| 1   | L     | 282 | LEU  | O-C-N      | -5.03 | 116.42      | 122.15   |
| 1   | L     | 387 | LEU  | CA-C-O     | -5.03 | 116.26      | 121.99   |
| 1   | P     | 297 | VAL  | CA-C-O     | -5.03 | 115.95      | 121.28   |
| 1   | S     | 433 | ALA  | O-C-N      | -5.03 | 115.54      | 121.32   |
| 1   | L     | 382 | LEU  | CA-C-O     | 5.02  | 125.67      | 120.40   |
| 1   | A     | 250 | ASP  | CA-CB-CG   | 5.02  | 117.62      | 112.60   |
| 1   | A     | 375 | ASN  | CA-C-N     | 5.02  | 126.12      | 119.84   |
| 1   | A     | 375 | ASN  | C-N-CA     | 5.02  | 126.12      | 119.84   |
| 1   | M     | 69  | THR  | N-CA-C     | 5.02  | 115.16      | 108.38   |
| 1   | P     | 299 | ILE  | O-C-N      | -5.02 | 117.75      | 123.18   |
| 1   | A     | 444 | VAL  | N-CA-CB    | 5.02  | 116.42      | 110.55   |
| 1   | E     | 168 | SER  | N-CA-C     | -5.02 | 106.00      | 112.68   |
| 1   | L     | 300 | CYS  | O-C-N      | -5.02 | 116.10      | 122.78   |
| 1   | Q     | 421 | VAL  | CA-C-N     | 5.02  | 127.28      | 120.65   |
| 1   | Q     | 421 | VAL  | C-N-CA     | 5.02  | 127.28      | 120.65   |
| 1   | S     | 296 | ASN  | CA-C-N     | -5.02 | 115.15      | 122.58   |
| 1   | S     | 296 | ASN  | C-N-CA     | -5.02 | 115.15      | 122.58   |
| 1   | B     | 482 | ASN  | OD1-CG-ND2 | -5.02 | 117.58      | 122.60   |
| 1   | C     | 205 | ASP  | CA-CB-CG   | 5.02  | 117.62      | 112.60   |
| 1   | F     | 252 | SER  | O-C-N      | -5.02 | 116.70      | 122.87   |
| 1   | I     | 119 | GLU  | CA-C-O     | 5.02  | 125.87      | 120.55   |
| 1   | O     | 306 | GLU  | CA-CB-CG   | -5.02 | 104.06      | 114.10   |
| 1   | Q     | 390 | LEU  | N-CA-CB    | -5.02 | 102.74      | 110.12   |
| 1   | S     | 355 | SER  | N-CA-C     | 5.02  | 116.75      | 111.28   |
| 1   | C     | 119 | GLU  | CA-C-O     | -5.02 | 115.23      | 120.55   |
| 1   | F     | 313 | ALA  | CA-C-O     | -5.02 | 115.53      | 120.70   |
| 1   | Q     | 335 | THR  | CA-CB-OG1  | 5.02  | 117.13      | 109.60   |
| 1   | D     | 484 | TRP  | CA-CB-CG   | 5.02  | 123.13      | 113.60   |
| 1   | M     | 146 | ILE  | CA-C-N     | 5.02  | 127.27      | 120.65   |
| 1   | M     | 146 | ILE  | C-N-CA     | 5.02  | 127.27      | 120.65   |
| 1   | Q     | 468 | ASP  | O-C-N      | -5.02 | 116.71      | 122.08   |
| 1   | A     | 360 | ARG  | NE-CZ-NH1  | -5.01 | 116.49      | 121.50   |
| 1   | C     | 94  | LYS  | O-C-N      | 5.01  | 127.24      | 122.03   |
| 1   | G     | 67  | THR  | O-C-N      | -5.01 | 116.86      | 123.28   |
| 1   | H     | 472 | LYS  | CA-C-O     | 5.01  | 125.56      | 119.49   |
| 1   | I     | 456 | SER  | CB-CA-C    | -5.01 | 103.01      | 110.88   |
| 1   | K     | 429 | LEU  | CA-C-N     | 5.01  | 126.96      | 120.44   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 429 | LEU  | C-N-CA     | 5.01  | 126.96      | 120.44   |
| 1   | A     | 86  | ALA  | N-CA-C     | -5.01 | 105.71      | 111.07   |
| 1   | L     | 465 | ASP  | CA-C-O     | -5.01 | 114.79      | 119.80   |
| 1   | P     | 219 | ASP  | CA-C-O     | 5.01  | 125.50      | 119.43   |
| 1   | Q     | 487 | ILE  | CB-CA-C    | -5.01 | 104.22      | 111.19   |
| 1   | B     | 340 | VAL  | N-CA-C     | 5.01  | 115.07      | 107.80   |
| 1   | D     | 467 | ILE  | N-CA-C     | 5.01  | 115.24      | 110.53   |
| 1   | E     | 66  | ILE  | CA-CB-CG1  | 5.01  | 118.92      | 110.40   |
| 1   | M     | 445 | GLU  | CA-C-N     | 5.01  | 127.27      | 120.65   |
| 1   | M     | 445 | GLU  | C-N-CA     | 5.01  | 127.27      | 120.65   |
| 1   | N     | 426 | ALA  | N-CA-CB    | 5.01  | 117.22      | 110.10   |
| 1   | R     | 362 | VAL  | O-C-N      | -5.01 | 117.85      | 122.71   |
| 1   | R     | 477 | HIS  | CB-CG-CD2  | -5.01 | 124.69      | 131.20   |
| 1   | C     | 280 | GLU  | CA-C-O     | 5.01  | 125.80      | 120.24   |
| 1   | D     | 355 | SER  | N-CA-C     | 5.01  | 117.47      | 111.71   |
| 1   | E     | 338 | ARG  | NE-CZ-NH2  | -5.01 | 114.69      | 119.20   |
| 1   | L     | 286 | LYS  | CA-C-N     | 5.01  | 126.87      | 120.56   |
| 1   | L     | 286 | LYS  | C-N-CA     | 5.01  | 126.87      | 120.56   |
| 1   | M     | 335 | THR  | CA-C-O     | 5.01  | 125.21      | 119.35   |
| 1   | N     | 42  | VAL  | CA-C-O     | -5.01 | 115.74      | 120.95   |
| 1   | S     | 508 | VAL  | N-CA-CB    | -5.01 | 104.69      | 110.55   |
| 1   | D     | 396 | ARG  | CD-NE-CZ   | 5.01  | 131.41      | 124.40   |
| 1   | E     | 370 | VAL  | CA-C-O     | 5.01  | 127.04      | 120.78   |
| 1   | G     | 122 | LEU  | O-C-N      | -5.01 | 116.81      | 122.12   |
| 1   | I     | 432 | TYR  | N-CA-C     | 5.01  | 116.59      | 111.03   |
| 1   | K     | 79  | MET  | O-C-N      | -5.01 | 115.67      | 122.48   |
| 1   | N     | 313 | ALA  | O-C-N      | -5.01 | 116.81      | 122.12   |
| 1   | S     | 461 | ASN  | CB-CG-ND2  | -5.01 | 108.89      | 116.40   |
| 1   | I     | 415 | ILE  | O-C-N      | -5.00 | 117.72      | 122.97   |
| 1   | S     | 171 | SER  | CB-CA-C    | -5.00 | 101.73      | 110.09   |
| 1   | S     | 439 | LYS  | CA-C-N     | 5.00  | 127.69      | 120.38   |
| 1   | S     | 439 | LYS  | C-N-CA     | 5.00  | 127.69      | 120.38   |
| 1   | C     | 35  | ASN  | CA-C-N     | 5.00  | 127.05      | 120.60   |
| 1   | C     | 35  | ASN  | C-N-CA     | 5.00  | 127.05      | 120.60   |
| 1   | G     | 323 | ALA  | O-C-N      | -5.00 | 117.34      | 122.94   |
| 1   | M     | 433 | ALA  | N-CA-C     | 5.00  | 120.87      | 109.81   |
| 1   | S     | 265 | ARG  | CG-CD-NE   | -5.00 | 100.99      | 112.00   |
| 1   | B     | 353 | TYR  | N-CA-CB    | -5.00 | 102.70      | 110.55   |
| 1   | B     | 477 | HIS  | CG-CD2-NE2 | 5.00  | 112.20      | 107.20   |
| 1   | E     | 182 | ALA  | CA-C-O     | 5.00  | 126.07      | 120.82   |
| 1   | G     | 111 | SER  | O-C-N      | 5.00  | 127.23      | 122.03   |
| 1   | H     | 525 | ARG  | NE-CZ-NH1  | -5.00 | 116.50      | 121.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | K     | 379 | ILE  | N-CA-C     | -5.00 | 101.50      | 108.80   |
| 1   | Q     | 36  | ILE  | CA-C-N     | 5.00  | 129.14      | 121.19   |
| 1   | Q     | 36  | ILE  | C-N-CA     | 5.00  | 129.14      | 121.19   |
| 1   | Q     | 73  | ALA  | CA-C-N     | 5.00  | 126.98      | 120.28   |
| 1   | Q     | 73  | ALA  | C-N-CA     | 5.00  | 126.98      | 120.28   |
| 1   | Q     | 234 | HIS  | CG-CD2-NE2 | 5.00  | 112.20      | 107.20   |

There are no chirality outliers.

All (207) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 135 | TYR  | Sidechain |
| 1   | A     | 178 | ARG  | Sidechain |
| 1   | A     | 234 | HIS  | Sidechain |
| 1   | A     | 240 | ARG  | Sidechain |
| 1   | A     | 322 | ARG  | Sidechain |
| 1   | A     | 33  | ARG  | Sidechain |
| 1   | A     | 353 | TYR  | Sidechain |
| 1   | A     | 430 | ARG  | Sidechain |
| 1   | A     | 474 | ARG  | Sidechain |
| 1   | B     | 162 | ARG  | Sidechain |
| 1   | B     | 322 | ARG  | Sidechain |
| 1   | B     | 333 | ARG  | Sidechain |
| 1   | B     | 353 | TYR  | Sidechain |
| 1   | B     | 360 | ARG  | Sidechain |
| 1   | B     | 384 | ARG  | Sidechain |
| 1   | B     | 389 | ARG  | Sidechain |
| 1   | B     | 430 | ARG  | Sidechain |
| 1   | B     | 447 | TYR  | Sidechain |
| 1   | B     | 464 | PHE  | Sidechain |
| 1   | B     | 474 | ARG  | Sidechain |
| 1   | B     | 477 | HIS  | Sidechain |
| 1   | B     | 485 | TYR  | Sidechain |
| 1   | B     | 50  | TYR  | Sidechain |
| 1   | B     | 525 | ARG  | Sidechain |
| 1   | B     | 53  | ARG  | Sidechain |
| 1   | C     | 135 | TYR  | Sidechain |
| 1   | C     | 162 | ARG  | Sidechain |
| 1   | C     | 180 | TYR  | Sidechain |
| 1   | C     | 196 | ARG  | Sidechain |
| 1   | C     | 224 | TYR  | Sidechain |
| 1   | C     | 321 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 333 | ARG  | Sidechain |
| 1   | C     | 338 | ARG  | Sidechain |
| 1   | C     | 360 | ARG  | Sidechain |
| 1   | C     | 384 | ARG  | Sidechain |
| 1   | C     | 430 | ARG  | Sidechain |
| 1   | C     | 432 | TYR  | Sidechain |
| 1   | C     | 485 | TYR  | Sidechain |
| 1   | C     | 490 | TYR  | Sidechain |
| 1   | C     | 53  | ARG  | Sidechain |
| 1   | D     | 110 | PHE  | Sidechain |
| 1   | D     | 135 | TYR  | Sidechain |
| 1   | D     | 178 | ARG  | Sidechain |
| 1   | D     | 224 | TYR  | Sidechain |
| 1   | D     | 234 | HIS  | Sidechain |
| 1   | D     | 275 | PHE  | Sidechain |
| 1   | D     | 338 | ARG  | Sidechain |
| 1   | D     | 360 | ARG  | Sidechain |
| 1   | D     | 413 | ARG  | Sidechain |
| 1   | D     | 432 | TYR  | Sidechain |
| 1   | D     | 50  | TYR  | Sidechain |
| 1   | D     | 53  | ARG  | Sidechain |
| 1   | E     | 178 | ARG  | Sidechain |
| 1   | E     | 240 | ARG  | Sidechain |
| 1   | E     | 338 | ARG  | Sidechain |
| 1   | E     | 360 | ARG  | Sidechain |
| 1   | E     | 389 | ARG  | Sidechain |
| 1   | E     | 474 | ARG  | Sidechain |
| 1   | E     | 490 | TYR  | Sidechain |
| 1   | F     | 123 | TYR  | Sidechain |
| 1   | F     | 135 | TYR  | Sidechain |
| 1   | F     | 240 | ARG  | Sidechain |
| 1   | F     | 321 | ARG  | Sidechain |
| 1   | F     | 333 | ARG  | Sidechain |
| 1   | F     | 369 | PHE  | Sidechain |
| 1   | F     | 389 | ARG  | Sidechain |
| 1   | F     | 474 | ARG  | Sidechain |
| 1   | F     | 53  | ARG  | Sidechain |
| 1   | G     | 135 | TYR  | Sidechain |
| 1   | G     | 178 | ARG  | Sidechain |
| 1   | G     | 180 | TYR  | Sidechain |
| 1   | G     | 321 | ARG  | Sidechain |
| 1   | G     | 33  | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | G     | 333 | ARG  | Sidechain |
| 1   | G     | 353 | TYR  | Sidechain |
| 1   | G     | 360 | ARG  | Sidechain |
| 1   | G     | 432 | TYR  | Sidechain |
| 1   | G     | 474 | ARG  | Sidechain |
| 1   | G     | 485 | TYR  | Sidechain |
| 1   | G     | 490 | TYR  | Sidechain |
| 1   | G     | 525 | ARG  | Sidechain |
| 1   | G     | 53  | ARG  | Sidechain |
| 1   | H     | 110 | PHE  | Sidechain |
| 1   | H     | 196 | ARG  | Sidechain |
| 1   | H     | 265 | ARG  | Sidechain |
| 1   | H     | 321 | ARG  | Sidechain |
| 1   | H     | 322 | ARG  | Sidechain |
| 1   | H     | 338 | ARG  | Sidechain |
| 1   | H     | 353 | TYR  | Sidechain |
| 1   | H     | 396 | ARG  | Sidechain |
| 1   | H     | 432 | TYR  | Sidechain |
| 1   | H     | 474 | ARG  | Sidechain |
| 1   | H     | 485 | TYR  | Sidechain |
| 1   | H     | 490 | TYR  | Sidechain |
| 1   | H     | 525 | ARG  | Sidechain |
| 1   | I     | 110 | PHE  | Sidechain |
| 1   | I     | 123 | TYR  | Sidechain |
| 1   | I     | 178 | ARG  | Sidechain |
| 1   | I     | 234 | HIS  | Sidechain |
| 1   | I     | 333 | ARG  | Sidechain |
| 1   | I     | 360 | ARG  | Sidechain |
| 1   | I     | 413 | ARG  | Sidechain |
| 1   | I     | 432 | TYR  | Sidechain |
| 1   | I     | 447 | TYR  | Sidechain |
| 1   | I     | 50  | TYR  | Sidechain |
| 1   | I     | 53  | ARG  | Sidechain |
| 1   | I     | 83  | HIS  | Sidechain |
| 1   | K     | 178 | ARG  | Sidechain |
| 1   | K     | 201 | TYR  | Sidechain |
| 1   | K     | 224 | TYR  | Sidechain |
| 1   | K     | 311 | TYR  | Sidechain |
| 1   | K     | 322 | ARG  | Sidechain |
| 1   | K     | 333 | ARG  | Sidechain |
| 1   | K     | 384 | ARG  | Sidechain |
| 1   | K     | 396 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | K     | 430 | ARG  | Sidechain |
| 1   | K     | 432 | TYR  | Sidechain |
| 1   | K     | 464 | PHE  | Sidechain |
| 1   | K     | 485 | TYR  | Sidechain |
| 1   | K     | 490 | TYR  | Sidechain |
| 1   | K     | 50  | TYR  | Sidechain |
| 1   | L     | 135 | TYR  | Sidechain |
| 1   | L     | 162 | ARG  | Sidechain |
| 1   | L     | 250 | ASP  | Mainchain |
| 1   | L     | 265 | ARG  | Sidechain |
| 1   | L     | 322 | ARG  | Sidechain |
| 1   | L     | 33  | ARG  | Sidechain |
| 1   | L     | 333 | ARG  | Sidechain |
| 1   | L     | 338 | ARG  | Sidechain |
| 1   | L     | 396 | ARG  | Sidechain |
| 1   | L     | 399 | ARG  | Sidechain |
| 1   | L     | 413 | ARG  | Sidechain |
| 1   | L     | 474 | ARG  | Mainchain |
| 1   | L     | 525 | ARG  | Sidechain |
| 1   | M     | 110 | PHE  | Sidechain |
| 1   | M     | 123 | TYR  | Sidechain |
| 1   | M     | 275 | PHE  | Sidechain |
| 1   | M     | 322 | ARG  | Sidechain |
| 1   | M     | 353 | TYR  | Sidechain |
| 1   | M     | 360 | ARG  | Sidechain |
| 1   | M     | 485 | TYR  | Sidechain |
| 1   | M     | 525 | ARG  | Sidechain |
| 1   | N     | 180 | TYR  | Sidechain |
| 1   | N     | 240 | ARG  | Sidechain |
| 1   | N     | 311 | TYR  | Sidechain |
| 1   | N     | 321 | ARG  | Sidechain |
| 1   | N     | 33  | ARG  | Sidechain |
| 1   | N     | 360 | ARG  | Sidechain |
| 1   | O     | 123 | TYR  | Sidechain |
| 1   | O     | 135 | TYR  | Sidechain |
| 1   | O     | 201 | TYR  | Sidechain |
| 1   | O     | 224 | TYR  | Sidechain |
| 1   | O     | 311 | TYR  | Sidechain |
| 1   | O     | 321 | ARG  | Sidechain |
| 1   | O     | 338 | ARG  | Sidechain |
| 1   | O     | 360 | ARG  | Sidechain |
| 1   | O     | 430 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | O     | 432 | TYR  | Sidechain |
| 1   | O     | 490 | TYR  | Sidechain |
| 1   | O     | 525 | ARG  | Sidechain |
| 1   | O     | 83  | HIS  | Sidechain |
| 1   | P     | 110 | PHE  | Sidechain |
| 1   | P     | 180 | TYR  | Sidechain |
| 1   | P     | 265 | ARG  | Sidechain |
| 1   | P     | 333 | ARG  | Sidechain |
| 1   | P     | 360 | ARG  | Sidechain |
| 1   | P     | 384 | ARG  | Sidechain |
| 1   | P     | 413 | ARG  | Sidechain |
| 1   | P     | 430 | ARG  | Sidechain |
| 1   | P     | 432 | TYR  | Sidechain |
| 1   | P     | 53  | ARG  | Sidechain |
| 1   | Q     | 123 | TYR  | Sidechain |
| 1   | Q     | 135 | TYR  | Sidechain |
| 1   | Q     | 178 | ARG  | Sidechain |
| 1   | Q     | 180 | TYR  | Sidechain |
| 1   | Q     | 196 | ARG  | Sidechain |
| 1   | Q     | 240 | ARG  | Sidechain |
| 1   | Q     | 311 | TYR  | Sidechain |
| 1   | Q     | 321 | ARG  | Sidechain |
| 1   | Q     | 33  | ARG  | Sidechain |
| 1   | Q     | 333 | ARG  | Sidechain |
| 1   | Q     | 396 | ARG  | Sidechain |
| 1   | Q     | 399 | ARG  | Sidechain |
| 1   | Q     | 413 | ARG  | Sidechain |
| 1   | Q     | 485 | TYR  | Sidechain |
| 1   | Q     | 50  | TYR  | Sidechain |
| 1   | Q     | 525 | ARG  | Sidechain |
| 1   | Q     | 98  | GLU  | Mainchain |
| 1   | R     | 135 | TYR  | Sidechain |
| 1   | R     | 162 | ARG  | Sidechain |
| 1   | R     | 178 | ARG  | Sidechain |
| 1   | R     | 196 | ARG  | Sidechain |
| 1   | R     | 240 | ARG  | Sidechain |
| 1   | R     | 311 | TYR  | Sidechain |
| 1   | R     | 353 | TYR  | Sidechain |
| 1   | R     | 360 | ARG  | Sidechain |
| 1   | R     | 396 | ARG  | Sidechain |
| 1   | R     | 413 | ARG  | Sidechain |
| 1   | R     | 430 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | R     | 432 | TYR  | Sidechain |
| 1   | S     | 135 | TYR  | Sidechain |
| 1   | S     | 180 | TYR  | Sidechain |
| 1   | S     | 265 | ARG  | Sidechain |
| 1   | S     | 311 | TYR  | Sidechain |
| 1   | S     | 430 | ARG  | Sidechain |
| 1   | S     | 490 | TYR  | Sidechain |
| 1   | S     | 83  | HIS  | Sidechain |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3849  | 0        | 3995     | 8       | 0            |
| 1   | B     | 3849  | 0        | 3995     | 19      | 0            |
| 1   | C     | 3849  | 0        | 3995     | 15      | 0            |
| 1   | D     | 3849  | 0        | 3995     | 14      | 0            |
| 1   | E     | 3849  | 0        | 3995     | 21      | 0            |
| 1   | F     | 3849  | 0        | 3995     | 13      | 0            |
| 1   | G     | 3849  | 0        | 3995     | 19      | 0            |
| 1   | H     | 3849  | 0        | 3995     | 11      | 0            |
| 1   | I     | 3849  | 0        | 3995     | 14      | 0            |
| 1   | K     | 3849  | 0        | 3995     | 18      | 0            |
| 1   | L     | 3849  | 0        | 3995     | 8       | 0            |
| 1   | M     | 3849  | 0        | 3995     | 13      | 0            |
| 1   | N     | 3849  | 0        | 3995     | 16      | 0            |
| 1   | O     | 3849  | 0        | 3995     | 12      | 0            |
| 1   | P     | 3849  | 0        | 3995     | 17      | 0            |
| 1   | Q     | 3849  | 0        | 3995     | 14      | 0            |
| 1   | R     | 3849  | 0        | 3995     | 7       | 0            |
| 1   | S     | 3849  | 0        | 3995     | 10      | 0            |
| 2   | A     | 31    | 0        | 12       | 0       | 0            |
| 2   | B     | 31    | 0        | 12       | 0       | 0            |
| 2   | C     | 31    | 0        | 12       | 0       | 0            |
| 2   | D     | 31    | 0        | 12       | 0       | 0            |
| 2   | E     | 31    | 0        | 12       | 0       | 0            |
| 2   | F     | 31    | 0        | 12       | 0       | 0            |
| 2   | G     | 31    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | H     | 31    | 0        | 12       | 0       | 0            |
| 2   | I     | 31    | 0        | 12       | 0       | 0            |
| 2   | K     | 31    | 0        | 12       | 0       | 0            |
| 2   | L     | 31    | 0        | 12       | 0       | 0            |
| 2   | M     | 31    | 0        | 12       | 0       | 0            |
| 2   | N     | 31    | 0        | 12       | 0       | 0            |
| 2   | O     | 31    | 0        | 12       | 0       | 0            |
| 2   | P     | 31    | 0        | 12       | 0       | 0            |
| 2   | Q     | 31    | 0        | 12       | 0       | 0            |
| 2   | R     | 31    | 0        | 12       | 0       | 0            |
| 2   | S     | 31    | 0        | 12       | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |
| 3   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 3   | S     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 69858 | 0        | 72126    | 241     | 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 (241) 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:F:246:ILE:HA   | 1:F:297:VAL:HG13 | 1.62                     | 0.79              |
| 1:P:88:LEU:HD13  | 1:Q:68:ILE:HD11  | 1.73                     | 0.71              |
| 1:K:189:VAL:HG11 | 1:K:405:VAL:HG12 | 1.76                     | 0.67              |
| 1:E:331:LEU:HD11 | 1:E:370:VAL:HG11 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:79:MET:HE2   | 1:C:81:LEU:HD21  | 1.79                     | 0.65              |
| 1:B:418:GLY:HA3  | 1:B:497:MET:HE2  | 1.79                     | 0.65              |
| 1:K:473:LEU:HD12 | 1:K:487:ILE:HG23 | 1.79                     | 0.64              |
| 1:M:106:THR:HG23 | 1:M:454:LEU:HD21 | 1.79                     | 0.62              |
| 1:M:222:LEU:HD11 | 1:M:379:ILE:HD12 | 1.80                     | 0.62              |
| 1:F:240:ARG:HG2  | 1:F:240:ARG:HH11 | 1.64                     | 0.61              |
| 1:K:104:THR:O    | 1:K:108:VAL:HG23 | 2.01                     | 0.61              |
| 1:I:164:ILE:HG21 | 1:I:408:VAL:HG21 | 1.82                     | 0.60              |
| 1:B:393:GLU:CD   | 1:B:396:ARG:HH22 | 2.11                     | 0.58              |
| 1:O:393:GLU:CD   | 1:O:396:ARG:HH21 | 2.12                     | 0.58              |
| 1:D:480:GLU:CD   | 1:D:480:GLU:H    | 2.11                     | 0.58              |
| 1:M:30:GLU:H     | 1:M:30:GLU:CD    | 2.10                     | 0.58              |
| 1:E:459:ILE:HD11 | 1:E:487:ILE:HB   | 1.87                     | 0.57              |
| 1:F:272:MET:HE3  | 1:F:276:LEU:HD11 | 1.86                     | 0.57              |
| 1:G:222:LEU:HD11 | 1:G:379:ILE:HD12 | 1.85                     | 0.56              |
| 1:Q:232:VAL:HG11 | 1:Q:318:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:507:LEU:HD23 | 1:D:507:LEU:H    | 1.71                     | 0.56              |
| 1:D:85:ALA:HB1   | 1:D:523:VAL:HG13 | 1.89                     | 0.55              |
| 1:I:241:LEU:HB3  | 1:I:244:ALA:HB2  | 1.88                     | 0.54              |
| 1:H:46:LEU:HD21  | 1:H:105:LYS:HA   | 1.90                     | 0.54              |
| 1:N:462:ALA:HB2  | 1:N:489:LEU:HD22 | 1.90                     | 0.54              |
| 1:O:177:ALA:HB3  | 1:O:217:ILE:HG13 | 1.88                     | 0.54              |
| 1:D:443:ALA:O    | 1:D:446:ALA:HB3  | 2.07                     | 0.54              |
| 1:C:305:ASP:OD2  | 1:C:307:VAL:HG22 | 2.08                     | 0.54              |
| 1:C:433:ALA:HB3  | 1:C:434:PRO:HD3  | 1.90                     | 0.53              |
| 1:G:138:ALA:HB1  | 1:G:429:LEU:HD21 | 1.91                     | 0.53              |
| 1:M:423:ILE:HD12 | 1:M:477:HIS:CG   | 2.44                     | 0.53              |
| 1:E:233:VAL:HG12 | 1:E:237:MET:SD   | 2.49                     | 0.53              |
| 1:A:162:ARG:HG3  | 1:A:186:VAL:HG21 | 1.91                     | 0.53              |
| 1:O:145:THR:HG21 | 1:O:425:ILE:HA   | 1.91                     | 0.53              |
| 1:O:234:HIS:CD2  | 1:O:236:GLY:H    | 2.28                     | 0.52              |
| 1:I:248:LEU:N    | 1:I:248:LEU:HD22 | 2.25                     | 0.52              |
| 1:N:155:ILE:HD12 | 1:N:190:THR:HG22 | 1.92                     | 0.52              |
| 1:I:136:LYS:HA   | 1:I:136:LYS:HE2  | 1.92                     | 0.51              |
| 1:H:473:LEU:HD11 | 1:H:487:ILE:HG23 | 1.91                     | 0.51              |
| 1:O:360:ARG:HB2  | 1:O:369:PHE:CE2  | 2.45                     | 0.51              |
| 1:Q:477:HIS:CG   | 1:Q:477:HIS:O    | 2.64                     | 0.51              |
| 1:Q:75:ILE:HG22  | 1:Q:75:ILE:O     | 2.11                     | 0.51              |
| 1:G:162:ARG:CG   | 1:G:186:VAL:HG21 | 2.41                     | 0.50              |
| 1:H:224:TYR:HA   | 1:H:379:ILE:HG22 | 1.93                     | 0.50              |
| 1:M:477:HIS:CG   | 1:M:477:HIS:O    | 2.63                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:185:VAL:HG13 | 1:L:402:LEU:HA   | 1.93                     | 0.50              |
| 1:A:189:VAL:HG21 | 1:A:405:VAL:HG12 | 1.93                     | 0.50              |
| 1:L:418:GLY:HA3  | 1:L:497:MET:HE2  | 1.94                     | 0.50              |
| 1:D:231:GLU:CD   | 1:D:231:GLU:H    | 2.19                     | 0.49              |
| 1:F:53:ARG:HH21  | 1:F:490:TYR:HA   | 1.77                     | 0.49              |
| 1:K:327:ASP:O    | 1:K:331:LEU:HB2  | 2.12                     | 0.49              |
| 1:H:184:ILE:HG23 | 1:H:222:LEU:HB2  | 1.94                     | 0.49              |
| 1:N:38:ALA:O     | 1:N:41:ALA:HB3   | 2.13                     | 0.49              |
| 1:Q:88:LEU:HD22  | 1:R:68:ILE:HD11  | 1.94                     | 0.49              |
| 1:F:248:LEU:H    | 1:F:248:LEU:HD12 | 1.78                     | 0.49              |
| 1:K:526:ILE:HG21 | 1:L:58:MET:HE2   | 1.95                     | 0.48              |
| 1:N:383:ILE:HD11 | 1:N:398:LEU:CD2  | 2.43                     | 0.48              |
| 1:K:185:VAL:HG12 | 1:K:405:VAL:HG21 | 1.94                     | 0.48              |
| 1:B:383:ILE:HD11 | 1:B:398:LEU:HD23 | 1.94                     | 0.48              |
| 1:G:47:LYS:HA    | 1:G:109:ILE:HD11 | 1.96                     | 0.48              |
| 1:I:222:LEU:HD11 | 1:I:379:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:430:ARG:HH21 | 1:A:452:GLU:CD   | 2.21                     | 0.48              |
| 1:O:251:ALA:HB2  | 1:O:341:SER:O    | 2.13                     | 0.48              |
| 1:P:30:GLU:CD    | 1:P:30:GLU:H     | 2.22                     | 0.48              |
| 1:O:338:ARG:HH21 | 1:O:350:ASP:CG   | 2.22                     | 0.47              |
| 1:A:55:MET:HB3   | 1:I:527:ASP:HB2  | 1.96                     | 0.47              |
| 1:B:430:ARG:HH21 | 1:B:452:GLU:CD   | 2.22                     | 0.47              |
| 1:B:496:ASP:CG   | 1:B:499:GLN:HE21 | 2.22                     | 0.47              |
| 1:C:161:LEU:HD11 | 1:C:409:ILE:HD11 | 1.95                     | 0.47              |
| 1:I:192:VAL:HG21 | 1:I:207:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:248:LEU:HD21 | 1:B:331:LEU:HD13 | 1.94                     | 0.47              |
| 1:K:244:ALA:HB1  | 1:K:297:VAL:HG23 | 1.96                     | 0.47              |
| 1:K:423:ILE:HD12 | 1:K:477:HIS:CG   | 2.50                     | 0.47              |
| 1:D:290:ILE:HG21 | 1:D:298:ILE:HD12 | 1.97                     | 0.47              |
| 1:I:102:ASP:HB3  | 1:I:508:VAL:HG11 | 1.96                     | 0.47              |
| 1:L:335:THR:HB   | 1:L:353:TYR:H    | 1.80                     | 0.47              |
| 1:B:39:VAL:HG22  | 1:B:89:LEU:HD22  | 1.97                     | 0.47              |
| 1:F:49:THR:HG22  | 1:F:49:THR:O     | 2.15                     | 0.47              |
| 1:M:234:HIS:CD2  | 1:M:236:GLY:H    | 2.33                     | 0.47              |
| 1:A:334:ALA:O    | 1:A:373:ALA:HB1  | 2.14                     | 0.46              |
| 1:N:452:GLU:CD   | 1:N:474:ARG:HH22 | 2.24                     | 0.46              |
| 1:C:415:ILE:HD12 | 1:C:421:VAL:HG21 | 1.96                     | 0.46              |
| 1:E:283:ILE:HD12 | 1:E:286:LYS:HD2  | 1.98                     | 0.46              |
| 1:L:329:GLU:O    | 1:L:332:ALA:HB3  | 2.16                     | 0.46              |
| 1:D:471:MET:HA   | 1:D:474:ARG:HG2  | 1.97                     | 0.46              |
| 1:P:433:ALA:O    | 1:P:436:VAL:HG22 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:362:VAL:HG21 | 1:N:367:MET:HE3  | 1.97                     | 0.46              |
| 1:S:393:GLU:CD   | 1:S:396:ARG:HH21 | 2.24                     | 0.46              |
| 1:G:30:GLU:CD    | 1:G:30:GLU:H     | 2.23                     | 0.46              |
| 1:H:185:VAL:HG13 | 1:H:402:LEU:HA   | 1.97                     | 0.46              |
| 1:P:398:LEU:C    | 1:P:398:LEU:HD23 | 2.41                     | 0.46              |
| 1:S:184:ILE:HG23 | 1:S:222:LEU:HB2  | 1.98                     | 0.46              |
| 1:Q:336:GLY:HA3  | 1:Q:374:LYS:HD3  | 1.98                     | 0.45              |
| 1:D:248:LEU:HD22 | 1:D:248:LEU:H    | 1.82                     | 0.45              |
| 1:N:473:LEU:HA   | 1:N:476:THR:HG22 | 1.98                     | 0.45              |
| 1:F:246:ILE:HD13 | 1:F:331:LEU:HD21 | 1.97                     | 0.45              |
| 1:G:162:ARG:HG2  | 1:G:186:VAL:HG21 | 1.97                     | 0.45              |
| 1:P:253:LEU:HD11 | 1:P:298:ILE:HD11 | 1.98                     | 0.45              |
| 1:R:161:LEU:HD22 | 1:R:405:VAL:HG13 | 1.99                     | 0.45              |
| 1:D:477:HIS:CD2  | 1:D:477:HIS:O    | 2.70                     | 0.45              |
| 1:N:208:GLN:HB3  | 1:N:380:SER:HB3  | 1.99                     | 0.45              |
| 1:E:242:GLU:HA   | 1:E:356:LEU:HD12 | 1.98                     | 0.45              |
| 1:P:212:LYS:O    | 1:P:384:ARG:HA   | 2.17                     | 0.45              |
| 1:E:155:ILE:HG13 | 1:E:190:THR:HG22 | 1.99                     | 0.45              |
| 1:E:425:ILE:O    | 1:E:429:LEU:HB2  | 2.17                     | 0.45              |
| 1:R:312:LEU:HD13 | 1:R:319:ALA:HB2  | 1.99                     | 0.45              |
| 1:B:329:GLU:O    | 1:B:332:ALA:HB3  | 2.16                     | 0.44              |
| 1:O:30:GLU:CD    | 1:O:30:GLU:H     | 2.25                     | 0.44              |
| 1:B:293:THR:HG21 | 1:B:346:ILE:HG22 | 1.98                     | 0.44              |
| 1:K:208:GLN:OE1  | 1:K:226:ILE:HG23 | 2.18                     | 0.44              |
| 1:P:531:SER:HA   | 1:Q:60:VAL:H     | 1.82                     | 0.44              |
| 1:C:164:ILE:HG21 | 1:C:408:VAL:HG21 | 2.00                     | 0.44              |
| 1:B:246:ILE:HA   | 1:B:297:VAL:HB   | 2.00                     | 0.44              |
| 1:K:246:ILE:HD12 | 1:K:246:ILE:H    | 1.83                     | 0.44              |
| 1:F:240:ARG:HG2  | 1:F:240:ARG:NH1  | 2.31                     | 0.44              |
| 1:G:237:MET:HB3  | 1:G:238:PRO:HD2  | 2.00                     | 0.44              |
| 1:Q:421:VAL:O    | 1:Q:425:ILE:HD12 | 2.18                     | 0.44              |
| 1:B:387:LEU:H    | 1:B:390:LEU:HB3  | 1.83                     | 0.44              |
| 1:B:76:LEU:HD11  | 1:B:108:VAL:HG21 | 1.98                     | 0.44              |
| 1:L:443:ALA:O    | 1:L:446:ALA:HB3  | 2.17                     | 0.43              |
| 1:E:76:LEU:HD11  | 1:E:108:VAL:HG21 | 2.00                     | 0.43              |
| 1:E:229:ASP:HA   | 1:E:367:MET:SD   | 2.58                     | 0.43              |
| 1:E:477:HIS:CG   | 1:E:477:HIS:O    | 2.71                     | 0.43              |
| 1:C:423:ILE:HD12 | 1:C:473:LEU:HD22 | 1.99                     | 0.43              |
| 1:S:161:LEU:HD22 | 1:S:405:VAL:HG13 | 2.01                     | 0.43              |
| 1:D:209:ILE:HG21 | 1:D:395:GLU:HG3  | 2.00                     | 0.43              |
| 1:E:250:ASP:HB2  | 1:E:339:VAL:CG1  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:287:VAL:HG13 | 1:E:312:LEU:HD21 | 2.00                     | 0.43              |
| 1:E:453:SER:O    | 1:E:457:ILE:HG13 | 2.18                     | 0.43              |
| 1:L:208:GLN:HE21 | 1:L:210:VAL:CG1  | 2.31                     | 0.43              |
| 1:P:459:ILE:O    | 1:P:462:ALA:HB3  | 2.18                     | 0.43              |
| 1:G:423:ILE:CD1  | 1:G:473:LEU:HD22 | 2.47                     | 0.43              |
| 1:G:473:LEU:HD12 | 1:G:487:ILE:HB   | 2.00                     | 0.43              |
| 1:M:526:ILE:HD13 | 1:N:58:MET:SD    | 2.59                     | 0.43              |
| 1:N:383:ILE:HD11 | 1:N:398:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:432:TYR:CZ   | 1:A:436:VAL:HG22 | 2.53                     | 0.43              |
| 1:E:429:LEU:HD11 | 1:E:444:VAL:HG13 | 2.01                     | 0.43              |
| 1:P:36:ILE:O     | 1:P:39:VAL:HB    | 2.19                     | 0.43              |
| 1:S:232:VAL:HG22 | 1:S:359:GLU:OE1  | 2.18                     | 0.43              |
| 1:C:477:HIS:O    | 1:C:477:HIS:CD2  | 2.71                     | 0.43              |
| 1:M:226:ILE:HD11 | 1:M:334:ALA:HB2  | 2.01                     | 0.43              |
| 1:N:207:ILE:HA   | 1:N:379:ILE:O    | 2.19                     | 0.43              |
| 1:F:226:ILE:HD11 | 1:F:378:SER:HB3  | 2.01                     | 0.43              |
| 1:H:306:GLU:CD   | 1:H:306:GLU:H    | 2.27                     | 0.43              |
| 1:B:433:ALA:HB3  | 1:B:434:PRO:HD3  | 2.01                     | 0.43              |
| 1:I:192:VAL:HG12 | 1:I:202:VAL:HG23 | 2.01                     | 0.43              |
| 1:M:338:ARG:HH21 | 1:M:350:ASP:CG   | 2.26                     | 0.43              |
| 1:N:249:ILE:HD11 | 1:N:290:ILE:HD13 | 2.01                     | 0.43              |
| 1:P:88:LEU:CD1   | 1:Q:68:ILE:HD11  | 2.44                     | 0.43              |
| 1:P:343:ILE:C    | 1:P:345:GLU:H    | 2.27                     | 0.43              |
| 1:Q:238:PRO:HG2  | 1:Q:241:LEU:HD21 | 1.99                     | 0.43              |
| 1:G:318:LEU:C    | 1:G:318:LEU:HD23 | 2.43                     | 0.43              |
| 1:K:323:ALA:HB3  | 1:K:328:LEU:HD21 | 2.01                     | 0.43              |
| 1:S:254:GLU:HG2  | 1:S:255:VAL:H    | 1.83                     | 0.43              |
| 1:P:433:ALA:HB3  | 1:P:434:PRO:HD3  | 2.02                     | 0.42              |
| 1:S:299:ILE:HG13 | 1:S:320:VAL:HB   | 2.01                     | 0.42              |
| 1:H:231:GLU:H    | 1:H:231:GLU:CD   | 2.28                     | 0.42              |
| 1:K:415:ILE:HG12 | 1:K:506:ALA:HB2  | 2.01                     | 0.42              |
| 1:L:213:ALA:HB2  | 1:L:391:VAL:HG11 | 2.01                     | 0.42              |
| 1:K:232:VAL:HG11 | 1:K:318:LEU:HD11 | 2.02                     | 0.42              |
| 1:K:30:GLU:CD    | 1:K:30:GLU:H     | 2.28                     | 0.42              |
| 1:F:185:VAL:HG13 | 1:F:402:LEU:HA   | 2.00                     | 0.42              |
| 1:N:486:GLY:O    | 1:N:494:PRO:HA   | 2.20                     | 0.42              |
| 1:G:290:ILE:HD13 | 1:G:298:ILE:HD11 | 2.00                     | 0.42              |
| 1:M:248:LEU:H    | 1:M:248:LEU:HD22 | 1.85                     | 0.42              |
| 1:Q:232:VAL:HA   | 1:Q:320:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:173:ALA:HB3  | 1:A:393:GLU:HG2  | 2.02                     | 0.42              |
| 1:C:150:ALA:HB1  | 1:C:413:ARG:HB3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:79:MET:HB3   | 1:E:81:LEU:HD21  | 2.02                     | 0.42              |
| 1:G:526:ILE:HA   | 1:H:56:ASP:O     | 2.19                     | 0.42              |
| 1:K:93:ALA:HB1   | 1:K:108:VAL:HG22 | 2.02                     | 0.42              |
| 1:O:477:HIS:NE2  | 1:O:483:LYS:HA   | 2.34                     | 0.42              |
| 1:F:272:MET:HE3  | 1:F:276:LEU:CD1  | 2.49                     | 0.41              |
| 1:M:433:ALA:HB3  | 1:M:434:PRO:HD3  | 2.01                     | 0.41              |
| 1:S:264:ILE:HD12 | 1:S:266:ILE:HD12 | 2.02                     | 0.41              |
| 1:C:161:LEU:HB3  | 1:C:186:VAL:HG22 | 2.02                     | 0.41              |
| 1:G:226:ILE:HG13 | 1:G:331:LEU:HA   | 2.01                     | 0.41              |
| 1:G:234:HIS:CD2  | 1:G:236:GLY:H    | 2.38                     | 0.41              |
| 1:K:42:VAL:O     | 1:K:45:ALA:HB3   | 2.21                     | 0.41              |
| 1:G:291:LEU:HD21 | 1:G:317:VAL:HG21 | 2.01                     | 0.41              |
| 1:S:47:LYS:HA    | 1:S:109:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:245:LYS:HB3  | 1:C:351:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:415:ILE:HB   | 1:D:421:VAL:HG21 | 2.03                     | 0.41              |
| 1:F:289:LYS:NZ   | 1:F:344:ASP:OD2  | 2.48                     | 0.41              |
| 1:G:249:ILE:O    | 1:G:300:CYS:HA   | 2.21                     | 0.41              |
| 1:N:287:VAL:CG1  | 1:N:312:LEU:HD21 | 2.51                     | 0.41              |
| 1:R:409:ILE:HD13 | 1:R:409:ILE:HA   | 1.96                     | 0.41              |
| 1:S:287:VAL:HG11 | 1:S:311:TYR:CD2  | 2.56                     | 0.41              |
| 1:C:388:GLU:H    | 1:C:388:GLU:CD   | 2.29                     | 0.41              |
| 1:G:162:ARG:HG3  | 1:G:186:VAL:HG21 | 2.03                     | 0.41              |
| 1:K:179:GLU:CD   | 1:K:179:GLU:H    | 2.27                     | 0.41              |
| 1:C:141:VAL:HG21 | 1:C:432:TYR:CE1  | 2.55                     | 0.41              |
| 1:H:181:ILE:CG2  | 1:H:398:LEU:HD23 | 2.51                     | 0.41              |
| 1:H:500:LYS:HG2  | 1:H:500:LYS:O    | 2.20                     | 0.41              |
| 1:O:46:LEU:HD23  | 1:O:46:LEU:HA    | 1.92                     | 0.41              |
| 1:O:219:ASP:HB3  | 1:O:384:ARG:HD3  | 2.01                     | 0.41              |
| 1:P:230:LYS:HG3  | 1:P:323:ALA:HA   | 2.02                     | 0.41              |
| 1:P:297:VAL:HG21 | 1:P:357:ILE:HD13 | 2.02                     | 0.41              |
| 1:B:485:TYR:HA   | 1:B:495:VAL:O    | 2.20                     | 0.41              |
| 1:E:248:LEU:HD12 | 1:E:328:LEU:HD23 | 2.02                     | 0.41              |
| 1:B:30:GLU:CD    | 1:B:30:GLU:H     | 2.29                     | 0.41              |
| 1:B:257:LYS:HB2  | 1:B:260:LEU:HD21 | 2.02                     | 0.41              |
| 1:D:30:GLU:H     | 1:D:30:GLU:CD    | 2.29                     | 0.41              |
| 1:E:460:GLU:OE2  | 1:E:466:PRO:HG2  | 2.21                     | 0.41              |
| 1:G:331:LEU:HD11 | 1:G:370:VAL:HG21 | 2.02                     | 0.41              |
| 1:H:246:ILE:HA   | 1:H:297:VAL:HG13 | 2.02                     | 0.41              |
| 1:I:227:VAL:HG22 | 1:I:369:PHE:CD1  | 2.56                     | 0.41              |
| 1:I:354:ALA:HB3  | 1:I:357:ILE:HD11 | 2.02                     | 0.41              |
| 1:K:416:ALA:HB3  | 1:K:484:TRP:CE3  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:201:TYR:CE1  | 1:P:410:LYS:HG2  | 2.56                     | 0.41              |
| 1:E:110:PHE:CE2  | 1:E:451:LEU:HD22 | 2.56                     | 0.41              |
| 1:G:312:LEU:HD13 | 1:G:319:ALA:HB2  | 2.03                     | 0.41              |
| 1:I:415:ILE:HD12 | 1:I:421:VAL:HG21 | 2.02                     | 0.41              |
| 1:M:49:THR:O     | 1:M:49:THR:HG22  | 2.20                     | 0.41              |
| 1:M:246:ILE:HA   | 1:M:297:VAL:HG13 | 2.02                     | 0.41              |
| 1:P:93:ALA:HB1   | 1:P:108:VAL:HG22 | 2.03                     | 0.41              |
| 1:Q:106:THR:HG23 | 1:Q:454:LEU:HD21 | 2.01                     | 0.41              |
| 1:B:250:ASP:HB2  | 1:B:339:VAL:HG12 | 2.03                     | 0.40              |
| 1:B:290:ILE:HD11 | 1:B:343:ILE:HD12 | 2.03                     | 0.40              |
| 1:B:425:ILE:HG21 | 1:B:425:ILE:HD13 | 1.81                     | 0.40              |
| 1:D:477:HIS:O    | 1:D:477:HIS:CG   | 2.74                     | 0.40              |
| 1:I:471:MET:HA   | 1:I:474:ARG:HG2  | 2.03                     | 0.40              |
| 1:P:211:LYS:HD2  | 1:P:391:VAL:HG22 | 2.03                     | 0.40              |
| 1:N:30:GLU:H     | 1:N:30:GLU:CD    | 2.30                     | 0.40              |
| 1:N:340:VAL:HG11 | 1:N:346:ILE:HB   | 2.04                     | 0.40              |
| 1:R:36:ILE:HG22  | 1:R:40:LYS:HE2   | 2.03                     | 0.40              |
| 1:S:234:HIS:CE1  | 1:S:309:GLN:OE1  | 2.74                     | 0.40              |
| 1:A:229:ASP:HA   | 1:A:367:MET:HG2  | 2.04                     | 0.40              |
| 1:D:150:ALA:HA   | 1:D:415:ILE:HG22 | 2.04                     | 0.40              |
| 1:E:383:ILE:HG22 | 1:E:384:ARG:N    | 2.36                     | 0.40              |
| 1:E:498:TRP:C    | 1:E:500:LYS:H    | 2.29                     | 0.40              |
| 1:R:28:GLY:N     | 1:R:30:GLU:OE2   | 2.55                     | 0.40              |
| 1:C:30:GLU:H     | 1:C:30:GLU:CD    | 2.30                     | 0.40              |
| 1:C:361:LYS:HG3  | 1:C:366:LYS:HG2  | 2.04                     | 0.40              |
| 1:F:297:VAL:HG23 | 1:F:318:LEU:HD22 | 2.03                     | 0.40              |
| 1:O:482:ASN:HB3  | 1:O:485:TYR:CD1  | 2.56                     | 0.40              |
| 1:Q:430:ARG:HH21 | 1:Q:452:GLU:CD   | 2.30                     | 0.40              |
| 1:E:46:LEU:O     | 1:E:47:LYS:C     | 2.65                     | 0.40              |
| 1:I:35:ASN:O     | 1:I:39:VAL:HG23  | 2.21                     | 0.40              |
| 1:Q:360:ARG:HH22 | 1:Q:371:GLU:CD   | 2.30                     | 0.40              |
| 1:R:87:LYS:HA    | 1:R:90:VAL:HG22  | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 503/553 (91%)   | 453 (90%)  | 46 (9%)  | 4 (1%)   | 16          | 54 |
| 1   | B     | 503/553 (91%)   | 451 (90%)  | 44 (9%)  | 8 (2%)   | 7           | 37 |
| 1   | C     | 503/553 (91%)   | 456 (91%)  | 44 (9%)  | 3 (1%)   | 21          | 59 |
| 1   | D     | 503/553 (91%)   | 459 (91%)  | 41 (8%)  | 3 (1%)   | 21          | 59 |
| 1   | E     | 503/553 (91%)   | 449 (89%)  | 50 (10%) | 4 (1%)   | 16          | 54 |
| 1   | F     | 503/553 (91%)   | 457 (91%)  | 42 (8%)  | 4 (1%)   | 16          | 54 |
| 1   | G     | 503/553 (91%)   | 449 (89%)  | 50 (10%) | 4 (1%)   | 16          | 54 |
| 1   | H     | 503/553 (91%)   | 459 (91%)  | 42 (8%)  | 2 (0%)   | 30          | 67 |
| 1   | I     | 503/553 (91%)   | 456 (91%)  | 44 (9%)  | 3 (1%)   | 21          | 59 |
| 1   | K     | 503/553 (91%)   | 457 (91%)  | 44 (9%)  | 2 (0%)   | 30          | 67 |
| 1   | L     | 503/553 (91%)   | 451 (90%)  | 46 (9%)  | 6 (1%)   | 10          | 43 |
| 1   | M     | 503/553 (91%)   | 456 (91%)  | 42 (8%)  | 5 (1%)   | 12          | 48 |
| 1   | N     | 503/553 (91%)   | 454 (90%)  | 43 (8%)  | 6 (1%)   | 10          | 43 |
| 1   | O     | 503/553 (91%)   | 452 (90%)  | 46 (9%)  | 5 (1%)   | 12          | 48 |
| 1   | P     | 503/553 (91%)   | 455 (90%)  | 43 (8%)  | 5 (1%)   | 12          | 48 |
| 1   | Q     | 503/553 (91%)   | 450 (90%)  | 50 (10%) | 3 (1%)   | 21          | 59 |
| 1   | R     | 503/553 (91%)   | 455 (90%)  | 43 (8%)  | 5 (1%)   | 12          | 48 |
| 1   | S     | 503/553 (91%)   | 451 (90%)  | 49 (10%) | 3 (1%)   | 21          | 59 |
| All | All   | 9054/9954 (91%) | 8170 (90%) | 809 (9%) | 75 (1%)  | 18          | 54 |

All (75) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 213 | ALA  |
| 1   | B     | 30  | GLU  |
| 1   | C     | 30  | GLU  |
| 1   | D     | 30  | GLU  |
| 1   | F     | 30  | GLU  |
| 1   | H     | 30  | GLU  |
| 1   | H     | 438 | GLY  |
| 1   | I     | 30  | GLU  |
| 1   | K     | 30  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 95  | GLY  |
| 1   | L     | 203 | ASP  |
| 1   | M     | 177 | ALA  |
| 1   | O     | 30  | GLU  |
| 1   | P     | 30  | GLU  |
| 1   | P     | 305 | ASP  |
| 1   | Q     | 30  | GLU  |
| 1   | S     | 30  | GLU  |
| 1   | A     | 30  | GLU  |
| 1   | A     | 438 | GLY  |
| 1   | B     | 149 | LEU  |
| 1   | B     | 203 | ASP  |
| 1   | B     | 438 | GLY  |
| 1   | C     | 438 | GLY  |
| 1   | D     | 149 | LEU  |
| 1   | D     | 438 | GLY  |
| 1   | E     | 30  | GLU  |
| 1   | E     | 149 | LEU  |
| 1   | G     | 30  | GLU  |
| 1   | L     | 30  | GLU  |
| 1   | M     | 30  | GLU  |
| 1   | N     | 30  | GLU  |
| 1   | N     | 438 | GLY  |
| 1   | P     | 149 | LEU  |
| 1   | R     | 30  | GLU  |
| 1   | S     | 438 | GLY  |
| 1   | B     | 56  | ASP  |
| 1   | C     | 149 | LEU  |
| 1   | E     | 438 | GLY  |
| 1   | G     | 149 | LEU  |
| 1   | G     | 438 | GLY  |
| 1   | I     | 438 | GLY  |
| 1   | K     | 438 | GLY  |
| 1   | L     | 438 | GLY  |
| 1   | M     | 149 | LEU  |
| 1   | N     | 177 | ALA  |
| 1   | N     | 229 | ASP  |
| 1   | O     | 203 | ASP  |
| 1   | O     | 438 | GLY  |
| 1   | P     | 257 | LYS  |
| 1   | P     | 438 | GLY  |
| 1   | R     | 47  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 438 | GLY  |
| 1   | S     | 251 | ALA  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 245 | LYS  |
| 1   | B     | 98  | GLU  |
| 1   | F     | 216 | SER  |
| 1   | G     | 148 | GLU  |
| 1   | I     | 149 | LEU  |
| 1   | M     | 499 | GLN  |
| 1   | N     | 149 | LEU  |
| 1   | N     | 363 | GLY  |
| 1   | O     | 149 | LEU  |
| 1   | O     | 216 | SER  |
| 1   | R     | 149 | LEU  |
| 1   | E     | 81  | LEU  |
| 1   | F     | 149 | LEU  |
| 1   | M     | 438 | GLY  |
| 1   | Q     | 149 | LEU  |
| 1   | Q     | 438 | GLY  |
| 1   | B     | 176 | GLY  |
| 1   | B     | 434 | PRO  |
| 1   | L     | 202 | VAL  |
| 1   | R     | 95  | GLY  |
| 1   | F     | 438 | GLY  |

### 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%) | 392 (96%) | 18 (4%)  | 25          | 47 |
| 1   | B     | 410/447 (92%) | 395 (96%) | 15 (4%)  | 30          | 51 |
| 1   | C     | 410/447 (92%) | 397 (97%) | 13 (3%)  | 34          | 56 |
| 1   | D     | 410/447 (92%) | 397 (97%) | 13 (3%)  | 34          | 56 |
| 1   | E     | 410/447 (92%) | 395 (96%) | 15 (4%)  | 30          | 51 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | F     | 410/447 (92%)   | 395 (96%)  | 15 (4%)  | 30          | 51 |
| 1   | G     | 410/447 (92%)   | 395 (96%)  | 15 (4%)  | 30          | 51 |
| 1   | H     | 410/447 (92%)   | 391 (95%)  | 19 (5%)  | 24          | 45 |
| 1   | I     | 410/447 (92%)   | 393 (96%)  | 17 (4%)  | 27          | 48 |
| 1   | K     | 410/447 (92%)   | 398 (97%)  | 12 (3%)  | 37          | 58 |
| 1   | L     | 410/447 (92%)   | 397 (97%)  | 13 (3%)  | 34          | 56 |
| 1   | M     | 410/447 (92%)   | 387 (94%)  | 23 (6%)  | 19          | 40 |
| 1   | N     | 410/447 (92%)   | 387 (94%)  | 23 (6%)  | 19          | 40 |
| 1   | O     | 410/447 (92%)   | 397 (97%)  | 13 (3%)  | 34          | 56 |
| 1   | P     | 410/447 (92%)   | 396 (97%)  | 14 (3%)  | 32          | 54 |
| 1   | Q     | 410/447 (92%)   | 395 (96%)  | 15 (4%)  | 30          | 51 |
| 1   | R     | 410/447 (92%)   | 399 (97%)  | 11 (3%)  | 39          | 60 |
| 1   | S     | 410/447 (92%)   | 399 (97%)  | 11 (3%)  | 39          | 60 |
| All | All   | 7380/8046 (92%) | 7105 (96%) | 275 (4%) | 31          | 51 |

All (275) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 144 | GLN  |
| 1   | A     | 239 | LYS  |
| 1   | A     | 246 | ILE  |
| 1   | A     | 301 | GLN  |
| 1   | A     | 343 | ILE  |
| 1   | A     | 356 | LEU  |
| 1   | A     | 366 | LYS  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 421 | VAL  |
| 1   | A     | 423 | ILE  |
| 1   | A     | 429 | LEU  |
| 1   | A     | 436 | VAL  |
| 1   | A     | 460 | GLU  |
| 1   | A     | 471 | MET  |
| 1   | A     | 473 | LEU  |
| 1   | A     | 483 | LYS  |
| 1   | A     | 487 | ILE  |
| 1   | A     | 511 | ASN  |
| 1   | B     | 30  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 89  | LEU  |
| 1   | B     | 114 | LEU  |
| 1   | B     | 183 | ASP  |
| 1   | B     | 209 | ILE  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 331 | LEU  |
| 1   | B     | 348 | GLU  |
| 1   | B     | 360 | ARG  |
| 1   | B     | 407 | ASP  |
| 1   | B     | 408 | VAL  |
| 1   | B     | 421 | VAL  |
| 1   | B     | 473 | LEU  |
| 1   | B     | 477 | HIS  |
| 1   | B     | 489 | LEU  |
| 1   | C     | 59  | LEU  |
| 1   | C     | 89  | LEU  |
| 1   | C     | 153 | VAL  |
| 1   | C     | 270 | THR  |
| 1   | C     | 296 | ASN  |
| 1   | C     | 333 | ARG  |
| 1   | C     | 366 | LYS  |
| 1   | C     | 368 | VAL  |
| 1   | C     | 378 | SER  |
| 1   | C     | 429 | LEU  |
| 1   | C     | 451 | LEU  |
| 1   | C     | 473 | LEU  |
| 1   | C     | 487 | ILE  |
| 1   | D     | 43  | GLU  |
| 1   | D     | 115 | VAL  |
| 1   | D     | 132 | ILE  |
| 1   | D     | 211 | LYS  |
| 1   | D     | 231 | GLU  |
| 1   | D     | 248 | LEU  |
| 1   | D     | 288 | ASP  |
| 1   | D     | 301 | GLN  |
| 1   | D     | 331 | LEU  |
| 1   | D     | 396 | ARG  |
| 1   | D     | 407 | ASP  |
| 1   | D     | 473 | LEU  |
| 1   | D     | 487 | ILE  |
| 1   | E     | 63  | LEU  |
| 1   | E     | 89  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 131 | ILE  |
| 1   | E     | 144 | GLN  |
| 1   | E     | 220 | THR  |
| 1   | E     | 234 | HIS  |
| 1   | E     | 282 | LEU  |
| 1   | E     | 321 | ARG  |
| 1   | E     | 366 | LYS  |
| 1   | E     | 390 | LEU  |
| 1   | E     | 421 | VAL  |
| 1   | E     | 473 | LEU  |
| 1   | E     | 485 | TYR  |
| 1   | E     | 487 | ILE  |
| 1   | E     | 502 | VAL  |
| 1   | F     | 30  | GLU  |
| 1   | F     | 131 | ILE  |
| 1   | F     | 164 | ILE  |
| 1   | F     | 167 | THR  |
| 1   | F     | 183 | ASP  |
| 1   | F     | 199 | LYS  |
| 1   | F     | 234 | HIS  |
| 1   | F     | 270 | THR  |
| 1   | F     | 356 | LEU  |
| 1   | F     | 366 | LYS  |
| 1   | F     | 423 | ILE  |
| 1   | F     | 470 | LEU  |
| 1   | F     | 473 | LEU  |
| 1   | F     | 485 | TYR  |
| 1   | F     | 531 | SER  |
| 1   | G     | 167 | THR  |
| 1   | G     | 293 | THR  |
| 1   | G     | 301 | GLN  |
| 1   | G     | 339 | VAL  |
| 1   | G     | 415 | ILE  |
| 1   | G     | 429 | LEU  |
| 1   | G     | 432 | TYR  |
| 1   | G     | 451 | LEU  |
| 1   | G     | 453 | SER  |
| 1   | G     | 473 | LEU  |
| 1   | G     | 485 | TYR  |
| 1   | G     | 487 | ILE  |
| 1   | G     | 489 | LEU  |
| 1   | G     | 523 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 525 | ARG  |
| 1   | H     | 59  | LEU  |
| 1   | H     | 84  | PRO  |
| 1   | H     | 128 | PRO  |
| 1   | H     | 153 | VAL  |
| 1   | H     | 155 | ILE  |
| 1   | H     | 167 | THR  |
| 1   | H     | 181 | ILE  |
| 1   | H     | 204 | LEU  |
| 1   | H     | 231 | GLU  |
| 1   | H     | 232 | VAL  |
| 1   | H     | 234 | HIS  |
| 1   | H     | 238 | PRO  |
| 1   | H     | 293 | THR  |
| 1   | H     | 421 | VAL  |
| 1   | H     | 434 | PRO  |
| 1   | H     | 436 | VAL  |
| 1   | H     | 466 | PRO  |
| 1   | H     | 484 | TRP  |
| 1   | H     | 487 | ILE  |
| 1   | I     | 50  | TYR  |
| 1   | I     | 84  | PRO  |
| 1   | I     | 89  | LEU  |
| 1   | I     | 97  | ASP  |
| 1   | I     | 153 | VAL  |
| 1   | I     | 160 | LEU  |
| 1   | I     | 185 | VAL  |
| 1   | I     | 235 | PRO  |
| 1   | I     | 293 | THR  |
| 1   | I     | 297 | VAL  |
| 1   | I     | 317 | VAL  |
| 1   | I     | 366 | LYS  |
| 1   | I     | 399 | ARG  |
| 1   | I     | 407 | ASP  |
| 1   | I     | 469 | LEU  |
| 1   | I     | 485 | TYR  |
| 1   | I     | 530 | VAL  |
| 1   | K     | 43  | GLU  |
| 1   | K     | 89  | LEU  |
| 1   | K     | 96  | GLN  |
| 1   | K     | 114 | LEU  |
| 1   | K     | 179 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 246 | ILE  |
| 1   | K     | 266 | ILE  |
| 1   | K     | 305 | ASP  |
| 1   | K     | 333 | ARG  |
| 1   | K     | 388 | GLU  |
| 1   | K     | 453 | SER  |
| 1   | K     | 473 | LEU  |
| 1   | L     | 79  | MET  |
| 1   | L     | 84  | PRO  |
| 1   | L     | 143 | LEU  |
| 1   | L     | 218 | ASN  |
| 1   | L     | 341 | SER  |
| 1   | L     | 356 | LEU  |
| 1   | L     | 428 | LYS  |
| 1   | L     | 429 | LEU  |
| 1   | L     | 442 | LEU  |
| 1   | L     | 458 | LEU  |
| 1   | L     | 466 | PRO  |
| 1   | L     | 487 | ILE  |
| 1   | L     | 505 | PRO  |
| 1   | M     | 30  | GLU  |
| 1   | M     | 43  | GLU  |
| 1   | M     | 76  | LEU  |
| 1   | M     | 89  | LEU  |
| 1   | M     | 143 | LEU  |
| 1   | M     | 159 | ASP  |
| 1   | M     | 220 | THR  |
| 1   | M     | 231 | GLU  |
| 1   | M     | 241 | LEU  |
| 1   | M     | 248 | LEU  |
| 1   | M     | 263 | GLU  |
| 1   | M     | 305 | ASP  |
| 1   | M     | 309 | GLN  |
| 1   | M     | 331 | LEU  |
| 1   | M     | 356 | LEU  |
| 1   | M     | 366 | LYS  |
| 1   | M     | 370 | VAL  |
| 1   | M     | 390 | LEU  |
| 1   | M     | 398 | LEU  |
| 1   | M     | 423 | ILE  |
| 1   | M     | 434 | PRO  |
| 1   | M     | 484 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 525 | ARG  |
| 1   | N     | 60  | VAL  |
| 1   | N     | 62  | SER  |
| 1   | N     | 67  | THR  |
| 1   | N     | 128 | PRO  |
| 1   | N     | 167 | THR  |
| 1   | N     | 181 | ILE  |
| 1   | N     | 204 | LEU  |
| 1   | N     | 231 | GLU  |
| 1   | N     | 234 | HIS  |
| 1   | N     | 297 | VAL  |
| 1   | N     | 305 | ASP  |
| 1   | N     | 318 | LEU  |
| 1   | N     | 329 | GLU  |
| 1   | N     | 357 | ILE  |
| 1   | N     | 370 | VAL  |
| 1   | N     | 409 | ILE  |
| 1   | N     | 445 | GLU  |
| 1   | N     | 451 | LEU  |
| 1   | N     | 473 | LEU  |
| 1   | N     | 484 | TRP  |
| 1   | N     | 485 | TYR  |
| 1   | N     | 487 | ILE  |
| 1   | N     | 511 | ASN  |
| 1   | O     | 297 | VAL  |
| 1   | O     | 298 | ILE  |
| 1   | O     | 305 | ASP  |
| 1   | O     | 326 | SER  |
| 1   | O     | 356 | LEU  |
| 1   | O     | 364 | GLU  |
| 1   | O     | 423 | ILE  |
| 1   | O     | 432 | TYR  |
| 1   | O     | 451 | LEU  |
| 1   | O     | 453 | SER  |
| 1   | O     | 469 | LEU  |
| 1   | O     | 489 | LEU  |
| 1   | O     | 511 | ASN  |
| 1   | P     | 89  | LEU  |
| 1   | P     | 155 | ILE  |
| 1   | P     | 185 | VAL  |
| 1   | P     | 222 | LEU  |
| 1   | P     | 233 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 241 | LEU  |
| 1   | P     | 252 | SER  |
| 1   | P     | 283 | ILE  |
| 1   | P     | 343 | ILE  |
| 1   | P     | 349 | GLN  |
| 1   | P     | 368 | VAL  |
| 1   | P     | 473 | LEU  |
| 1   | P     | 476 | THR  |
| 1   | P     | 511 | ASN  |
| 1   | Q     | 84  | PRO  |
| 1   | Q     | 89  | LEU  |
| 1   | Q     | 153 | VAL  |
| 1   | Q     | 183 | ASP  |
| 1   | Q     | 202 | VAL  |
| 1   | Q     | 283 | ILE  |
| 1   | Q     | 347 | SER  |
| 1   | Q     | 390 | LEU  |
| 1   | Q     | 421 | VAL  |
| 1   | Q     | 424 | GLU  |
| 1   | Q     | 440 | GLU  |
| 1   | Q     | 453 | SER  |
| 1   | Q     | 476 | THR  |
| 1   | Q     | 489 | LEU  |
| 1   | Q     | 507 | LEU  |
| 1   | R     | 47  | LYS  |
| 1   | R     | 82  | GLN  |
| 1   | R     | 89  | LEU  |
| 1   | R     | 153 | VAL  |
| 1   | R     | 230 | LYS  |
| 1   | R     | 233 | VAL  |
| 1   | R     | 234 | HIS  |
| 1   | R     | 293 | THR  |
| 1   | R     | 396 | ARG  |
| 1   | R     | 408 | VAL  |
| 1   | R     | 473 | LEU  |
| 1   | S     | 88  | LEU  |
| 1   | S     | 174 | VAL  |
| 1   | S     | 223 | VAL  |
| 1   | S     | 234 | HIS  |
| 1   | S     | 301 | GLN  |
| 1   | S     | 356 | LEU  |
| 1   | S     | 368 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 407 | ASP  |
| 1   | S     | 451 | LEU  |
| 1   | S     | 494 | PRO  |
| 1   | S     | 528 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | ASN  |
| 1   | A     | 234 | HIS  |
| 1   | A     | 493 | GLN  |
| 1   | B     | 191 | GLN  |
| 1   | B     | 221 | GLN  |
| 1   | B     | 499 | GLN  |
| 1   | C     | 83  | HIS  |
| 1   | C     | 234 | HIS  |
| 1   | C     | 243 | ASN  |
| 1   | C     | 511 | ASN  |
| 1   | D     | 83  | HIS  |
| 1   | D     | 156 | ASN  |
| 1   | D     | 206 | ASN  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 281 | ASN  |
| 1   | D     | 301 | GLN  |
| 1   | E     | 243 | ASN  |
| 1   | E     | 267 | ASN  |
| 1   | F     | 144 | GLN  |
| 1   | F     | 147 | GLN  |
| 1   | F     | 191 | GLN  |
| 1   | F     | 206 | ASN  |
| 1   | F     | 349 | GLN  |
| 1   | F     | 493 | GLN  |
| 1   | G     | 147 | GLN  |
| 1   | G     | 234 | HIS  |
| 1   | G     | 441 | GLN  |
| 1   | G     | 482 | ASN  |
| 1   | H     | 91  | GLN  |
| 1   | H     | 206 | ASN  |
| 1   | H     | 221 | GLN  |
| 1   | H     | 499 | GLN  |
| 1   | H     | 511 | ASN  |
| 1   | I     | 82  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 83  | HIS  |
| 1   | I     | 147 | GLN  |
| 1   | I     | 191 | GLN  |
| 1   | I     | 243 | ASN  |
| 1   | I     | 267 | ASN  |
| 1   | I     | 511 | ASN  |
| 1   | K     | 243 | ASN  |
| 1   | K     | 349 | GLN  |
| 1   | K     | 482 | ASN  |
| 1   | M     | 83  | HIS  |
| 1   | M     | 218 | ASN  |
| 1   | M     | 234 | HIS  |
| 1   | M     | 309 | GLN  |
| 1   | M     | 499 | GLN  |
| 1   | N     | 144 | GLN  |
| 1   | N     | 156 | ASN  |
| 1   | N     | 221 | GLN  |
| 1   | N     | 375 | ASN  |
| 1   | N     | 479 | ASN  |
| 1   | N     | 481 | ASN  |
| 1   | N     | 499 | GLN  |
| 1   | O     | 234 | HIS  |
| 1   | O     | 309 | GLN  |
| 1   | P     | 156 | ASN  |
| 1   | P     | 191 | GLN  |
| 1   | P     | 243 | ASN  |
| 1   | P     | 342 | ASN  |
| 1   | P     | 435 | GLN  |
| 1   | P     | 441 | GLN  |
| 1   | Q     | 218 | ASN  |
| 1   | Q     | 221 | GLN  |
| 1   | Q     | 267 | ASN  |
| 1   | Q     | 441 | GLN  |
| 1   | Q     | 481 | ASN  |
| 1   | R     | 96  | GLN  |
| 1   | R     | 273 | GLN  |
| 1   | R     | 349 | GLN  |
| 1   | R     | 499 | GLN  |
| 1   | R     | 511 | ASN  |
| 1   | S     | 82  | GLN  |
| 1   | S     | 83  | HIS  |
| 1   | S     | 91  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 234 | HIS  |
| 1   | S     | 375 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | ATP  | S     | 800 | 3    | 32,33,33     | 2.21 | 8 (25%)     | 48,52,52    | 1.37 | 8 (16%)     |
| 2   | ATP  | E     | 800 | 3    | 32,33,33     | 1.61 | 7 (21%)     | 48,52,52    | 1.49 | 9 (18%)     |
| 2   | ATP  | D     | 800 | 3    | 32,33,33     | 2.18 | 3 (9%)      | 48,52,52    | 1.35 | 5 (10%)     |
| 2   | ATP  | K     | 800 | 3    | 32,33,33     | 2.00 | 8 (25%)     | 48,52,52    | 1.20 | 6 (12%)     |
| 2   | ATP  | M     | 800 | 3    | 32,33,33     | 2.58 | 7 (21%)     | 48,52,52    | 1.53 | 8 (16%)     |
| 2   | ATP  | H     | 800 | 3    | 32,33,33     | 1.71 | 5 (15%)     | 48,52,52    | 1.48 | 5 (10%)     |
| 2   | ATP  | R     | 800 | 3    | 32,33,33     | 1.09 | 1 (3%)      | 48,52,52    | 1.55 | 9 (18%)     |
| 2   | ATP  | G     | 800 | 3    | 32,33,33     | 2.78 | 6 (18%)     | 48,52,52    | 1.55 | 10 (20%)    |
| 2   | ATP  | P     | 800 | 3    | 32,33,33     | 1.61 | 5 (15%)     | 48,52,52    | 1.14 | 2 (4%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ATP  | L     | 800 | 3    | 32,33,33     | 2.72 | 5 (15%)  | 48,52,52    | 1.31 | 6 (12%)  |
| 2   | ATP  | F     | 800 | 3    | 32,33,33     | 1.64 | 7 (21%)  | 48,52,52    | 1.52 | 10 (20%) |
| 2   | ATP  | Q     | 800 | 3    | 32,33,33     | 2.02 | 6 (18%)  | 48,52,52    | 1.30 | 5 (10%)  |
| 2   | ATP  | O     | 800 | 3    | 32,33,33     | 1.76 | 3 (9%)   | 48,52,52    | 1.31 | 6 (12%)  |
| 2   | ATP  | A     | 800 | 3    | 32,33,33     | 1.58 | 3 (9%)   | 48,52,52    | 1.60 | 9 (18%)  |
| 2   | ATP  | C     | 800 | 3    | 32,33,33     | 1.65 | 6 (18%)  | 48,52,52    | 1.19 | 5 (10%)  |
| 2   | ATP  | B     | 800 | 3    | 32,33,33     | 2.14 | 3 (9%)   | 48,52,52    | 1.29 | 6 (12%)  |
| 2   | ATP  | I     | 800 | 3    | 32,33,33     | 2.30 | 6 (18%)  | 48,52,52    | 1.28 | 7 (14%)  |
| 2   | ATP  | N     | 800 | 3    | 32,33,33     | 2.56 | 6 (18%)  | 48,52,52    | 1.39 | 8 (16%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | ATP  | S     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | E     | 800 | 3    | -       | 5/22/38/38 | 0/3/3/3 |
| 2   | ATP  | D     | 800 | 3    | -       | 3/22/38/38 | 0/3/3/3 |
| 2   | ATP  | K     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | M     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | H     | 800 | 3    | -       | 8/22/38/38 | 0/3/3/3 |
| 2   | ATP  | R     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | G     | 800 | 3    | -       | 5/22/38/38 | 0/3/3/3 |
| 2   | ATP  | P     | 800 | 3    | -       | 2/22/38/38 | 0/3/3/3 |
| 2   | ATP  | L     | 800 | 3    | -       | 3/22/38/38 | 0/3/3/3 |
| 2   | ATP  | F     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | Q     | 800 | 3    | -       | 3/22/38/38 | 0/3/3/3 |
| 2   | ATP  | O     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | A     | 800 | 3    | -       | 6/22/38/38 | 0/3/3/3 |
| 2   | ATP  | C     | 800 | 3    | -       | 5/22/38/38 | 0/3/3/3 |
| 2   | ATP  | B     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | I     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |
| 2   | ATP  | N     | 800 | 3    | -       | 4/22/38/38 | 0/3/3/3 |

All (95) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | G     | 800 | ATP  | PA-O3A  | -13.74 | 1.44        | 1.59     |
| 2   | L     | 800 | ATP  | PA-O3A  | -12.46 | 1.46        | 1.59     |
| 2   | N     | 800 | ATP  | PA-O3A  | -12.16 | 1.46        | 1.59     |
| 2   | M     | 800 | ATP  | PA-O3A  | -11.93 | 1.46        | 1.59     |
| 2   | I     | 800 | ATP  | PA-O3A  | -10.58 | 1.48        | 1.59     |
| 2   | D     | 800 | ATP  | PA-O3A  | -10.05 | 1.48        | 1.59     |
| 2   | B     | 800 | ATP  | PA-O3A  | -9.66  | 1.49        | 1.59     |
| 2   | S     | 800 | ATP  | PA-O3A  | -8.22  | 1.50        | 1.59     |
| 2   | K     | 800 | ATP  | PA-O3A  | -7.92  | 1.50        | 1.59     |
| 2   | O     | 800 | ATP  | PA-O3A  | -6.99  | 1.52        | 1.59     |
| 2   | A     | 800 | ATP  | PA-O3A  | -6.89  | 1.52        | 1.59     |
| 2   | Q     | 800 | ATP  | PB-O3B  | 6.33   | 1.66        | 1.59     |
| 2   | P     | 800 | ATP  | PA-O3A  | -6.21  | 1.52        | 1.59     |
| 2   | H     | 800 | ATP  | PA-O3A  | -6.01  | 1.53        | 1.59     |
| 2   | L     | 800 | ATP  | PB-O3A  | 5.34   | 1.65        | 1.59     |
| 2   | C     | 800 | ATP  | PB-O3B  | 5.11   | 1.65        | 1.59     |
| 2   | Q     | 800 | ATP  | O4'-C1' | -5.08  | 1.30        | 1.42     |
| 2   | E     | 800 | ATP  | PA-O3A  | -4.83  | 1.54        | 1.59     |
| 2   | S     | 800 | ATP  | PB-O3A  | 4.72   | 1.64        | 1.59     |
| 2   | Q     | 800 | ATP  | PB-O3A  | -4.49  | 1.54        | 1.59     |
| 2   | F     | 800 | ATP  | PA-O3A  | -4.34  | 1.54        | 1.59     |
| 2   | B     | 800 | ATP  | PB-O3B  | 3.86   | 1.63        | 1.59     |
| 2   | S     | 800 | ATP  | C2'-C3' | 3.82   | 1.63        | 1.53     |
| 2   | N     | 800 | ATP  | C5-N7   | -3.72  | 1.32        | 1.39     |
| 2   | N     | 800 | ATP  | PB-O3A  | 3.59   | 1.63        | 1.59     |
| 2   | D     | 800 | ATP  | C5-N7   | -3.47  | 1.32        | 1.39     |
| 2   | Q     | 800 | ATP  | PA-O3A  | -3.36  | 1.55        | 1.59     |
| 2   | G     | 800 | ATP  | O4'-C4' | 3.34   | 1.52        | 1.45     |
| 2   | M     | 800 | ATP  | C8-N9   | 3.31   | 1.43        | 1.37     |
| 2   | E     | 800 | ATP  | C6-N6   | 3.27   | 1.42        | 1.34     |
| 2   | C     | 800 | ATP  | PA-O3A  | -3.25  | 1.56        | 1.59     |
| 2   | O     | 800 | ATP  | PB-O3A  | -3.19  | 1.56        | 1.59     |
| 2   | K     | 800 | ATP  | C5-N7   | 3.18   | 1.44        | 1.39     |
| 2   | F     | 800 | ATP  | C2-N3   | -3.09  | 1.28        | 1.33     |
| 2   | N     | 800 | ATP  | PB-O3B  | 3.00   | 1.62        | 1.59     |
| 2   | F     | 800 | ATP  | C5-C4   | -2.95  | 1.33        | 1.39     |
| 2   | L     | 800 | ATP  | C8-N7   | -2.83  | 1.26        | 1.31     |
| 2   | G     | 800 | ATP  | C5-N7   | -2.77  | 1.34        | 1.39     |
| 2   | C     | 800 | ATP  | C5-N7   | -2.71  | 1.34        | 1.39     |
| 2   | M     | 800 | ATP  | C2'-C1' | -2.70  | 1.45        | 1.53     |
| 2   | H     | 800 | ATP  | C5'-C4' | 2.69   | 1.59        | 1.51     |
| 2   | G     | 800 | ATP  | C8-N9   | 2.64   | 1.42        | 1.37     |
| 2   | S     | 800 | ATP  | C5-C4   | 2.63   | 1.43        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | M     | 800 | ATP  | C4-N3   | 2.63  | 1.39        | 1.34     |
| 2   | E     | 800 | ATP  | O2'-C2' | 2.62  | 1.49        | 1.43     |
| 2   | C     | 800 | ATP  | C5-C4   | 2.60  | 1.43        | 1.39     |
| 2   | G     | 800 | ATP  | PB-O3A  | -2.59 | 1.56        | 1.59     |
| 2   | I     | 800 | ATP  | C6-N6   | 2.57  | 1.40        | 1.34     |
| 2   | Q     | 800 | ATP  | C5-N7   | 2.56  | 1.43        | 1.39     |
| 2   | I     | 800 | ATP  | C6-N1   | 2.54  | 1.42        | 1.35     |
| 2   | M     | 800 | ATP  | C2-N3   | 2.52  | 1.38        | 1.33     |
| 2   | I     | 800 | ATP  | PB-O3A  | 2.52  | 1.62        | 1.59     |
| 2   | A     | 800 | ATP  | C4-N9   | -2.51 | 1.32        | 1.37     |
| 2   | I     | 800 | ATP  | C8-N9   | 2.51  | 1.41        | 1.37     |
| 2   | C     | 800 | ATP  | PA-O2A  | -2.50 | 1.43        | 1.55     |
| 2   | P     | 800 | ATP  | PB-O3B  | 2.50  | 1.62        | 1.59     |
| 2   | S     | 800 | ATP  | PB-O3B  | 2.47  | 1.62        | 1.59     |
| 2   | D     | 800 | ATP  | C2-N3   | 2.44  | 1.38        | 1.33     |
| 2   | L     | 800 | ATP  | C5'-C4' | 2.41  | 1.58        | 1.51     |
| 2   | F     | 800 | ATP  | C8-N7   | 2.41  | 1.36        | 1.31     |
| 2   | F     | 800 | ATP  | C3'-C4' | -2.32 | 1.47        | 1.53     |
| 2   | E     | 800 | ATP  | C8-N9   | -2.32 | 1.33        | 1.37     |
| 2   | F     | 800 | ATP  | PB-O3A  | 2.31  | 1.62        | 1.59     |
| 2   | N     | 800 | ATP  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | E     | 800 | ATP  | O3'-C3' | 2.30  | 1.48        | 1.43     |
| 2   | S     | 800 | ATP  | C8-N9   | -2.30 | 1.33        | 1.37     |
| 2   | G     | 800 | ATP  | C4-N9   | 2.25  | 1.42        | 1.37     |
| 2   | P     | 800 | ATP  | PB-O1B  | 2.25  | 1.58        | 1.50     |
| 2   | K     | 800 | ATP  | C4-N9   | 2.24  | 1.42        | 1.37     |
| 2   | K     | 800 | ATP  | PB-O3A  | 2.22  | 1.61        | 1.59     |
| 2   | P     | 800 | ATP  | C3'-C4' | 2.20  | 1.58        | 1.53     |
| 2   | H     | 800 | ATP  | PG-O2G  | -2.19 | 1.46        | 1.54     |
| 2   | F     | 800 | ATP  | C1'-N9  | 2.18  | 1.52        | 1.46     |
| 2   | B     | 800 | ATP  | C4-N3   | 2.16  | 1.38        | 1.34     |
| 2   | K     | 800 | ATP  | PB-O3B  | 2.15  | 1.61        | 1.59     |
| 2   | H     | 800 | ATP  | PB-O3A  | -2.14 | 1.57        | 1.59     |
| 2   | K     | 800 | ATP  | C2-N3   | 2.14  | 1.37        | 1.33     |
| 2   | A     | 800 | ATP  | PB-O3B  | 2.14  | 1.61        | 1.59     |
| 2   | K     | 800 | ATP  | C3'-C4' | 2.13  | 1.58        | 1.53     |
| 2   | R     | 800 | ATP  | PA-O3A  | -2.13 | 1.57        | 1.59     |
| 2   | M     | 800 | ATP  | C3'-C4' | 2.11  | 1.58        | 1.53     |
| 2   | N     | 800 | ATP  | C4-N3   | 2.10  | 1.38        | 1.34     |
| 2   | I     | 800 | ATP  | C2'-C1' | -2.09 | 1.46        | 1.53     |
| 2   | C     | 800 | ATP  | PA-O5'  | -2.08 | 1.51        | 1.59     |
| 2   | S     | 800 | ATP  | O4'-C4' | 2.08  | 1.49        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 800 | ATP  | C2-N1   | -2.08 | 1.30        | 1.33     |
| 2   | S     | 800 | ATP  | PG-O3G  | -2.07 | 1.47        | 1.54     |
| 2   | M     | 800 | ATP  | C4-N9   | 2.07  | 1.42        | 1.37     |
| 2   | K     | 800 | ATP  | C6-N6   | -2.06 | 1.29        | 1.34     |
| 2   | L     | 800 | ATP  | C2-N1   | 2.04  | 1.37        | 1.33     |
| 2   | Q     | 800 | ATP  | C2-N3   | 2.02  | 1.37        | 1.33     |
| 2   | E     | 800 | ATP  | C4-N9   | 2.02  | 1.41        | 1.37     |
| 2   | H     | 800 | ATP  | C6-N1   | -2.02 | 1.30        | 1.35     |
| 2   | O     | 800 | ATP  | PG-O3G  | -2.01 | 1.47        | 1.54     |
| 2   | P     | 800 | ATP  | O4'-C1' | 2.01  | 1.46        | 1.42     |

All (124) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | G     | 800 | ATP  | O4'-C1'-N9  | 4.98  | 117.65      | 108.09   |
| 2   | F     | 800 | ATP  | O2A-PA-O3A  | 4.87  | 120.43      | 107.27   |
| 2   | M     | 800 | ATP  | C4-N9-C8    | -4.81 | 100.69      | 105.74   |
| 2   | H     | 800 | ATP  | O4'-C1'-N9  | 4.08  | 115.93      | 108.09   |
| 2   | A     | 800 | ATP  | N6-C6-N1    | 4.07  | 127.44      | 118.38   |
| 2   | A     | 800 | ATP  | O2A-PA-O3A  | 3.86  | 117.70      | 107.27   |
| 2   | E     | 800 | ATP  | O2B-PB-O3B  | 3.83  | 117.64      | 107.27   |
| 2   | O     | 800 | ATP  | O4'-C1'-N9  | 3.67  | 115.14      | 108.09   |
| 2   | Q     | 800 | ATP  | O4'-C4'-C3' | -3.66 | 97.90       | 105.15   |
| 2   | M     | 800 | ATP  | C3'-C2'-C1' | 3.63  | 108.33      | 101.46   |
| 2   | I     | 800 | ATP  | O4'-C1'-N9  | 3.61  | 115.02      | 108.09   |
| 2   | G     | 800 | ATP  | O2B-PB-O3B  | 3.57  | 116.93      | 107.27   |
| 2   | L     | 800 | ATP  | O4'-C1'-N9  | 3.48  | 114.78      | 108.09   |
| 2   | D     | 800 | ATP  | O4'-C1'-N9  | 3.41  | 114.63      | 108.09   |
| 2   | R     | 800 | ATP  | C6-C5-C4    | -3.38 | 112.57      | 117.18   |
| 2   | H     | 800 | ATP  | C5-C4-N3    | -3.36 | 122.09      | 126.72   |
| 2   | E     | 800 | ATP  | O2G-PG-O3B  | 3.36  | 115.90      | 104.64   |
| 2   | A     | 800 | ATP  | O3A-PA-O1A  | -3.29 | 100.79      | 110.70   |
| 2   | F     | 800 | ATP  | O2B-PB-O3B  | 3.29  | 116.16      | 107.27   |
| 2   | E     | 800 | ATP  | N6-C6-N1    | 3.28  | 125.67      | 118.38   |
| 2   | A     | 800 | ATP  | C4-C5-N7    | 3.22  | 114.27      | 110.58   |
| 2   | S     | 800 | ATP  | C5-C6-N6    | -3.16 | 115.46      | 123.29   |
| 2   | Q     | 800 | ATP  | O3A-PB-O1B  | -3.14 | 101.27      | 110.70   |
| 2   | D     | 800 | ATP  | N3-C2-N1    | 3.11  | 133.28      | 128.58   |
| 2   | O     | 800 | ATP  | O3A-PA-O1A  | 3.10  | 120.04      | 110.70   |
| 2   | N     | 800 | ATP  | O3B-PB-O1B  | 3.08  | 119.97      | 110.70   |
| 2   | G     | 800 | ATP  | C4-N9-C8    | -3.05 | 102.53      | 105.74   |
| 2   | G     | 800 | ATP  | O3G-PG-O2G  | 3.05  | 119.22      | 107.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | K     | 800 | ATP  | C2-N1-C6    | -2.99 | 113.82      | 118.73   |
| 2   | R     | 800 | ATP  | O3B-PB-O1B  | 2.96  | 119.61      | 110.70   |
| 2   | M     | 800 | ATP  | C4'-O4'-C1' | -2.93 | 103.00      | 109.47   |
| 2   | S     | 800 | ATP  | O4'-C4'-C3' | -2.89 | 99.42       | 105.15   |
| 2   | B     | 800 | ATP  | O4'-C1'-N9  | 2.89  | 113.63      | 108.09   |
| 2   | D     | 800 | ATP  | O2A-PA-O3A  | 2.88  | 115.06      | 107.27   |
| 2   | N     | 800 | ATP  | C4'-O4'-C1' | -2.87 | 103.12      | 109.47   |
| 2   | B     | 800 | ATP  | C4'-O4'-C1' | -2.86 | 103.14      | 109.47   |
| 2   | R     | 800 | ATP  | N6-C6-N1    | -2.86 | 112.01      | 118.38   |
| 2   | R     | 800 | ATP  | C5-C4-N3    | 2.85  | 130.63      | 126.72   |
| 2   | L     | 800 | ATP  | C2-N1-C6    | -2.84 | 114.06      | 118.73   |
| 2   | I     | 800 | ATP  | O2A-PA-O3A  | 2.83  | 114.93      | 107.27   |
| 2   | N     | 800 | ATP  | O2G-PG-O1G  | 2.80  | 121.75      | 110.83   |
| 2   | A     | 800 | ATP  | O2B-PB-O3B  | 2.77  | 114.76      | 107.27   |
| 2   | E     | 800 | ATP  | O4'-C1'-N9  | 2.76  | 113.40      | 108.09   |
| 2   | E     | 800 | ATP  | O3B-PG-O1G  | -2.75 | 96.59       | 111.04   |
| 2   | K     | 800 | ATP  | N3-C4-N9    | 2.71  | 131.78      | 127.17   |
| 2   | N     | 800 | ATP  | O3G-PG-O3B  | -2.71 | 95.55       | 104.64   |
| 2   | E     | 800 | ATP  | C5-C6-N6    | -2.69 | 116.61      | 123.29   |
| 2   | C     | 800 | ATP  | O2A-PA-O3A  | 2.69  | 114.53      | 107.27   |
| 2   | F     | 800 | ATP  | N9-C8-N7    | -2.66 | 110.16      | 113.94   |
| 2   | M     | 800 | ATP  | C5-N7-C8    | 2.66  | 107.63      | 103.45   |
| 2   | R     | 800 | ATP  | C3'-C2'-C1' | 2.65  | 106.47      | 101.46   |
| 2   | A     | 800 | ATP  | C5-C6-N6    | -2.65 | 116.73      | 123.29   |
| 2   | F     | 800 | ATP  | C4-C5-N7    | 2.64  | 113.59      | 110.58   |
| 2   | H     | 800 | ATP  | O4'-C4'-C3' | -2.59 | 100.01      | 105.15   |
| 2   | S     | 800 | ATP  | N6-C6-N1    | 2.59  | 124.14      | 118.38   |
| 2   | B     | 800 | ATP  | O3A-PA-O1A  | 2.58  | 118.47      | 110.70   |
| 2   | C     | 800 | ATP  | O4'-C1'-N9  | 2.56  | 113.01      | 108.09   |
| 2   | C     | 800 | ATP  | C2'-C1'-N9  | -2.55 | 106.96      | 113.30   |
| 2   | R     | 800 | ATP  | O4'-C4'-C5' | 2.53  | 117.44      | 109.33   |
| 2   | F     | 800 | ATP  | O3A-PB-O1B  | -2.50 | 103.20      | 110.70   |
| 2   | O     | 800 | ATP  | O4'-C4'-C5' | 2.50  | 117.33      | 109.33   |
| 2   | N     | 800 | ATP  | O3'-C3'-C2' | 2.48  | 119.77      | 111.82   |
| 2   | K     | 800 | ATP  | O5'-C5'-C4' | 2.48  | 117.43      | 108.99   |
| 2   | I     | 800 | ATP  | O3B-PG-O1G  | -2.47 | 98.05       | 111.04   |
| 2   | R     | 800 | ATP  | O2B-PB-O3A  | -2.47 | 100.61      | 107.27   |
| 2   | K     | 800 | ATP  | C4'-O4'-C1' | -2.45 | 104.06      | 109.47   |
| 2   | I     | 800 | ATP  | O4'-C4'-C3' | -2.45 | 100.30      | 105.15   |
| 2   | O     | 800 | ATP  | O3'-C3'-C2' | 2.43  | 119.62      | 111.82   |
| 2   | B     | 800 | ATP  | O4'-C4'-C5' | 2.40  | 117.02      | 109.33   |
| 2   | F     | 800 | ATP  | O3G-PG-O2G  | 2.39  | 116.75      | 107.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 800 | ATP  | O3B-PG-O1G  | -2.38 | 98.52       | 111.04   |
| 2   | O     | 800 | ATP  | O2B-PB-O3A  | -2.38 | 100.84      | 107.27   |
| 2   | K     | 800 | ATP  | C5-C4-N3    | -2.38 | 123.44      | 126.72   |
| 2   | I     | 800 | ATP  | C4-N9-C8    | -2.37 | 103.25      | 105.74   |
| 2   | E     | 800 | ATP  | C5-C4-N9    | -2.37 | 103.23      | 105.81   |
| 2   | S     | 800 | ATP  | N9-C8-N7    | 2.37  | 117.29      | 113.94   |
| 2   | M     | 800 | ATP  | C5-C4-N9    | 2.36  | 108.38      | 105.81   |
| 2   | C     | 800 | ATP  | C4'-O4'-C1' | -2.34 | 104.31      | 109.47   |
| 2   | B     | 800 | ATP  | O3B-PG-O1G  | -2.33 | 98.78       | 111.04   |
| 2   | L     | 800 | ATP  | O3B-PB-O1B  | -2.32 | 103.71      | 110.70   |
| 2   | F     | 800 | ATP  | O3'-C3'-C4' | 2.31  | 117.73      | 111.08   |
| 2   | N     | 800 | ATP  | O3A-PA-O1A  | 2.29  | 117.61      | 110.70   |
| 2   | G     | 800 | ATP  | C4'-O4'-C1' | -2.29 | 104.41      | 109.47   |
| 2   | M     | 800 | ATP  | O3B-PB-O1B  | 2.26  | 117.51      | 110.70   |
| 2   | S     | 800 | ATP  | C6-C5-C4    | -2.26 | 114.10      | 117.18   |
| 2   | E     | 800 | ATP  | O4'-C4'-C3' | -2.25 | 100.69      | 105.15   |
| 2   | L     | 800 | ATP  | O3'-C3'-C2' | 2.24  | 119.01      | 111.82   |
| 2   | H     | 800 | ATP  | C5-C4-N9    | 2.24  | 108.25      | 105.81   |
| 2   | N     | 800 | ATP  | C4-N9-C8    | -2.24 | 103.39      | 105.74   |
| 2   | F     | 800 | ATP  | O2B-PB-O3A  | 2.23  | 113.30      | 107.27   |
| 2   | I     | 800 | ATP  | O2B-PB-O3B  | 2.23  | 113.30      | 107.27   |
| 2   | C     | 800 | ATP  | O3A-PB-O1B  | -2.21 | 104.06      | 110.70   |
| 2   | P     | 800 | ATP  | O2B-PB-O3A  | -2.21 | 101.31      | 107.27   |
| 2   | K     | 800 | ATP  | C5-C6-N1    | 2.19  | 123.06      | 117.51   |
| 2   | G     | 800 | ATP  | C4-C5-N7    | 2.18  | 113.07      | 110.58   |
| 2   | I     | 800 | ATP  | O3A-PA-O1A  | -2.17 | 104.17      | 110.70   |
| 2   | S     | 800 | ATP  | O2B-PB-O3A  | -2.17 | 101.40      | 107.27   |
| 2   | N     | 800 | ATP  | O2G-PG-O3B  | 2.15  | 111.85      | 104.64   |
| 2   | Q     | 800 | ATP  | O3G-PG-O2G  | 2.15  | 115.86      | 107.80   |
| 2   | Q     | 800 | ATP  | C4-C5-N7    | -2.15 | 108.13      | 110.58   |
| 2   | P     | 800 | ATP  | C5'-C4'-C3' | 2.15  | 122.93      | 115.21   |
| 2   | H     | 800 | ATP  | O2A-PA-O3A  | 2.14  | 113.06      | 107.27   |
| 2   | A     | 800 | ATP  | O3A-PB-O1B  | -2.13 | 104.28      | 110.70   |
| 2   | Q     | 800 | ATP  | C4-N9-C1'   | -2.13 | 121.64      | 126.63   |
| 2   | M     | 800 | ATP  | C5-C6-N6    | -2.11 | 118.06      | 123.29   |
| 2   | G     | 800 | ATP  | O3B-PG-O1G  | -2.11 | 99.94       | 111.04   |
| 2   | A     | 800 | ATP  | O2G-PG-O1G  | 2.10  | 119.03      | 110.83   |
| 2   | G     | 800 | ATP  | N3-C2-N1    | 2.10  | 131.76      | 128.58   |
| 2   | R     | 800 | ATP  | N3-C4-N9    | -2.07 | 123.64      | 127.17   |
| 2   | G     | 800 | ATP  | C2-N1-C6    | -2.07 | 115.32      | 118.73   |
| 2   | G     | 800 | ATP  | C5-C4-N3    | 2.07  | 129.57      | 126.72   |
| 2   | L     | 800 | ATP  | C5-C6-N1    | 2.06  | 122.73      | 117.51   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 800 | ATP  | O4'-C4'-C5' | 2.05  | 115.91      | 109.33   |
| 2   | S     | 800 | ATP  | O4'-C1'-C2' | 2.05  | 110.99      | 106.62   |
| 2   | D     | 800 | ATP  | C5-N7-C8    | 2.04  | 106.66      | 103.45   |
| 2   | B     | 800 | ATP  | O3A-PB-O1B  | -2.04 | 104.57      | 110.70   |
| 2   | O     | 800 | ATP  | O5'-PA-O1A  | -2.03 | 100.88      | 108.94   |
| 2   | S     | 800 | ATP  | O4'-C1'-N9  | 2.03  | 111.98      | 108.09   |
| 2   | R     | 800 | ATP  | O2A-PA-O3A  | 2.03  | 112.75      | 107.27   |
| 2   | A     | 800 | ATP  | C5-N7-C8    | -2.03 | 100.27      | 103.45   |
| 2   | M     | 800 | ATP  | C2-N1-C6    | -2.02 | 115.42      | 118.73   |
| 2   | E     | 800 | ATP  | O2A-PA-O3A  | 2.02  | 112.72      | 107.27   |
| 2   | L     | 800 | ATP  | PA-O5'-C5'  | 2.01  | 132.89      | 121.35   |
| 2   | F     | 800 | ATP  | C2-N1-C6    | -2.01 | 115.43      | 118.73   |

There are no chirality outliers.

All (76) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | B     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | B     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | B     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | C     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | C     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | C     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | D     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | E     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | E     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | E     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | F     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | F     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | G     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | H     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | H     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | H     | 800 | ATP  | O4'-C4'-C5'-O5' |
| 2   | I     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | I     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | K     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | L     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | L     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | M     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | N     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | O     | 800 | ATP  | C5'-O5'-PA-O2A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | Q     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | R     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | R     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | R     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | S     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | H     | 800 | ATP  | C3'-C4'-C5'-O5' |
| 2   | P     | 800 | ATP  | O4'-C4'-C5'-O5' |
| 2   | P     | 800 | ATP  | C3'-C4'-C5'-O5' |
| 2   | A     | 800 | ATP  | PB-O3A-PA-O2A   |
| 2   | A     | 800 | ATP  | C5'-O5'-PA-O2A  |
| 2   | A     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | D     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | F     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | G     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | H     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | I     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | K     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | K     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | L     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | M     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | M     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | N     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | N     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | O     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | O     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | Q     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | Q     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | S     | 800 | ATP  | C5'-O5'-PA-O1A  |
| 2   | S     | 800 | ATP  | C5'-O5'-PA-O3A  |
| 2   | F     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | H     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | A     | 800 | ATP  | PB-O3A-PA-O1A   |
| 2   | B     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | D     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | E     | 800 | ATP  | PG-O3B-PB-O1B   |
| 2   | E     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | G     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | G     | 800 | ATP  | PB-O3A-PA-O1A   |
| 2   | H     | 800 | ATP  | PB-O3A-PA-O1A   |
| 2   | H     | 800 | ATP  | PB-O3A-PA-O2A   |
| 2   | N     | 800 | ATP  | PG-O3B-PB-O2B   |
| 2   | R     | 800 | ATP  | PG-O3B-PB-O2B   |

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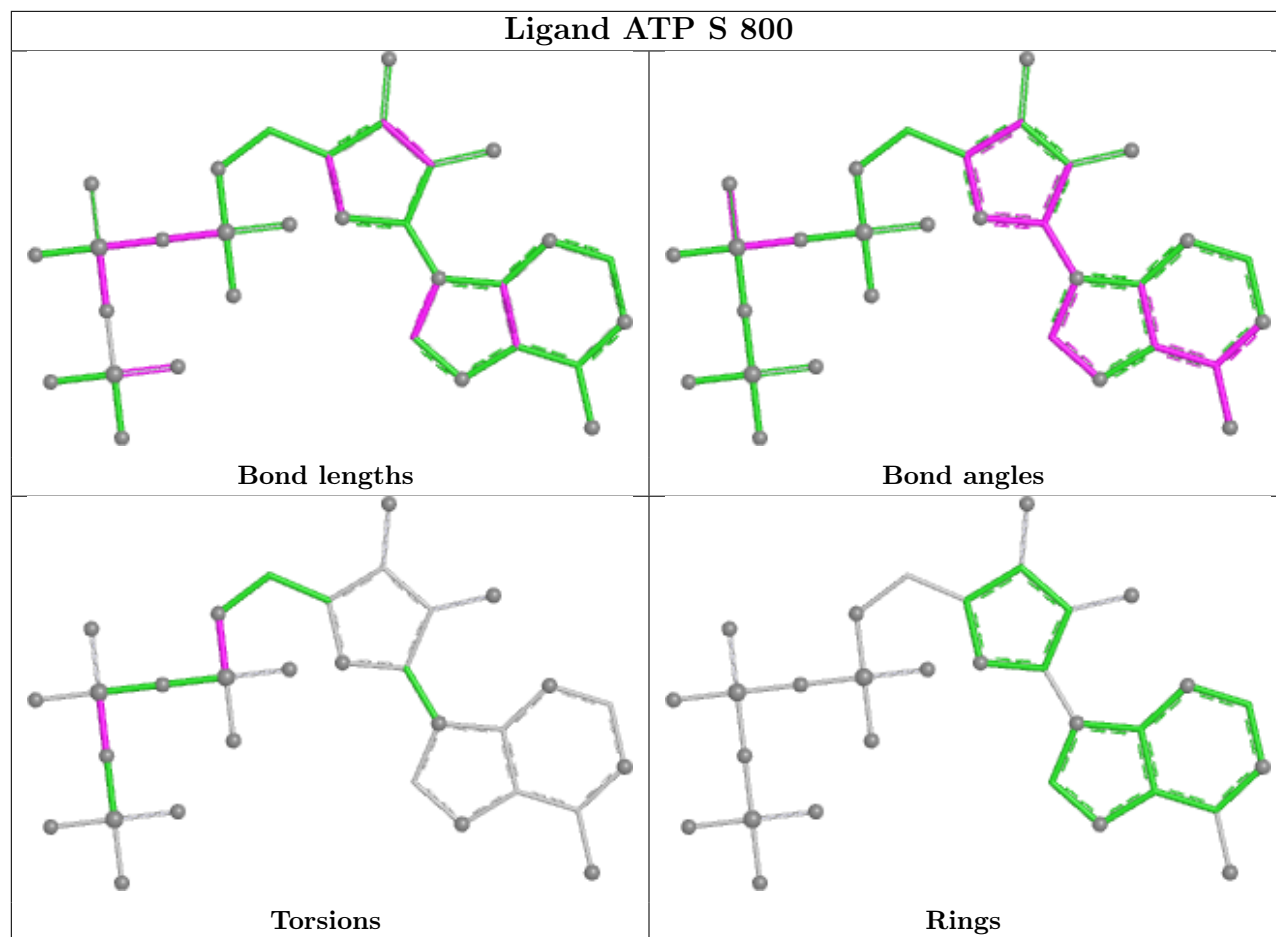
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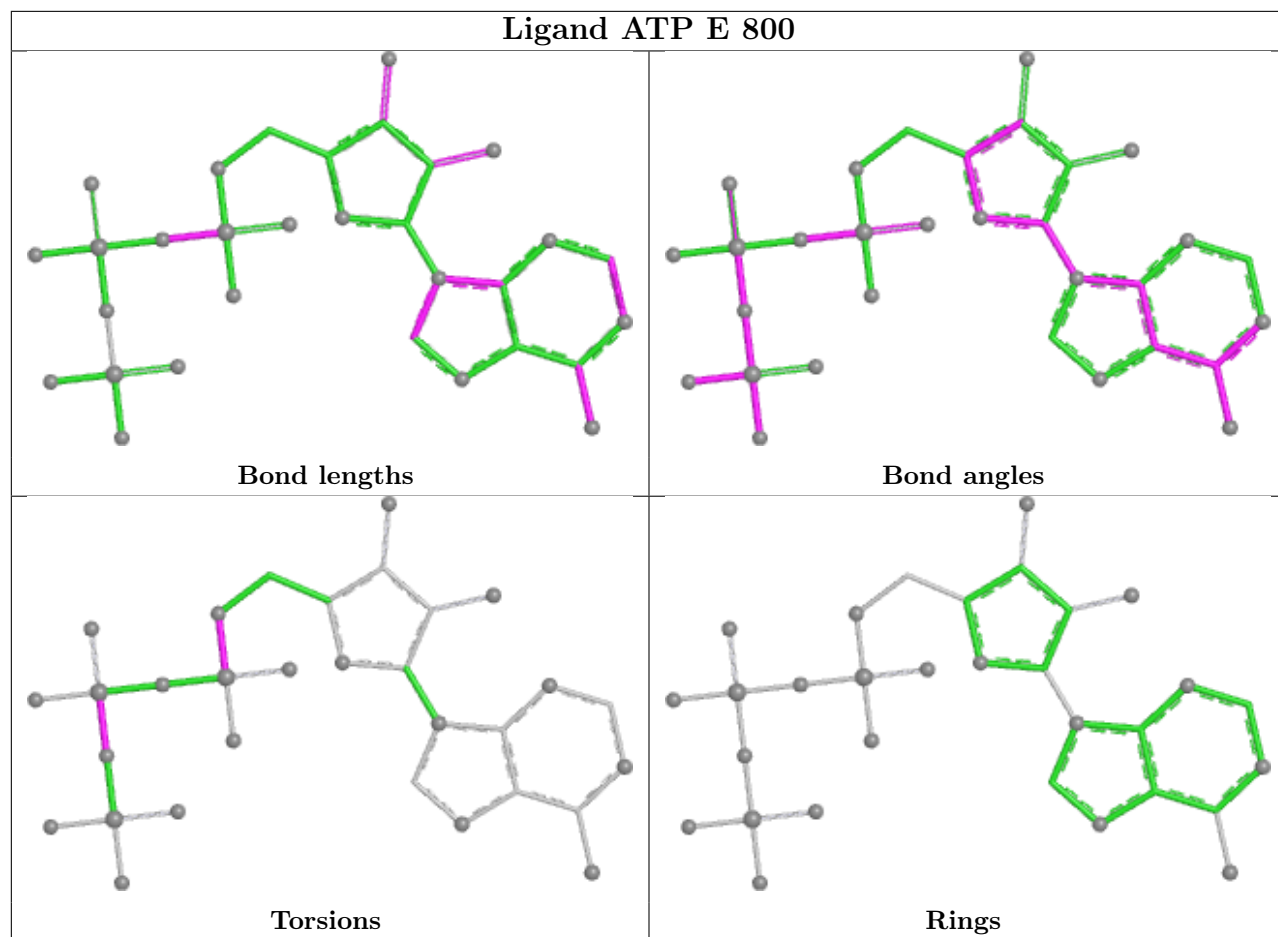
| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | K     | 800 | ATP  | C2'-C1'-N9-C8 |
| 2   | A     | 800 | ATP  | PG-O3B-PB-O1B |
| 2   | C     | 800 | ATP  | PG-O3B-PB-O1B |
| 2   | C     | 800 | ATP  | PG-O3B-PB-O2B |
| 2   | G     | 800 | ATP  | PG-O3B-PB-O1B |
| 2   | I     | 800 | ATP  | PG-O3B-PB-O2B |
| 2   | M     | 800 | ATP  | PG-O3B-PB-O2B |
| 2   | O     | 800 | ATP  | PG-O3B-PB-O2B |
| 2   | S     | 800 | ATP  | PG-O3B-PB-O2B |

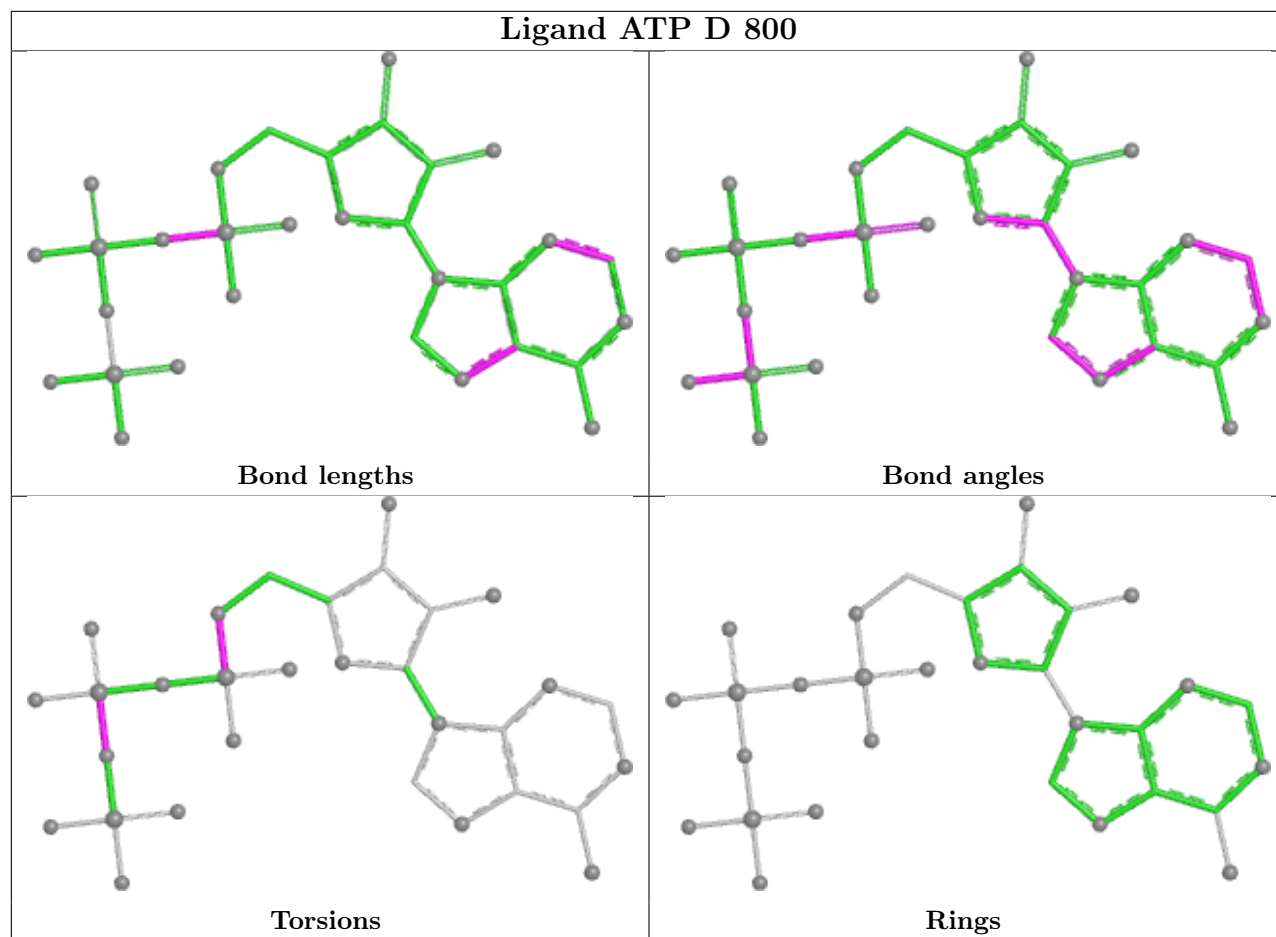
There are no ring outliers.

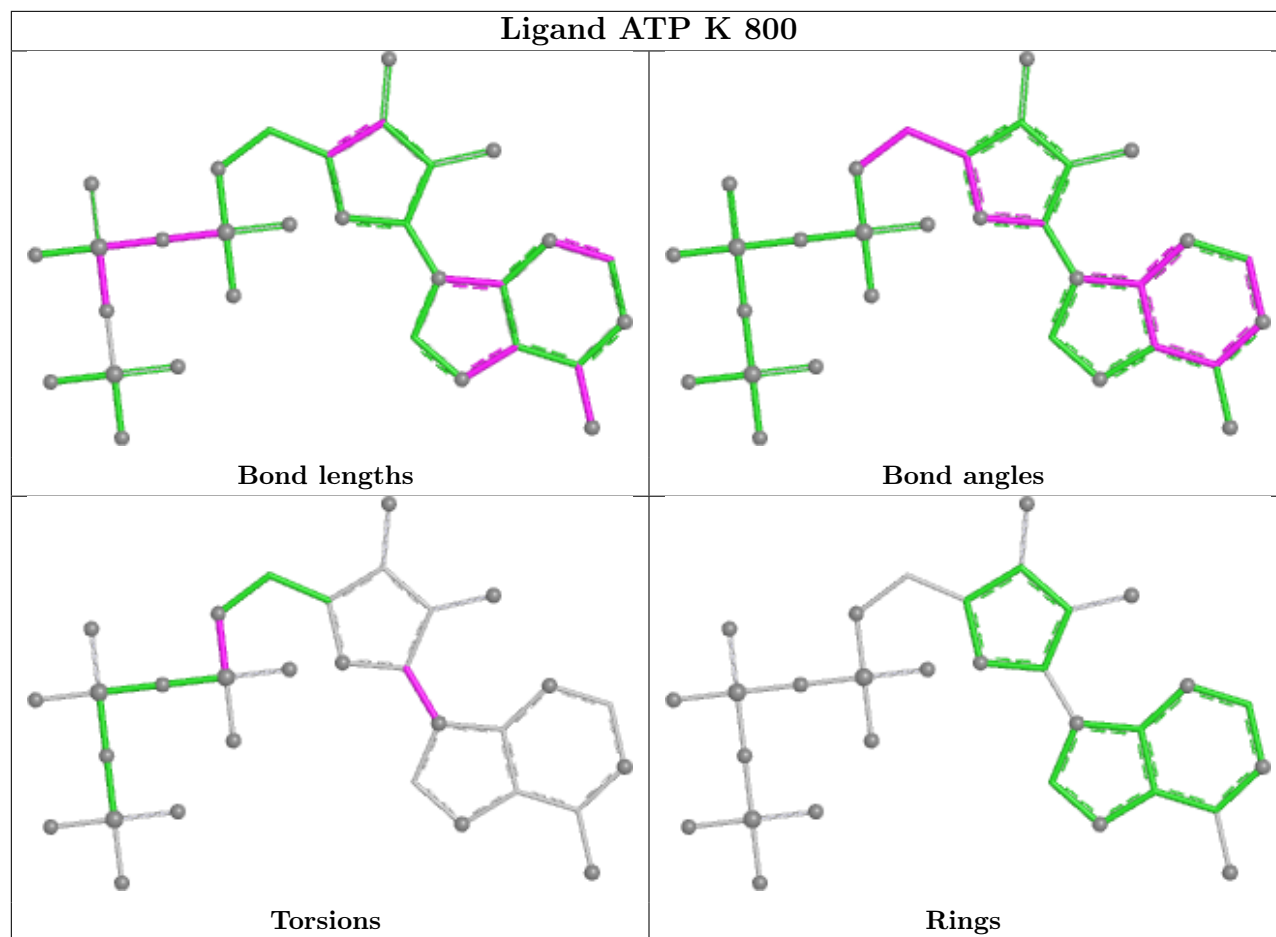
No monomer is involved in short contacts.

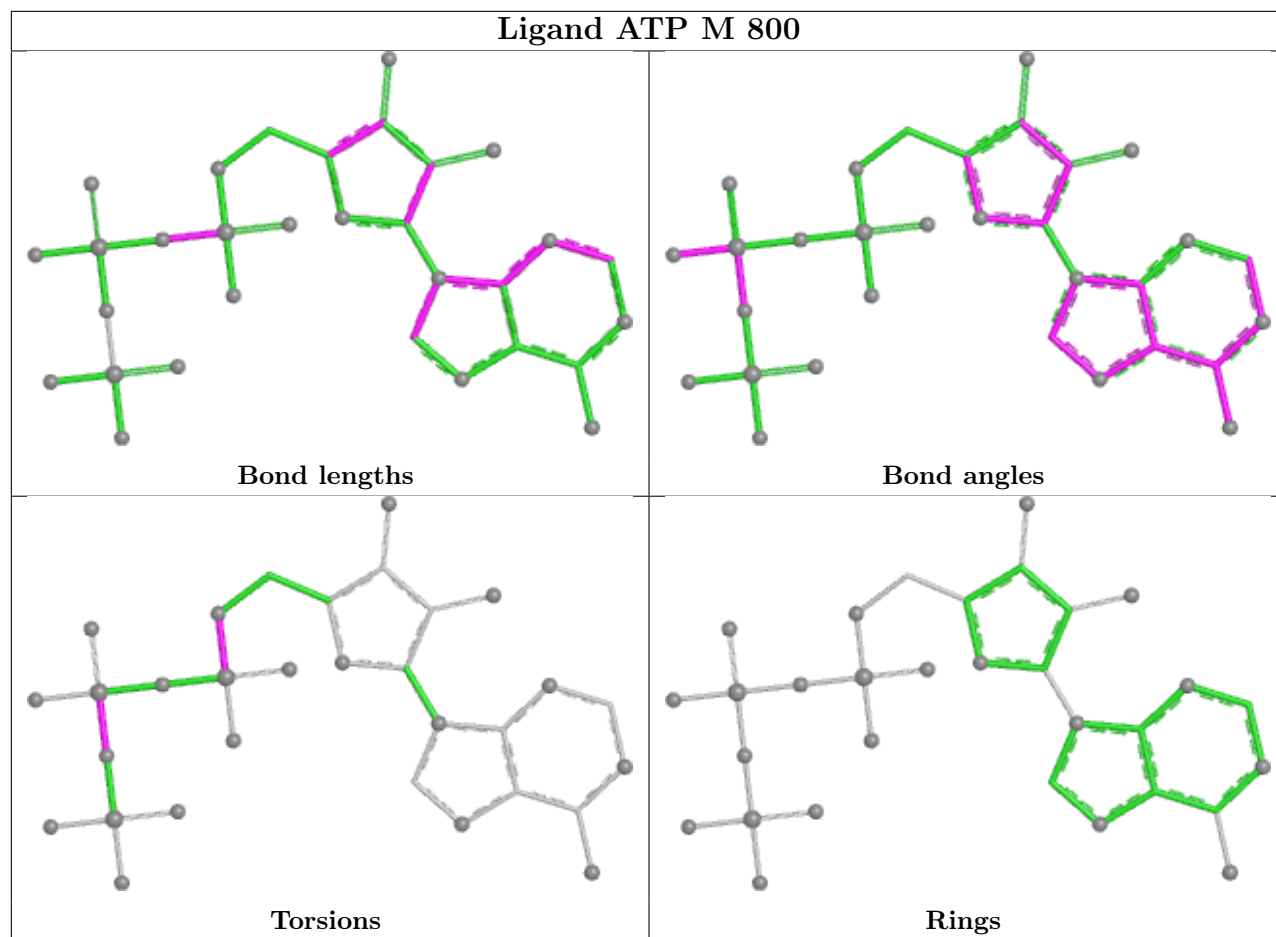
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

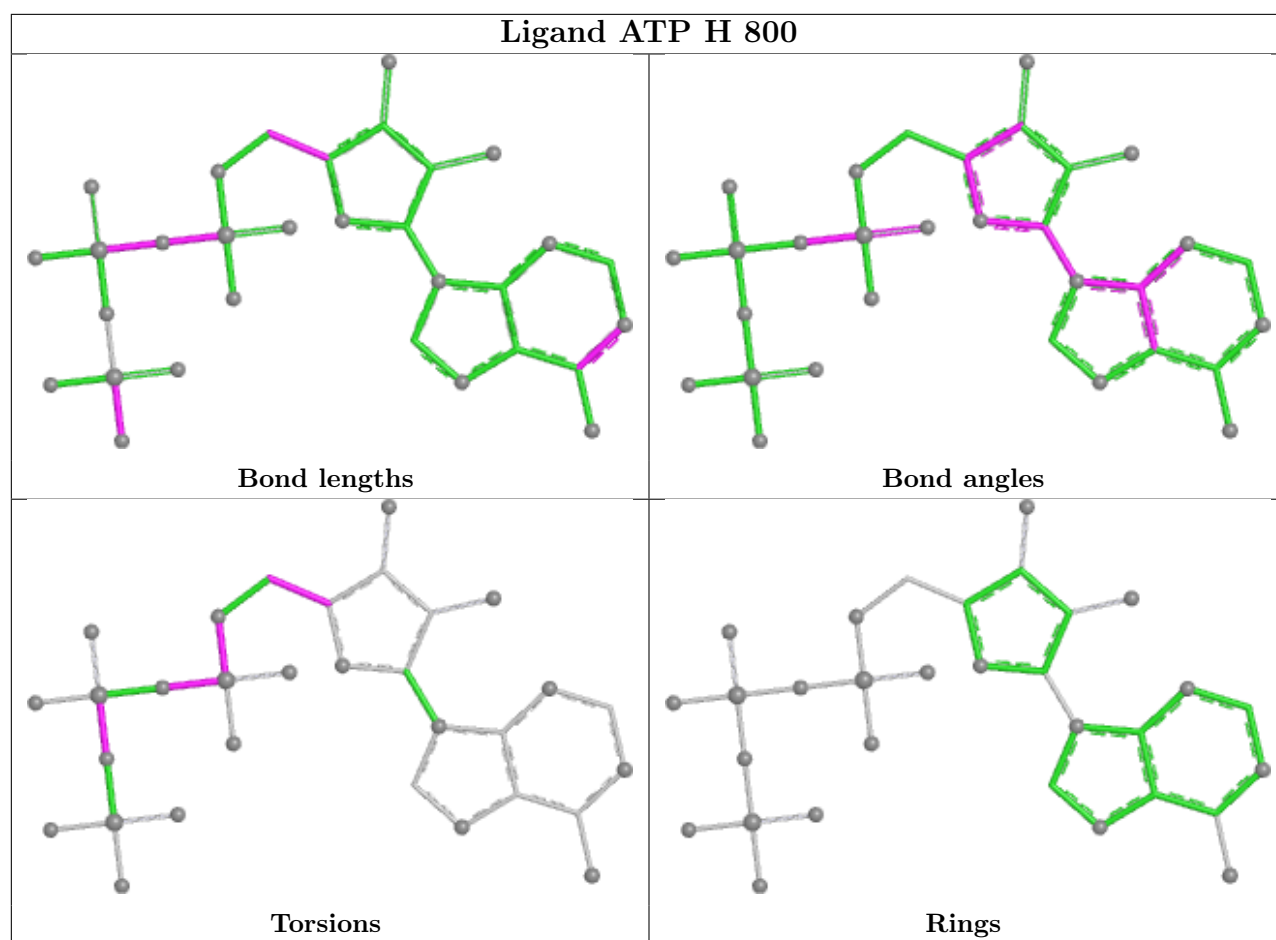


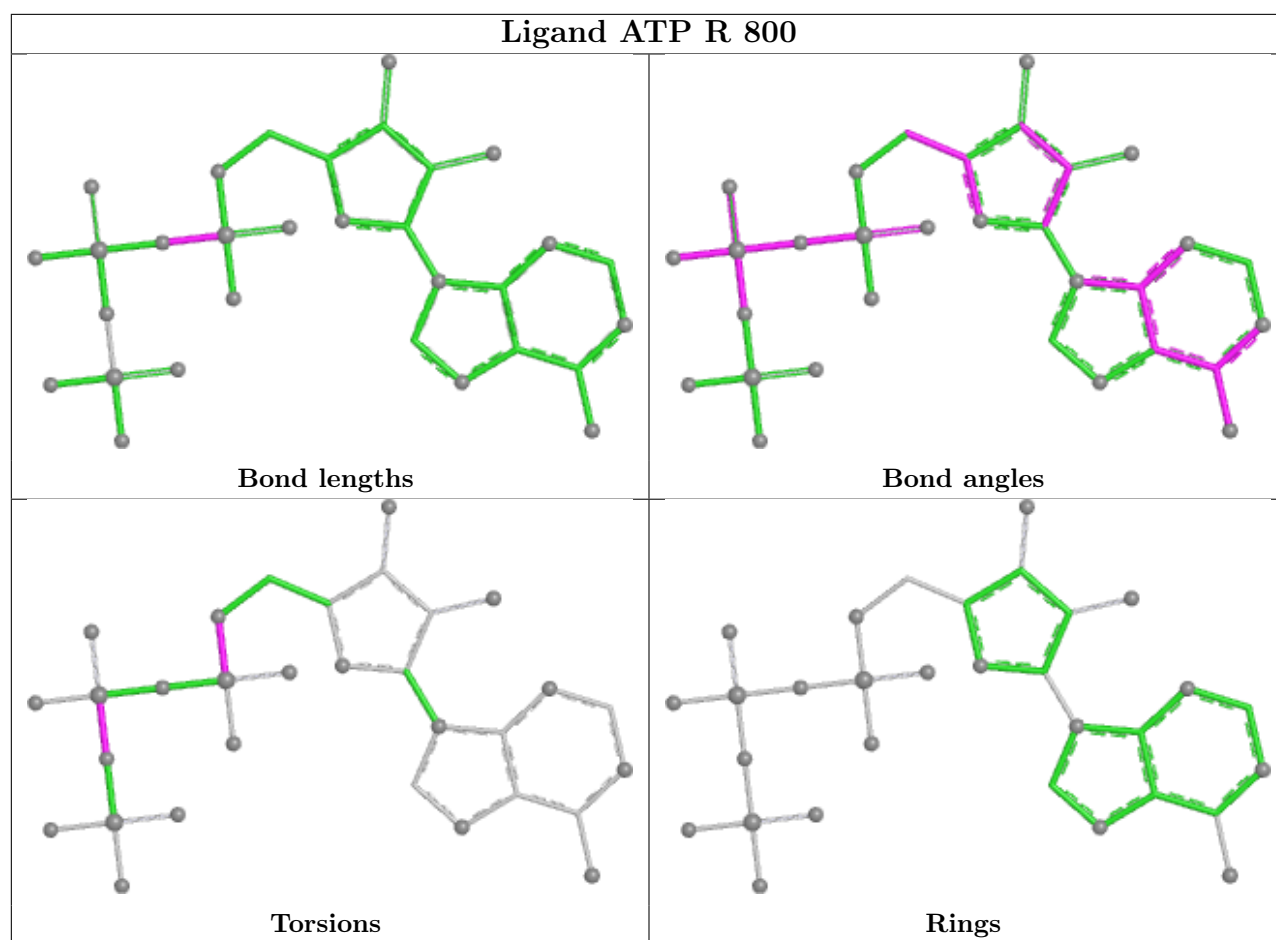


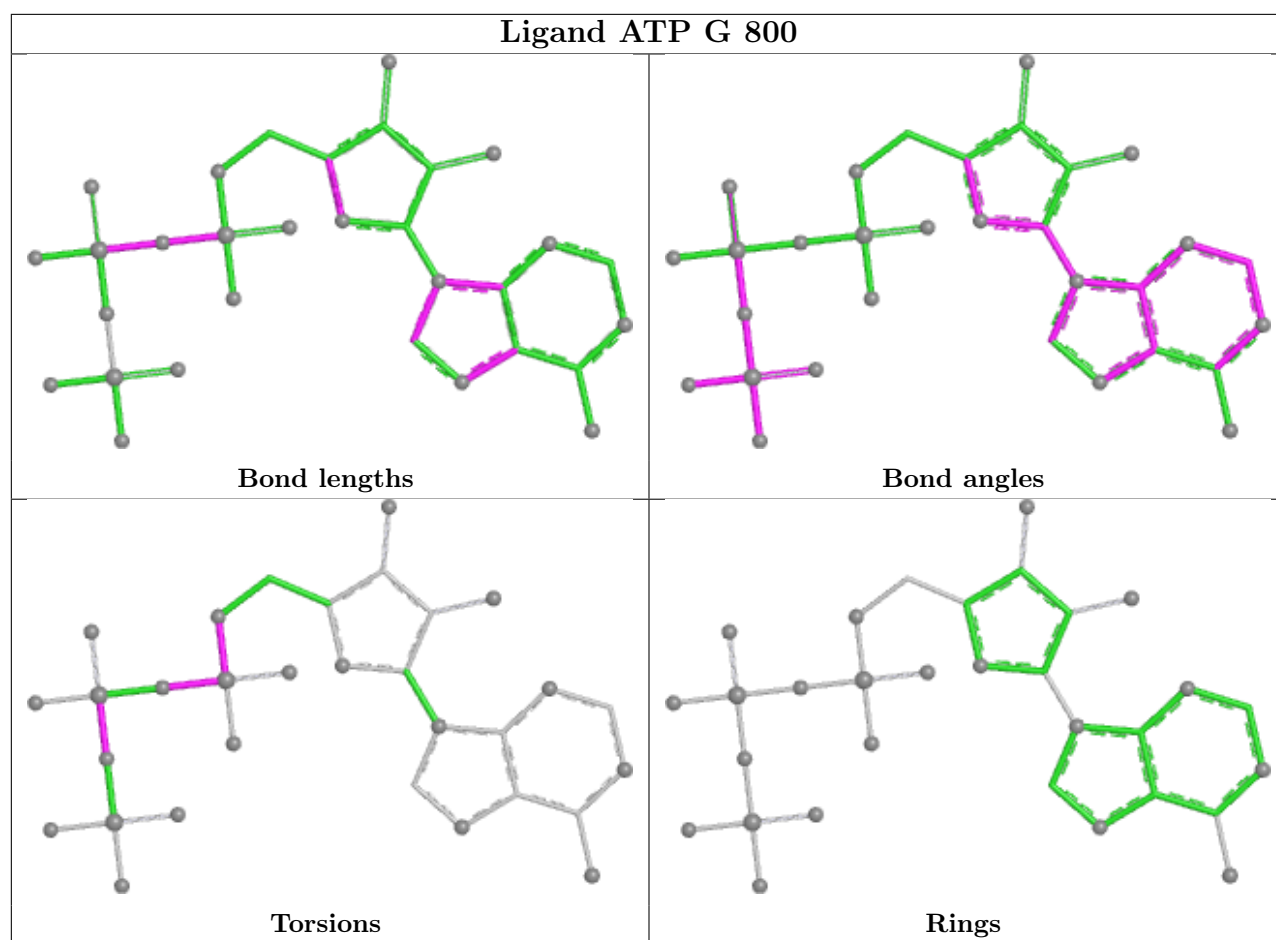


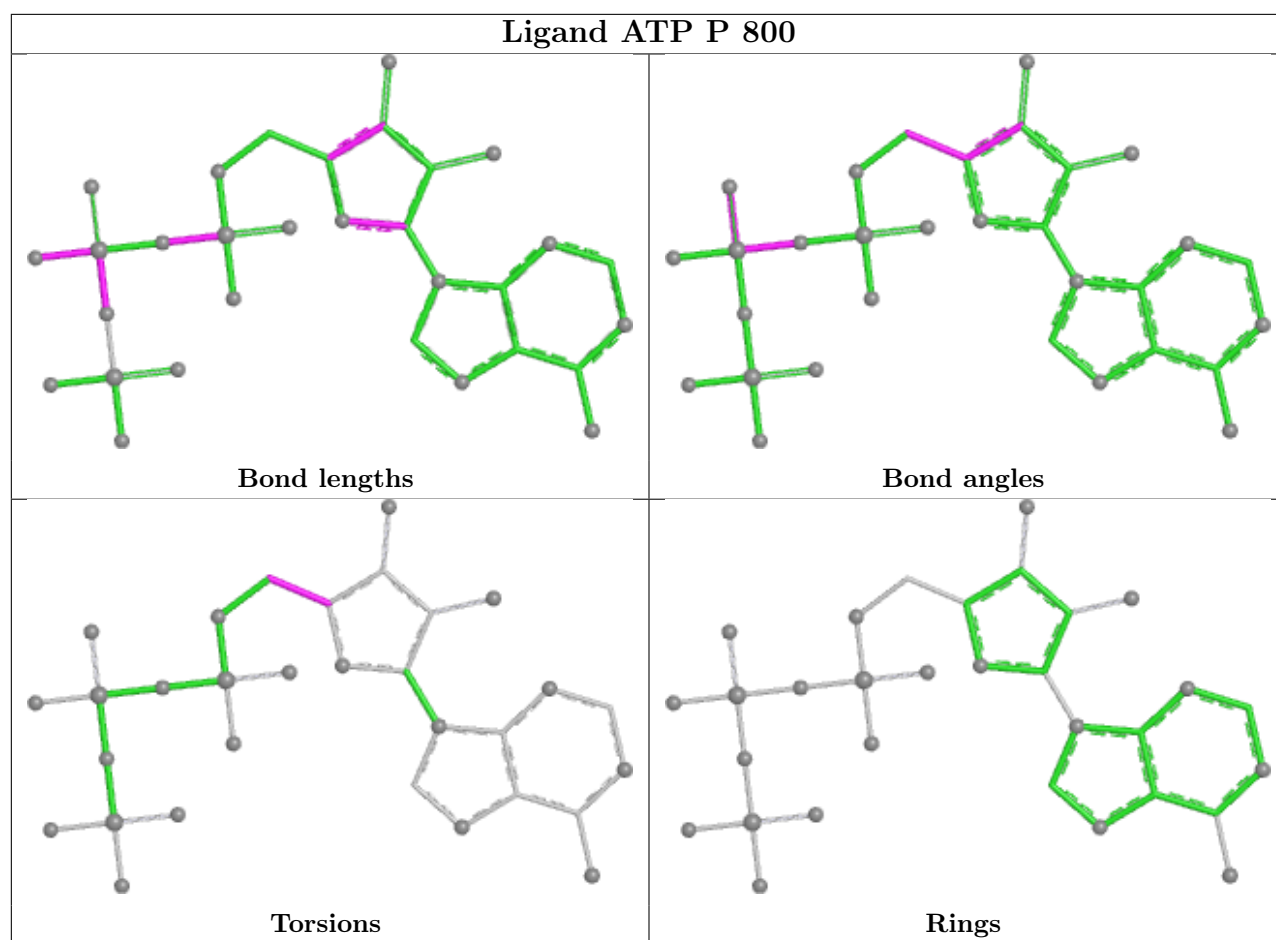


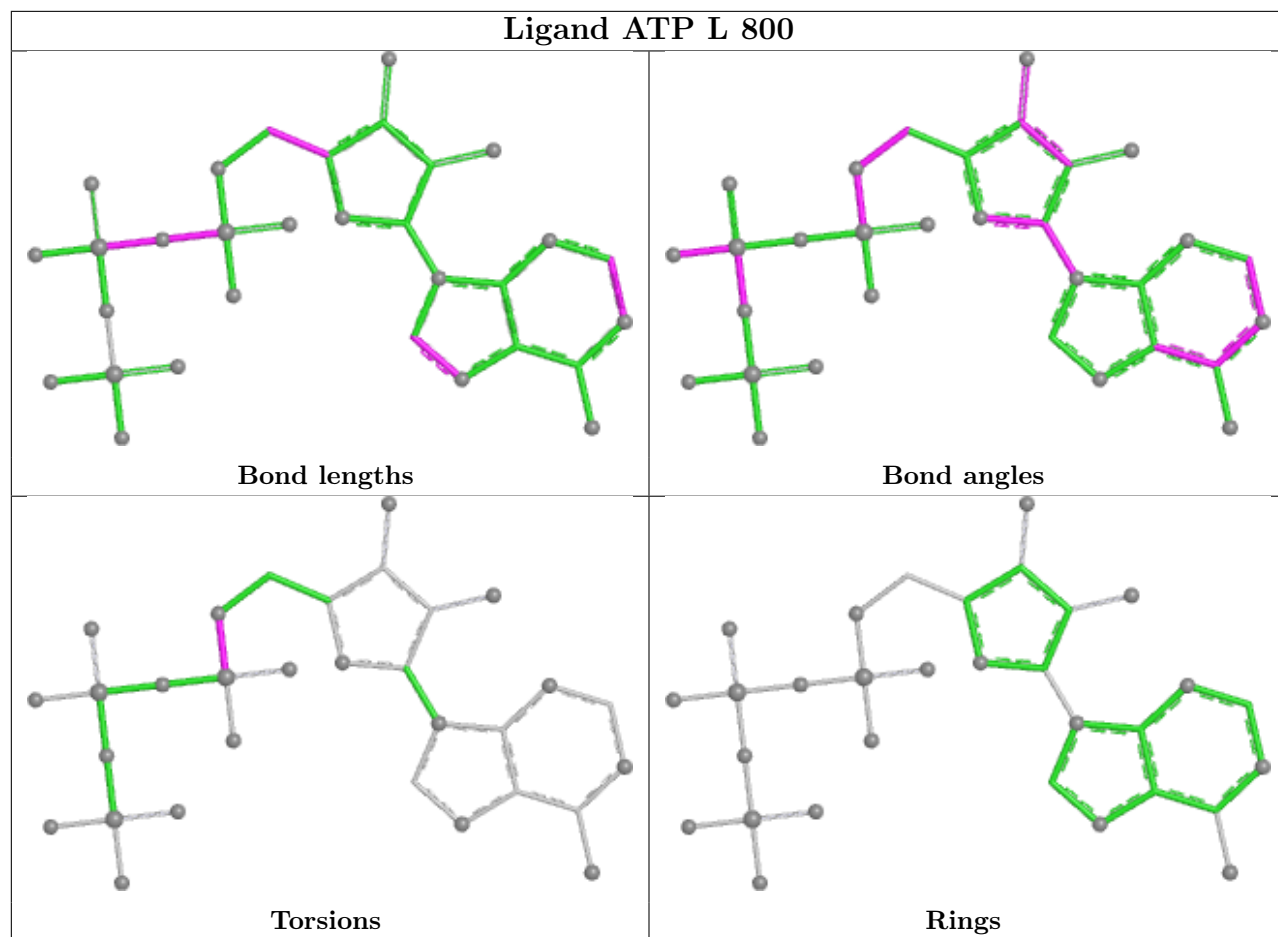


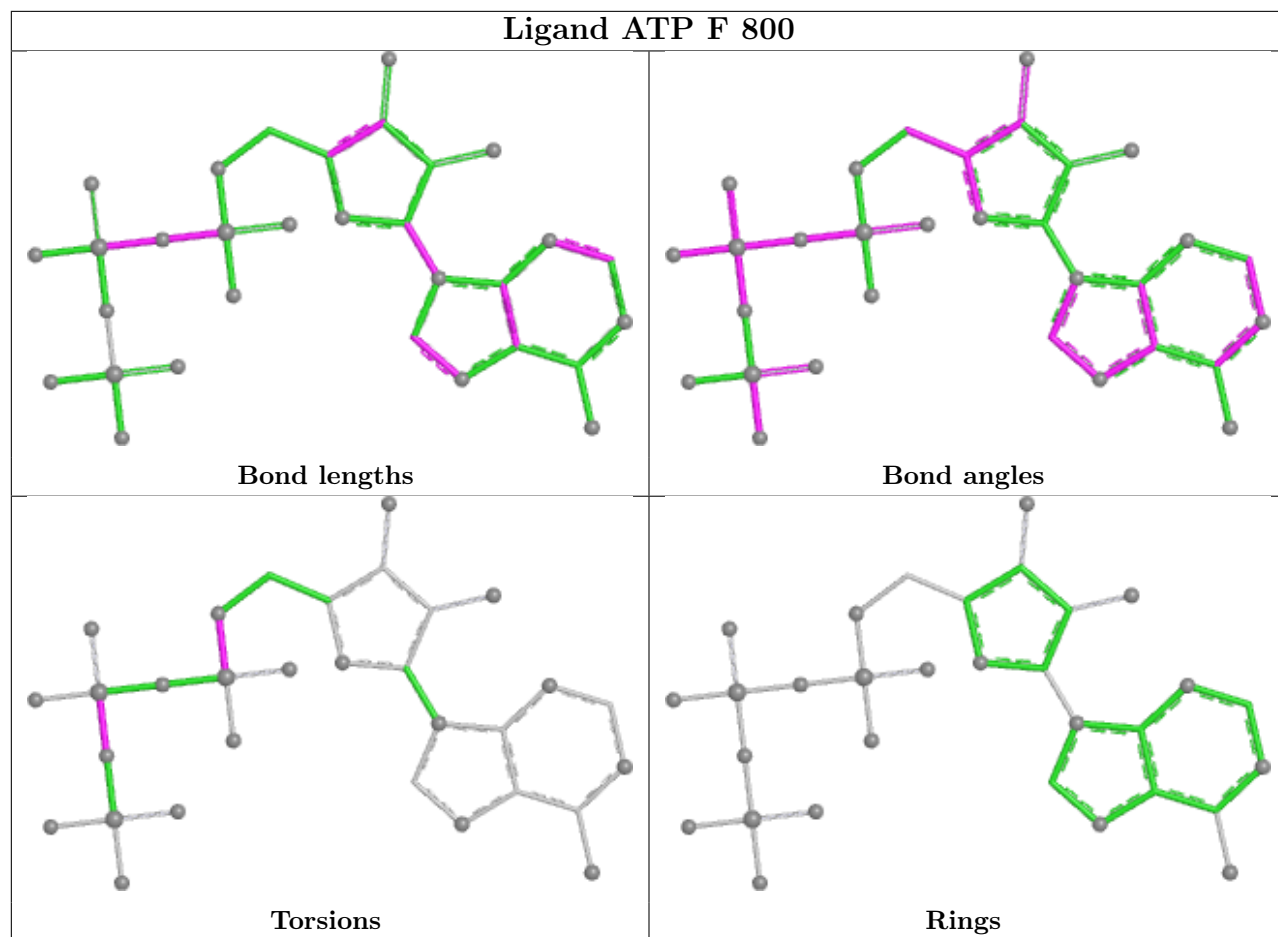


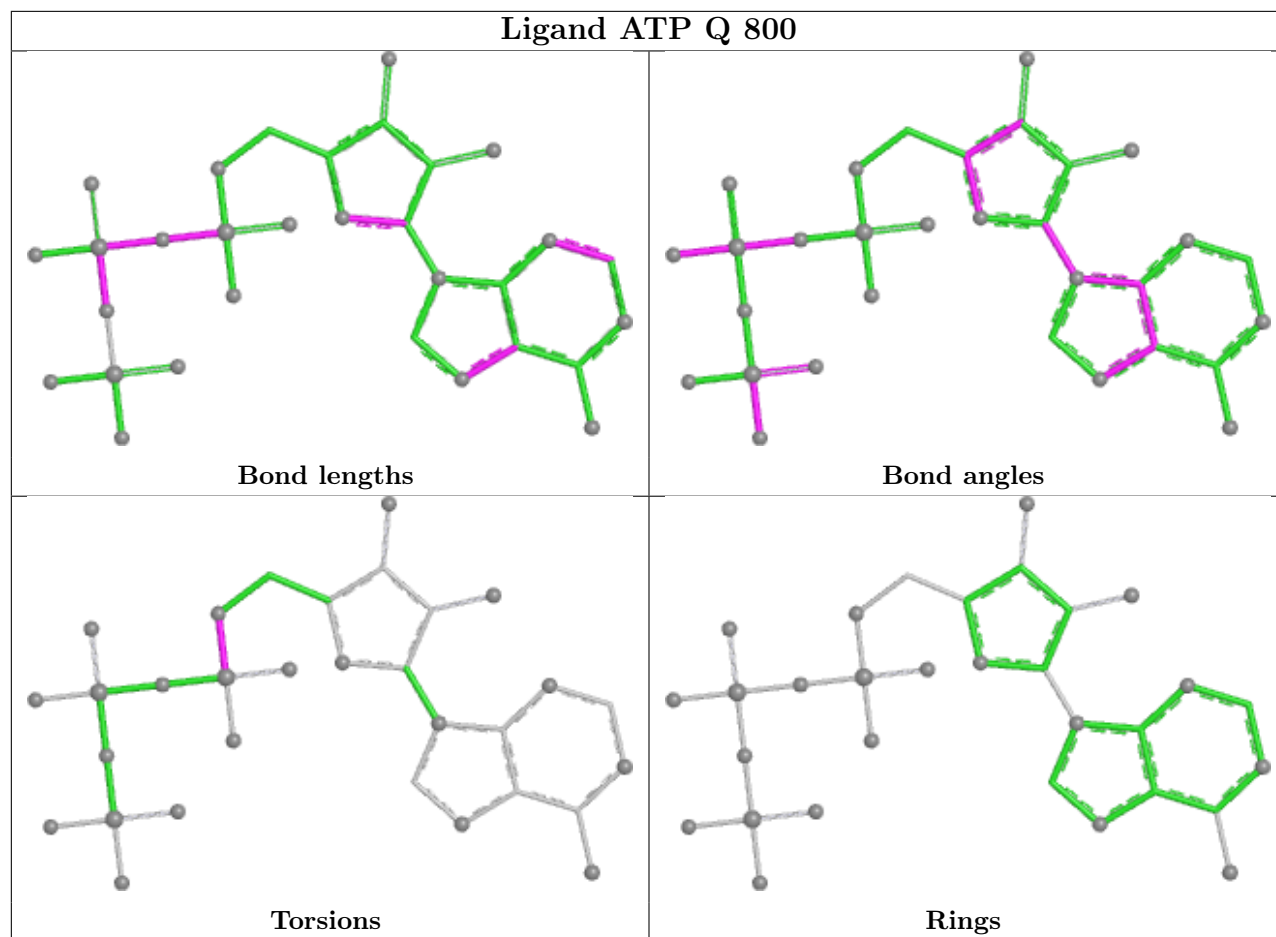


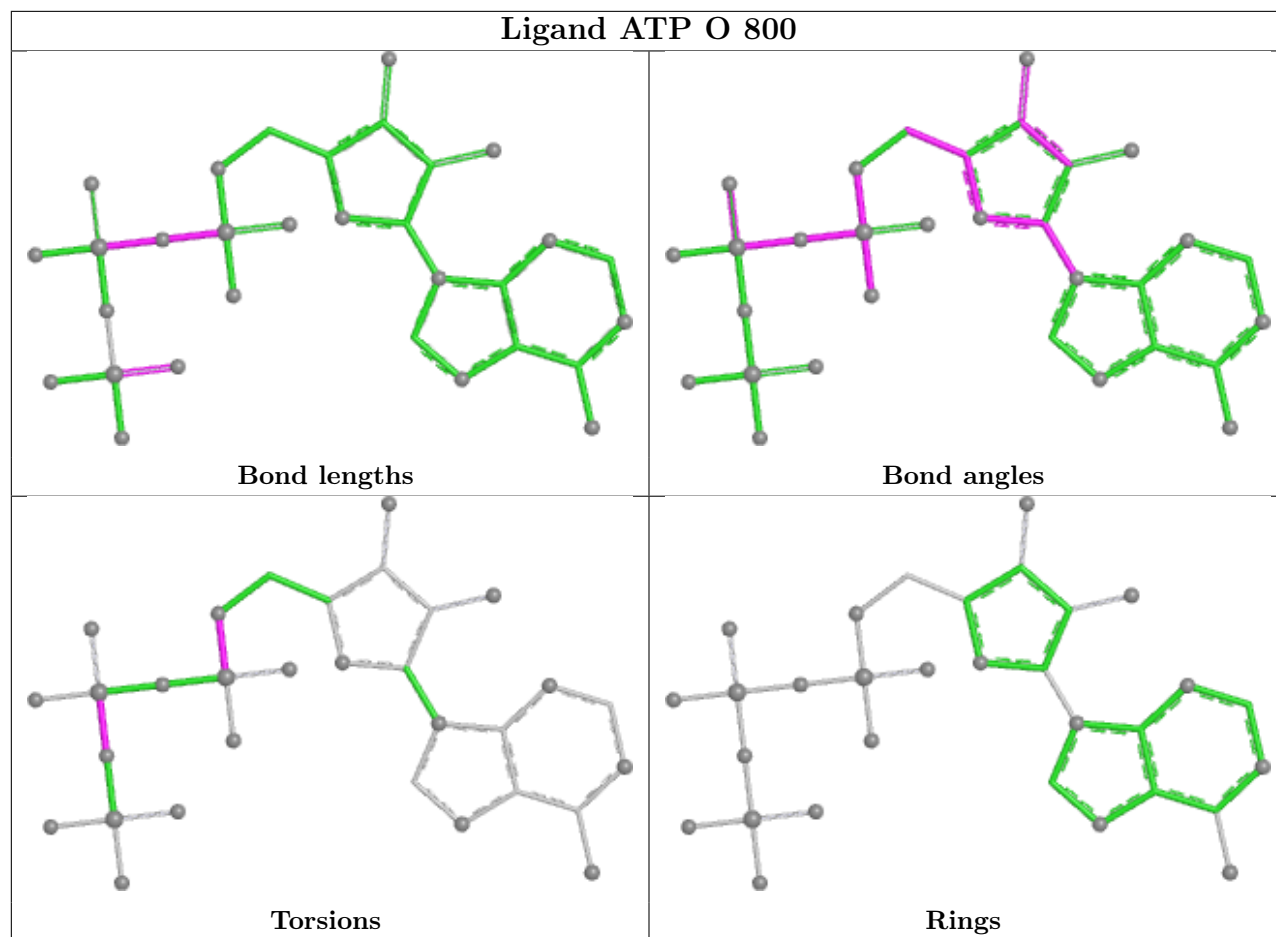


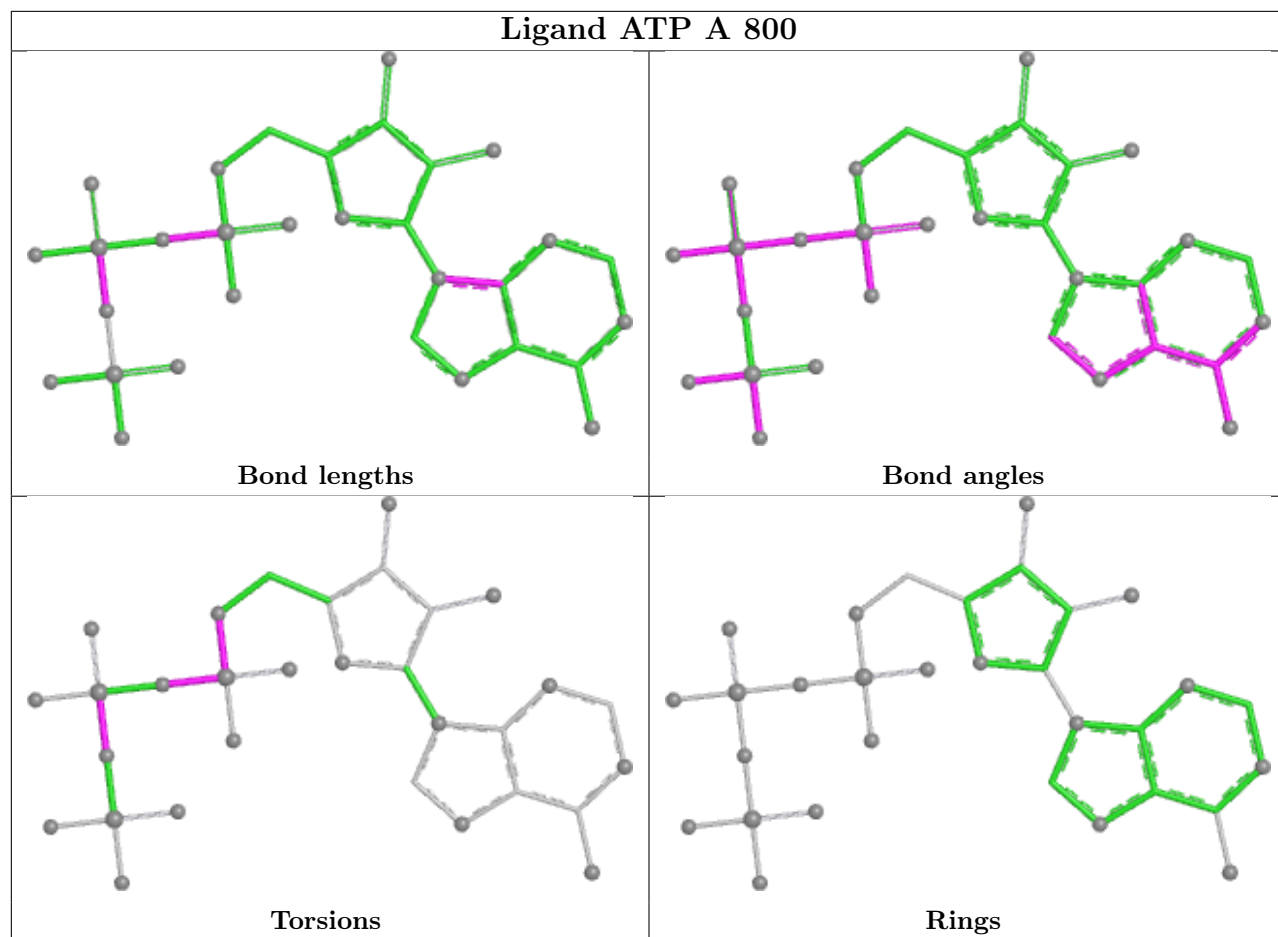


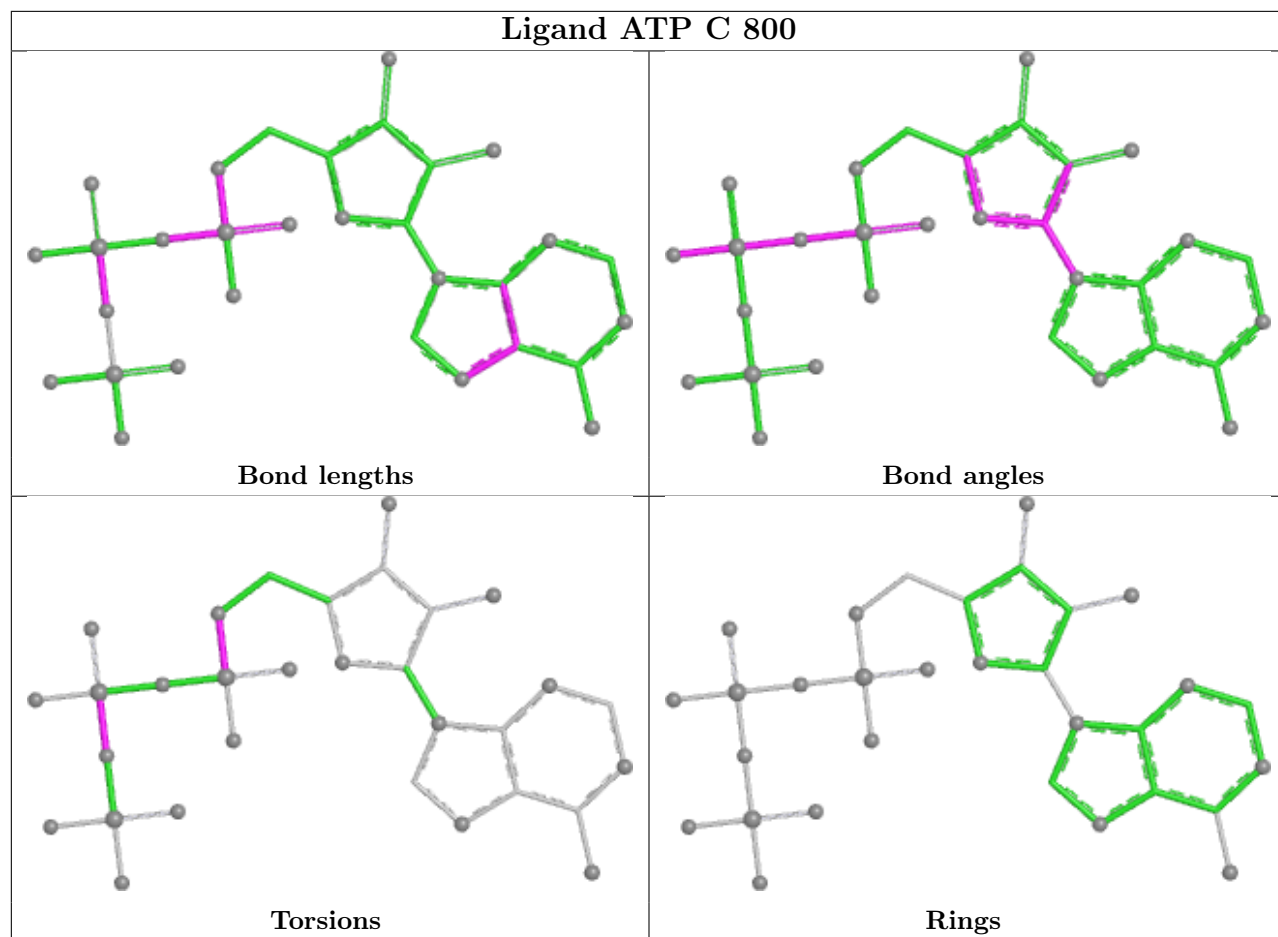


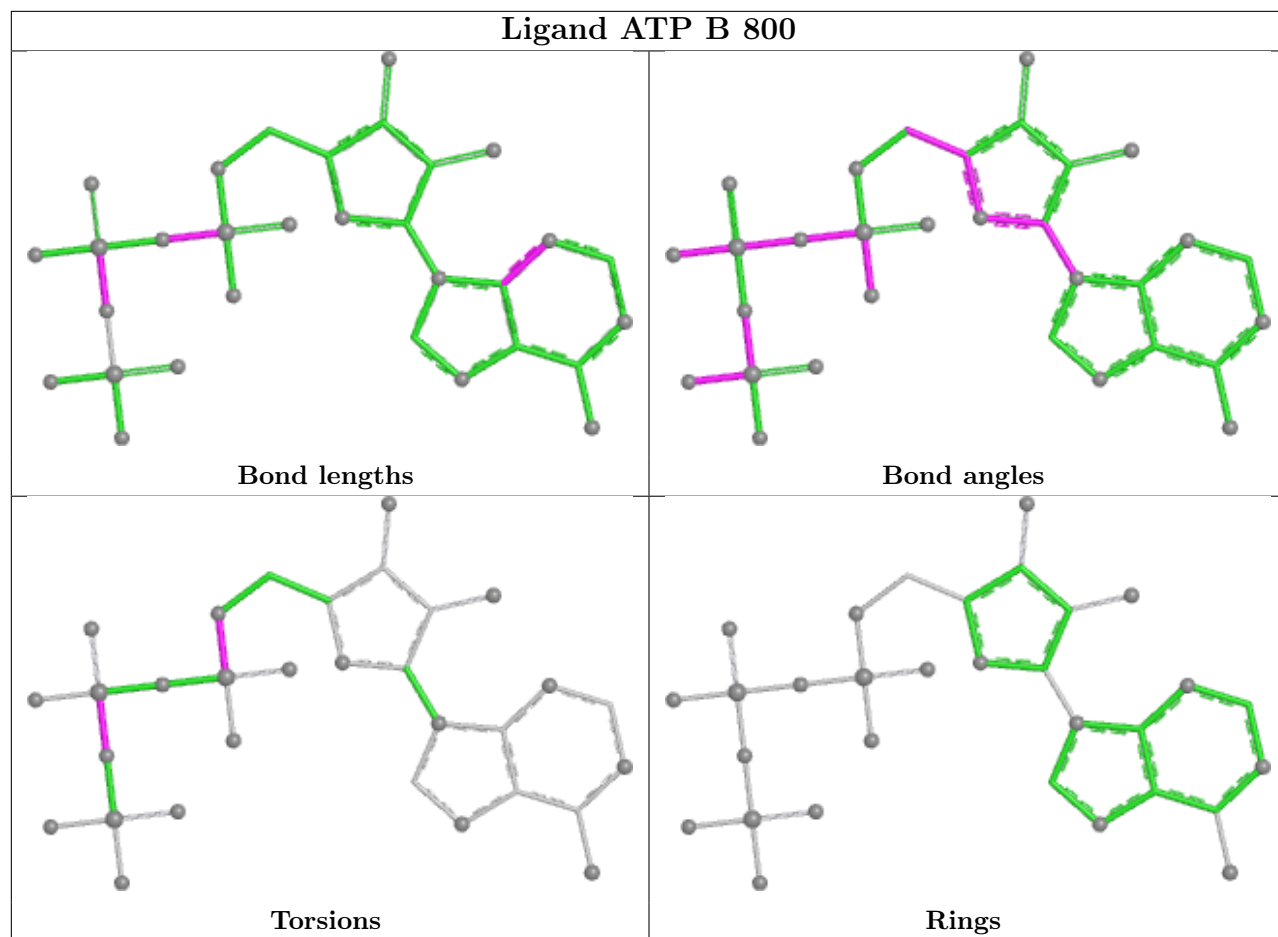


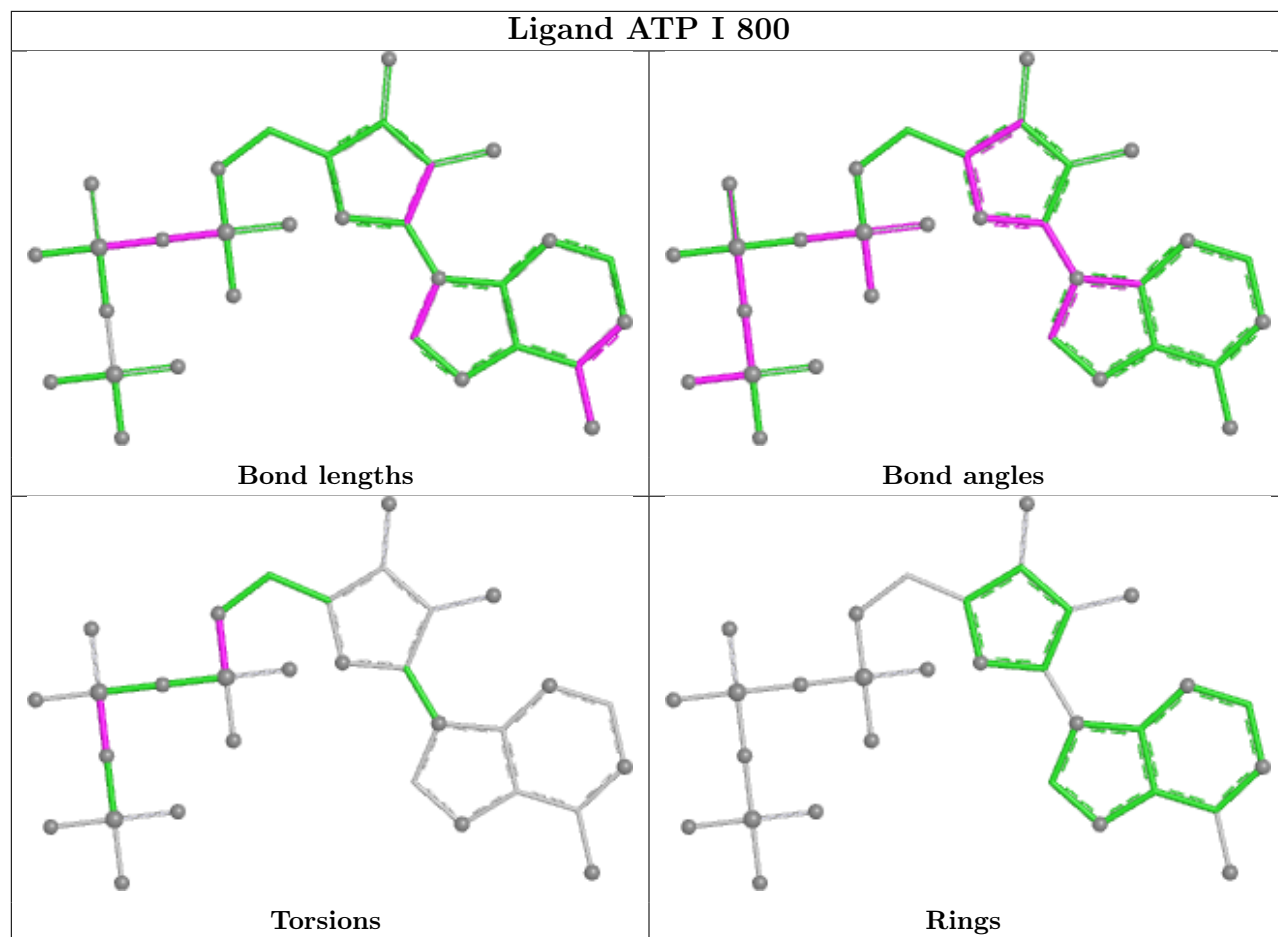


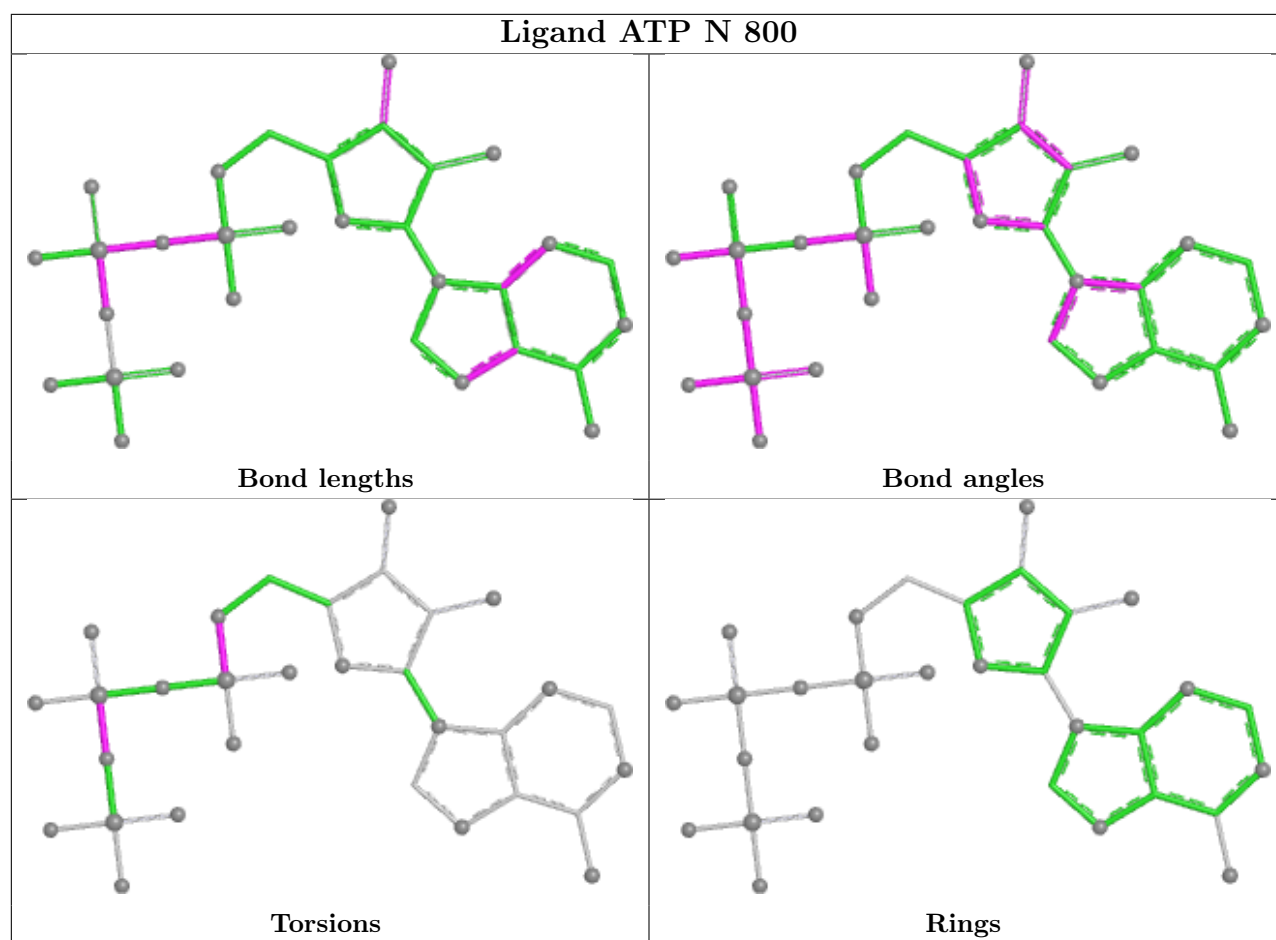












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

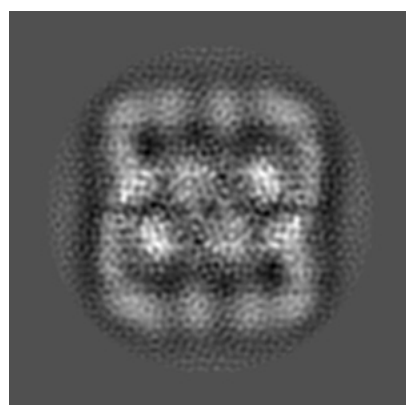
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5396. These allow visual inspection of the internal detail of the map and identification of artifacts.

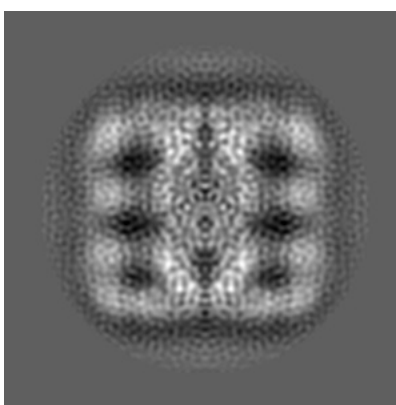
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

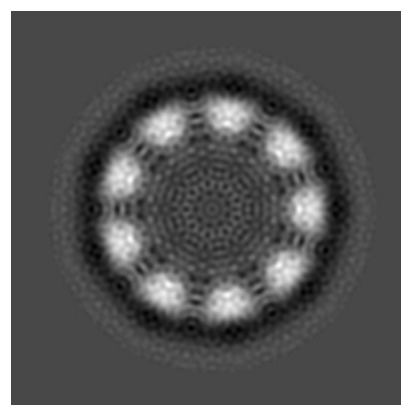
#### 6.1.1 Primary map



X



Y

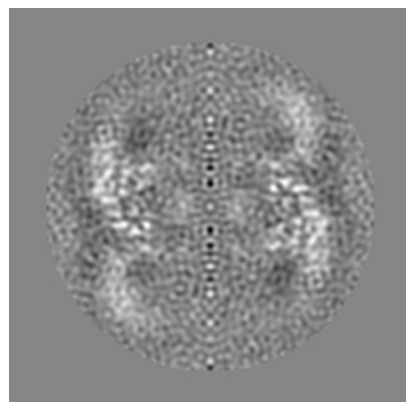


Z

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

### 6.2 Central slices [i](#)

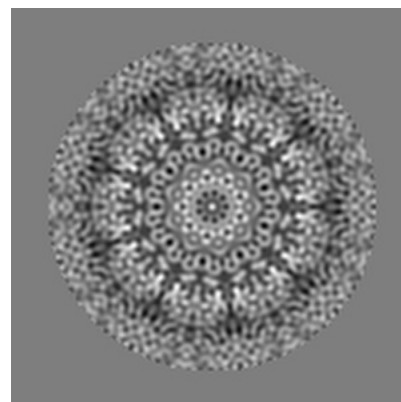
#### 6.2.1 Primary map



X Index: 80



Y Index: 80

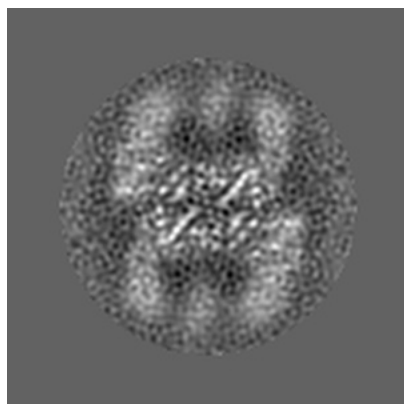


Z Index: 80

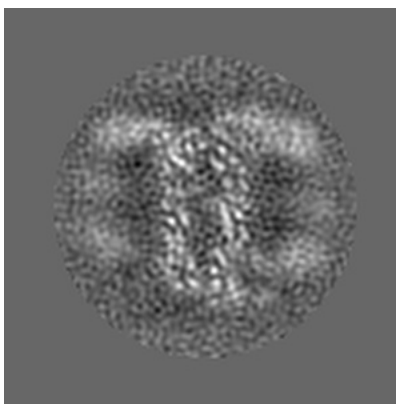
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

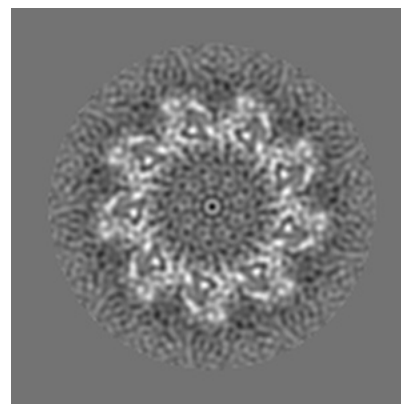
### 6.3.1 Primary map



X Index: 109



Y Index: 106

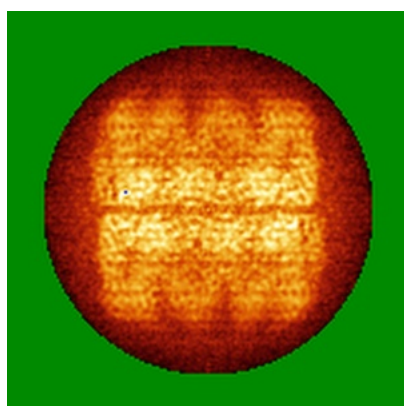


Z Index: 90

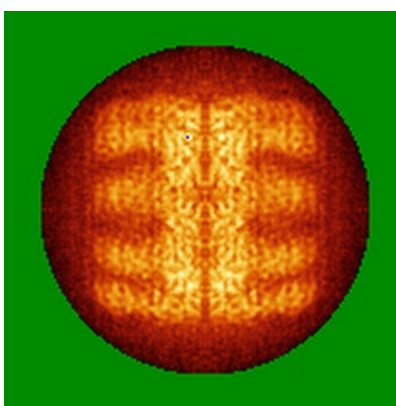
The images above show the largest variance slices of the map in three orthogonal directions.

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

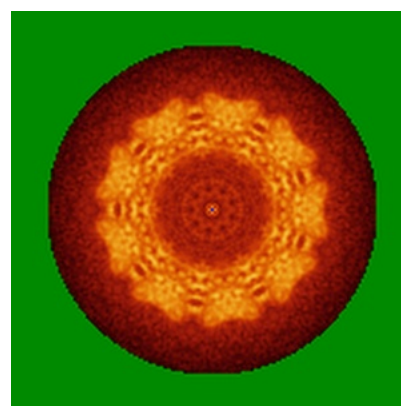
### 6.4.1 Primary map



X



Y

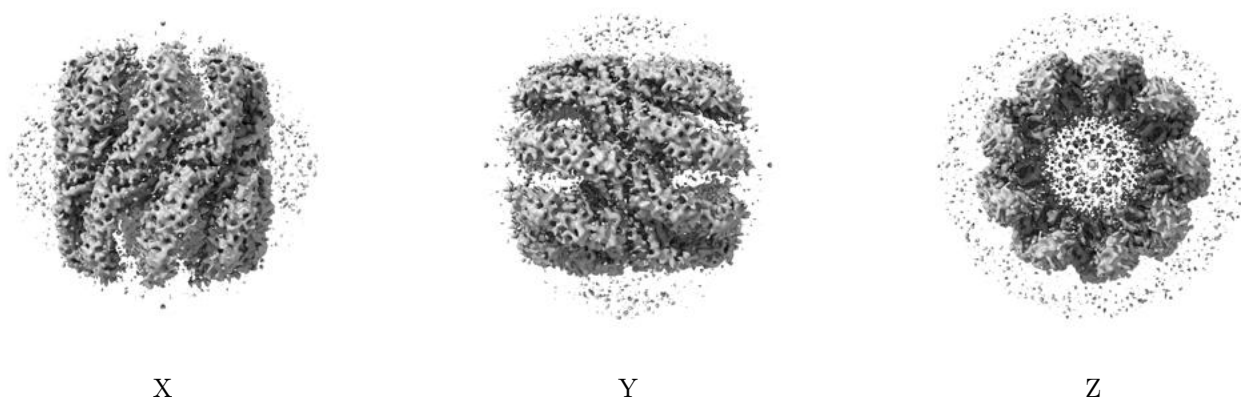


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

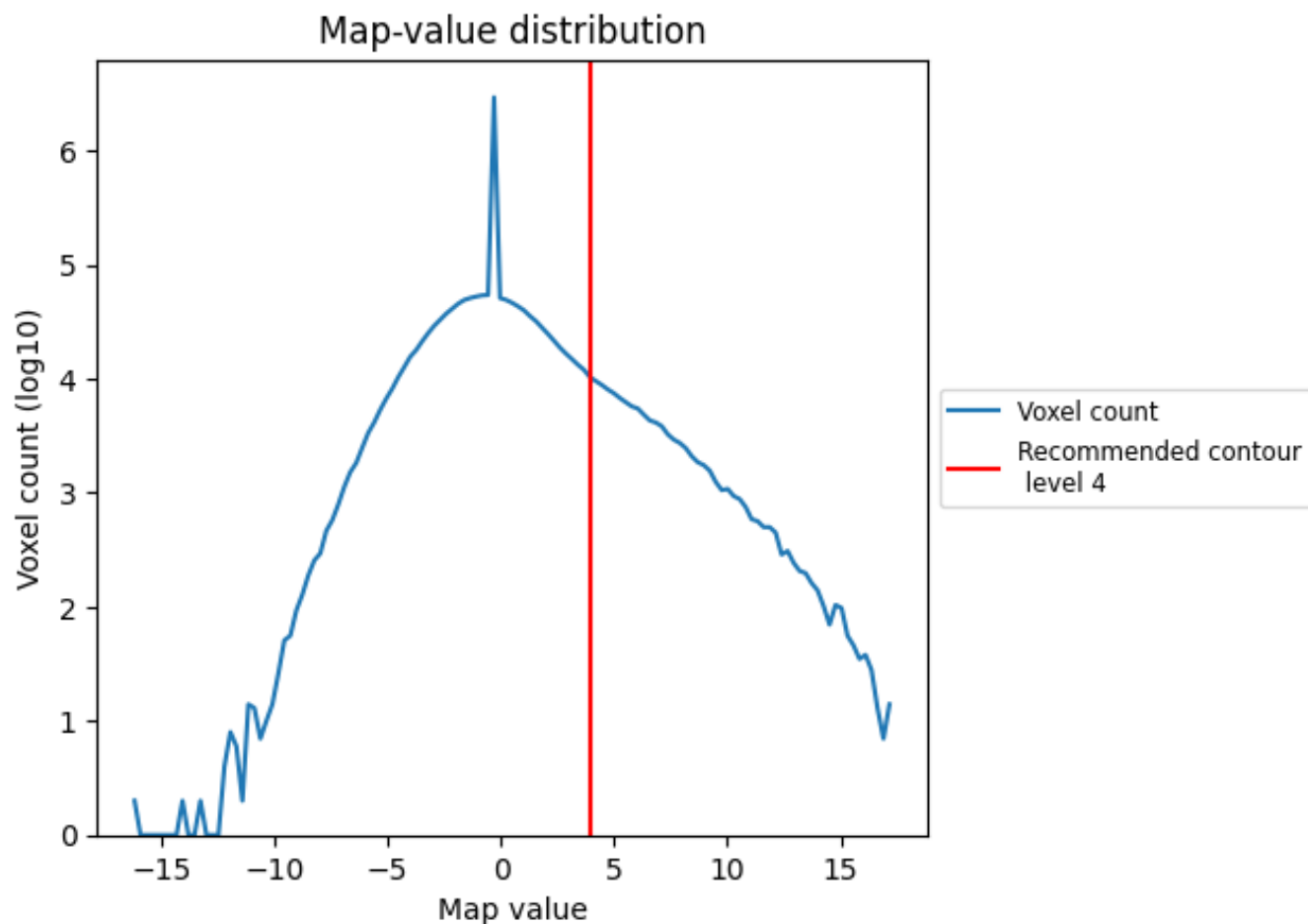
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

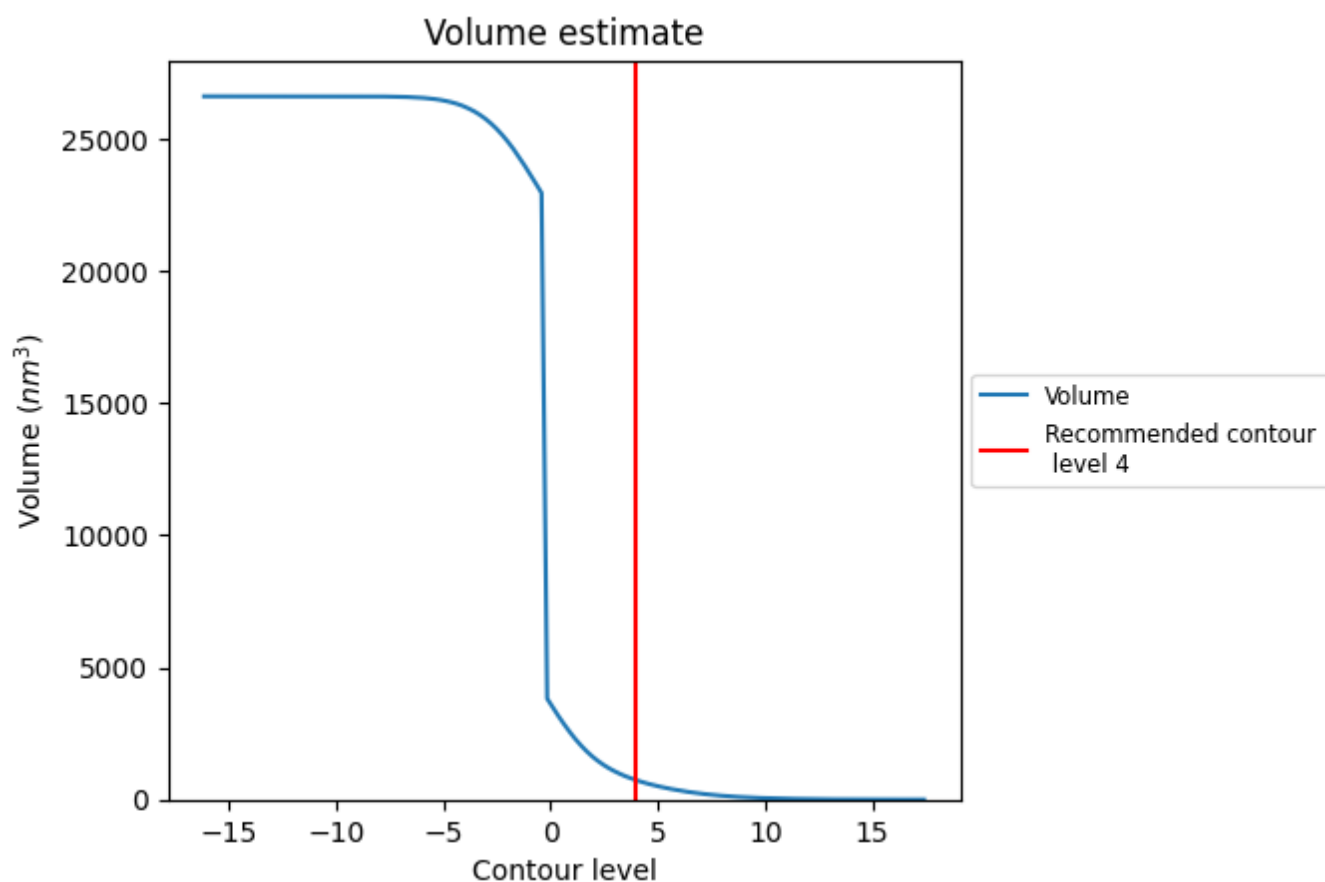
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

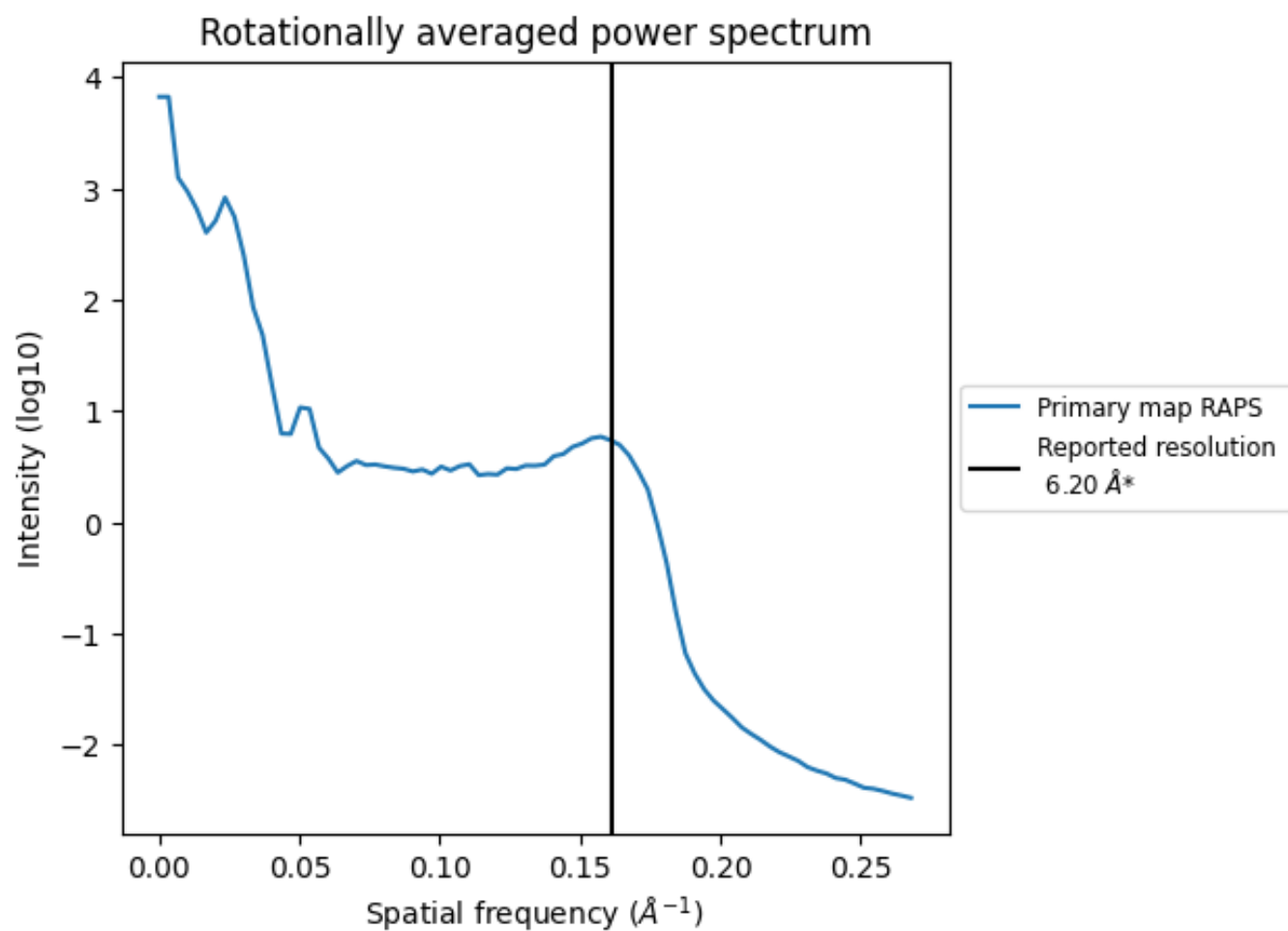
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 731 nm<sup>3</sup>; this corresponds to an approximate mass of 660 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.161 Å<sup>-1</sup>

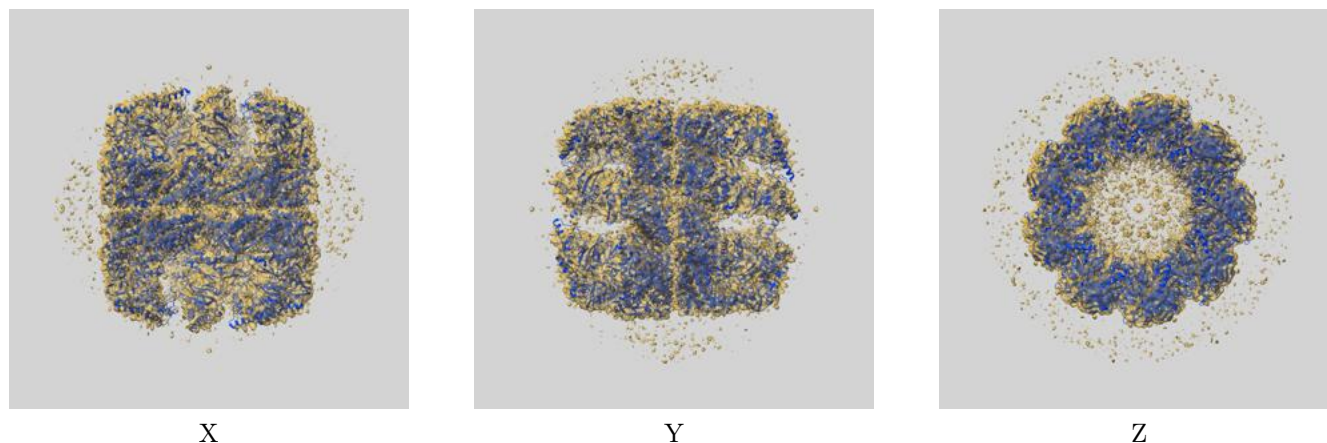
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

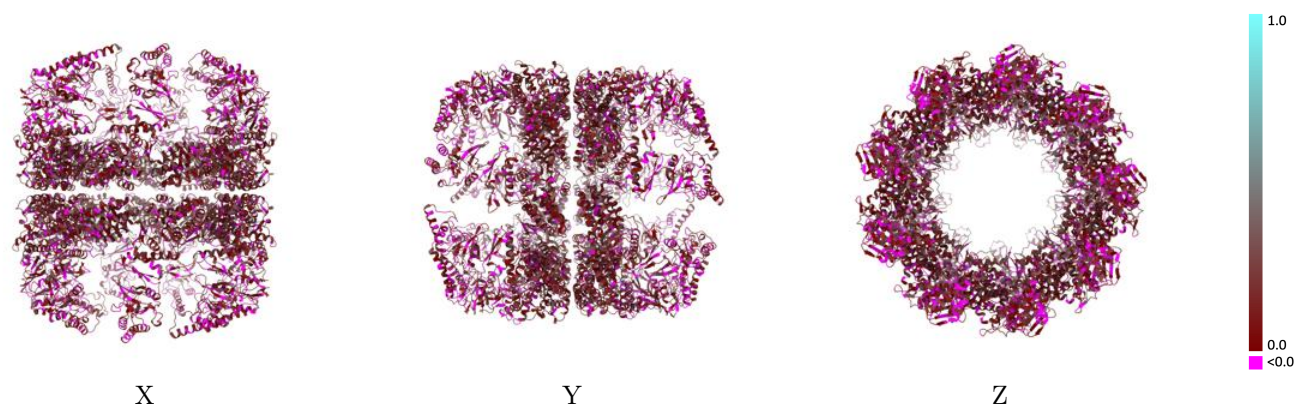
This section contains information regarding the fit between EMDB map EMD-5396 and PDB model 3J1F. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



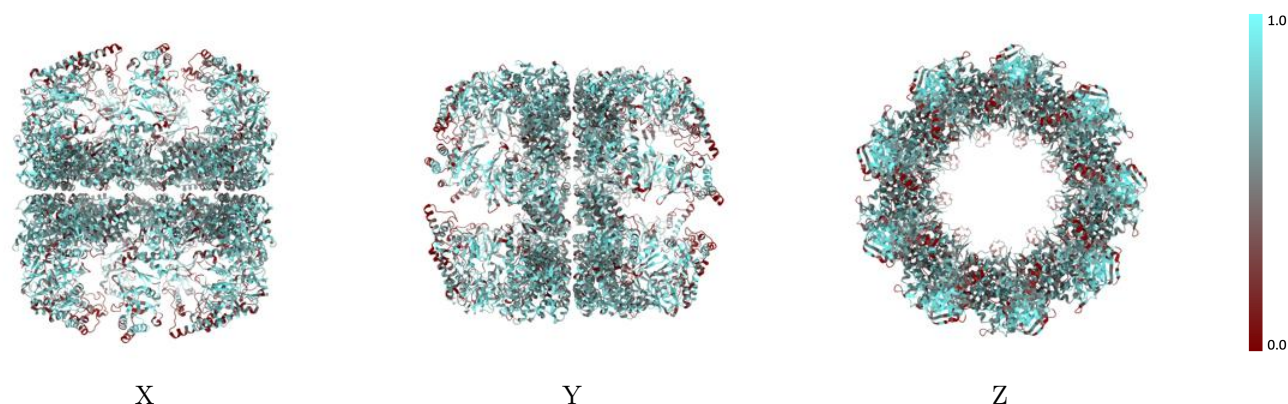
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



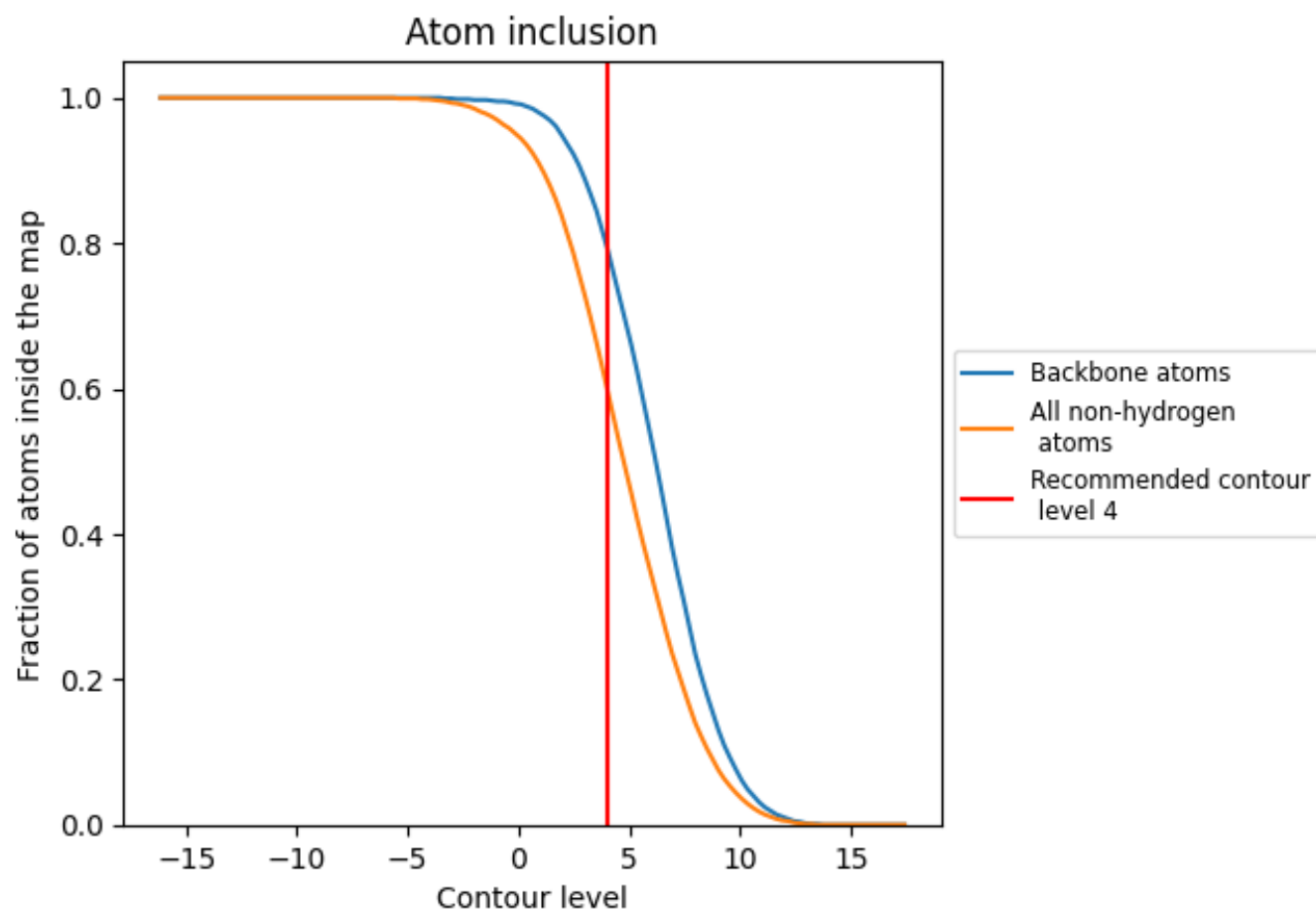
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.6000 | <div><div></div></div> 0.1410 |
| A     | <div><div></div></div> 0.6040 | <div><div></div></div> 0.1420 |
| B     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.1430 |
| C     | <div><div></div></div> 0.6020 | <div><div></div></div> 0.1430 |
| D     | <div><div></div></div> 0.6020 | <div><div></div></div> 0.1410 |
| E     | <div><div></div></div> 0.6000 | <div><div></div></div> 0.1380 |
| F     | <div><div></div></div> 0.6000 | <div><div></div></div> 0.1350 |
| G     | <div><div></div></div> 0.6010 | <div><div></div></div> 0.1390 |
| H     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.1410 |
| I     | <div><div></div></div> 0.6030 | <div><div></div></div> 0.1410 |
| K     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.1410 |
| L     | <div><div></div></div> 0.6010 | <div><div></div></div> 0.1420 |
| M     | <div><div></div></div> 0.6030 | <div><div></div></div> 0.1400 |
| N     | <div><div></div></div> 0.6020 | <div><div></div></div> 0.1450 |
| O     | <div><div></div></div> 0.5970 | <div><div></div></div> 0.1400 |
| P     | <div><div></div></div> 0.5950 | <div><div></div></div> 0.1410 |
| Q     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.1410 |
| R     | <div><div></div></div> 0.5990 | <div><div></div></div> 0.1450 |
| S     | <div><div></div></div> 0.6000 | <div><div></div></div> 0.1420 |

1.0

0.0

<0.0